STEREOCHEMICAL ASPECTS IN THE INTERRUPTED NAZAROV REACTION OF ALLENYL VINYL KETONES: A COMPUTATIONAL STUDY

by

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"It is far from simple to show the truth, yet the truth is simple." – Dziga Vertov

"All truth passes through three stages. First, it is ridiculed. Second, it is violently opposed. Third, it is accepted as being self-evident." – Arthur Schopenhauer

"All I know, is that I know nothing." – Socratic Paradox

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ABSTRACT

Transition state models are often invoked to explain stereochemical outcomes in chemical reactions. The relevance of these models to correctly predict these outcomes can be further validated by studying reactions where multiple stereocenters are formed sequentially. Through the use of computational methods, insight is provided on some sterochemical aspects of a two-step cascade reaction, i.e., a Nazarov/homologous Mukaiyama reaction sequence.

The torquoselectivity in the thermal, Lewis acid-mediated Nazarov reaction of a series of terminally substituted allenyl vinyl ketones has been subjected to a computational investigation using density functional methods. In this conrotatory electrocyclization reaction, the preferred mode of rotation of the termini was found to be by outward rotation of the allenyl substituent. This leads to products that are not the lower-energy isomers because there are large steric interactions present in the kinetic products. However, the torquoselectivity is shown to be decided at the transition state more by steric interactions between the termini of the allenyl and the vinyl moieties than by the competing steric interactions between between substituents on the allene of the substrate. These steric interactions cause the transition state for the inward rotation of allenyl substituent to be more distorted than that for outward rotation, resulting in high levels of torquoselectivity (>20:1) in favor of outward rotation of the allenyl terminus.

The diastereoselectivity in the trapping of an oxyallyl cation by a series silyloxy enol ethers and their corresponding enols through open-type transition states has also been assessed computationally. Perhaps as a consequence of the high reactivity of oxyallyl cations for addition by such electron-rich alkenes, multiple, nearly iso-energetic, reaction pathways were found. This should lead to low levels of diastereoselectivity. The results allowed some discussion with respect to how these transition states are ordered in terms of energy. However, the complexity of these open-type transition states, as opposed to the well-known cyclic aldol transition states, limits the interpretation of the results to a simplistic level. However, some published experimental results indicated that the diastereoselectivity could be quite high. Therefore, it is postulated that the observed diastereoselectivity must be due to equilibration of the products after the carbon-carbon forming event of the homologous Mukaiyama aldol addition.

Overall, the results presented in this thesis show that the conventional use of steric and/or electronic arguments based on generally accepted models may not provide correct predictions in terms of the developing stereochemistry in a complex organic reaction, and that the use of computational methods is demonstrated herein to be crucial for attaining a better understanding of reaction mechanisms.

LIST OF ABBREVIATIONS AND SYMBOLS USED

Abbreviations	*Description*
AVK	allenyl vinyl ketone
B3LYP	Becke's hybrid exhange-correlation functional
B88	Becke's B88 exchange functional
B97	Becke's B97 exchange-correlation functional
ωB97X, ωB97X-D	Head-Gordon's range-separated B97 functionals
c	clockwise
cc	counterclockwise
CC	coupled cluster
CI	configuration interaction
disp	dispersion
DFT-D	dispersion-corrected density functional theory
ENL	enol
HF	Hartree-Fock
HOMO	highest-occupied molecular orbital
^{i}Pr	isopropyl
IRC	intrinsic reaction coordinate
KS-DFT	Kohn-Sham density functional theory
DFT-D	dispersion-corrected density functional theory
L	Lewis acid
LR	long-range
LSDA	local spin density approximation
LUMO	lowest-unoccupied molecular orbital
LYP	Lee-Yang-Parr's correlation functional
Me	methyl
MPBT	many-body perturbation theory
MPn	n-th order Møller-Plesset perturbation theory
M06, M06-2X	Truhlar's Minnesota functionals
OAC	oxyallyl cation
PC	product complex

PCM	polarizable continuum model
PDC	pentadienyl cation
PES	potential energy surface
Ph	phenyl
PT	product
RC	reactant complex
RT	reactant
SEE	silyl enol ether
SR	short-range
^{t}Bu	*tert*-butyl
TBS	*tert*-butyldimethylsilyl
TMS	trimethylsilyl
TS	transition state
ZPE	zero point energy

Symbols	***Description***
A(*,*,*)	angle
D	Slater determinant
D(*,*,*,*)	dihedral angle
E	energy
E_c	correlation energy functional
E_s	Taft steric substituent constant
E_x	exchange energy functional
E_{xc}	exchange-corrrelation energy functional
F_{rs}	Fock matrix elements
$\hat{F}$	Fock operator
G	Gibbs energy
G_{corr}	thermal correction to Gibbs energy
H_{ij}	one-electron core integral
H_{rs}	one-electron core matrix elements

$\hat{H}$	Hamiltonian operator
J_{ij}	Coulomb integral
$\hat{J}_j$	Coulomb operator
k	force constant
k_{12}	rate constant
K	equilibrium constant
K_{ij}	exchange integral
$\hat{K}_j$	exchange operator
m_s	spin coordinates
$q_i \equiv (x_i, y_i, z_i, m_s)$	spatial and spin coordinates
r_{ij}	Euclidean distance between particles i and j
$\mathbf{r}_i \equiv (x_i,y_i,z_i)$	spatial coordinates
R(*,*)	bond length / distance between two centers
S_{ij}	overlap integral
S_{rs}	overlap matrix elements
$\hat{T}$	kinetic energy operator
T	temperature
$\hat{U}$ or $\hat{V}$	potential energy operator
W	variational integral
Z	nuclear charge
Ψ	state (or wave) function
ψ	stationary state (or wave) function
ϕ	trial state (or wave) variation function
$u_i \equiv \sigma_i\theta_i$	spin-orbital (product of spin, σ_i, and spatial, θ_i, orbitals)
ε_i	orbital energy
χ_j	basis functions
ρ	electronic density
ρ_{tr}	trial density function

$v(\mathbf{r}_i)$	external potential

Units	**Description**
m	metre (length)
Å	angstrom (length), 10^{-10} m
kg	kilogram (mass)
mol	mole (amount of substance)
C	coulomb (electric charge)
J	joule (enegy, work or heat)
cal	calorie (energy, work or heat), 4.184 J
Ha	hartree (atomic unit for energy work or heat), 2625.500 kJ/mol
s	second (time)
min	minute (time), 60 s
K	kelvin (temperature)
^{o}C	degrees Celsius (temperature relative to 273.15 K)
atm	atmosphere (pressure)

Constants	**Description**
a_0	Bohr radius (5.29×10^{-11} m)
m_e	electron rest mass (9.019×10^{-31} kg)
e	elementary charge (1.602×10^{-19} C)
ε	relative permittivity (or dielectric constant)
ϵ_0	permittivity of free space
$\hbar$	reduced Planck's constant (1.055×10^{-34} J s)
R	gas constant (8.3145 J K^{-1} mol^{-1})

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CHAPTER 1 INTRODUCTION

Cascading reactions[1,2] in organic synthesis (also referred to as domino, tandem or sequential reactions) have served, and are continuing to serve, chemists well in preparing highly complex structures. In these types of reactions, multiple new stereocenters, functionalities and bonds are introduced consecutively in a sequence of reactions where there is ideally no 'intervention' by the chemist until the very last steps (workup, purification, characterization, etc.).

The success of these cascading reactions relies heavily on producing structures in high yields and with the desired features. Understanding the regio-, chemo- and stereoselective aspects of each of the individual reaction steps in cascade reactions is therefore important. However, intermediates resulting from each step are often not isolable and so gaining mechanistic insight from each reaction step can be rather difficult experimentally. Furthermore, being able to predict what will become of a particular set of reactants following a sequence of reactions is also invaluable in the elaboration of synthetic procedures.

Computational chemistry allows the chemist to study these intermediates and to explore reaction paths and potential energy surfaces through the use of computers, algorithms, procedures and theory. When one does not have access or the means to observe or measure properties of reactive intermediates, it can be useful to turn to computations in order to gain more mechanistic insight into what is potentially happening during a given reaction. The advantages of using computational chemistry to study cascade reactions should be obvious to the reader.

Pericyclic domino processes[3] are examples of cascading reactions in which at least one reaction of the sequence consists of a pericyclic reaction. Much work has been done in recent years on these types of reactions.[4] The aim of the work presented in this thesis is to provide insight into various stereochemical aspects of two sequential steps of a pericyclic cascade reaction, namely the interrupted Nazarov reaction,[5,6] using computational

methods. More specifically, the sequence studied can be further described as a Nazarov/homologous Mukaiyama reaction sequence.[6,7]

The thesis is divided as follows. Chapter 2 serves as a brief introduction to the theoretical foundations of the computational methods used in the subsequent chapters. Chapters 3 and 4 deal with exploring the two reaction steps of the sequence, i.e., the Nazarov cyclization and the homologous Mukaiyama reaction, respectively. Chapter 5 serves as conclusion to the thesis.

CHAPTER 2 COMPUTATIONAL METHODS

This chapter provides a brief introduction to the theoretical background of the computational methods used in Chapters 3 and 4. More detailed information on theoretical[8-11] and/or practical[12,13] aspects of these computational methods is provided elsewhere.

Dirac notation will be used throughout this chapter to simplify some of the equations. More specifically, the (definite) integral over all space of the product of the complex conjugate of f, f^*, and of an operator, $\widehat{A}$, acting on f can be written as follows:

$$\int f^* \widehat{A} f d\tau \equiv \langle f | \widehat{A} | f \rangle \qquad (2.\ 1)$$

Unless otherwise stated, quantum-mechanical operators and/or properties explicitly defined will be given in atomic units throughout this chapter. The electron's mass, m_e, the elementary charge, e, the reduced Planck's constant, $\hbar$ and $4\pi\epsilon_0$ are set to 1. In these units, the ground-state energy of the H atom, $-\frac{m_e e^4}{2(4\pi\varepsilon_0)^2\hbar^2}$, equals -0.5 "hartrees" or -0.5 Ha.

Discussion will also be restricted to systems whose ground-states are non-degenerate and to systems in which there are no unpaired electrons, also known as closed-shell systems.

2.1 The Schrödinger Equation

Quantum chemistry applies the laws of quantum mechanics to problems of interest in chemistry. These laws describe the non-classical behavior of small particles, such as electrons and nuclei. It is important to note that quantum mechanics is statistical in nature and is based on a set of postulates.

The time-dependent Schrödinger equation is the quantum-mechanical analogue to the classical Newton's laws and describes how the state of a system of small particles, Ψ, changes with time. Of greater interest to chemists is the time-independent Schrödinger equation[14] for stationary states,

$$\hat{H}\Psi_n = E_n\Psi_n \tag{2. 2}$$

where $\hat{H}$ is the Hamiltonian operator. The wave function, Ψ_n, is postulated to contain all information pertaining to the system. The Born postulate states that $|\Psi|^2 \equiv \Psi^*\Psi$ is the probability density. Moreover, for Ψ normalized, $\langle\Psi|\Psi\rangle = 1$. With the correct quantum-mechanical operator, physicochemical properties can be extracted from the wave function. For example, by subjecting the wave function to the Hamiltonian operator, the energy of the system for that state is extracted.

By imposing boundary conditions on the wave function and by imposing that the wave function be well-behaved (single-valuedness, continuity and quadratic integrability), the (time-independent) Schrödinger equation can be solved exactly for Ψ and E for a number of simplistic and/or ideal systems, e.g. the particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen-like atom.

However, for systems of many interacting particles, i.e., for atoms and molecules, approximations need to be made in order to solve the Schrödinger equation as interelectronic repulsion terms prevent the equation from being separable and solved analytically. The following subsections deal with two of the basic principles behind these approximation methods, the variation method and perturbation theory.

2.1.1 The Variation Method

By applying the variation method, one can obtain an upper bound to the ground-state energy of the system of interest. This method is based on the variation theorem, which is stated as follows:

The variation theorem For any well-behaved trial variation function, ϕ, that satisfies the boundary conditions of the problem, the variational integral $W = \frac{\langle\phi|\hat{H}|\phi\rangle}{\langle\phi|\phi\rangle} \geq E_0$. The closer the trial variation function is to the true ground-state wave function, Ψ_0, the closer the variational integral will be to the ground state-energy, E_0.

By expanding the trial variation function as a linear combination of basis functions, χ_j, that satisfies the same boundary conditions as the problem, $\phi = \sum_{j=1}^{n} c_j\chi_j$, and minimizing the variational integral by setting $\frac{\partial W}{\partial c_j} = 0$, one obtains a set of simultaneous, linear homogeneous equations in the n unknowns $c_1, c_2, \dots, c_n$,

$$\sum_{j=1}^{n}\left[\left(H_{ij} - WS_{ij}\right)c_j\right] = 0, \qquad i = 1,2,\dots,n \tag{2. 3}$$

where $H_{ij} \equiv \langle\chi_i|\hat{H}|\chi_j\rangle$ and $S_{ij} \equiv \langle\chi_i|\chi_j\rangle$. For there to be a non-trivial solution, e.g., $c_{ij} \neq 0$, to this set of equations, the secular equation must vanish, i.e., $|H_{ij} - WS_{ij}| = 0$, where the vertical bars represent a determinant. Expanding the determinant and solving for W yields the upper bounds to the true energies of the lowest n bound states of the systems, such that $E_0 \leq W_0, E_2 \leq W_2, \dots, E_{n-1} \leq W_{n-1}$.

Including more basis functions in the expansion of the trial variation function yields upper bounds that become closer to the true energies of the states of the systems. Ideally, a complete set (often an infinite number) of basis functions would be needed to obtain the

true ground-state wave function and the true ground-state energies of the system, which is, of course, not practical. Thus, basis functions have to be chosen wisely in order to best represent the molecular orbitals. An example of commonly used basis sets in quantum mechanical calculations are the Pople-type basis sets (e.g., 6-31G(d), 6-31+G(d,p), etc.).[15]

2.1.2 Perturbation Theory

Another method of approximating the solution to the Schrödinger equation is to use a perturbative approach. Here, the Hamiltonian operator for a system that cannot be solved exactly is written as $\hat{H} = \hat{H}^0 + \lambda\hat{H}'$ where $\hat{H}^0$ is the Hamiltonian operator for a system whose solution is known exactly (the unperturbed system) and where $\hat{H}'$ is the perturbation. The factor λ ranges from 0 to 1 and serves to apply the perturbation to the unperturbed system gradually. This relationship therefore relates the wave functions and energies of the perturbed to the unperturbed systems.

For the perturbed state, the Schrödinger equation in written as follows:

$$\hat{H}\Psi_n = \left(\hat{H}^0 + \lambda\hat{H}'\right)\Psi_n = E_n \qquad (2.\ 4)$$

The wave function and the energy are then expanded in a Taylor series in powers of λ, $\Psi_n = \Psi_n^{(0)} + \lambda\Psi_n^{(1)} + \cdots + \lambda^k\Psi_n^{(k)}$ and $E_n = E_n^{(0)} + \lambda E_n^{(1)} + \cdots + \lambda^k E_n^{(k)}$, where $\Psi_n^{(k)} = \frac{1}{k!}\frac{\partial^k\Psi_n}{\partial\lambda^k}\Big|_{\lambda=0}$ and $E_n^{(k)} = \frac{1}{k!}\frac{\partial^k E_n}{\partial\lambda^k}\Big|_{\lambda=0}$, respectively. $\Psi_n^{(0)}$ and $E_n^{(0)}$ are the wave function and the energy of the unperturbed system (since $\lambda = 0$) and $\Psi_n^{(k)}$ and $E_n^{(k)}$ are the k-th order corrections to the wave function and energy. Expanding Ψ_n and E_n in the Schrödinger equation and ensuring that $\Psi_n^{(0)}$ is normalized and that Ψ_n satisfies $\left\langle\Psi_n^{(0)}\middle|\Psi_n\right\rangle = 1$, the k-th order corrections to the wave function and to the energy can be obtained.

For example, truncating the Taylor series after the first-order correction to the wave function yields:

$$\Psi_n \approx \Psi_n^{(0)} + \Psi_n^{(1)} = \Psi_n^{(0)} + \sum_{m \neq n} \frac{H'_{mn}}{E_n^{(0)} - E_m^{(0)}} \Psi_m^{(0)} \quad (2.5)$$

and truncating it after the second-order correction to the energy yields:

$$E_n \approx E_n^{(0)} + E_n^{(1)} + E_n^{(2)} = E_n^{(0)} + H'_{nn} + \sum_{m \neq n} \frac{|H'_{mn}|^2}{E_n^{(0)} - E_m^{(0)}} \quad (2.6)$$

where H'_{nn} and H'_{mn} have similar definitions to H_{ij} in Section **2.1.1** with f replaced by $\Psi^{(0)}$.

2.2 Many-Electron Systems and Hartree-Fock Theory

The wave function representing an n-electron system must not be able to distinguish between electrons (a consequence of the Heisenberg uncertainty principle), and must therefore be antisymmetric with respect to interchange of any two electrons (or for any particles with half-integral spin). Particles with integral spin are represented by a symmetric wave function. This is known as the spin statistics theorem.

A wave function satisfying this criterion and that describes an n-electron system was suggested by Slater as the determinant of the form:

$$D = \frac{1}{\sqrt{n!}} \begin{vmatrix} u_1(1) & \bar{u}_1(1) & u_2(1) & \cdot\cdot & \cdot\cdot & \bar{u}_{n/2}(1) \\ u_1(2) & \bar{u}_1(2) & u_2(2) & & & \bar{u}_{n/2}(2) \\ \vdots & & \cdot\cdot & & & \vdots \\ \vdots & & & \cdot\cdot & & \vdots \\ \vdots & & & & \cdot\cdot & \vdots \\ u_1(n) & \bar{u}_1(n) & u_2(n) & \cdot\cdot & \cdot\cdot & \bar{u}_{n/2}(n) \end{vmatrix}$$

(2. 7)

where the u_i are spin-orbitals (products of spin, σ_i, and spatial orbitals, θ_i). Elements of the same row involve the same electron and elements in the same column involve the same spin-orbital. These types of wave functions are known as Slater determinants.[16]

Hartree-Fock calculations[17] for establishing self-consistent field wavefunctions for many-electrons systems, i.e., for atoms and molecules, have served as a cornerstone for performing calculations on a many-electron system. These types of procedures are as follows:

The "molecular" Hamiltonian is first defined as:

$$\hat{H} = \hat{H}_{el} + \hat{V}_{NN} = \left[-\frac{1}{2}\sum_i \nabla_i^2 - \sum_\alpha \sum_i \frac{Z_\alpha}{r_{i\alpha}} + \sum_j \sum_{i>j} \frac{1}{r_{ij}} \right] + \sum_\alpha \sum_{\beta>\alpha} \frac{Z_\alpha Z_\beta}{r_{\alpha\beta}}$$

(2. 8)

where the first three terms are the operators for the kinetic energy of the n-electron system, $\hat{T}_e$, the potential energy for nuclear-electronic repulsion between each electron i and each nucleus α, $\hat{V}_{Ne}$, and the potential energy for electron-electron repulsions between each electrons i and j, $\hat{V}_{ee}$, respectively. These constitute the purely electronic Hamiltonian, $\hat{H}_{el}$. The last term consists of the nuclear-nuclear repulsion between each pair of nuclei α and β, $\hat{V}_{NN}$. The formulation of this Hamiltonian assumes the validity of the Born-Oppenheimer approximation,[18] which is discussed in more detail in Section **2.4**.

By the variation theorem, the Hartree-Fock molecular energy, E_{HF}, is then given by the variational integral:

$$E_{HF} = \langle D|\hat{H}|D\rangle = \langle D|\hat{H}_{el} + \hat{V}_{NN}|D\rangle = \langle D|\hat{H}_{el}|D\rangle + \hat{V}_{NN} \tag{2. 9}$$

where D is the (normalized) Slater determinant defined earlier. By the use of Condon-Slater rules,[8] the Hartree-Fock energy for a closed-shell system can be rewritten as the sum of one- and two-electron terms as follows:

$$E_{HF} = 2\sum_{i=1}^{\frac{n}{2}} H_{ii}^{core} + \sum_{i=1}^{\frac{n}{2}}\sum_{j=1}^{\frac{n}{2}} (2J_{ij} - K_{ij}) + V_{NN} \tag{2. 10}$$

where

$$H_{ii}^{core} \equiv \langle u_i(1)|\hat{H}^{core}(1)|u_i(1)\rangle \equiv \left\langle u_i(1)\left|-\tfrac{1}{2}\nabla_i^2 - \textstyle\sum_\alpha \frac{Z_\alpha}{r_{1\alpha}}\right|u_i(1)\right\rangle, \tag{2. 11}$$

$$J_{ij} \equiv \left\langle u_i(1)u_j(2)\left|\frac{1}{r_{12}}\right|u_i(1)u_j(2)\right\rangle, \tag{2. 12}$$

$$\text{and } K_{ij} \equiv \left\langle u_i(1)u_j(2)\left|\frac{1}{r_{12}}\right|u_j(1)u_i(2)\right\rangle \tag{2. 13}$$

are the one-electron core Hamiltonian, the Coulomb and the exchange integrals, respectively. The sums extend over all occupied orbitals and the integrals, over all spatial

coordinates of electrons 1 and 2. The (orthonormal) spin-orbitals, u_i, that minimize the variational integral, and thus E_{HF}, are found to satisfy the Fock equations

$$\hat{F}(1)u_i(1) = \varepsilon_i u_i(1), \qquad i = 1,2,\dots,n$$

(2. 14)

where the Fock operator, $\hat{F}$, is defined as:

$$\hat{F}(1) \equiv \hat{H}^{core}(1) + \sum_{j=1}^{\frac{n}{2}} \left[2\hat{J}_j(1) - \hat{K}_j(1)\right]$$

(2. 15)

and where $\hat{J}_j(1)f(1) = f(1)\int \frac{|u_j(2)|^2}{r_{12}} dv_2$ and $\hat{K}_j(1)f(1) = u_j(1)\int \frac{u_j^*(2)f(2)}{r_{12}} dv_2$ are the Coulomb and exchange operators, respectively. The ε_i's are the energies of the orbitals u_i.

One must solve the Fock equations iteratively as the Fock operator depends on its own eigenfunctions, u_i. By solving for H_{ii}^{core} in terms of the ε_i's, the Hartree-Fock energy can be rewritten as:

$$E_{HF} = 2\sum_{i=1}^{\frac{n}{2}} \varepsilon_i - \sum_{i=1}^{\frac{n}{2}}\sum_{j=1}^{\frac{n}{2}} \left(2J_{ij} - K_{ij}\right) + V_{NN}\,.$$

(2. 16)

By further expanding each orbital in terms of a linear combination of basis functions, $u_i = \sum_{s=1}^{b} c_{si}\,\chi_s$, and substituting into the Hartree-Fock equations, one can arrive at the Roothaan-Hall equations:[19]

$$\sum_{s=1}^{b} c_{si}(F_{rs} - \varepsilon_i S_{rs}) = 0, \qquad r = 1,2,\dots,b$$

(2. 17)

where $F_{rs} \equiv \langle \chi_r | \hat{F} | \chi_s \rangle = H_{rs}^{core} + \sum_{t=1}^{b} \sum_{u=1}^{b} \sum_{j=1}^{\frac{n}{2}} c_{rj}^{*} c_{uj} [2(rs|tu) - (ru|ts)]$ and $S_{rs} \equiv \langle \chi_r | \chi_s \rangle$.

The two-electron repulsion integrals are defined as follows:

$$(rs|tu) \equiv \iint \frac{\chi_r^{*}(1)\chi_s(1)\chi_t^{*}(2)\chi_u(2)}{r_{12}} d\nu_1 d\nu_2 \, .$$

(2. 18)

Similarly to the results for linear variation functions in Section **2.1.1**, the orbital energies, ε_i, can be obtained from the roots of the secular equation $|F_{rs} - \varepsilon_i S_{rs}| = 0$. Once again, these sets of equations must be solved iteratively as F_{rs} depends on the expanded orbitals in terms of basis functions, χ_s, and their associated unknown coefficients, c_{si}, through the Fock operator, $\hat{F}$.

This iterative process is usually conducted in the following way. (1) Guesses are initially made for the spin-orbitals in terms of a linear combination of basis functions. (2) The Fock operator and the matrix elements, F_{rs}, are then computed. (3) The secular equation is solved for the orbital energies, ε_i. (4) The orbitals energies are used to obtain improved coefficients from the Roothaan-Hall equations, c_{si}, and the process returns to point (2). When there is no further improvement in the coefficients and orbital energies, the calculations are complete and the Hartree-Fock energy is obtained. Other information can then be obtained from the wave function expanded in terms of the basis functions with improved coefficients.

Compared to the Hartree-Fock equations, which can be solved numerically only for atoms, the Roothaan-Hall equations have facilitated the computations of molecules as these equations are solved more easily through the use of matrix methods and which can be easily implemented in computer programs.[8]

2.3 Electron Correlation Methods

An approximation made in Hartree-Fock theory is that each electron is considered to be subjected to an averaged potential from all other electrons. However, as electrons repel one another, the motion of any one electron is correlated to the motion of all other electrons. These instantaneous interactions are not included in Hartree-Fock theory, excluding the fact that the wave function must obey the antisymmetry principle.[20] The correlation energy, E_{corr}, is defined as:

$$E_{corr} = E - E_{HF} \tag{2. 19}$$

where E_{HF} is the Hartree-Fock energy and E is the exact energy.

Methods of including electron correlation have been developed. Such methods include configuration interaction (CI) methods, coupled cluster (CC) methods, many-body perturbation theory (MPBT or MPn), density functional theory (DFT), etc. The underlying principles behind Møller-Plesset perturbation theory and density functional theory will now be discussed as these are the methods that have been used in subsequent chapters to perform electronic structure calculations.

2.3.1 Møller-Plesset Perturbation Theory

Møller-Plesset perturbation theory[21a] is a type of many-body perturbation theory which applies the principles discussed in Section **2.1.2**, to a system containing many interacting particles.

Taking the unperturbed wave function as the Hartree-Fock wave function and the unperturbed Hamiltonian as the sum of one-electron Fock operators described earlier gives:

$$\hat{H}^0 D = \left(\sum_{i=1}^{n} \varepsilon_i \right) D = E^{(0)} D$$

(2. 20)

The perturbation is given by the difference between the Hamiltonian operators for the unperturbed system, essentially the sum of the one-electron Fock operators, and the perturbed system, which includes interelectronic repulsions. It is therefore equal to the difference between the true interelectronic potential between electrons and the averaged Hartree-Fock potential between any one electron and the other electrons in the system.

The sum of the zeroth-order energy and first-order correction to the energy can be shown to be equal to the Hartree-Fock molecular energy of the system, i.e.,

$$E_0^{(0)} + E_0^{(1)} = E_{HF}$$

(2. 21)

To improve upon these energies, second-, third-, and higher order corrections can be added to the Hartree-Fock molecular energy. MPn calculations denote Hartree-Fock calculations that have been subjected to a Møller-Plesset perturbative treatment and have had corrections up to the n-th order added to the energies and to the wave functions. For example, in MP2 calculations,[21b-h] the second-order energy correction,

$$E_0^{(2)} = \sum_{s \neq 0} \frac{\left| \left\langle \psi_s^{(0)} \middle| \hat{H}' \middle| D \right\rangle \right|^2}{E_0^{(0)} - E_s^{(0)}}$$

(2. 22)

is added to the Hartree-Fock energy to obtain the molecular energy. The $\psi_s^{(0)}$'s that will not make the numerator in the expression for $E_0^{(2)}$ vanish, are doubly-excited determinants, D_{ij}^{ab}, in which electrons in the occupied spin-orbitals i and j have been excited to virtual spin-orbitals a and b. This expression can be rewritten as:

$$E_0^{(2)} = \sum_{b=a+1}^{\infty} \sum_{a=n+1}^{\infty} \sum_{i=j+1}^{n-1} \sum_{j=1}^{n-1} \frac{|\langle ab|r_{12}^{-1}|ij\rangle - \langle ab|r_{12}^{-1}|ji\rangle|^2}{\varepsilon_i + \varepsilon_j - \varepsilon_a - \varepsilon_b} \qquad (2.\ 23)$$

where n is the number of electrons in the system and definitions of the two-electron repulsion integrals have been used (cf. Section **2.2**).

2.3.2 Density Functional Theory

In order to reduce the number of variables in functions used to derive molecular energies and other electronic properties of an n-electron system, density functional theory (DFT) methods were developed. These methods take advantage of functions of the ground-state electronic density, defined as:

$$\rho_0(\mathbf{r}) = n \sum_{\text{all } m_s} \int \dots \int |\Psi_0(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_n, m_{s1}, \dots, m_{s2})|^2 \, d\mathbf{r}_2 \dots d\mathbf{r}_n \, . \qquad (2.\ 24)$$

This reduces the number of coordinates to consider from 4n spatial and spin coordinates of the usual wave function, $\Psi_0(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_n, m_{s1}, \dots, m_{s2})$, to the three coordinates, $\mathbf{r} \equiv (x, y, z)$, of $\rho_0(\mathbf{r})$.

Once the ground-state electronic density is found, both the external potential, defined as the potential energy between the electron i and the nuclei, or $v(r_i) = -\sum_\alpha \frac{Z_\alpha}{r_{1\alpha}}$, and the number of electrons, n, can be determined as stated by the Hohenberg-Kohn theorem.[22a]

Hohenberg-Kohn theorem The ground state molecular energy, wave function and all other electronic properties are uniquely determined by the ground-state electron probability, $\rho_0(x, y, z)$. The ground-state molecular energy, E_0, is thus a functional of the ground-state electronic density, ρ_0, and is denoted by $E_0 = E_v[\rho_0]$.

The Schrödinger equation can then be solved to determine the ground-state electronic energy and other electronic properties. The purely electronic Hamiltonian for this n-electron system is given by:

$$\hat{H}_{el} = \hat{T}_e + \hat{V}_{Ne} + \hat{V}_{ee} = -\frac{1}{2}\sum_{i=1}^{n}\nabla_i^2 + \sum_{i=1}^{n} v(\mathbf{r}_i) + \sum_{j}\sum_{i>j}\frac{1}{r_{ij}}$$

(2. 25)

and so the ground-state electronic energy is the sum of averaged kinetic-energy, electron-nuclear attraction and electron-electron repulsion terms for the ground state:

$$E_0 = E_v[\rho_0] = \overline{T}[\rho_0] + \overline{V}_{Ne}[\rho_0] + \overline{V}_{ee}[\rho_0] = \overline{T}[\rho_0] + \int \rho_0(\mathbf{r})v(\mathbf{r})d\mathbf{r} + \overline{V}_{ee}[\rho_0]\,.$$

(2. 26)

The Hohenberg-Kohn theorem does not, however, specify how to calculate E_0 or how to find ρ_0 without first finding the wave function. The Kohn-Sham method[22b] was developed to achieve this. A fictitious system of n non-interacting particles is first postulated to have the same ground state electronic density as the system of interest, $\rho_s = \rho_0$. The expression for E_0 is then rewritten as:

$$E_0 = E_v[\rho] = \int \rho(\mathbf{r})v(\mathbf{r})d\mathbf{r} + \overline{T}_s[\rho] + \frac{1}{2}\iint \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{r_{12}}d\mathbf{r}_1 d\mathbf{r}_2 + E_{xc}[\rho]$$

(2. 27)

where $E_{xc} \equiv \Delta\overline{T}[\rho] + \Delta\overline{V}_{ee}[\rho]$ and is known as the exchange-correlation energy functional. $\Delta\overline{T}[\rho]$ and $\Delta\overline{V}_{ee}[\rho]$ are defined as the differences in average ground-state electronic kinetic and electrostatic interelectronic repulsion energies between the actual molecular system and the reference system of non-interacting particles.

The ground-state electronic energy and the ground-state electron density can be expressed in terms of Kohn-Sham spin-orbitals, $u_i^{KS} \equiv \theta_i^{KS}\sigma_i^{KS}$, for which the Slater determinant of these orbitals, $\psi_{s,0} = \left|u_1^{KS}u_2^{KS} \ldots u_n^{KS}\right|$ satisfies the Schrödinger equation with Hamiltonian

$$\hat{H}_s = \sum_{i=1}^{n} \hat{h}_i^{KS} = \sum_{i=1}^{n} \left[-\frac{1}{2}\nabla_i^2 + v_s(\mathbf{r}_i)\right] \qquad (2.\ 28)$$

By varying the electron density (or in this case, the Kohn-Sham orbitals) to minimize $E_v[\rho]$ (see the Hohenberg-Kohn variational theorem),[22a] one finds that the Kohn-Sham equations must be satisfied, i.e.,

$$\left[-\frac{1}{2}\nabla_1^2 - \sum_{\alpha}\frac{Z_\alpha}{r_{1\alpha}} + \int \frac{\rho(\mathbf{r}_2)}{r_{12}}d\mathbf{r}_2 + v_{xc}(1)\right]\theta_i^{KS}(1) = \varepsilon_i^{KS}\theta_i^{KS}(1) \qquad (2.\ 29)$$

where $v_{xc} \equiv \frac{\delta E_{xc}[\rho(r)]}{\delta\rho(r)}$, the "functional" derivative of $E_{xc}[\rho(r)]$,[11] is the exchange-correlation potential. From these Kohn-Sham orbitals, both the ground-state electron density and the ground-state electronic energy can be determined by knowing that:

$$\rho_0 = \rho_s = \sum_{i=1}^{n}\left|\theta_i^{KS}\right|^2 \qquad (2.\ 30)$$

and that:

$$E_0 = E_v[\rho] = -\sum_{\alpha} Z_\alpha \int \frac{\rho(\mathbf{r}_1)}{r_{1\alpha}} d\mathbf{r}_1 - \frac{1}{2}\sum_{i=1}^{n} \langle \theta_i^{KS}(1) | \nabla_1^2 | \theta_i^{KS}(1) \rangle + \frac{1}{2}\iint \frac{\rho(\mathbf{r}_1)\rho(\mathbf{r}_2)}{r_{12}} d\mathbf{r}_1 d\mathbf{r}_2 + E_{xc}[\rho] \,. \quad (2.\ 31)$$

To account for nuclear repulsion, $\hat{V}_{NN} \equiv \sum_\alpha \sum_{\beta>\alpha} \frac{Z_\alpha Z_\beta}{r_{\alpha\beta}}$ is added to the purely electronic Hamiltonian, just as V_{NN} is added to the electronic energy.

Hohenberg-Kohn variational theorem For a trial density function $\rho_{tr}(\mathbf{r})$ that satisfies $\int \rho_{tr}(\mathbf{r}) d\mathbf{r} = n$ and $\rho_{tr} \geq 0$ for all $\mathbf{r}$, the following inequality holds: $E_0 \leq E_v[\rho_{tr}]$. In other words, the true ground-state electron density, ρ_0, minimizes the energy functional $E_v[\rho_{tr}]$.

Performing Kohn-Sham DFT calculations amounts to: (1) making an initial guess at the ground-state electron density, (2) estimating the exchange-correlation potential, v_{xc}, from an approximation made to establish the exchange-correlation functional, $E_{xc}[\rho]$, (3) obtaining Kohn-Sham orbitals from the Kohn-Sham equations, and (4) obtaining an improved electron density, an improved exchange-correlation potential, … and so on until self-consistency is achieved in the electron density and Kohn-Sham orbitals. The ground-state molecular energy (and other properties) can then be calculated from the resulting ground-state electron density.

The Kohn-Sham orbitals can also be expanded in terms of basis sets, in a similar manner to the Roothaan-Hall method presented in Section **2.2**.

The exchange-correlation functional, E_{xc}, is not known and must be approximated in order to solve for $E_v[\rho]$. If it was not for the unknown exchange-correlation functional, Kohn-Sham density functional theory (KS DFT) would yield exact results for the ground state

molecular energy, electronic density and other molecular properties. This, and the fact that there is no systematic way of improving upon the exchange-correlation functionals, remains one of the main drawbacks to DFT calculations.[23,24]

DFT methods have been, and are currently being, used extensively to determine the molecular energies and other electronic properties and to explore the potential energy surfaces for fairly large systems.[8] Despite the fact that MPn, CC, and CI methods can potentially yield more accurate results, most DFT functionals yield fairly good results and require a significantly lower computational cost for larger systems than what would be needed by the other methods.[13]

The DFT functionals used for electronic structure calculations in subsequent chapters are now briefly discussed.

The B3LYP[25] exchange-correlation functional, E_{xc}^{B3LYP}, has the form:

$$E_{xc}^{B3LYP} = E_x^{LSDA} + a_0(E_x^{HF} - E_x^{LSDA}) + a_x\Delta E_x^{B88} + a_c\Delta E_c^{LYP} \quad (2.\ 32)$$

Like typical "hybrid" functionals, B3LYP is a combination of exchange and correlation functionals mixed with some Hartree-Fock exchange, ΔE_x^{HF}. This is done to partially correct for the non-local self-interaction energy present in the Coulomb correlation term of $E_v[\rho]$.[24] For B3LYP, Becke's B88[25a] exchange functional, ΔE_x^{B88}, and Lee, Yang and Parr's LYP[25b] correlation functional, ΔE_x^{LYP}, are mixed with 20% Hartree-Fock exchange. The remainder is described by a functional, E_x^{LSDA}, based on the local spin density approximation (LSDA), which assumes the electron density at each point in space to be that of a homogeneous electron gas.

Problems associated with this functional include a decrease in accuracy as the system size increases[26] (although errors are often reduced in isodesmic reactions[27]), underestimation of medium- and long-range interactions, e.g., 1,3-interactions and dispersion,

respectively.[26,28] Despite these issues, the B3LYP functional has been one of the most used functionals in the past two decades due to its economical and fairly balanced description of organic chemical reactions.[29,30] The good performance of the B3LYP functional has often been attributed to error compensation.[30]

The M06-2X[31] functional along with the other "Minnesota" functionals developed by Truhlar and co-workers,[24] are also gaining momentum in the study of organic reactions.[28c] M06-2X has been recommended for main-group thermochemistry and kinetics and is capable of treating medium-range correlation better than B3LYP.[32] It is important to note, though, that these functionals are heavily parametrized through the combination of many functional forms, constraint satisfaction and semi-empirical fits.[32]

In order to treat long-range interactions, e.g. dispersion or London forces, an approach that is often taken is to include an empirical dispersion correction term, E_{disp} to previously existing functionals, E_{KS-DFT},[33] i.e.,

$$E_{DFT-D} = E_{KS-DFT} + E_{disp} \tag{2. 33}$$

For example, the ωB97X[33a] functional is a "range-separated hybrid" functional and is the modified form of the B97[34] exchange-correlation functional, i.e.,

$$E_{xc}^{\omega B97X} = E_x^{LR-HF} + c_x E_x^{SR-HF} + E_x^{SR-B97} + E_c^{B97} \tag{2. 34}$$

where the exchange was partitioned into short-, $c_x E_x^{SR-HF} + E_x^{SR-B97}$, and long-range, E_x^{LR-HF} terms. By adding an empirical atomic-pairwise dispersion correction term to the ωB97X functional, the ωB97X-D[33b] functional is obtained, which in turn corrects for long-range interactions.

2.4 Potential Energy Surfaces

The potential energy surface (PES) of a non-linear molecule corresponds to the potential energy function, U, as a function of the 3N-6 independent coordinates.

Exploring the PES of molecules is of interest to chemists as it allows, to some degree, the elucidation of mechanisms of chemical reactions, establishing rates of reactions, performing conformational analysis of molecules, etc.

Finding points of interest on the PES (reactants, transition states, products, etc.) is the focus of geometry optimization procedures (Berny optimization algorithm, synchronous transit-guided quasi-Newton methods, etc.).[8,35] Reactants and products correspond to structures that are local minima on the PES in which any small displacement in nuclear coordinates results in an increase in energy of the system. Transition state structures that connect the reactant and product minima are first-order saddle points, in which the displacement of the nuclei along one and only one mode of vibration results in a decrease in energy. All other displacements of the nuclear coordinates yield an increase in energy.

In mathematical terms, the gradient, $\nabla U = \left\{\frac{\partial U}{\partial q_i}\right\}$ is zero for all coordinates q_i for stationary points (minima, maxima, first-order saddle points) on the PES. The Hessian matrix, whose elements are those corresponding to the set of second-order partial derivatives of U with respect to the nuclear coordinates for nuclei i and j, $\nabla^2 U = \left\{\frac{\partial^2 U}{\partial q_i^2}, \frac{\partial^2 U}{\partial q_i \partial q_j}, \frac{\partial^2 U}{\partial q_j \partial q_i}, \frac{\partial^2 U}{\partial q_j^2}, \dots\right\}$, can be used to determine the nature of these stationary points. The elements of the Hessian matrix will be positive for a minimum, whereas n of these elements will be negative for an nth-order saddle point (a first-order saddle point, transition states that are of greater interest for chemists, has one element that is negative).

The second-order derivatives of U can be related to the force constants, k, and therefore to the vibrational frequencies of all (normal) modes of vibration in a molecule.[8] Thus, by

performing a vibrational frequency analysis on a stationary point, its nature can be determined in an analogous manner to what was just discussed.

Generally, transition states (or first-order saddle points), connect one reactant-product pair only. Whereas it may be easy to conclude which reactant or product structure corresponds to a particular transition state when visualizing the imaginary frequency on a graphical interface software, it may sometimes lead a chemist to erroneously interpret the said minima.

The intrinsic reaction co-ordinate (IRC),[35c,36] also known as the reaction path, corresponds to a "least energy" path that connects the transition state to the minima on each side. The calculation of the IRC can be used to ensure that the transition state links the reactant with the product. Caution should be taken here as the points along the path when descending to the reactant and product do not describe how the reactant arrives at the transition state nor how the transition state arrives at the product.

On a final note to this chapter, the Born-Oppenheimer approximation is discussed.[18] The molecular Hamiltonian operator corresponding to a system consisting of electrons and nuclei is given by:

$$\begin{aligned}\hat{H} &= \hat{T}_N + \hat{T}_e + \hat{V}_{NN} + \hat{V}_{Ne} + \hat{V}_{ee} \\ &= -\frac{1}{2}\sum_{\alpha}\frac{\nabla_\alpha^2}{m_\alpha} - \frac{1}{2}\sum_{i}\nabla_i^2 + \sum_{\alpha}\sum_{\beta>\alpha}\frac{Z_\alpha Z_\beta}{r_{\alpha\beta}} - \sum_{\alpha}\sum_{i}\frac{Z_\alpha}{r_{i\alpha}} + \sum_{i}\sum_{j>i}\frac{1}{r_{ij}}\end{aligned} \qquad (2.\ 35)$$

where the only term that differs from the Hamiltonian defined in Section 2.2 is the nuclear kinetic energy operator, $\hat{T}_N$. This operator corresponds to the motion of the nuclei in the system of interest. Why does the Hamiltonian defined earlier not contain this term?

As electrons are significantly smaller than the nuclei (by a factor of at least ~1800), nuclei can be considered fixed relative to the electrons. Thus, $\widehat{T}_N \approx 0$ and one can write the Schrödinger equation for electronic motion as:

$$\widehat{H}\Psi = \left(\widehat{H}_{el} + \widehat{V}_{NN}\right)\Psi = (E_{el} + V_{NN})\Psi = U\Psi\,.$$

(2. 36)

CHAPTER 3 TORQUOSELECTIVITY IN THE THERMAL LEWIS ACID-MEDIATED NAZAROV REACTION OF ALLENYL VINYL KETONES

Since its discovery in 1941, the Nazarov reaction[37] has received much attention on the experimental front as highlighted by a number of reviews.[5,38] The use of this reaction in natural product synthesis has been particularly interesting due to its ability to produce a cyclopentenoid core with a high degree of stereoselectivity (FIGURE 3.1).[38c]

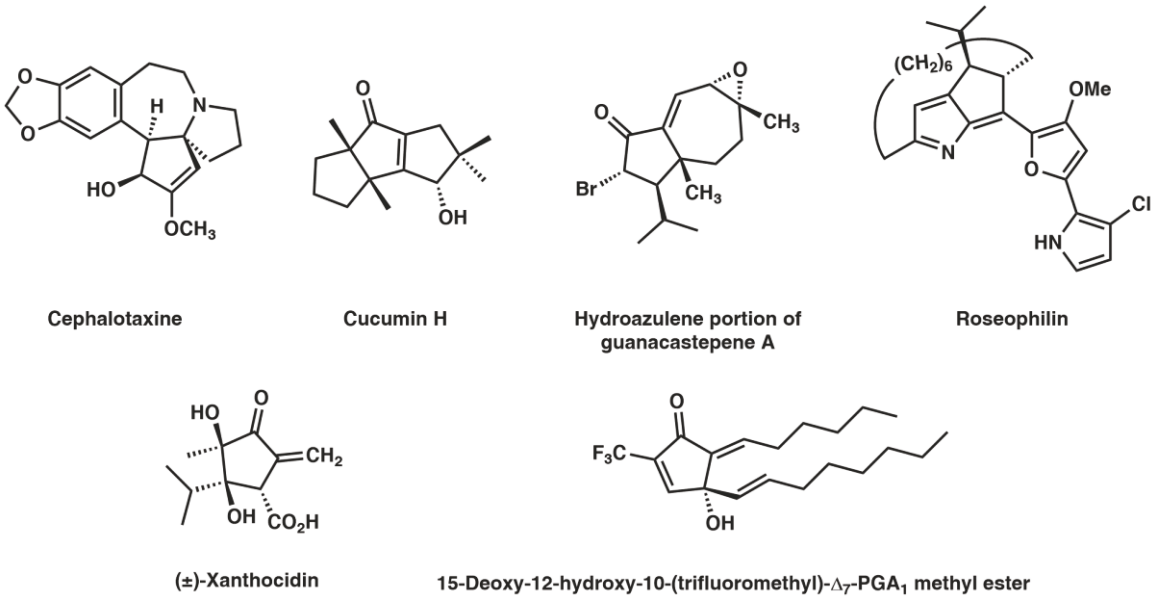


FIGURE 3.1 Examples of natural products where a key step in their syntheses is a Nazarov reaction.

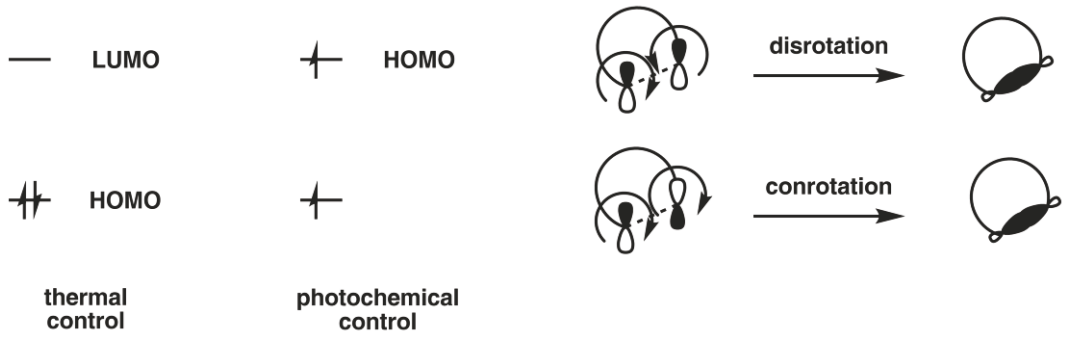
In this chapter, the conversion of allenyl vinyl ketones into oxyallyl cations by the Nazarov reaction will be examined. More specifically, the preferential formation of one stereoisomer over the other during the cyclization will be rationalized by the use of computational methods.

3.1 Electrocyclic Processes and Corresponding Woodward-Hoffmann Rules of Conservation of Orbital Symmetry

The rearrangement of a fully conjugated linear π-electron system so that a σ-bond is formed between two termini, which results in the loss of one π bond in the process, is known as an electrocyclic reaction.[39a]

Orbital symmetry is conserved in such concerted reactions. Woodward and Hoffmann devised their theory of conservation of orbital symmetry in order to explain the outcomes of electrocyclic reactions and related processes.[39b] They postulated that the symmetry of the highest occupied molecular orbital (HOMO) of the cyclizing substrate determines the outcome of the reaction.

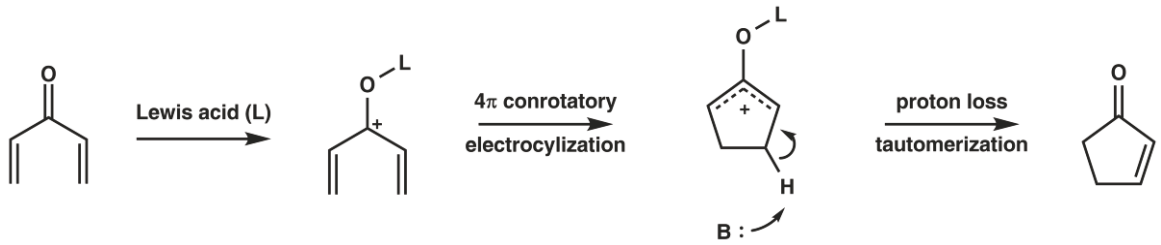
For example, in the cases of 4k π-electron systems under thermal control (k being a non-negative integer), the individual orbitals of the atoms at the incipient bond must rotate in a conrotatory fashion to form a σ bond. Conversely, in photochemically excited systems, the HOMO of the π system is now what was the lowest unoccupied molecular orbital (LUMO) of the system under thermal control. The σ bond is then formed by disrotation of the orbitals of the two carbon termini (SCHEME 3.1). These relationships are reversed for 4k+2 π-electron systems.



SCHEME 3.1 Conrotatory and disrotatory modes of rotation in electrocyclic reactions under thermal and photochemical control.

3.2 The Nazarov Reaction

In the simplest Nazarov reaction, a divinyl ketone undergoes 4π-electrocyclization to ultimately form a cyclopentenone in the presence of an acid (usually a Lewis acid but sometimes a proton, H^+) (SCHEME 3.2). The divinyl ketone complexes with the acid to form a pentadienyl cation, which then undergoes orbital reorganization to form an oxyallyl cation. The oxyallyl cation converts to a cyclopentenone by loss of a proton and tautomerization.



SCHEME 3.2 The Lewis acid-mediated Nazarov reaction of a divinyl ketone.

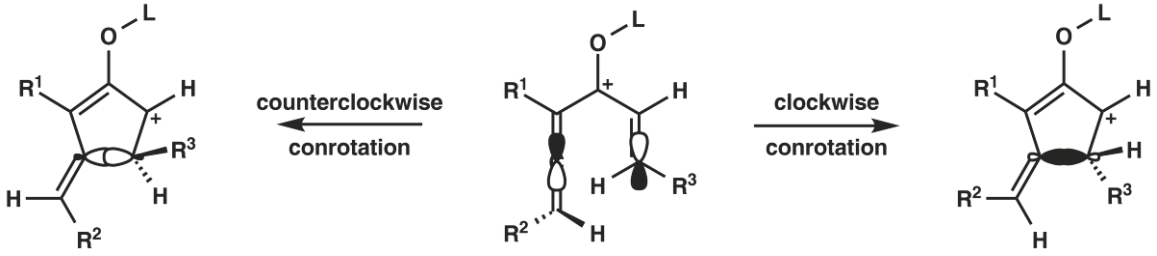
Allenyl vinyl ketones undergo the same process[40] more easily largely because there is less steric hindrance between the termini during cyclization.[38a,41] Allenyl vinyl ketones also appear to be more suitable for a variant of the Nazarov reaction, namely the "interrupted" Nazarov reaction[6] (SCHEME 3.3), in which the oxyallyl cation intermediate is trapped by a nucleophile in order to introduce additional σ-bond(s) onto the five-membered ring.

SCHEME 3.3 The "interrupted" Nazarov reaction of an allenyl vinyl ketone

As a side note, butatrienyl vinyl ketones have also been shown to cyclize efficiently by way of a Nazarov reaction.[42]

Some simple Nazarov reactions have problems stemming from the lack of reactivity necessitating highly acidic reaction conditions, and non-specific proton elimination during the final stage of the reaction can lead to a mixture of isomeric products. These problems have been addressed experimentally by employing different Lewis acids and introducing substituents to facilitate the cyclization or to direct the proton loss. In Denmark's silicon-directed variant of the Nazarov reaction, a silicon group is positioned such that the new double-bond is generated by the loss of the silicon rather than by deprotonation.[43]

Another issue in the Nazarov reaction and its variants is what is known as torquoselectivity.[44] This is a form of stereoselectivity that arises by a preferential direction of rotation of the π-bonds during the formation, or the rupture, of bonds during electrocyclic reactions. The Nazarov reaction is an electrocyclic process and is conrotatory under thermal conditions, as predicted by the Woodward-Hoffmann rules for conservation of orbital symmetry. The two termini can therefore rotate in either a clockwise or a counterclockwise fashion (SCHEME 3.4), and a preference for rotation in one direction is the torquoselectivity of the Nazarov reaction.



SCHEME 3.4 Conrotatory ring closure of the pentadienyl cation undergoing the thermal acid-mediated Nazarov reaction.

3.3 Torquoselectivity: Steric or Stereoelectronic Effects?

A few of theories have been put forward in order to explain the torquoselectivity observed in electrocyclic reactions. Houk's theory of torquoselectivity[44] and Inagaki's geminal bond participation theory[45] are two such examples.

Houk and co-workers[44] first developed their theory for cyclobutene ring-opening reactions. The central tenet of this theory is that the orbitals from π-donor or π-acceptor substituents vicinal to the breaking or forming bond and their interactions with the frontier molecular orbitals of the reactant π-systems cause a preference for inward or outward rotation of substituents. The extent to which the substituents overlap with the breaking bond determines the level of torquoselectivity due to electronic effects. [44e] To illustrate this, the transition states for butadiene-cyclobutene interconversions (a 4π electron system)[44a,b] with those of larger six and eight π-electron systems in electrocylic reactions (i.e., hexatriene-cyclohexadiene[44e] and octatetraenes-cyclooctatrienes interconversions, respectively[44d]) were compared (FIGURE 3.2).

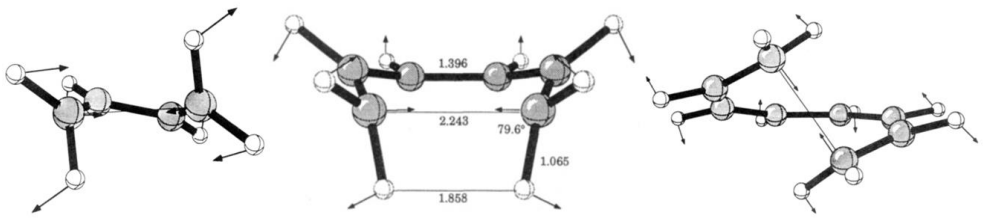


FIGURE 3.2 Transition states (with transition vectors) for the butadiene-cyclobutene[44a,b,d], hexatriene-cyclohexadiene[44e] and octatetraene-cyclooctatriene[44d] interconversions.

In these larger systems, the inside and outside substituents at the interacting termini have approximately the same relationship with the forming/breaking bond. In contrast, the rotation about each terminus is more pronounced for the butadiene-cyclobutene interconversion, and one substituent is therefore more capable of overlap with the frontier molecular orbitals of the π-system than the other substituent germinal to it. Smaller electronic effects are therefore expected for these larger systems than in the butadiene-cyclobutene interconversion and steric effects are predicted to be important in dictating the torquoselectivity.[44d,e]

On the other hand, Inagaki's theory of geminal bond participation,[45] as the name suggests, rationalizes torquoselectivity in electrocyclic reactions by looking at the interactions between orbitals at bonds geminal to the reacting center and the breaking or forming bond.

Bonding/anti-bonding properties of the delocalizations from geminal σ bonds are found to be opposite to each other. By comparing the inter-bond energies and inter-bond populations between the '*in*' and '*out*' substituents and the reacting centers, one finds that delocalization from electron-donating substituents is bonding whereas from electron-withdrawing substituents, it is anti-bonding. This leads to the conclusion that electropositive substituents prefer inward rotation, whereas electronegative substituents prefer outward rotation.

Many experimental and computational studies have been carried out to elucidate the cause of the torquoselectivity for various types of the Nazarov reaction.[46-55] While some have concluded that stereoelectronic effects are mainly the cause of the observed torquoselectivity,[47,48,50a] others have shown that differences in energy barriers for the different modes of conrotation can be primarily attributed to steric effects between substituents during cyclization.[47b, 52,53]

According to Houk and co-workers,[44b,d] steric effects should have an effect of no more than a few kcal mol^{-1} on the differences in barrier energies for the transition states that lead to the two possible isomers in a conrotatory electrocyclization, whereas stereoelectronic effects would be responsible for much larger differences in energies (i.e., an order of magnitude larger, or more).

For example, He *et al.*[50a] showed how substitution of divinyl ketones undergoing Nazarov cyclization affect reactivity, and that the torquoselectivity results from stereoelectronic effects. In contrast to this study, Marcus *et al.*[50b] presented evidence for significant steric effects between α- and γ-substituents of aryl dienyl ketones (1,3-allylic strain). This strain was found to be a primary factor that affected the cyclization step of the Nazarov reaction.

Flynn and co-workers[52] used an oxazolidinone-controlled Nazarov cyclization process in the enantioselective synthesis of (+)- and (–)-pauciflorol F, which produced these enantiomers with high enantiomeric ratios. They rationalized the torquoselectivity in this auxiliary-based Nazarov reaction to the presence of allylic strain and steric interactions between the pentadienyl and oxazolidinone substituents. As opposed to traditional coplanar

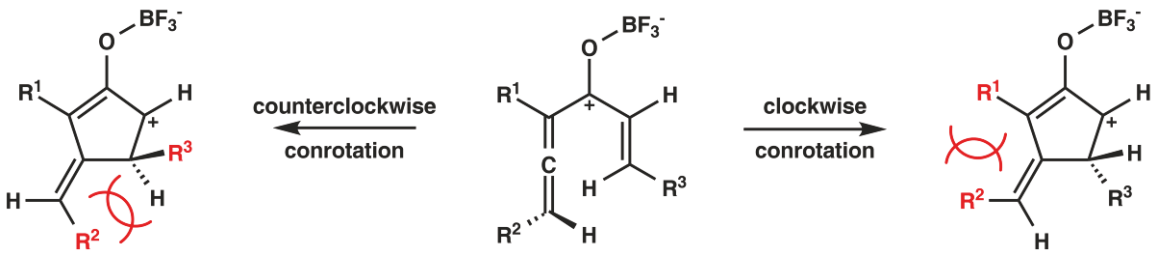
transition states, the reaction was found to proceed through a noncoplanar transition state where minimization of this allylic strain dictated the preferred pathway to obtaining the experimentally observed product.

Sanz *et al.*[53] showed that torquoselectivity in the gold-catalyzed Nazarov cyclization of 3-propargylindoles results from the minimization of some steric/developing allylic strain between the indole and propargyl substituents.

de Lera and co-workers as well as Tius and co-workers have shown similar results in their studies of the ring closures of vinylallenes,[54a,b] vinylallene acetals[54c,d] and allene ethers.[55] Steric interactions between substituents on the allene moiety or between the substituents on the distal carbons of the allene and vinyl moieties is thought to be responsible for the observed torquoselectivities, rather than stereoelectronic effects.

3.4 Project Objective and Motivation

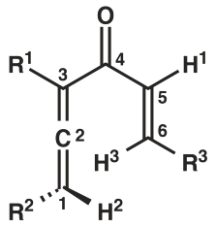
The torquoselectivity in the Nazarov reaction of allenyl vinyl ketones has not been systematically studied. Experimental research in the Burnell group[56] led to results showing that the favored product (obtained by clockwise mode of conrotation of the termini, as drawn in SCHEME 3.5) is that in which there are seemingly larger steric interactions between the R^1 and R^2 substituents, whereas the product obtained by counterclockwise mode of conrotation is disfavored. Moreover, as the steric interactions between these two positions increase (i.e., when the 'size' of the substituents increases), the ratio between products increases dramatically, up to the point where the only observed product is the one obtained by clockwise mode of conrotation (i.e., 3:1 versus >20:1 diastereomeric ratios in favor of the clockwise conrotation products for R^1, R^2, R^3 = Me and R^1, R^3 = Me, R^2 = ^{t}Bu, respectively).



SCHEME 3.5 Steric interactions present in the products of the Nazarov reaction.

The aim of the work in this chapter was to study this torquoselectivity computationally. This was to be more than a confirmation of experimental results. The real motivation was to explain the torquoselectivity in terms of the factors that determine this form of selectivity.

The systems of interest for this study are shown in FIGURE 3.3. Some of the substrates were chosen in order to corroborate the results obtained experimentally in the Burnell group, but also there are substrates that, unfortunately, were synthetically inaccessible but that computationally would provide valuable information regarding torquoselectivity.



	R^1	R^2	R^3
1	Me	Me	**a** H; **b** Me; **c** ^{i}Pr; **d** Ph
2	^{t}Bu	Me	
3	Me	^{t}Bu	
4	^{t}Bu	^{t}Bu	
5	Me	Ph	
6	^{t}Bu	Ph	

FIGURE 3.3 Allenyl vinyl ketones studied.

In the interest of brevity and consistency, the following conventions are used throughout this chapter: Structures are drawn of the same enantiomeric series showing the allenyl moiety to the left of the vinyl moiety so that "clockwise" and "counterclockwise" modes of conrotation in the Nazarov reaction are unambiguous to the reader. Thus, clockwise means that the terminal substituent on the allene is rotating away from the vinyl group. The substitution pattern shown also applies for the remainder of this discussion. Varying

degrees of substitution at the R^1, R^2 and R^3 positions of the allenyl vinyl ketones range from hydrogen (H), methyl (Me), isopropyl (^{i}Pr), *tert*-butyl (^{t}Bu) to phenyl (Ph) in order to evaluate the effect varying steric effects on the torquoselectivity in the thermal Lewis acid-mediated Nazarov reactions of these substrates.

3.5 Computational Methods

All of the quantum mechanical calculations were performed using the Gaussian 09 software package.[57] Stationary points were fully optimized in their ground states at the specified level of theory (B3LYP,[25] M06-2X,[31] or ωB97X-D[33] DFT functionals or the MP2[21b-g] perturbative approach), with the 6-31G(d), or a larger Pople basis set.[15] Minima and first-order saddle points were characterized by their number of imaginary frequencies (0 for minima and 1 for first-order saddle points) following normal-mode vibrational analysis. All first-order saddle points underwent intrinsic reaction coordinate calculations[36] in order to identify the minima on either side of the saddle point. All geometries and thermodynamic data were obtained from calculations done in the gas phase at 298.15 K and 1.0 atm unless otherwise indicated.

(Cartesian coordinates, energies and geometrical parameters for systems **1**-**6** presented in this chapter are given in Appendix 1.)

3.6 Preliminaries

Before undertaking the study of systems **1**-**6**, a few preliminary analyses were performed on selected systems (FIGURE 3.4) to verify a number of points.

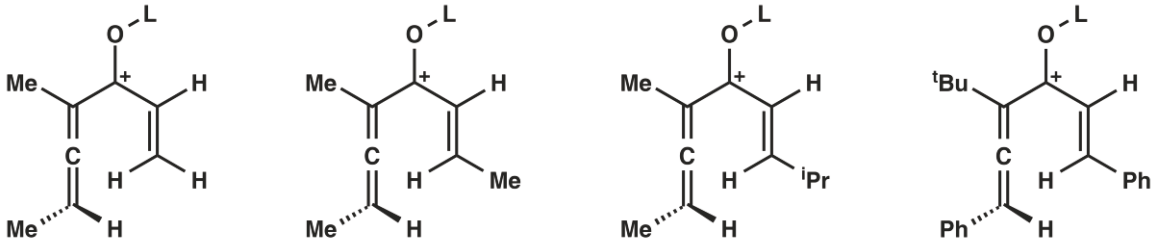


FIGURE 3.4 1a, **1b**, **1c** and **6d**, where L = BF_3 or H^+.

A conformational analysis of the pentadienyl cation **1b** was carried out in order to observe how substituents interact with each other and/or with the Lewis acid (or proton) complexed to the carbonyl oxygen. The relative energies of each conformer were then examined. Furthermore, the impact of exchanging the Lewis acid with a proton on the relative energy barrier heights for the Nazarov reaction pathways of the initial pentadienyl cation was evaluated.

A conformational analysis of systems containing an isopropyl substituent at the R^3 position was also carried out. The analysis of **1c** will be given as a representative example for all other systems containing an isopropyl substituent at this position.

Lastly, the relative energy barriers and geometries of **1a** and **6d** for the initial pentadienyl cation undergoing the Nazarov cyclization were computed and compared at different levels of theory in order to choose an appropriate method for further calculations.

3.6.1 Conformational Analysis of Pentadienyl Cations

Allenyl vinyl ketones (and their corresponding pentadienyl cations) exist in a variety of conformations, as illustrated for system **1b** in FIGURE 3.5. This is to be expected from the rotational flexibility about the carbon-carbon bonds with respect to the carbonyl carbon and proximal carbons of the vinyl and allenyl moieties. Furthermore, the Lewis acid can be complexed to the carbonyl oxygen *syn* or *anti* to the allenyl moiety. These conformers can further exist in either planar or nonplanar forms.

The relative energies of the conformers presented for pentadienyl cation **1b** are also shown in TABLE 3.1. The difference in energies of these conformers can be attributed to interactions between the substituents and the Lewis acid or the substituents with each other.

For example, consider the u-shaped conformers. The *anti*-L conformers are lower in energy compared to their *syn*-L counterparts, the methyl at the R^1 position interacts more with the Lewis acid or proton in the former than in the latter. The effect is larger for BF_3 than for H^+, as expected from the relative size of these two groups. The relative energies of the other conformers can be deduced accordingly by looking at the other interactions present, such as substituents on the allenyl moiety interacting with the ones on the vinyl moiety, or the Lewis acid (or proton) interacting with the substituents on carbons α or β to the ketone.

While it is the sickle-shaped conformer (**s-v**) that is of lowest energy in the case of the thermal boron trifluoride-mediated Nazarov reaction (and the w-shaped conformer (**w**) in the case of the proton-mediated Nazarov reaction), the reactive form of the pentadienyl cation in the Nazarov reaction can only be the u-shaped conformer (**u**).[6a,46,47,58] This conformer was therefore modelled as the starting reactant in this study.

In the two nonplanar forms (**cRT** and **ccRT**), the interactions between substituents are not the same. For instance, in the u-shaped conformers the interactions between substituents at the distal carbons are not equivalent in the **cRT** and **ccRT** forms. The fact that these differences exist between the nonplanar forms proved to be a deciding factor in which mode of conrotation is favored.

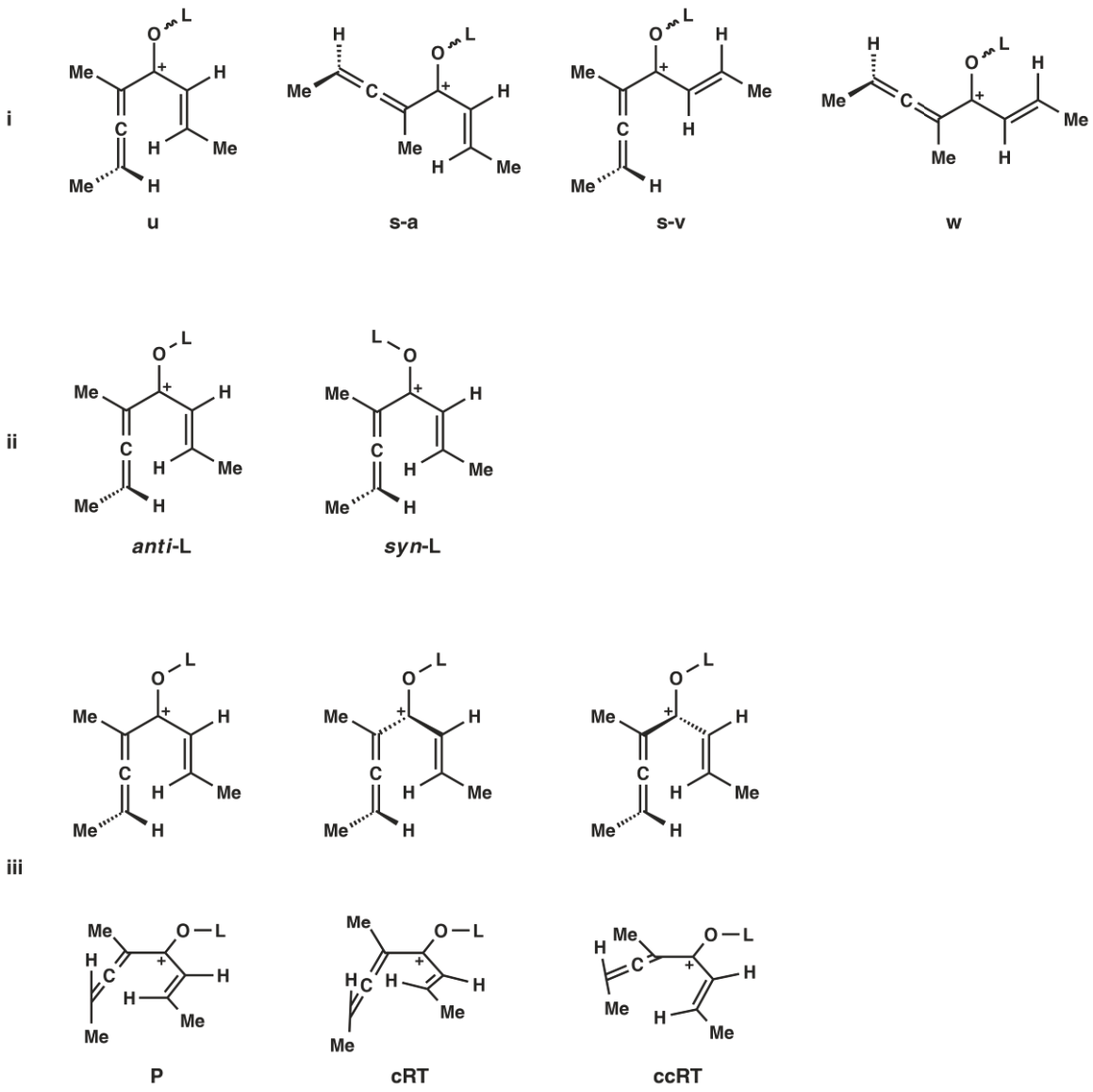


FIGURE 3.5 Conformational analysis of **1b** at the B3LYP/6-31G(d) level of theory. (i) Conformers of **1b** are the u-shaped conformer (**u**), the sickle-shaped conformers (**s-a** and **s-v**, indicating which moiety is pointing up, **a**llenyl or **v**inyl) and the w-shaped conformer (**w**).[6a,46,47,58] (ii) *Syn* or *anti* complexation to the carbonyl oxygen is possible by part of the Lewis acid or proton (denoted by L). (iii) As an example, planar (**P**) and nonplanar forms (**cRT** and **ccRT**) of the u-shaped conformer are shown.

TABLE 3.1 Conformational analysis of **1b** at the B3LYP/6-31G(d) level of theory.

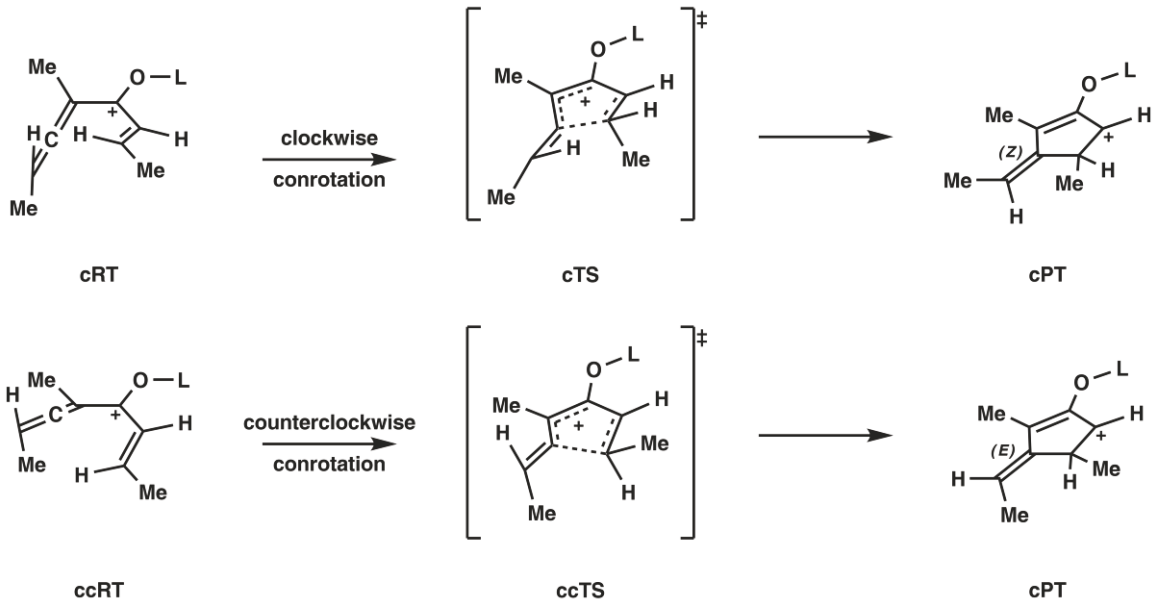
Conformer	Planar? [a]	Δ(E+ZPE) [b] (kJ mol^{-1})	Planar? [a]	Δ(E+ZPE) [b] (kJ mol^{-1})
anti-L		H^+		BF_3
u	No	0.0 / 0.3	No	0.0 / 0.2
s-a	No	9.2 / 9.3	No	17.7 / 17.3
s-v	Yes	-9.8	No	-4.7 / -4.7
w	No	0.1 / 0.1	No	9.8 / 9.8
syn-L		H^+		BF_3
u	No	0.6 / 0.8	No	14.8 / 15.9
s-a	Yes	-1.9	No	23.2 / 27.2
s-v	Yes	-18.2	Yes	2.5
w	Yes	-20.4	Yes	8.4

[a] When a conformer is nonplanar, the energies of both possible structures are indicated as follows: **cRT** / **ccRT**. [b] Energies are relative to the energy of the *anti*-L u-shaped conformer (**P** or **cRT**).

While searching for the transition states associated with the two conrotatory pathways of **1b**, it was found that the **cRT** form of the reactant led to the *Z* isomer (**cPT**), whereas the **ccRT** form led to the *E* isomer (**ccPT**) (SCHEME 3.6 and TABLE 3.2). Product distribution was assumed to be dependent only on relative transition state energies because the energy barrier for the interconversion between the **cRT** and **ccRT** structures was significantly smaller than the energy barriers for the formation of both products, **cPT** and **ccPT**.[59] (This is confirmed for systems **1a** and **6d** in Section **3.6.3**.)

Let us now take a look at the effect of exchanging boron trifluoride as the Lewis acid for a proton on the relative energy barriers between the two modes of conrotation.

Whether the Lewis acid or proton is *syn* or *anti* with respect to the allenyl moiety of the allenyl vinyl ketone poses no significant difference on the relative energy barriers between the clockwise and counterclockwise modes of conrotation. Exchanging H^+ for BF_3 has the effect of increasing the relative barrier heights (TABLE 3.2), which is to be expected from



SCHEME 3.6 Pathways associated to the two conrotatory modes of system **1b** undergoing a thermal boron trifluoride- or proton-mediated Nazarov reaction.

the size of BF_3 compared to H^+; BF_3 interacts more with the neighbouring substituents than does H^+. Most importantly, the clockwise mode of conrotation is preferred in all cases, which is in agreement with experiment for the boron trifluoride-mediated Nazarov reaction of the allenyl vinyl ketones studied here.

To summarize, conformational analysis of **1b** has shown that the *anti*-L u-shaped conformers are of lower energy compared to their *syn*-L counterparts. This would likely continue to be true for systems where the R^1, R^2 and R^3 substituents are larger than methyl. Exchanging boron trifluoride for a proton as the acid did not significantly affect relative barrier heights of the reaction or structural features of the reactants, transition states and products. Boron trifluoride was used as the Lewis acid experimentally, and so all subsequent calculations were done on systems with *anti*-BF_3 complexed allenyl vinyl ketones.

TABLE 3.2 Differences in transition state energies, $\Delta(E+ZPE)^{\ddagger}$, between clockwise and counterclockwise modes of conrotation for system **1b** undergoing a thermal boron trifluoride- and proton-mediated Nazarov reactions at the B3LYP/6-31G(d) level of theory.

Structure	$\Delta(E+ZPE)$ [a] (kJ mol^{-1})	
anti-L	H^+	BF_3
cRT / **ccRT**	0.0 / 0.3	0.0 / 0.2
cTS / **ccTS**	44.2 / 48.6	74.5 / 80.0
cPT / **ccPT**	-74.4 / -86.2	-20.5 / -29.7
$\Delta(E+ZPE)^{\ddagger}$ [b]	-4.3	-5.5
syn-L	H^+	BF_3
cRT / **ccRT**	0.0 / 0.2	0.0 / 1.1
cTS / **ccTS**	48.1 / 52.4	71.9 / 79.1
cPT / **ccPT**	-64.3 / -76.1	-25.5 / -36.1
$\Delta(E+ZPE)^{\ddagger}$ [b]	-4.3	-7.2

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, **cRT** or **ccRT**. [b] By convention, $\Delta(E+ZPE)^{\ddagger} = \Delta(E+ZPE)_{cTS} - \Delta(E+ZPE)_{ccTS}$, and so $\Delta(E+ZPE)^{\ddagger} < 0$ is indicative of the clockwise mode of conrotation being favored or the counterclockwise mode of conrotation.

3.6.2 Conformational Analysis of Systems Containing an Isopropyl Substituent at the R^3 Position

The systems studied were composed of allenyl vinyl ketones bearing various alkyl groups at the R^1, R^2 and R^3 positions. These alkyl groups (Me, ^{i}Pr, ^{t}Bu) were chosen so that the effect of increasing the steric bulk of these groups on relative interactions at these positions could be evaluated.

The methyl and *tert*-butyl groups had the advantage of having equivalent staggered conformations, which reduced the number of possibilities for reactant, transition state and product-like structures. This was, unfortunately, not the case with the isopropyl group. As can be seen from FIGURE 3.6 and TABLE 3.3, it can exist in three non-equivalent staggered conformations, which could react through three distinct transition states.

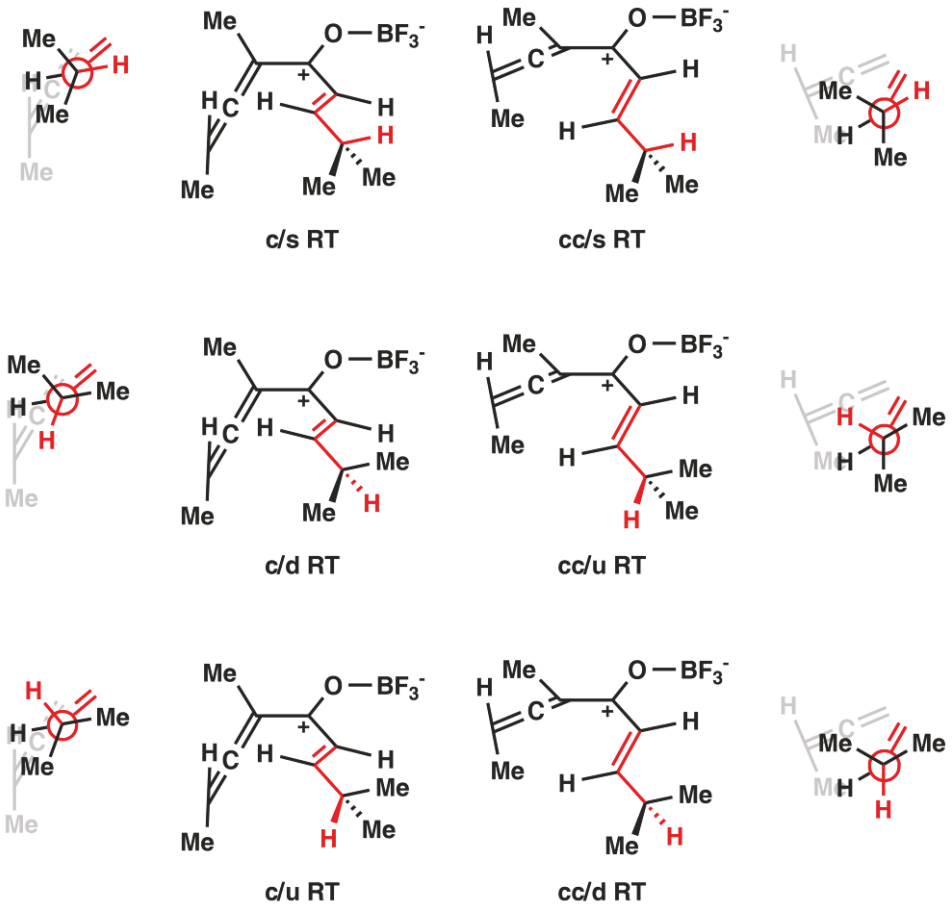


FIGURE 3.6 Conformational analysis of the isopropyl substituent for system **1c** undergoing a thermal boron trifluoride-mediated Nazarov reaction.

The **c**/**s** and **cc**/**s** are the conformers where the isopropyl hydrogen is approximately ***s****yn* to the double-bond and where the methyls are interacting with the remote allenyl moiety of the pentadienyl cation (shown in grey in FIGURE 3.6).

As for the **c**/**u**,**cc**/**u** and **c**/**d**,**cc**/**d** pairs of conformers, they depict the central isopropyl hydrogen pointing **u**p or **d**own, respectively. One of the isopropyl methyls interacted more with the allenyl moiety than the other. The reason for pairing the **c**/**d** structures with the **cc**/**u** structures and the **c**/**u** structures with the **cc**/**u** structures in FIGURE 3.6 was so that the relative interactions between substituents remained the same when comparing **c** and **cc** structures. In other words, the isopropyl fragments were assumed to remain in the same conformation during the cyclization.

TABLE 3.3 Differences in transition state energies, $\Delta(E+ZPE)^{\ddagger}$, between clockwise and counterclockwise modes of conrotation for system **1c** undergoing a thermal boron trifluoride-mediated Nazarov reaction at the B3LYP/6-31G(d) level of theory.

Structure	$\Delta(E+ZPE)$ [a] (kJ mol^{-1})	D(R^3(H),R^3,C_6, C_5) [b] (degrees)
1c, R^3 = ^{i}Pr		
c/s RT / **cc/s RT**	0.0 / 0.2	-4.8 / 4.5
c/s TS / **cc/s TS**	84.4 / 99.7	-39.2 / 35.5
c/s PT / **cc/s PT**	-10.9 / -14.8	-72.5 / 69.1
$\Delta(E+ZPE)^{\ddagger}$	-15.2	
c/d RT / **cc/u RT**	0.0 / 0.3	-124.6 / 124.7
c/d TS / **cc/u TS**	74.0 / 80.1	-156.3 / 173.4
c/d PT / **cc/u PT**	-22.9 / -31.3	-173.4 / 172.8
$\Delta(E+ZPE)^{\ddagger}$	-6.1	
c/u RT / **cc/d RT**	0.0 / 0.3	120.5 / -120.4
c/u TS / **cc/d TS**	79.8 / 90.9	55.8 / -38.9
c/u PT / **cc/d PT**	-17.7 / -20.9	59.5 / -58.4
$\Delta(E+ZPE)^{\ddagger}$	-11.1	

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, **cRT** or **ccRT**. [b] R^3(H) = central isopropyl hydrogen.

The **c/s** and **cc/s** structures led to higher energy transition state structures compared to the **c/d**,**cc/u** and **c/u**,**cc/d** pairs. The preferred pathway for the isopropyl-containing systems was the **c/d**,**cc/u** pair, where the isopropyl hydrogen interacted the most with the allenyl moiety and where the methyls were pointing away from it. The relative energy barriers for this pair were approximately equal to that of system **1b** (TABLE 3.2, *anti*-BF_3), which has a methyl group at the R^3 position.

The **c/s**,**cc/s** pair where both methyls are interacting with the allenyl moiety could be approximated to a system containing a *tert*-butyl group at the R^3 position, and energy barriers for these conformers should be similar to a system containing *tert*-butyl groups at the R^3 position.

3.6.3 Choosing an Adequate Level of Theory and Basis Set for Further Calculations

The B3LYP functional has been widely used to explore potential energy surfaces of systems similar to the ones presented here.[46,47a,48cd,49,50b,51a,52d,53,54cd] In this section, an explanation will be provided to why this functional and the 6-31G(d) basis set were chosen for the study of torquoselectivity in the thermal Lewis acid-mediated Nazarov reaction of systems **1**-**6**.

Reactant, transition state and product structures of **1a** and **6d**, the smallest and largest systems studied, respectively, were located at a variety of levels of theory and basis sets for both pathways and the differences in transition state energies were computed. Results are shown in TABLE 3.4 and TABLE 3.5.

The B3LYP/6-31G(d) level of theory was found to be an adequate choice for modelling the Nazarov reaction of allenyl vinyl ketones. The differences in transition state energies calculated at other levels of theory (full optimizations as well as single-point energy calculations on B3LYP/6-31G(d) geometries) were not significantly different to the ones calculated at the B3LYP/6-31G(d) level of theory for system **1a** (TABLE 3.4).

Including polarization and/or diffuse functions on hydrogen atoms or using a split-valence triple zeta basis set, for example, did not improve upon or disagree with the results found with the 6-31G(d) basis set. Calculations in the solvent phase were also performed to ensure that gas phase calculations are representative of experiment. Dielectric constants were chosen to represent the experimentally used solvent, dichloromethane, and a more polar solvent, methanol, to verify that polarity would not significantly affect geometries or computed energies in the reaction profiles.

TABLE 3.4 Differences in transition state energies, $\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$), between clockwise and counterclockwise modes of conrotation for systems **1a** at different levels of theory and basis sets.

Level of theory and basis set	$\Delta E^{\ddagger}$ (kJ mol^{-1})	$\Delta(E+ZPE)^{\ddagger}$ [a] (kJ mol^{-1})
1a		
B3LYP/6-31G(d)	-2.2	-1.9
B3LYP/6-31+G(d,p)	-2.4	-2.2
B3LYP/6-31+G(d,p)//B3LYP/6-31G(d)	-2.5	-2.2
B3LYP/6-311G(d)	-2.6	-2.3
B3LYP/6-311+G(d,p)	-2.8	-2.5
B3LYP/6-31G(d)/SCRF=(PCM, CH_2Cl_2, $\varepsilon = 8.93$) [b]	-2.2	-2.0
B3LYP/6-31G(d)/SCRF=(PCM, CH_3OH, $\varepsilon = 32.613$) [b]	-2.3	-1.9
M06-2X/6-31+G(d,p)	-1.3	-1.2
M06-2X/6-31+G(d,p)//B3LYP/6-31G(d)	-1.5	-1.2
MP2/6-31+G(d,p)	-1.7	-1.5
MP2/6-31+G(d,p)//B3LYP/6-31G(d)	-1.9	-1.6
ωB97X-D/6-31+G(d,p)	-1.5	-1.4
ωB97X-D/6-31+G(d,p)//B3LYP/6-31G(d)	-1.7	-1.4

[a] Zero-point energy (ZPE) corrections from the B3LYP/6-31G(d) level of theory were included in single-point energy calculations. [b] Calculations were done in the specified solvent phase using the default polarizable continuum model (PCM) method as implemented in Gaussian 09.[60]

As some of the systems studied here contained substituents that might interact by van der Waals forces, a verification for dispersion was made on **6d**, a system containing phenyl rings at the R^2 and R^3 positions (*cf.* FIGURE 3.3). As can be seen from TABLE 3.5, calculations performed with a method accounting for dispersion (e.g., ωB97X-D, M06-2X and MP2) were not in agreement with those performed at B3LYP/6-31G(d) level of theory.

TABLE 3.5 Differences in transition state energies, $\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$), between clockwise and counterclockwise modes of conrotation for systems **6d** at different levels of theory and basis sets.

Level of theory and basis set	$\Delta E^{\ddagger}$ (kJ mol^{-1})	$\Delta(E+ZPE)^{\ddagger}$ [a] (kJ mol^{-1})
6d		
B3LYP/6-31G(d)	-11.5	-10.3
B3LYP/6-31+G(d,p)	-11.7	-10.5
B3LYP/6-31+G(d,p)//B3LYP/6-31G(d)	-11.7	-10.5
B3LYP/6-31G(d) SCRF=(CH_2Cl_2, ε=8.93)	-10.4	-9.3
B3LYP/6-31+G(d,p) SCRF=(CH_2Cl_2, ε=8.93)	-11.7	-10.5
M06-2X/6-31G(d)	-1.5	-0.6
M06-2X/6-31+G(d,p)	-1.5	-0.5
M06-2X/6-31+G(d,p)//B3LYP/6-31G(d)	-7.8	-6.6
M06-2X/6-31G(d) SCRF=(CH_2Cl_2, ε=8.93)	-0.7	0.0
M06-2X/6-31+G(d,p) SCRF=(CH_2Cl_2, ε=8.93)	-0.4	0.5
MP2/6-31+G(d,p)//B3LYP/6-31G(d)	-0.8	0.3
ωB97X-D/6-31G(d)	-1.5	-0.6
ωB97X-D/6-31+G(d,p)	-1.7	-1.4
ωB97X-D/6-31+G(d,p)//B3LYP/6-31G(d)	-7.2	-6.0
ωB97X-D/6-31G(d) SCRF=(CH_2Cl_2, ε=8.93)	-0.6	0.6
ωB97X-D/6-31+G(d,p) SCRF=(CH_2Cl_2, ε=8.93)	-0.4	1.0

[a] Zero-point energy (ZPE) corrections from the B3LYP/6-31G(d) level of theory were included in single-point energy calculations. [b] Calculations were done in the specified solvent phase using the default polarizable continuum model (PCM) method as implemented in Gaussian 09.[60]

By comparing the two energy diagrams of **6d** at the B3LYP/6-31G(d) and ωB97X-D/6-31+G(d,p) levels of theory (FIGURE 3.7), one can clearly see that the reactant, transition and product-like structures for the counterclockwise mode of conrotation computed at the latter level of theory are significantly shifted down in terms of energy. The phenyl rings are closer to one another and in a parallel arrangement, suggesting π-π stacking,[28a,b] which could explain stabilization of the reactant and transition state structures (FIGURE 3.8).

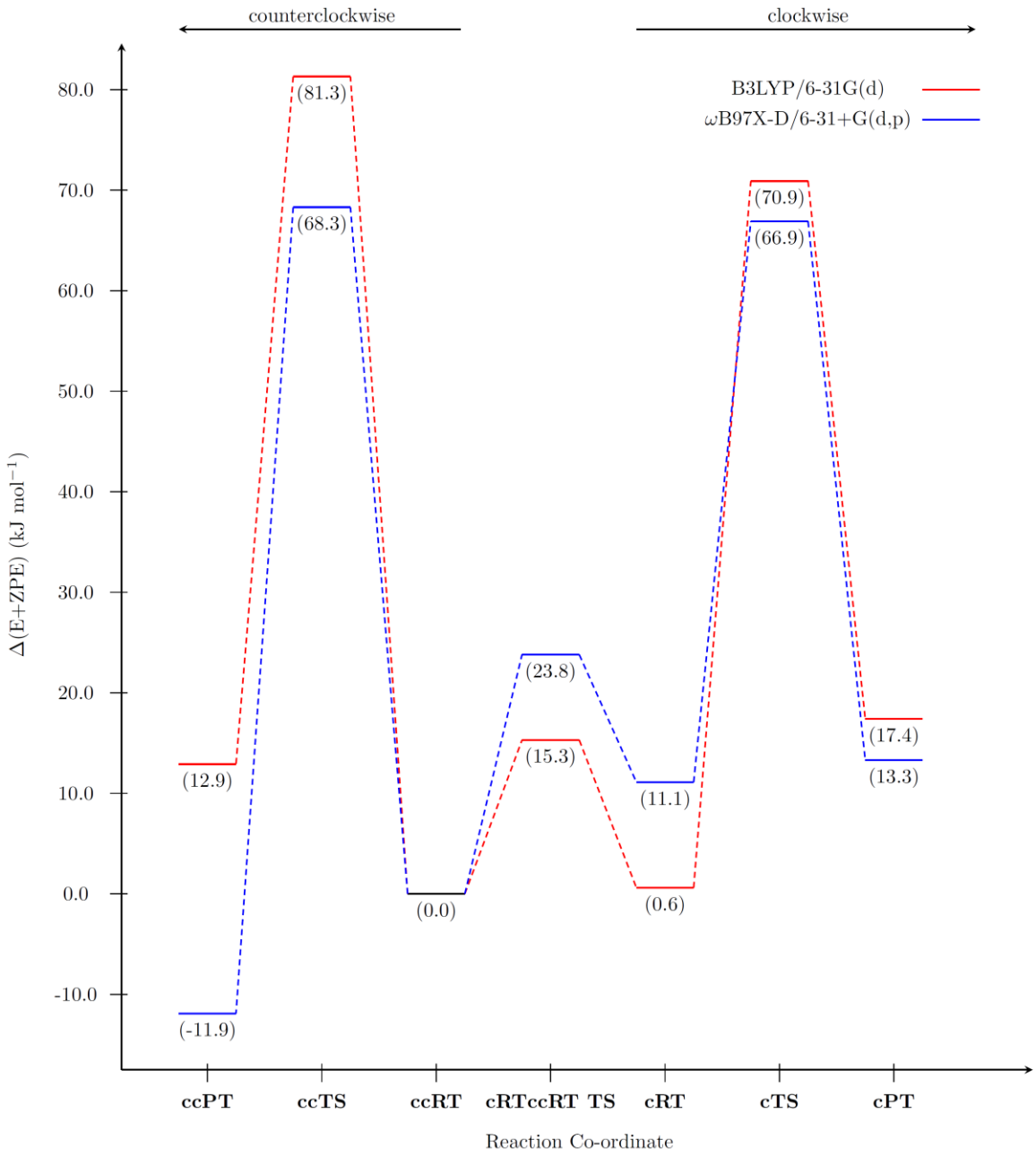


FIGURE 3.7 Energy diagrams for system **6d**, R^3 = Ph, at the B3LYP/6-31G(d) and ωB97X-D/6-31+G(d,p) levels of theory. All energies are relative to that of the **ccRT** reactant structure at the corresponding level of theory.

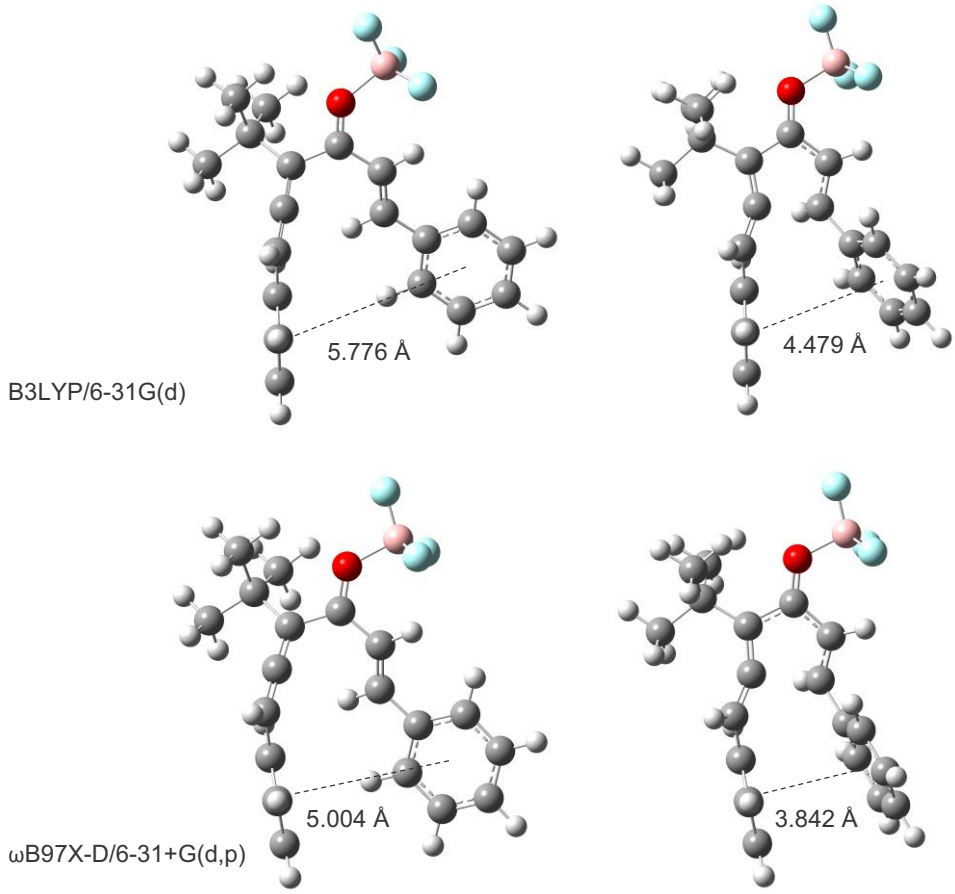


FIGURE 3.8 Interactions between the phenyl rings at the R^2 and R^3 positions in the reactant and transition state structures for the counterclockwise mode of conrotation of **6d** at the B3LYP/6-31G(d) and ωB97X-D/6-31+G(d,p) levels of theory.

This effect is much less evident in the clockwise mode of conrotation as the rings are further apart from each other throughout the reaction.

The calculations at the ωB97X-D/6-31+G(d,p) level of theory for **6d** predicted that there should be little selectivity between both modes of conrotation, while calculations performed at the B3LYP/6-31G(d) level of theory predicted a diastereomeric ratio of ~100:0 in favor of **cPT**. This prompted experiments in order to verify if calculations including dispersion were valid or not. As it turned out, performing a Nazarov reaction with **6d** yielded **cPT**:**ccPT** in a greater than 20:1 diastereomeric ratio. Influence of dispersion appears by experiment to be overestimated in calculations performed at the

ωB97X-D/6-31+G(d,p) level of theory and therefore justifies the use of the B3LYP/6-31G(d) level of theory for further calculations.

On another matter, one may have noticed that the difference in transition state energies between the two conrotatory pathways was used to establish which pathway was favored over the other for the results presented in previous tables. The systems studied here were found to follow Curtin-Hammett/Winstein-Holness kinetics.[59] In general, a compound existing in two interconverting isomeric forms, A_2 and A_3, that react by first order kinetics to produce two different products, A_1 and A_4, can be described as follows:

$$A_1 \overset{k_{21}}{\longleftarrow} A_2 \underset{k_{32}}{\overset{k_{23}}{\rightleftharpoons}} A_3 \overset{k_{34}}{\longrightarrow} A_4 \qquad (3.\ 1)$$

It is generally the case for organic reactions, that interconversion between isomeric forms is rapid compared to the reactions themselves ($k_{23}, k_{32} \gg k_{21}, k_{34}$). The product distribution can then be described as:

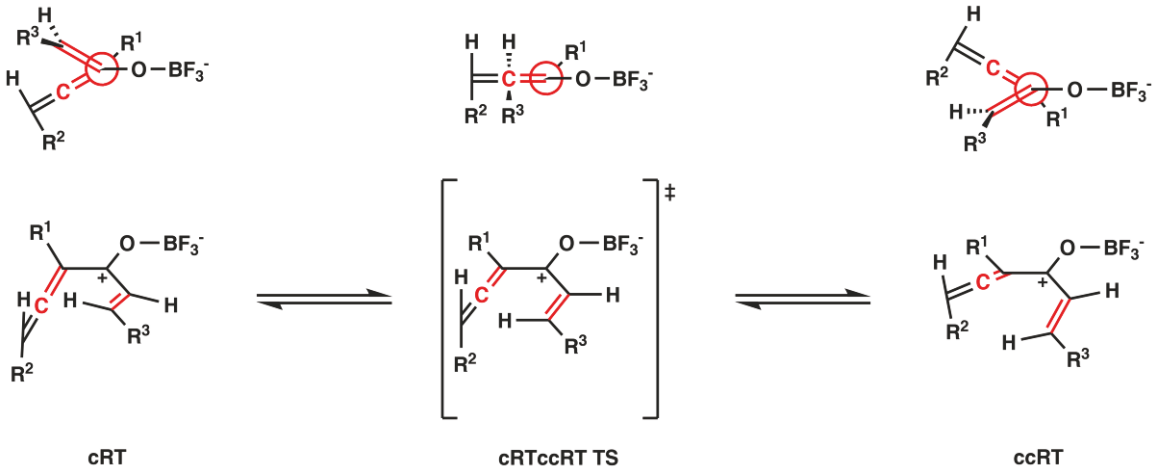
$$\frac{[A_4]}{[A_1]} = K\frac{k_{34}}{k_{21}} = e^{\frac{-(\Delta G_{34}{}^{\ddagger} + \Delta G^0 - \Delta G_{21}{}^{\ddagger})}{RT}} = e^{\frac{-\Delta G^{\ddagger}}{RT}} \qquad (3.\ 2)$$

where $K = \frac{[A_3]}{[A_2]}$ is constant as imposed by the fact that $k_{23}, k_{32} \gg k_{21}, k_{34}$, $\Delta G_{21}{}^{\ddagger}$ and $\Delta G_{34}{}^{\ddagger}$ are the activation barriers for the formation of A_1 and A_4, respectively, ΔG^0 is the difference between reactant energies and $\Delta G^{\ddagger}$ is the difference between transition state energies. The product distribution is therefore a function of the relative transition state energies, $\Delta G^{\ddagger}$, of the two associated pathways for the formation of the products (not just the difference in activations barriers, $\Delta\Delta G^{\ddagger}$). Of course, if the difference in energy between the two reactant conformers, **cRT** and **ccRT**, is nil ($\Delta G^0 = 0$), (3.2) can be rewritten as a function of $\Delta\Delta G^{\ddagger}$, or the difference in activation barriers for the two pathways:

$$\frac{[A_4]}{[A_1]} = e^{\frac{-(\Delta G_{34}{}^{\ddagger} - \Delta G_{21}{}^{\ddagger})}{RT}} = e^{\frac{-\Delta\Delta G^{\ddagger}}{RT}}$$

(3. 3)

Take for example, systems **1a** and **6d** (SCHEME 3.7 and TABLE 3.6). Energy diagrams of **6d** at the B3LYP/6-31G(d) and ωB97X-D/6-31+G(d,p) levels of theory were given in FIGURE 3.7.



SCHEME 3.7 Interconversion between **cRT** and **ccRT** structures.

For **1a** and **6d** at the B3LYP/6-31G(d) level of theory, both ΔE_o and $E_{cRT,ccRT}{}^{\ddagger}$ are significantly smaller than the activation barriers, $\Delta E_{cRT,cPT}{}^{\ddagger}$ and $\Delta E_{ccRT,ccPT}{}^{\ddagger}$. In fact, there is at least a 50 kJ mol^{-1} difference between $E_{cRT,ccRT}{}^{\ddagger}$ and the two activation barriers, indicating that the rate constant for interconversion between the **cRT** and **ccRT** would be roughly 5.8 x 10^8 times greater than that for the electrocyclic reactions leading to **cPT** and **ccPT**. Thus, one can assume that the two isomeric forms are at rapid equilibrium and that the reactions leading to the product oxyallyl cations are significantly slower. The Curtin-Hammet/Winstein-Holness principle holds, and so the product distribution should be described by the relative transition state energies, $\Delta E_{TS}{}^{\ddagger}$.

TABLE 3.6 Differences in transition state energies, $\Delta(E+ZPE)^{\ddagger}$, between clockwise and counterclockwise modes of conrotation for systems **1a** and **6d** undergoing a thermal boron trifluoride-mediated Nazarov reaction.

Structure	$\Delta(E+ZPE)$ [a] (kJ mol^{-1})	D(C_2,C_3,C_5,C_6) (degrees)
1a, R^3 = H (B3LYP/6-31G(d))		
cRT / **ccRT**	0.0 / 0.0	-45.1 / 44.6
cTS / **ccTS**	69.3 / 71.3	-26.4 / 26.7
cPT / **ccPT**	-45.1 / -57.2	0.0 / 0.0
cRTccRT TS	8.5	-2.1
$\Delta(E+ZPE)^{\ddagger}$	-1.9	
6d, R^3 = Ph (B3LYP/6-31G(d))		
cRT / **ccRT**	0.6 / 0.0	-54.3 / 47.7
cTS / **ccTS**	70.9 / 81.3	-25.6 / 20.7
cPT / **ccPT**	17.4 / 12.9	-9.2 / 1.3
cRTccRT TS	15.3	-4.7
$\Delta(E+ZPE)^{\ddagger}$	-10.3	
6d, R^3 = Ph (RωB97X-D/6-31+G(d,p))		
cRT / **ccRT**	11.1 / 0.0	-54.6 / 48.7
cTS / **ccTS**	66.9 / 68.3	-28.1 / 24.7
cPT / **ccPT**	13.3 / -11.9	-11.7 / 3.2
cRTccRT TS	23.8	-10.1
$\Delta(E+ZPE)^{\ddagger}$	-1.4	

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, **cRT** or **ccRT**.

3.7 Results and Discussion

Calculations at the B3LYP/6-31G(d) level fo theory predict in all cases that the clockwise mode of conrotation is favored in the thermal boron trifluoride-mediated Nazarov reactions

of systems **1-6**, resulting in the formation of the kinetically favored product (TABLE 3.7, *cf.* SCHEMES 3.5 and 3.6).

TABLE 3.7 Differences in transition state energies, $\Delta(E+ZPE)^{\ddagger}$ / and in Gibbs energies of activation, $\Delta(E+G_{corr})^{\ddagger}$ (kJ mol^{-1}), between clockwise and counterclockwise modes of conrotation for systems **1-6** at the B3LYP/6-31G(d) level of theory.

R^1,R^2 =	**1** Me,Me	**2** ^{t}Bu,Me	**3** Me,^{t}Bu	**4** ^{t}Bu,^{t}Bu	**5** Me,Ph	**6** ^{t}Bu,Ph
R^3 =						
a H	-1.9 / -2.1	-1.7 / -1.7	-10.3 / -10.1	-5.0 / -3.7	-5.1 / -5.5	-4.3 / -3.9
b Me	-5.5 / -5.7	-6.0 / -5.9	-19.5 / -20.1	-15.8 / -15.4	-5.2 / -5.8	-4.3 / -4.3
c ^{i}Pr ~ Me [a]	-6.1 / -6.6	-6.8 / -7.6	-20.3 / -21.4	-15.8 / -15.7	-5.9 / -6.0	-5.1 / -4.5
c ^{i}Pr	-11.1 / -11.3	-12.7 / -13.8	-32.4 / -35.2	-29.9 / -31.6	-13.9 / -13.6	-13.7 / -13.8
c ^{i}Pr ~ ^{t}Bu [a]	-15.2 / -15.7	-17.5 / -18.1	-32.8 / 34.8	-38.7 / -39.8	-16.1 / -16.6	-15.9 / -16.4
d Ph	-6.2 / -6.2	-6.6 / -6.6	-20.9 / -22.3	-16.9 / -17.3	-10.9 / -11.8	-10.3 / -10.6

[a] *cf.* Section **3.6.2**. The **c/d**,**cc/u** and **c/s**,**cc/s** pairs are approximated as having R^3 = Me and R^3 = ^{t}Bu, respectively instead of R^3 = ^{i}Pr.

Recall from Section **3.4**, SCHEME 3.5, that experimental results showed that **1b** underwent a Nazarov reaction to produce both isomers **cPT** and **ccPT** in a 3:1 ratio, whereas **3b** produced **cPT** in upwards of a 20:1 ratio with respect to another product, assumed to be **ccPT**. In fact, this turns out to be true for all other systems studied experimentally other than **1b**. It should quickly be noted that systems containing R^3 = H could not be studied experimentally since the allenyl vinyl ketones cannot be prepared by procedures similar to those used to synthesize the other Nazarov substrates. Furthermore, the products obtained by Nazarov cyclization of system **4** decomposed very quickly and therefore could not be analyzed spectroscopically. This is thought to be due to the fact that the two ^{t}Bu groups being very close to one another in the product led to considerable instability.

Calculations for systems **1-6** were also performed at the ωB97X-D/6-31+G(d,p) level of theory following the results on **6d** from Section **3.6.3**. These results are presented in TABLE 3.8. There are no significant differences between values of $\Delta(E+ZPE)^{\ddagger}$ (or $\Delta(E+G_{corr})^{\ddagger}$) calculated at the B3LYP/6-31G(d) and ωB97X-D/6-31+G(d,p) levels of theory for systems **1-4**, with the exception of **1-4d** (R^3 = Ph) and both **5** and **6** (which contain R^2 = Ph). Dispersion seems to have a greater effect on systems containing a phenyl substituent at either the R^2 or R^3 positions and seems to cause a decrease in torquoselectivity

TABLE 3.8 Differences in transition state energies, $\Delta(E+ZPE)^{\ddagger}$ / and in Gibbs energies of activation, $\Delta(E+G_{corr})^{\ddagger}$ (kJ mol^{-1}), between clockwise and counterclockwise modes of conrotation for systems **1**-**6** at the ωB97X-D/6-31+G(d,p) level of theory.

R^1,R^2 =	**1** Me,Me	**2** ^{t}Bu,Me	**3** Me,^{t}Bu	**4** ^{t}Bu,^{t}Bu	**5** Me,Ph	**6** ^{t}Bu,Ph
R^3 =						
a H	-1.4 / -1.8	-2.6 / -1.7	-11.1 / -11.3	-9.4 / -7.1	-3.3 / -3.7	-6.2 / -5.9
b Me	-4.5 / -4.3	-6.4 / -5.5	-20.0 / -21.5	-19.9 / -20.6	-1.3 / -3.7	-4.1 / -5.5
c ^{i}Pr ~ Me [a]	-3.9 / -5.5	-6.5 / -7.6	-19.4 / -22.4	-17.5 / -17.7	0.8 / -0.5	-2.3 / 3.0
c ^{i}Pr	-10.1 / -12.5	-13.2 / -13.7	-33.6 / -36.6	-33.8 / -36.0	-5.5 / -9.6	-9.5 / -13.6
c ^{i}Pr ~ ^{t}Bu [a]	-15.0 / -15.8	-18.3 / -18.7	-31.3 / -32.3	-41.0 / -42.6	-11.3 / -13.9	-13.2 / -13.5
d Ph	-3.0 / -4.7	-5.2 / -6.4	-17.5 / -21.7	-16.8 / -18.0	2.2 / -2.2	-1.4 / -5.0

[a] *cf.* Section **3.6.2**. The **c/d**,**cc/u** and **c/s**,**cc/s** pairs are approximated as having R^3 = Me and R^3 = ^{t}Bu, respectively instead of R^3 = ^{i}Pr.

compared to the results at the B3LYP/6-31G(d) level of theory. Results with the B3LYP/6-31G(d) level of theory are in better accord with experiment than those at the ωB97X-D/6-31+G(d,p) level of theory. Because of this, the remainder of this discussion will be based solely on the results at the B3LYP/6-31G(d) level of theory.

Some general observations can be made from TABLE 3.7. As the 'size' of the R^3 substituents increases, so does the difference between the transition state energies for the clockwise and counterclockwise modes of conrotation. When varying the R^2 substituent from Me to ^{t}Bu while keeping R^1 and R^3 constant, this difference in energy increases even more than when R^3 is varied. For example, there is a three- to five-fold increase when R^1 = Me and R^2 varies from Me to ^{t}Bu (systems **1** and **3**). Similarly, there is a roughly two- to three-fold increase when R^1 = ^{t}Bu and R^2 varies from Me to ^{t}Bu (systems **2** and **4**). Notice that when R^1 gets larger in these two scenarios (comparing systems **1** and **3** with systems **2** and **4**), that the relative increase is smaller. Comparison with systems **5** and **6** is more difficult because these contain a phenyl substituent at the R^2 position. However, they seem to have roughly the same effect as when a methyl was placed at these positions. It seems that interactions between the R^1, R^2 and R^3 are dictating the sense of torquoselectivity in the acid-mediated Nazarov reactions of allenyl vinyl ketones.

3.7.1 Origins of Torquoselectivity in the Thermal Acid-Mediated Nazarov Reaction of Allenyl Vinyl Ketones

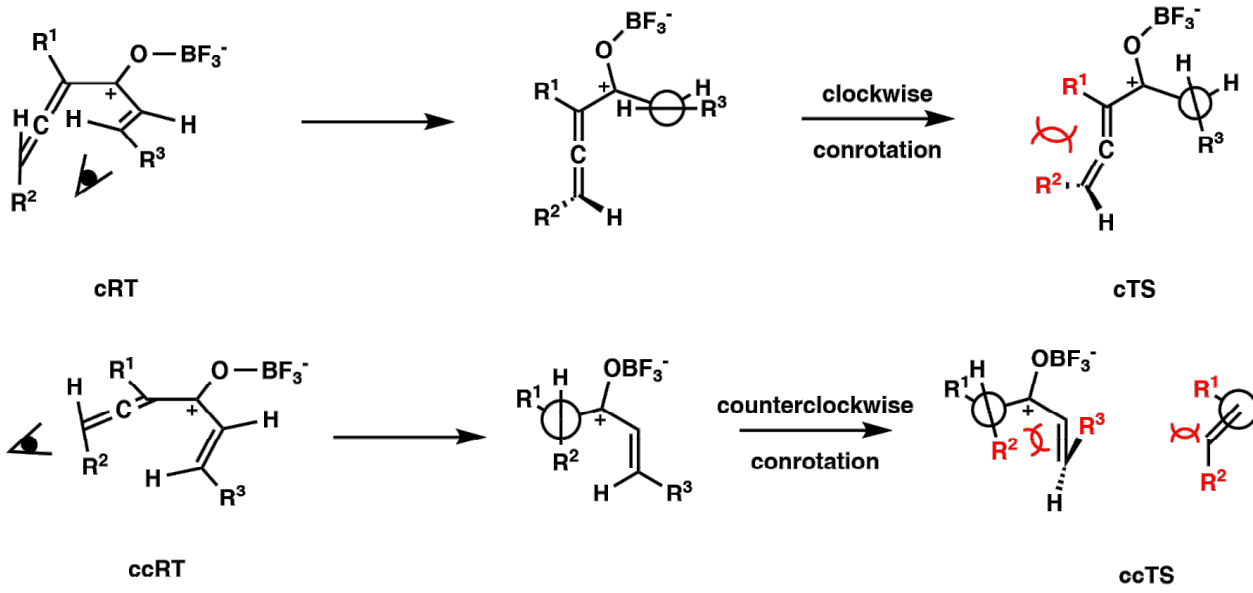
How can the torquoselectivity be rationalized for allenyl vinyl ketones in systems **1**-**6**? Kallel and Houk[44c] predicted that electronic effects should be important in the electrocyclization of pentadienyl cations. However, as discussed earlier for larger 6π- and 8π-electron systems (*cf.* Section **3.3**), electronic effects are diminished as the substituents on the cyclizing carbons have the same geometrical relationship to the breaking/forming bond. For systems **1**-**6**, the R^3 substituent on the vinyl moiety in the **cTS** and **ccTS** structures have similar geometries to the forming bond. Values of the dihedral angle, $D(R^3,C_6,C_5,C_4)$, can be verified to be approximately equal in **cTS** and **ccTS** structures (see Appendix 1, TABLES A1.4-A1.9). As such, even if there were electronic effects at play here, they should be very similar for both modes of conrotation and should not affect the degree of torquoselectivity.

It is thus assumed that the torquoselectivity in the acid-mediated Nazarov of allenyl vinyl ketones is due mostly to steric effects between substituents on the allenyl vinyl ketone framework. The hypothesis in terms of what steric interactions are dictating the sense of torquoselectivity is depicted in SCHEME 3.8.

The remainder of this discussion focuses on steric interactions between substituents at the R^1, R^2 and R^3 substituents based on their steric bulk. Steric bulk was estimated by the use of Taft steric substituent constants (TABLE 3.9).[61] Furthermore, the plots in FIGURES 3.9-3.12 have been constructed to represent the effect of varying the R^3 substituent (H, Me, ^{i}Pr, ^{t}Bu or Ph) on systems **1**-**6**. The effects of varying R^1 (Me or ^{t}Bu) can be observed from these plots by comparing systems **1** with **2, 3** with **4** or **5** with **6**, respectively. For the effects of varying R^2 (Me, ^{t}Bu or Ph), compare systems **1**, **3** with **5** or **2**, **4** with **6**, respectively. The trendlines shown have been fit to the data points in each series using the method of least squares / linear regression model.

Clockwise mode of conrotation

Steric interactions develop between R^1 and R^2 as the allene terminus rotates in a clockwise fashion. Interactions between R^2 and R^3 are negligeable.



Counterclockwise mode of conrotation

Steric interactions develop between R^2 and R^3 as both termini rotate in a counterclockwise fashion. Bending supercedes twisting of the allene to counteract these steric interactions. Steric interactions then start to develop between R^1 and R^2.

SCHEME 3.8 Hypothesis for the steric interactions dictating the sense of torquoselectivity in the acid-mediated Nazarov reaction of allenyl vinyl ketones.

TABLE 3.9 Taft steric substituent constants, E_s, relative to hydrogen.[61]

Substituent	System	Steric Substituent Constant, E_S
H	**a**	0.00
Me	**b, c** [a]	-1.24
^{i}Pr	**c** [b]	-1.71
^{t}Bu	**c** [c]	-2.78
Ph	**d**	-1.01

[a] **c/d** and **cc/u**, [b] **c/u** and **cc/d**, [c] **c/s** and **cc/s** structures are used as approximations for corresponding substituent (*cf.* Sections **3.6.2** and **3.7**).

First, consider the reactant structures associated with both modes of conrotation in the Nazarov reaction of allenyl vinyl ketones. In order for the clockwise and counterclockwise modes of conrotation to occur, the allenyl vinyl ketone must adopt **cRT** and **ccRT** conformations, respectively. The R^2 substituent is further separated from the R^3 substituent in the **cRT** structure than in the **ccRT**. Conversely, the two hydrogens geminal to these substituents, H^2 and H^3, are closer in the **cRT** than in the **ccRT** structures by approximately 1.0-1.5 Å for all systems studied (see Appendix 1, TABLES A1.4-A1.9 for distances between H^2 and H^3 or R^2 and H^3).

Now, consider how both reactant structures could proceed to their corresponding transition states, **cTS** and **ccTS**. For **cRT**, as the central carbon of the allene rehybridizes from sp to sp^2, the R^2 substituent gets closer to the R^1 substituent, while minimally interacting with R^3 as it too, rotates in a clockwise fashion. However, in the counterclockwise mode of conrotation (**ccRT** → **ccTS**), the same statement is not always true. There are two possible situations that can be considered. (i) If, at the transition state, the distance between the R^1 and R^2 substituents has increased from that in the reactant structure, rotation (or twisting) about the central carbon of the allene is more advanced than the bending of that carbon towards the product geometry. (ii) If, however, the bending of the allene is more advanced than the rotation of R^2 about the termini, then the distance between the R^1 and R^2 substituents will decrease at the transition state.

As can be seen in FIGURE 3.9, clockwise conrotation of the **cRT** structure for systems **1-6** leads to the R^1 and R^2 substituents approaching each other. In contrast to this, counterclockwise conrotation of the **ccRT** structure either brings together or separates R^1

and R^2 depending on whether the bending of the allene is more advanced than the twisting of the substituents at the transition state or not.

When the bending of the allene is more advanced than the twisting of substituents (i.e., when $\Delta R(R^1,R^2) < 0$), R^1 and R^2 are interacting as they would in the clockwise conrotation of **cRT**. However, when the opposite is true (i.e., when $\Delta R(R^1,R^2) > 0$), it is R^2 and R^3 that are interacting most. It is of no surprise that, when the steric bulk of the substituent increases at the R^2 and R^3 positions, the allene has to bend more at the transition state before conrotation of the termini can occur in a counterclockwise fashion (FIGURE 3.10).

Note also that the degree of separation of the allenyl and vinyl moieties varies when the steric bulk of R^1 increases in the clockwise mode of conrotation (FIGURE 3.11). It should be expected that as R^1 increases in size, the starting conformation of the reactant pentadienyl cation, **cRT**, will have both moieties more separated as the interactions between R^1 and the neighbouring oxygen-boron trifluoride group become larger. However, in the counterclockwise mode of conrotation, the R^2 and R^3 substituents further accentuate this effect in the **ccRT** structure as their steric bulk also increases as these are interacting more than in the **cRT** structure.

In general, the transition state for the counterclockwise mode of conrotation seems to be later than the one for the clockwise mode of conrotation as shown by a larger decrease in the $A(C_1,C_2,C_3)$ angle and the $D(C_2,C_3,C_5,C_6)$ dihedral angle (FIGURE 3.12). This, accompanied by additional R^2-R^3 steric interactions, seems to disfavor the counterclockwise mode of conrotation for the Nazarov reaction of allenyl vinyl ketones.

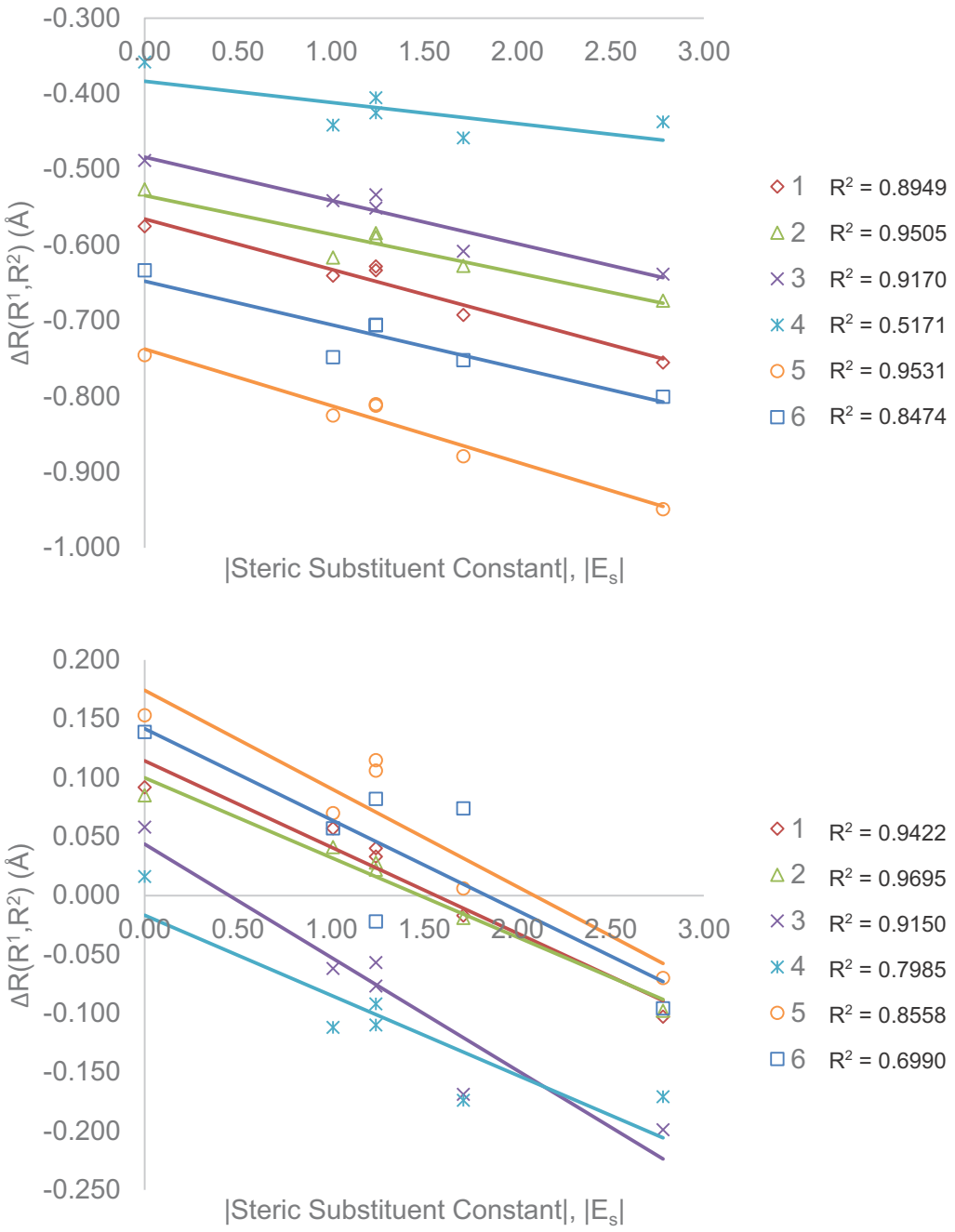


FIGURE 3.9 Variation in $R(R^1,R^2)$ for the clockwise (top) and counterclockwise (bottom) modes of conrotation. $\Delta R(R^1,R^2)$ is defined as the change in distance between R^1 and R^2 centers from the reactant to the transition state structure for systems **1**-**6**.

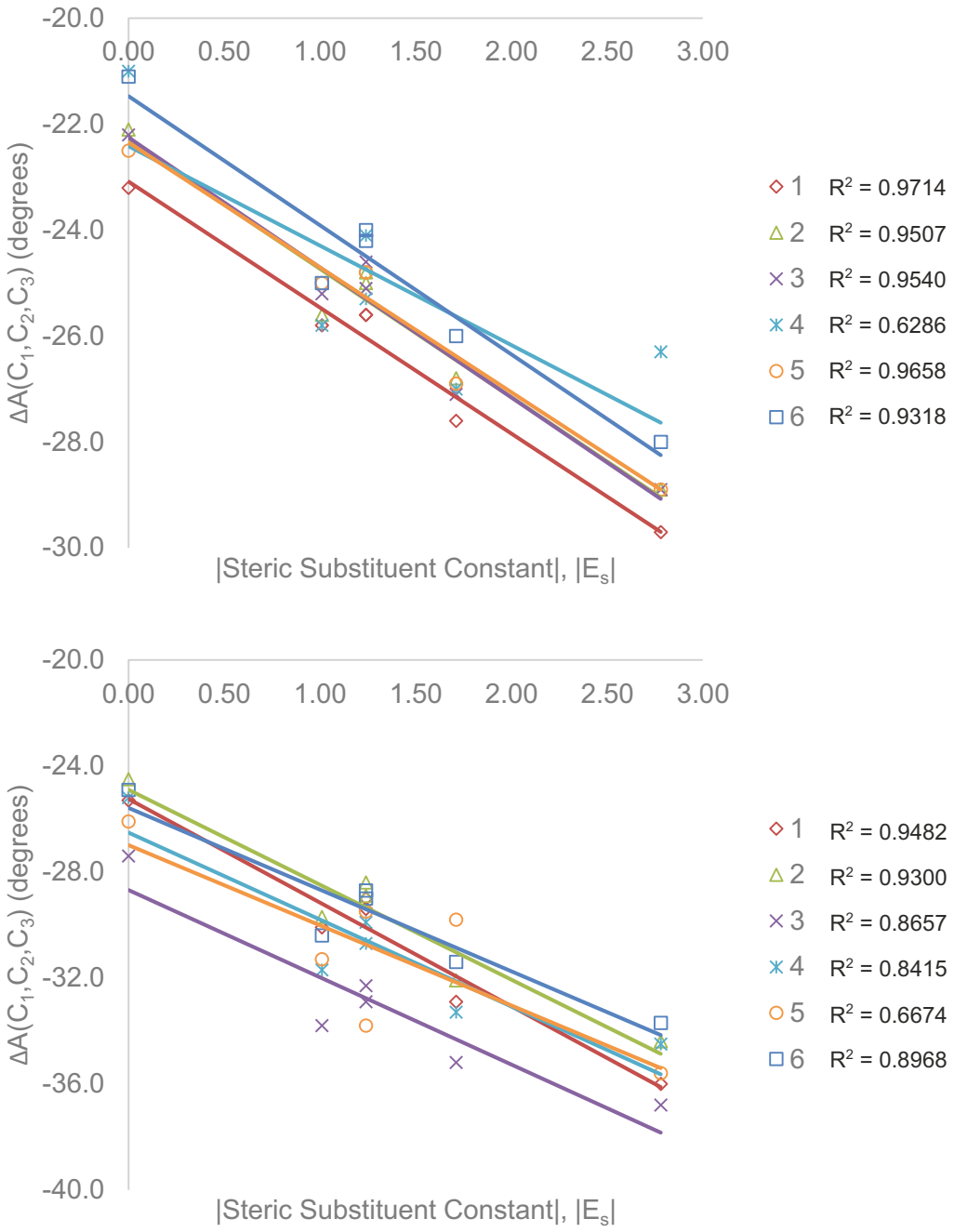
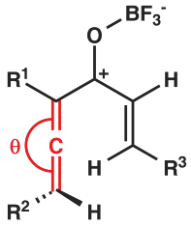


FIGURE 3.10 Variation in A(C_1,C_2,C_3) for the clockwise (top) and counterclockwise (bottom) modes of conrotation. ΔA(C_1,C_2,C_3) is defined as the change in the A(C_1,C_2,C_3) angle from the reactant to the transition state structure for systems **1**-**6**.



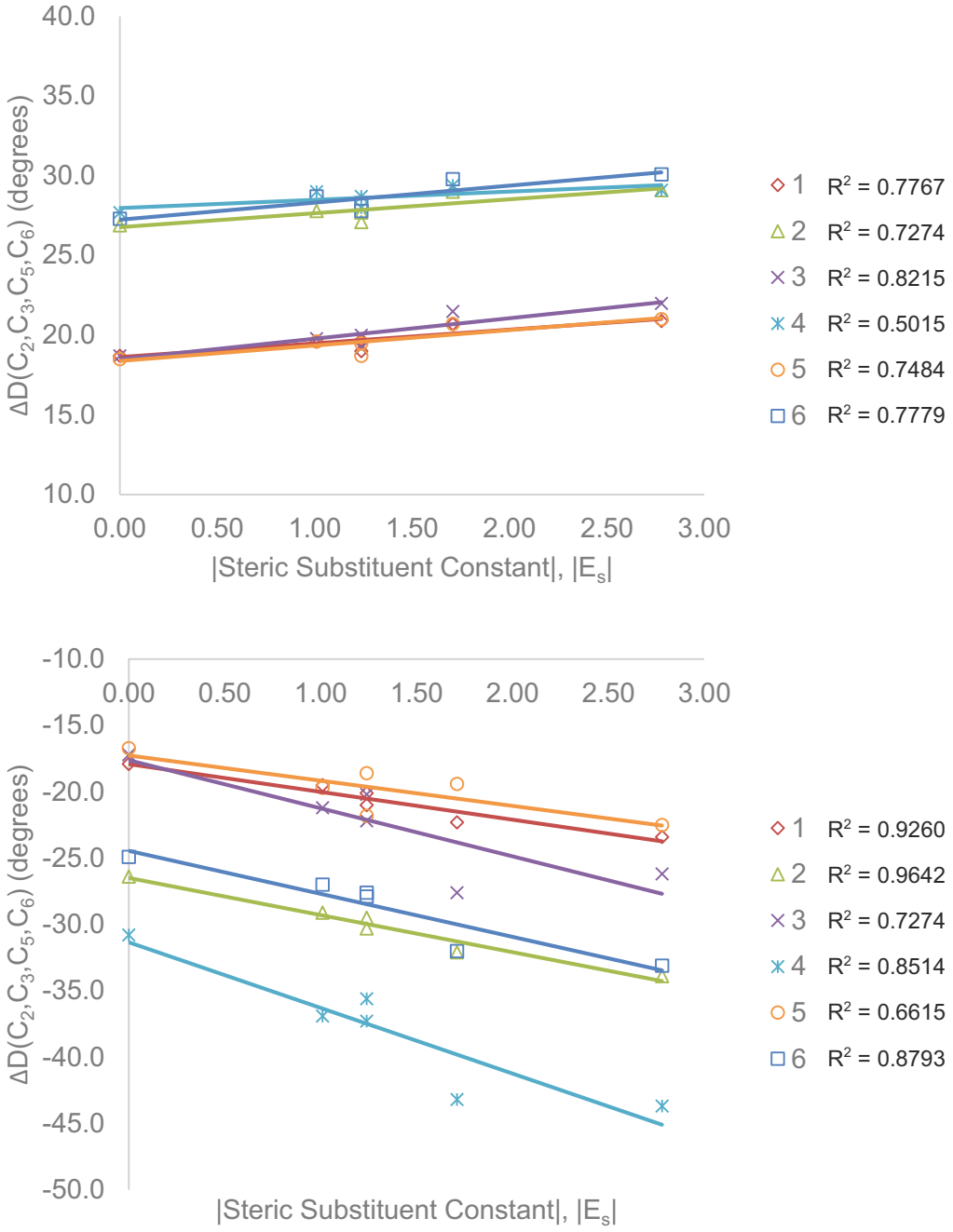
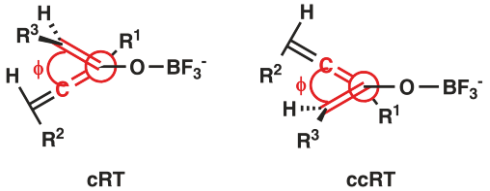


FIGURE 3.11 Variation in $D(C_2,C_3,C_5,C_6)$ for the clockwise (top) and counterclockwise (bottom) modes of conrotation. $\Delta D(C_2,C_3,C_5,C_6)$ is defined as the change in dihedral angle between the carbons at the incipient bond, $D(C_2,C_3,C_5,C_6)$, from the reactant to the transition state structure for systems **1**-**6**.



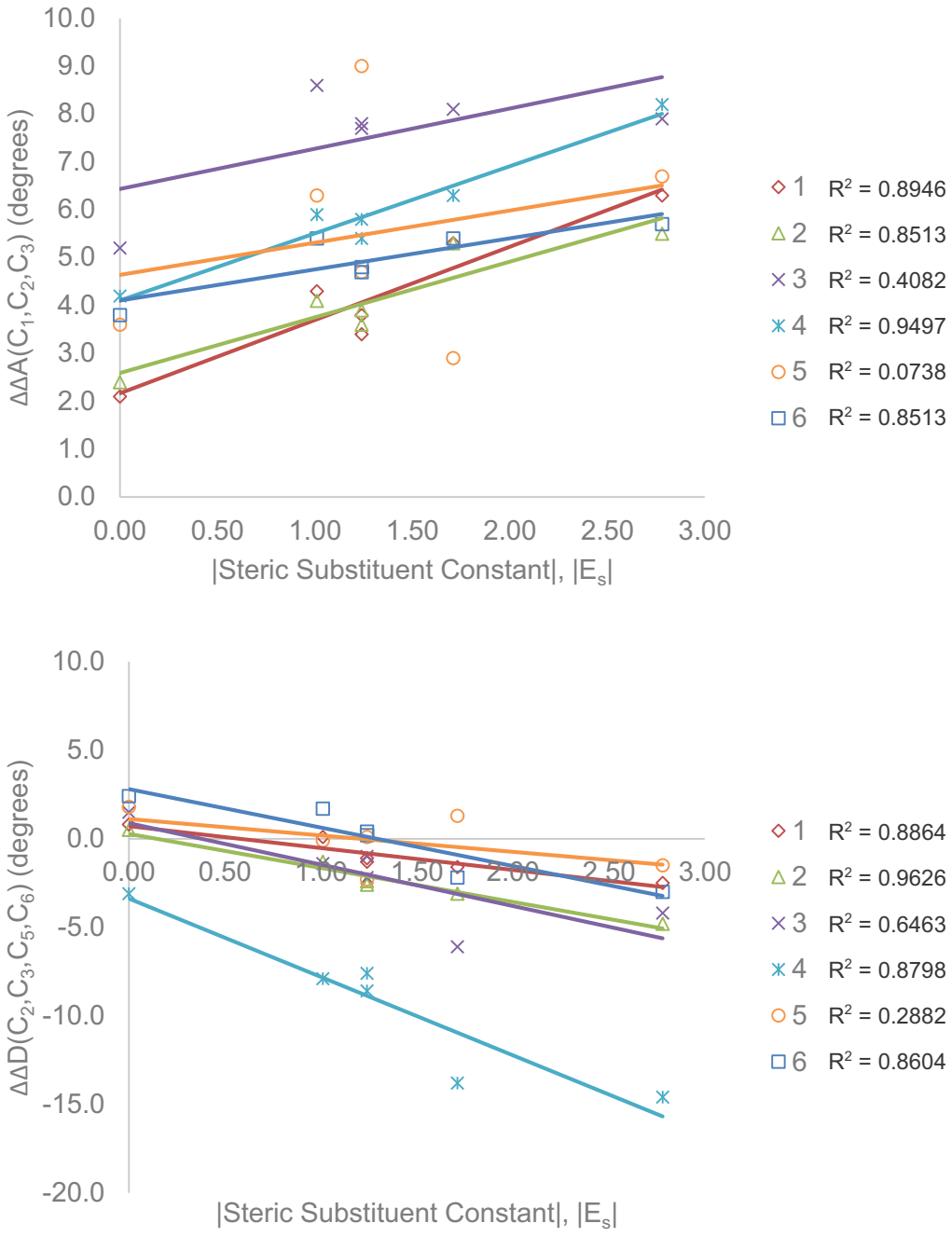


FIGURE 3.12 Differences in $\Delta A(C_1,C_2,C_3)$ (top) and $\Delta D(C_2,C_3,C_5,C_6)$ (bottom) between clockwise and counterclockwise modes of conrotation for systems **1-6**.

FIGURES 3.13-3.15 show how these geometrical parameters and steric interactions between the substituents on the allenyl vinyl ketone framework affect energy barriers for each mode of conrotation.

Larger steric interactions between the R^2 and R^3 substituents in the counterclockwise mode of conrotation bring about more bending of the allene so that twisting of its substituents can occur. Subsequently, interactions between R^1 and R^2 start to develop. In contrast, the R^2 and R^3 substituents rotate away from each other in the clockwise mode of conrotation, minimally interacting with one another. The allene does not need to bend as much, as these interactions are not as great as in the converse pathway. Only steric interactions between R^1 and R^2 substituents are significant.

This can be seen more clearly from FIGURE 3.16, where a scatter plot of the amounts of twisting and bending in the reactant, transition state and product structures for both modes of conrotation is superimposed on the potential energy surface of an allene at the B3LYP/6-31G(d) level of theory. This was done in order to illustrate that the bending of the allene is more energetically costly than the twisting of its substituents in the counterclockwise mode of conrotation.

The potential energy surface of the allene was obtained by performing single-point energy calculations at the B3LYP/6-31G(d) level of theory with varying values of ϕ and θ (depicted in the top right portion of FIGURE 3.16). Similar results were obtained at higher levels of theory, i.e., ωB97X-D/6-31+G(d,p), and are therefore excluded from this discussion. Of course, alleviation of some strain during rehybridization and other factors during the cyclization will cause the energy fluctuations of these systems to be different than that of an allene being distorted 'manually' as represented by the potential energy surface. However, it should nonetheless provide an estimate to how bending and twisting of the allenyl moiety affect the energy in these systems during cyclization.

It is more costly to bend the allene without much twisting of the substituents (**ccTS** structures) than it is to twist substituents with less bending (**cTS** structures). Energy barriers

for the counterclockwise mode of conroration as opposed to the clockwise mode of conrotation should therefore be larger when comparing where the transition state structures are on the potential energy surface.

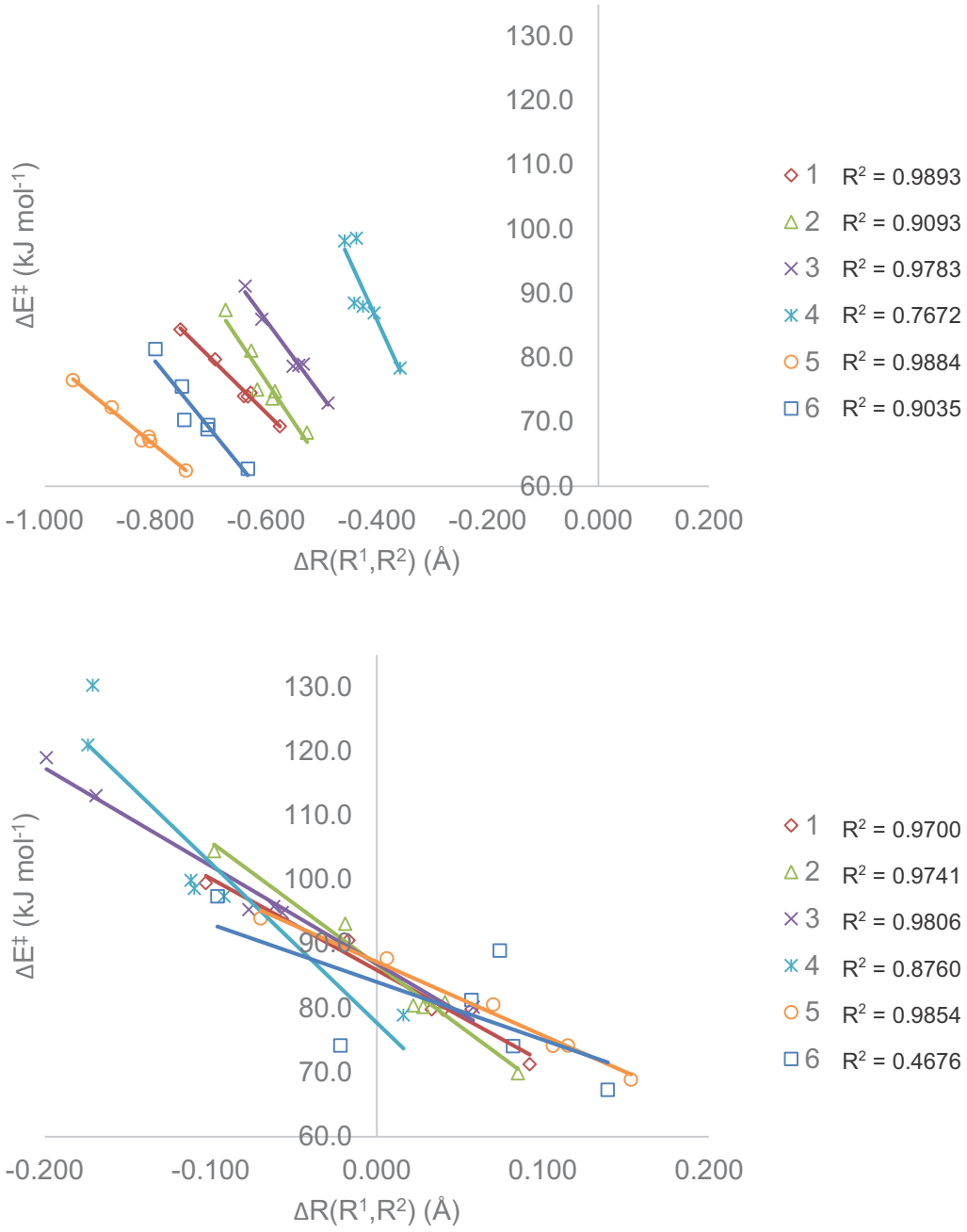


FIGURE 3.13 Effect of the variation of $\Delta R(R^1,R^2)$ on energy barriers for the clockwise (top) and counterclockwise (bottom) modes of conrotation for systems **1-6**.

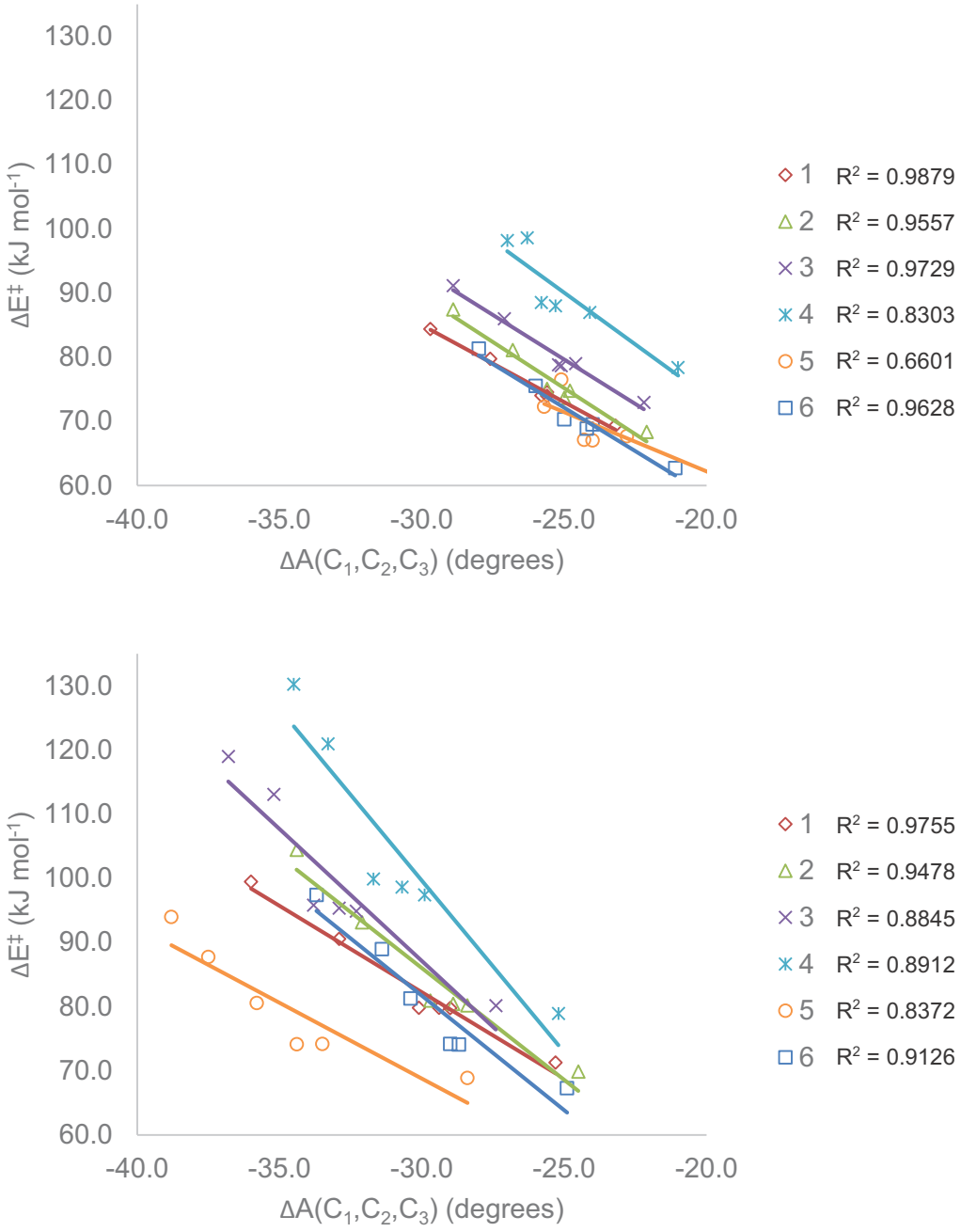


FIGURE 3.14 Effect of the variation of $\Delta A(C_1,C_2,C_3)$ on energy barriers for the clockwise (top) and counterclockwise (bottom) modes of conrotation for systems **1-6**.

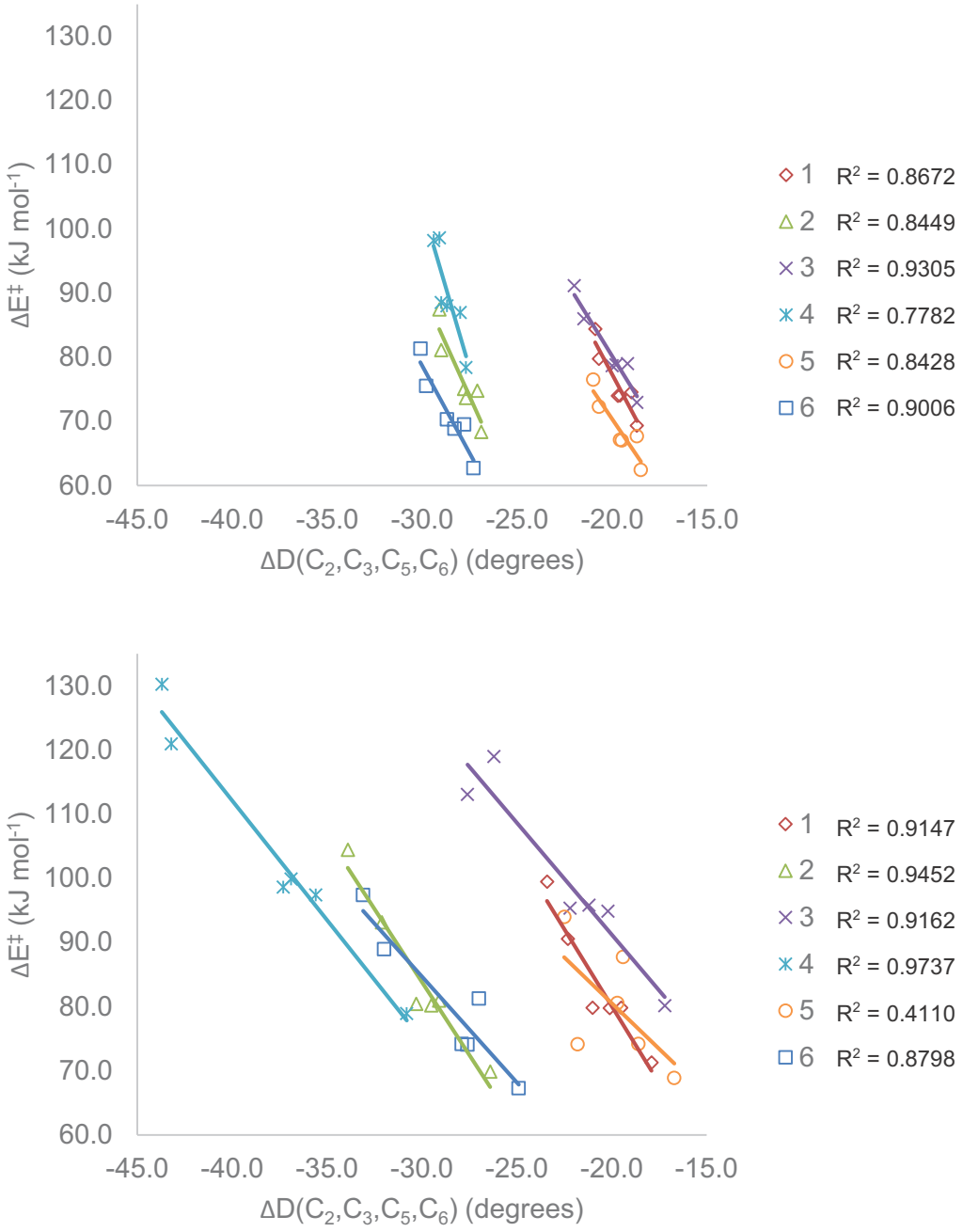


FIGURE 3.15 Effect of the variation of $\Delta D(C_2,C_3,C_5,C_6)$ on energy barriers for the clockwise (top) and counterclockwise (bottom) modes of conrotation for systems **1**-**6**.

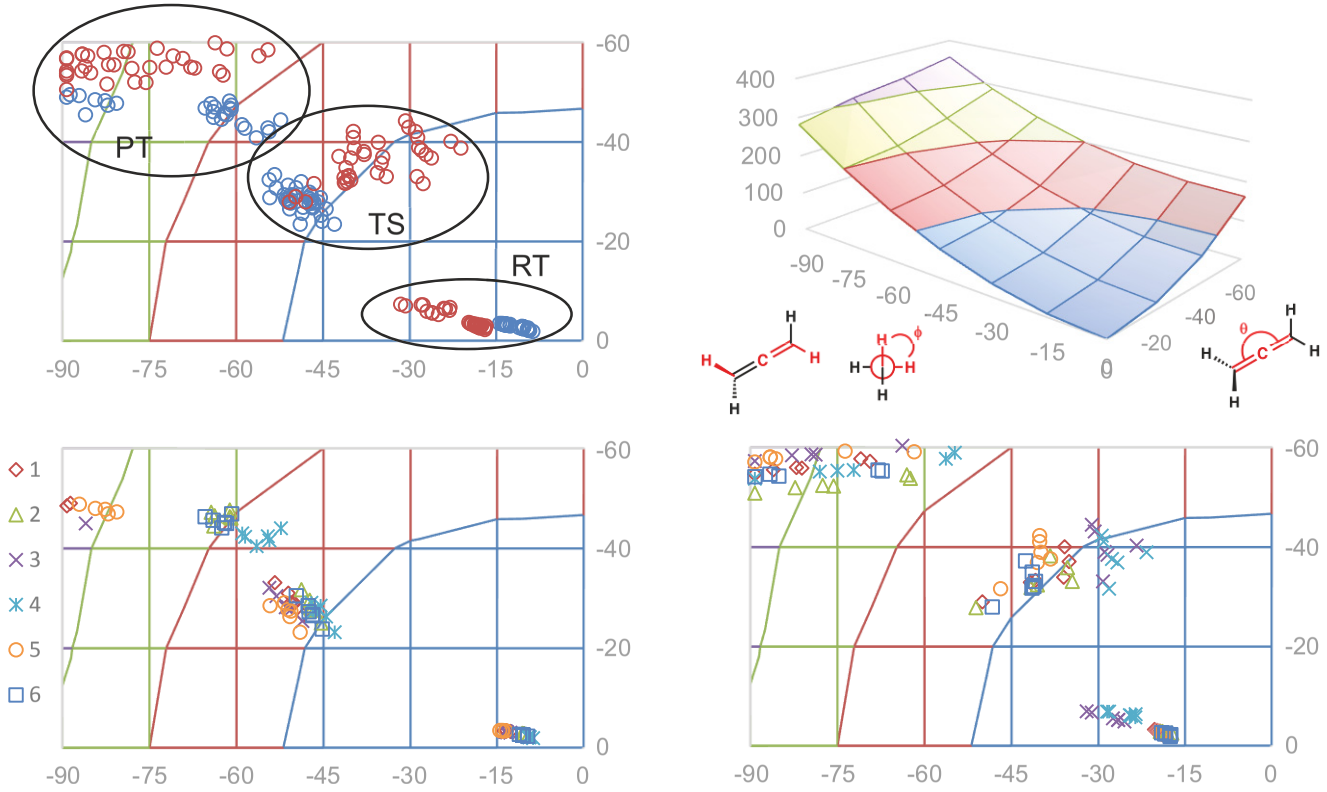
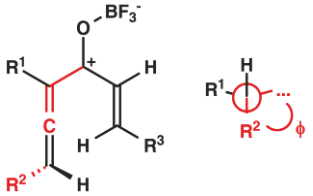


FIGURE 3.16 Superimposition of a ($D(R^2,C_2,C_3,C_4)$, $A(C_1,C_2,C_3)$) scatter plot on the potential energy surface (PES) of allene. $D(R^2,C_2,C_3,C_4)$ (x-axis) and $A(C_1,C_2,C_3)$ (y-axis) are in degrees. The (x,y) origin for the allene PES is set to ($\phi = 90°$, $\theta = 180°$). Energies in kJ mol^{-1} (z-axis) are relative to the lowest lying allene structure, $\theta = 180°$ and $\phi = 90°$. Top left: Clockwise (blue) and counterclockwise (red) modes of conrotation. Top right: Allene PES. Bottom left and bottom right: Clockwise and counterclockwise modes of conrotation for systems **1-6**, respectively.



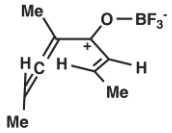
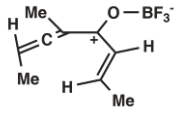
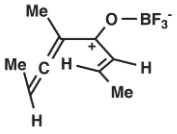
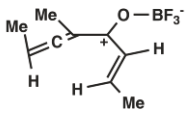
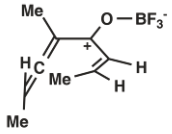
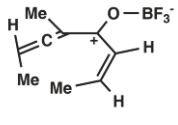
3.7.2 Allenyl Vinyl Ketones with Other Substitution Patterns

For systems bearing different substitution patterns than the ones presented in this study, it is still possible to predict the sense of torquoselectivity when they undergo a thermal Lewis acid-mediated Nazarov reaction. Systems **1b'** and **1b"** serve as a means of comparison with system **1b** (R^3 = Me) to show how changing the substituents on each of the termini affects the torquoselectivity. Data and associated structures are shown in FIGURE 3.17. (Energies and geometrical parameters can be found in TABLE A1.17 of Appendix 1.)

Interchanging the R^2 substituent of an allenyl vinyl ketone with the hydrogen geminal to it, H^2, produces the enantiomer of the original structure. Upon a 180^o degree out-of-plane rotation of structures **cRT 1b'** and **ccRT 1b'**, one notices that these two structures are enantiomeric with **ccRT 1b** and **cRT 1b**, respectively. Energies for each member of these two pairs of enantiomers are the same as expected. By inspecting the differences in transition state energies for the enantiomeric counterparts of system **1b**, **1b'**, one finds that it is the counterclockwise rotation which is favored. Note that both **1b** and **1b'** lead to the same product; it is only the sense of torquoselectivity which is reversed.

In contrast, interchanging the R^3 substituent of an allenyl vinyl ketone with the hydrogen geminal to it, H^3, produces a diastereomer of the original structure which also favors the same sense of rotation as its parent. For example, **cRT 1b** and **cRT 1b"** as well as **ccRT 1b** and **ccRT 1b"** are diastereomeric pairs. The pathway for clockwise conrotation is even more favored for **1b"** as it was for **1b** as **ccRT** and **ccTS** are further destabilized. This can surely be attributed to the fact that the methyl on the double-bond is now pointing inwards initially and interacts more with the other methyl substituent at the R^2 position as the reaction progresses and that it also distorts the **ccRT** and **ccTS** structures more than it does **cRT** and **cTS**.

FIGURE 3.17 Differences in transition state energies between clockwise and counterclockwise modes of conrotations, $\Delta(E+ZPE)^{\ddagger}$ of systems **1b**, **1b'** and **1b"** at the B3LYP/6-31G(d) level of theory.

Structure	$\Delta(E+ZPE)$ [a] (kJ mol^{-1})	
1b, R^2, R^3 = Me		
cRT / **ccRT**	0.0 / 0.2	 
cTS / **ccTS**	74.5 / 80.0	
cPT / **ccPT**	-20.5 / -29.7	
		cRT 1b ccRT 1b
$\Delta(E+ZPE)^{\ddagger}$	-5.5	
1b', R^2 = Me, H^3 ↬ R^3 = Me		
cRT / **ccRT**	0.2 / 0.0	 
cTS / **ccTS**	80.0 / 74.5	
cPT / **ccPT**	-29.7 / -20.5	
		cRT 1b' ccRT 1b'
		enantiomers of 1b
$\Delta(E+ZPE)^{\ddagger}$	5.5	
1b", H^2 ↬ R^2 = Me, R^3 = Me		
cRT / **ccRT**	0.0 / 2.5	 
cTS / **ccTS**	80.9 / 87.9	
cPT / **ccPT**	-37.0 / -46.1	
		cRT 1b" ccRT 1b"
		diastereomers of 1b
$\Delta(E+ZPE)^{\ddagger}$	-7.1	

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, **cRT** or **ccRT**.

3.8 Conclusions and Future Work

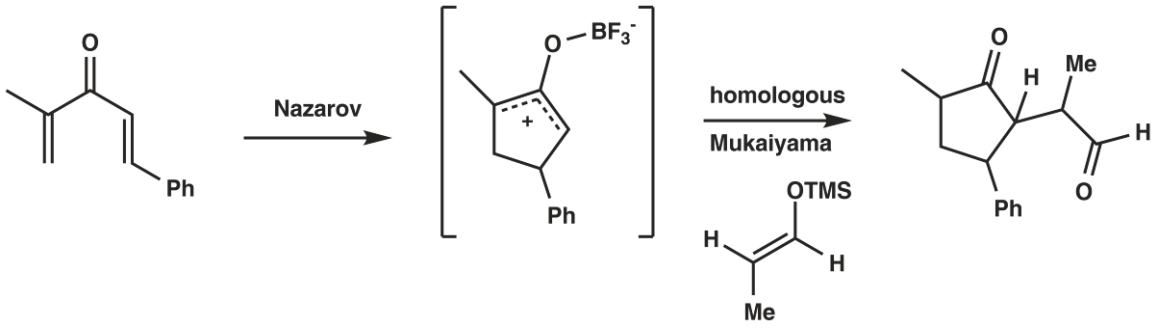
The rationale provided here based on results at the B3LYP/6-31G(d) level of theory can be used as a way of predicting which sense of conrotation predominates in the acid-mediated Nazarov reaction of allenyl vinyl ketones with varying degrees of substitution at the termini. Provided that no electronic effects are at play, the steric interactions between the substituents on the two termini seem to be dictating which mode of conrotation is preferred, i.e., the torquoselectivity in this reaction.

Calculations with functionals accounting for dispersion, e.g., M06-2X and ωB97X-D, turned out not to be representative of experiments, as diastereomeric ratios of greater than 20:1 in favor of **cPT** were obtained experimentally for **5d** and **6d**. The M06-2X and the ωB97X-D geometries are consistent with a π-π stacking phenomenon, which would not be evident in a calculation without dispersion correction such as B3LYP/6-31G(d). Calculations are underway to confirm the importance of dispersion with these diphenyl systems. The lack of agreement between the calculations and the experimental result might be related to some selectivity in the tandem (4+3)-cyclization step that is only present in the experiment.

Future work for this project should focus on better defining what is meant by steric bulk and how interactions between these substituents are measured or established computationally with a good degree of accuracy. Extending these findings to other substituents other than hydrogen, methyl, isopropyl, *tert*-butyl and phenyl could also be of interest. Furthermore, when allenyl vinyl ketones with R^3 = H are able to be synthesized and subjected to a Nazarov cyclization, it would be interesting to see if the model presented herein correctly predicts the correct torquoselectivity, e.g., for **1a** or **2a**, the torquoselectivity should be roughly 60:40 in favor of **ccPT**.

CHAPTER 4 RATIONALIZATION OF THE DIASTEREOSELECTIVITY IN THE THERMAL ACID-MEDIATED HOMOLOGOUS MUKAIYAMA ALDOL ADDITION OF SILYL ENOL ETHERS TO OXYALLYL CATIONS

The oxyallyl cation produced by the Nazarov cyclization usually undergoes deprotonation by a base in the reaction medium to give a cyclopentenone ring.[5,38] However, if a nucleophile is present in the reaction medium, it can add to the oxyallyl cation to give a more substituted cyclopentanone. This is known as an "interrupted" Nazarov reaction.[6] In this chapter, the addition of silicon-masked enolates to oxyallyl cations will be examined (SCHEME 4.1). This addition can be viewed as a homologous Mukaiyama aldol addition.[7]

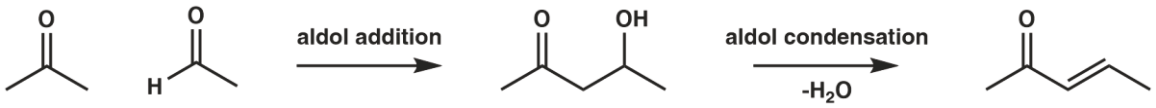


SCHEME 4.1 The Nazarov/homologous Mukaiyama reaction sequence.

4.1 Aldol Additions

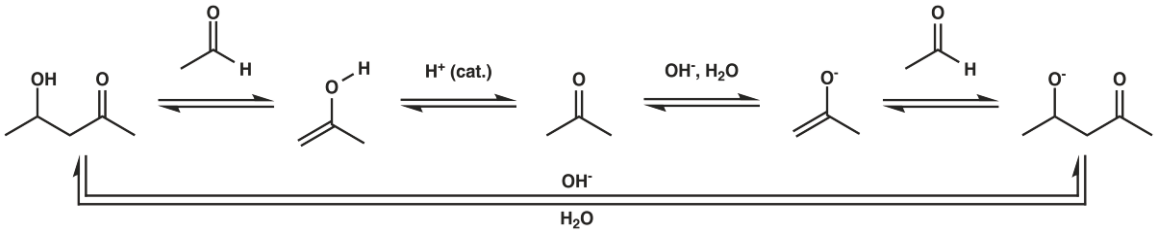
This preliminary section overviews the underlying principles of the aldol addition reactions.[62]

Aldol additions involve two reacting compounds, one possessing an enolizable carbonyl (a carbonyl functional group with at least one hydrogen atom on the α-carbon) and the other having an electrophilic carbonyl functional group (most often an aldehyde or a ketone). These reactions form β-hydroxycarbonyl compounds (aldol additions), which may subsequently eliminate water to provide α,β-unsaturated carbonyl compounds (aldol condensations) (SCHEME 4.2).



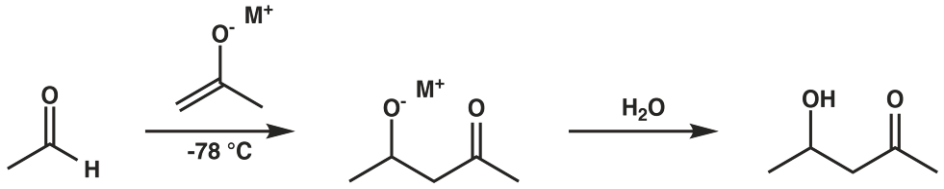
SCHEME 4.2 Illustrative example of an aldol addition and condensation between a ketone and an aldehyde.

Traditionally, the aldol addition occurs in a protic solvent, is mediated by an acid or base, and is reversible. Enols or enolates (the nucleophiles) add to aldehydes or ketones (the electrophiles). The reaction follows the qualitative mechanism shown in SCHEME 4.3.



SCHEME 4.3 Qualitative mechanism of acid- and base-mediated aldol additions.

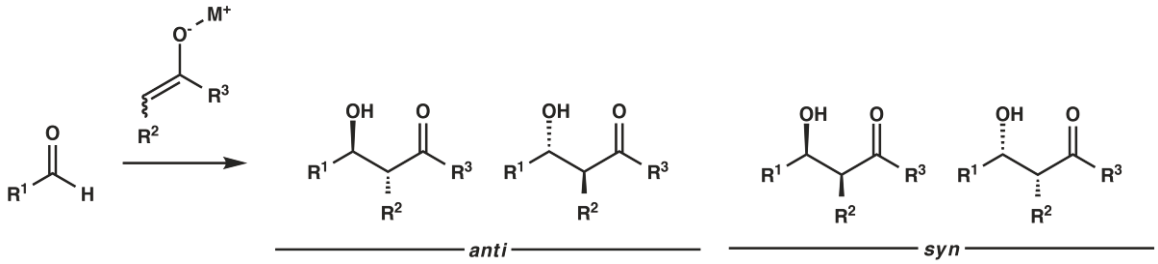
However, under these simple conditions it is often difficult to determine which of the two reacting components will be the electrophile and which will be the nucleophile. Also, controlling the stereochemical outcome in these reactions is problematic. To address these issues, today most aldol additions are carried out with preformed enolates at low temperatures. More specifically, the olefinic carbon of the preformed enolate acts irreversibly as the nucleophile and the carbonylic carbon of the aldehyde or ketone acts as the electrophile (SCHEME 4.3).



SCHEME 4.4 Aldol addition between a preformed enolate and an aldehyde.

In the course of an aldol addition, carbon-carbon bond formation is accompanied by the formation of one or more new stereocenters in the product. Diastereoselectivity can result from the formation of two new stereocenters when one reactant interacts preferentially with one of the two π faces of the other reactant.[63]

The Masamune nomenclature[64] has been widely used to describe the relative configuration of newly formed asymmetric centres resulting from an addition reaction when two stereocenters are formed. Here, the carbon chain containing the two new stereocenters and the remaining carbonyl carbon is drawn in a zig-zag fashion. A *syn* configuration refers to both substituents on the new stereocenters directed toward or away from the viewer, whereas an *anti* configuration refers to substituents facing in the opposite directions (SCHEME 4.5).

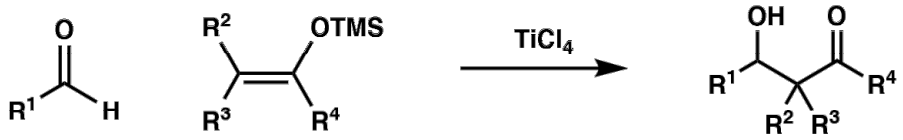


SCHEME 4.5 Masamune nomenclature for aldol additions.

The Masamune nomenclature will be used throughout this chapter when discussing possible reaction pathways and the associated products of aldol additions.

4.2 The Mukaiyama Aldol Addition and Associated Transition State Models

The reaction between silicon-masked enolates (further referred to as silyl enol ethers)[65] and aldehydes (or some other carbonyl containing derivatives) to form new carbon-carbon bonds has proven to be very useful for the creation of two new stereocenters in a simple step, as shown by the appearance of recent reviews.[66] This reaction serves as a synthetic method to form β-hydroxycarbonyl compounds (SCHEME 4.6).



SCHEME 4.6 Mukaiyama aldol addition of a silyl enol ether and a Lewis acid-activated aldehyde.

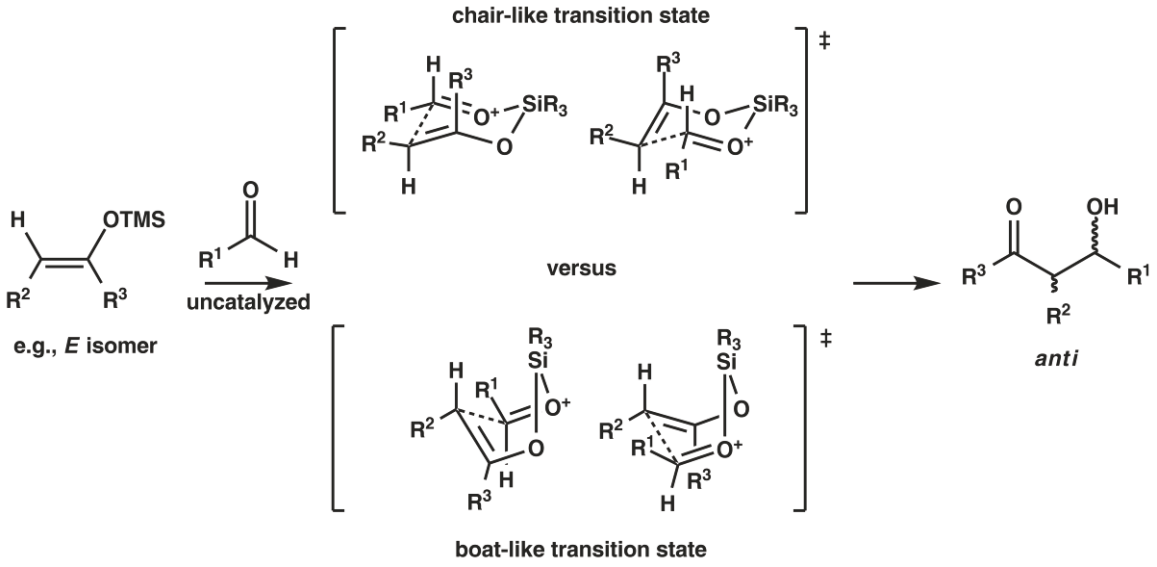
The reaction shown in SCHEME 4.6, pioneered and developed by T. Mukaiyama, is known as the Mukaiyama aldol addition.[67] Since its initial discovery in 1973, there have been many studies on this reaction and its variants. Much research focused on understanding the diastereoselectivity sometimes observed in this addition. Transition state models are often invoked to explain stereochemical outcomes of chemical reactions. As there are many variants to this reaction in addition to a wide range of reaction conditions (solvent, catalyst/mediator, substrate, etc.), it has often been stated in the literature that it is unlikely that a single transition state model could explain all the experimental results. In other words, the Mukaiyama aldol reaction and its variants may not proceed by one pathway.[62,66b,68]

The transition state models discussed in the next section represent the ones that have been used to explain stereochemical outcomes in the uncatalyzed and achiral Lewis acid-mediated versions of the Mukaiyama aldol additions. 1,2 and 1,3-Asymmetric induction models[69a] will not be taken into account as the systems studied in this project possess no chiral centres α or β to the incipient carbon-carbon bond. As such, this chapter will not focus on asymmetric variants of the reaction such as chiral Lewis acid-mediated Mukaiyama aldol additions.[69b]

4.2.1 The Silicon-Directed Mukaiyama Aldol Addition

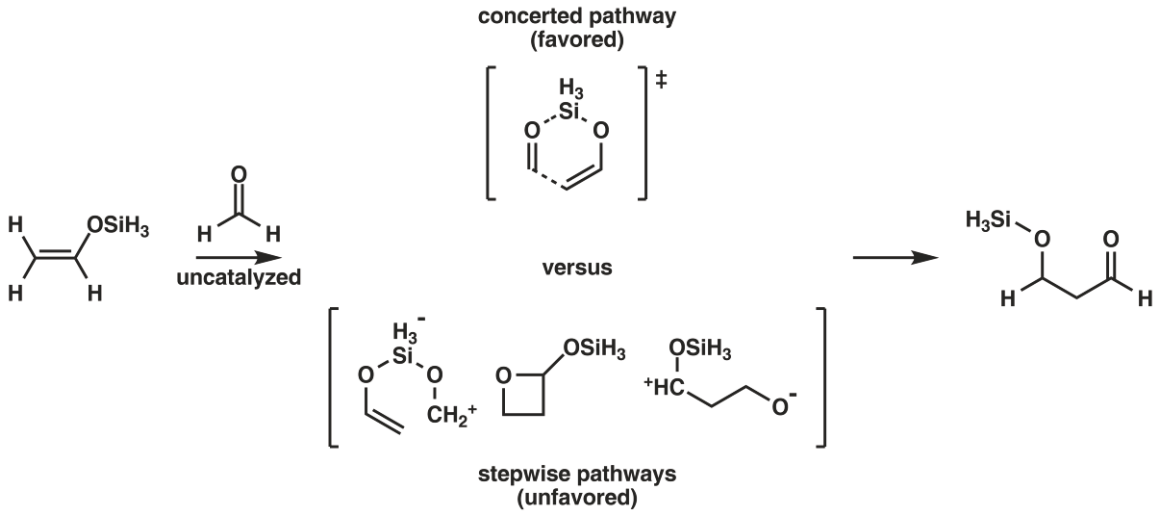
The silicon-directed Mukaiyama aldol addition is an uncatalyzed version of the reaction. Cyclic transition state models have been used to explain the observed distributions of *syn* and *anti* adducts. Experimental studies by Myers and co-workers[70a-c] and Denmark and co-workers[70d,e] and theoretical studies by Gung *et al.*[70f] have indicated that this version

of the reaction goes through chair-like or boat-like six-membered cyclic transition state structures with a hypervalent trigonal bipyramidal silicon species coordinated to the oxygens of both the enol and aldehyde. During the reaction the silicon is transferred from the enol to the oxygen of the aldehyde. The preference for boat- or chair-like geometries and the relative orientations of the reactants determine the diastereoseletivity in the reaction (SCHEME 4.7).



SCHEME 4.7 Chair- and boat-like transition state models for the uncatalyzed silicon-directed Mukaiyama aldol addition.

A computational study by Wong and Wong[71a] explored the possibility of stepwise pathways over concerted ones for this uncatalyzed reaction. Such potential pathways included the formation of an oxetane intermediate via [2+2] cycloaddition followed by a carbon-oxygen cleavage and a 1,3-silyl group shift.[71b] However, in their study Wong and Wong showed that this pathway is significantly disfavored over the concerted pathway (SCHEME 4.8).

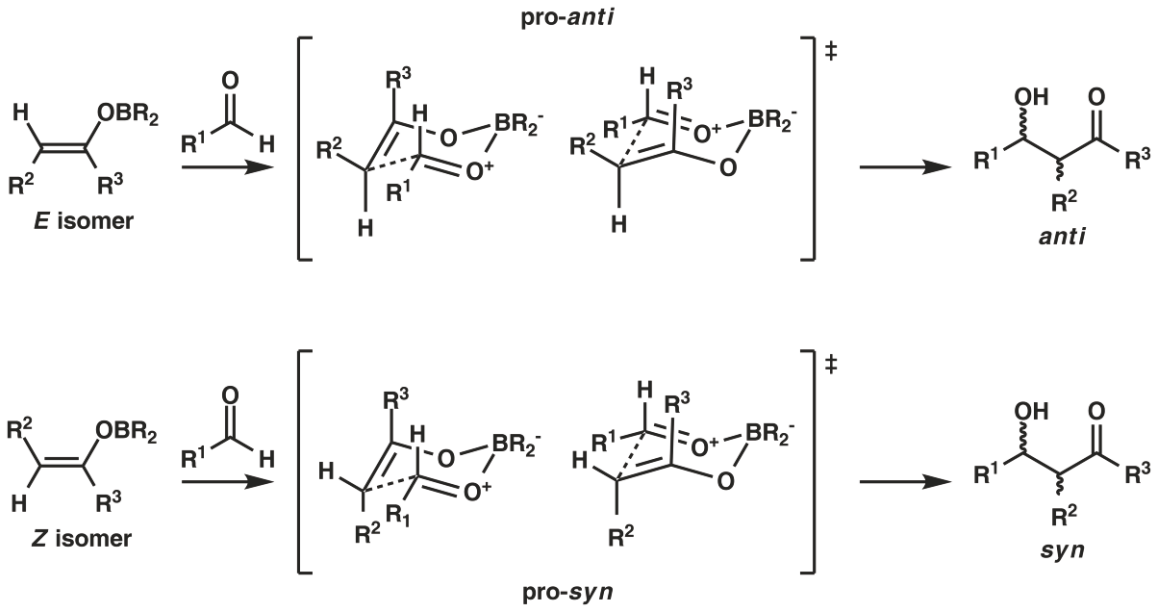


SCHEME 4.8 Concerted and stepwise pathways in the uncatalyzed silicon-directed Mukaiyama aldol addition.

Aldol additions going through cyclic transition states, such silicon-directed Mukaiyama aldol additions or reactions of vinyloxyboranes[72,73] (SCHEME 4.9), have the advantage that the diastereoselectivity can be predicted easily. *(E)*-Enolates lead to *anti* isomers and *(Z)*-enolates to *syn* isomers. (It is assumed that no equilibration between the *(E)*-enolates and the *(Z)*-enolates takes place.)

4.2.2 The Lewis Acid-Mediated Mukaiyama Aldol Addition

Most Mukaiyama aldol additions are mediated by a Lewis acid. It is accepted that the Lewis acid activates the electrophilic carbonyl substrate by coordinating to the carbonyl oxygen. This makes that carbon more susceptible to nucleophilic attack by the silyl enol ether (*cf.* SCHEME 4.4). The reaction takes place solely between the olefinic carbon of the silyl enol ether and the carbonylic carbon of the activated aldehyde.[67b]



SCHEME 4.9 Cyclic (chair) transition state models for the Mukaiyama aldol addition between vinyloxyboranes and aldehydes.

The Lewis acid-mediated additions of silyl enol ethers and additions of Lewis acid enolates with electrophiles are two very different reactions. These two reactions are thought to go through different pathways and stereochemical outcomes are often not comparable.[69b,74] For instance, when aldol additions are performed with lithium enolates (which can complex to the carbonyl oxygen of the aldehyde or ketone), the diastereoselectivity is found to be highly dependent of the starting lithium enolate geometry. However, when the corresponding reaction with the silyl enol ether is mediated by boron trifluoride, a decrease and in some cases a reversal, of the diastereoselectivity is observed.[75]

Cyclic (or Zimmerman-Traxler type)[76] transition state models do not fit the diastereoselectivies for the Lewis acid-mediated Mukaiyama aldol reaction, as shown by the extensive experimental studies.[77-84] Instead, open (or acyclic, "extended") transition state models seem to be in better agreement with the diastereoselectivities observed. Some relevant published findings are now summarized.

The diastereoselectivities are independent of enolate geometry, which supports the fact that cyclic transition states are unlikely.[77-81]

Varying the Lewis acid as the mediator of the Mukaiyama aldol reaction (boron trifluoride, titanium(IV) tetrachloride or tin(IV) tetrachloride) has little or no effect on the diastereoselectivity of reactions.[82] This implies that the Lewis acid is not intimately involved in the transition state with the silyl enol ether. It serves, however, to activate the aldehyde by complexing the carbonyl oxygen. Furthermore, the silyl group on the silyl enol ether does not transfer to the oxygen of the aldehyde as it would in the uncatalyzed Mukaiyama aldol addition. By treating a silylated aldol with titanium(IV) tetrachloride, the exchange of the silyl group with the titanium tetrachloride was found to be slow when compared to the formation of the aldol itself. This disproves a mechanism involving a transfer of the silyl group to the aldehyde oxygen concomitant with a silicon/titanium exchange.[83]

An open transition state model has been developed by Heathcock *et al.*[84a] and Denmark and Henke[84b] to rationalize the diastereoselectivity. This model relies upon minimization of both the non-bonded interactions between substituents around the incipient carbon-carbon bond as well as of the dipole moments in the transition state structures, which is largely due to the relative orientations of the carbon-oxygen bonds in the incoming nucleophile and in the activated electrophile. Staggered conformations are assumed at the incipient bond between the reactant pair, allowing for three geometries (pro-*anti*) leading to the *anti* product and three geometries (pro-*syn*) leading to the *syn* products. Also, the Lewis acid is assumed to be complexed *cis* to the aldehydic hydrogen (FIGURE 4.1).

Following this model, one can eliminate geometries A^2 and S^3 by arguing that dipole-dipole interactions would be unfavorable. A^2 and S^1 would be destabilized by non-bonded interactions between the ^{t}Bu and Ph groups. A^3 can probably be eliminated because of non-bonded interactions between ^{t}Bu and the Lewis acid, BF_3. This leaves two candidates: A^1 and S^2. The *anti* selectivity of Lewis acid-mediated Mukaiyama aldol additions is most possibly due to the fact that the antiperiplanar arrangement, A^1, is favored over the synclinal

arrangement, S^2, as the latter incorporates unfavorable interactions between the Ph/TMSO and ^{t}Bu/OBF_3 groups, whereas the former does not.

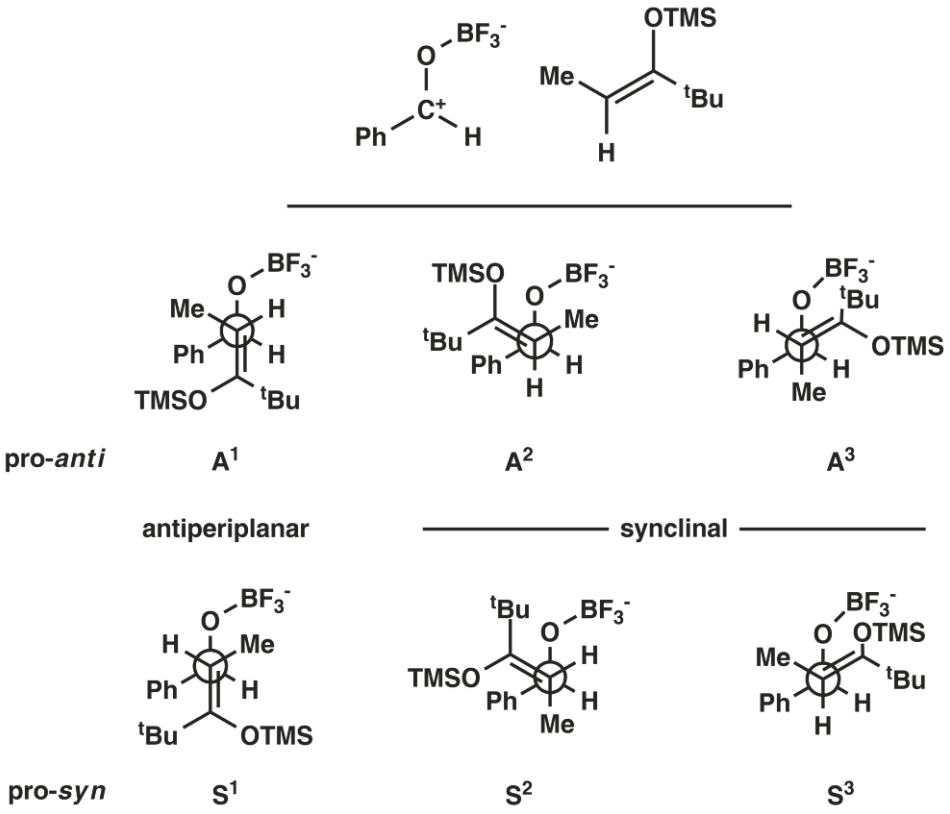
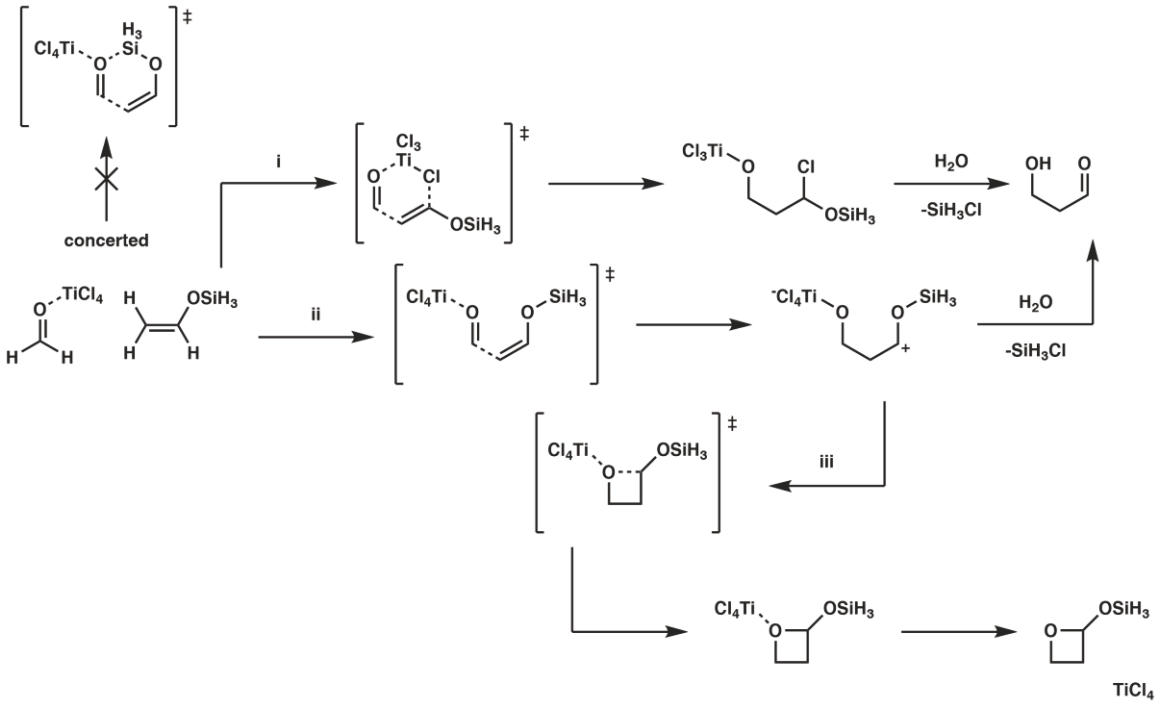


FIGURE 4.1 Possible staggered transition state geometries for the Lewis acid-mediated Mukaiyama aldol addition of silyl enol ethers to aldehydes

A small number of computational studies have dealt with the mechanism of the Lewis acid-mediated Mukaiyama aldol addition. These will now be discussed.

Wong and Wong[68b] explored the metal chloride-promoted Mukaiyama aldol addition between the simplest trihydrosilyl enol ether and formaldehyde. The metal was varied from titanium(IV), boron, aluminum to gallium. The calculations were done in the gas phase at the MP2/6-311+G(d,p)//B3LYP/6-31G(d) level of theory. The authors were unable to locate a concerted transition state after an extensive search, but they identified possible stepwise pathways (SCHEME 4.10).



SCHEME 4.10 Stepwise pathways in the Lewis acid-mediated Mukaiyama aldol addition.

The stepwise pathways in question are: (i) a simultaneous carbon-carbon bond formation and a chloride shift followed by hydrolysis, (ii) carbon-carbon bond formation followed by an elimination of trihydrosilyl chloride with the formation of the aldehyde, and (iii) the formation of an oxetane intermediate from a carbon-carbon bond formation followed by a carbon-oxygen ring closure. Pathway (i) was found to be the lowest energy pathway, whereas pathways (ii) and (iii) were energetically competitive with one another.

On another note, the observation of pre-transition state intermolecular complexes was also postulated to be important in understanding the reactivity and stereoselectivity in Lewis acid-promoted reactions.[68b,85] Wong and Wong[68b] supported the idea that the silyl enol ether forms an intermolecular complex with the Lewis acid-activated formaldehyde, the result of π-π stacking interactions between the reacting pair. These complexes have significant interaction energies (>30 kJ mol^{-1}) that result in negative energy barriers for the reactions if these complexes are not taken into account (FIGURE 4.2). The energy barriers from the intermolecular complexes to the transition states are less than 15 kJ mol^{-1} and were

rationalized by considering that the intermolecular complexes strongly resembles the transition state structures and therefore little distortion is needed to attain the transition state.

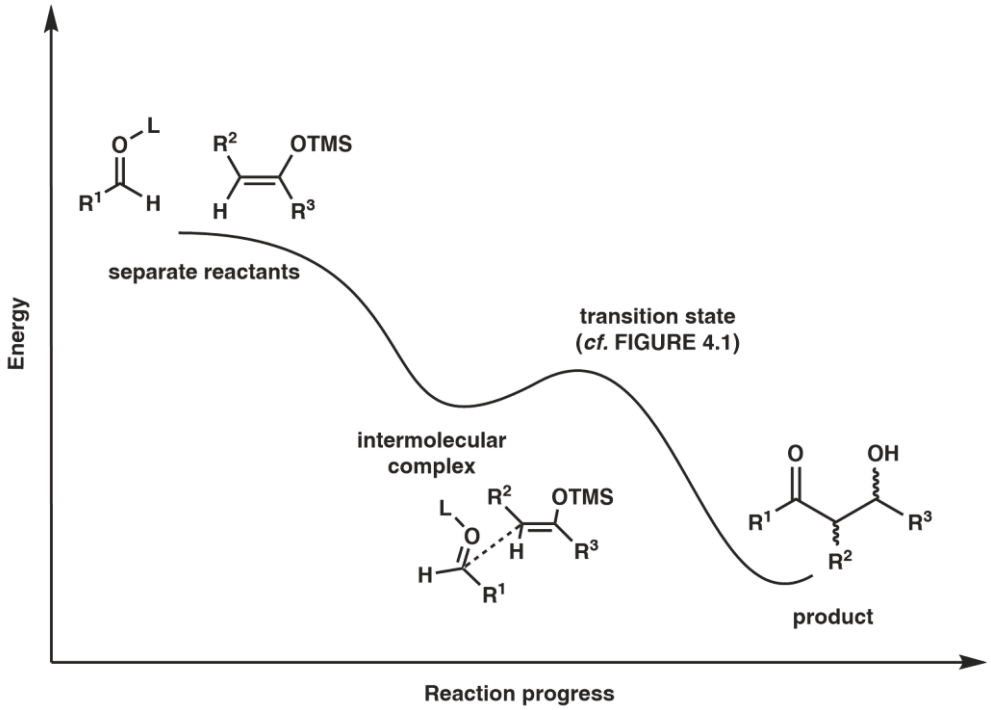


FIGURE 4.2 Reaction pathway between silyl enol ethers and Lewis activated aldehydes.

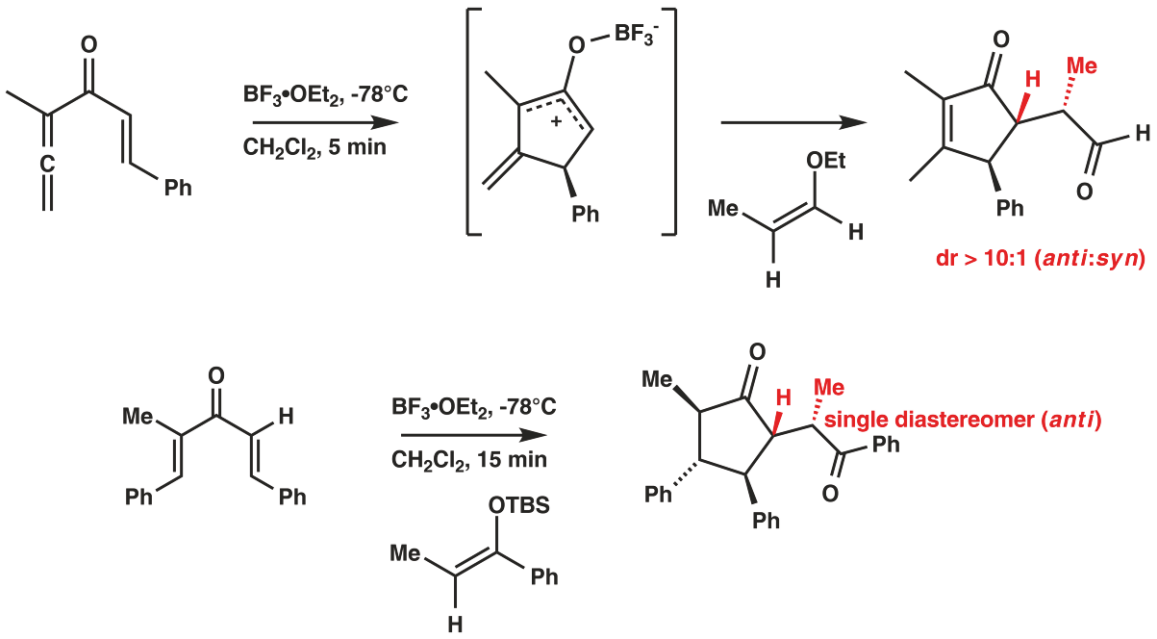
Lee *et al.*[86a] expanded on the models proposed by Heathcock *et al.*[84a] and Denmark and Henke[84b] and also on the work done by Wong and co-workers[68b,85b,c] by developing a "quantitative" model for predicting diastereoselectivity in the Lewis acid-mediated Mukaiyama aldol addition. Their model system included boron trichloride-activated aldehydes reacting with silyl enol ethers bearing different substituents. The calculations were done at the M06/6-311G(d)//B3LYP/6-31G(d) level of theory using a solvation model to represent the dielectric of diethyl ether. Their rationale for using boron trichloride instead of the experimentally used boron trifluoride was that fluorine is purported to cause difficulties in computation due to its high electronegativity[86b] as well as for the sake of comparison with the previous work done by Wong and Wong.[68b]

After locating transition states and comparing their results to the earlier models, they found that their computed geometries did not correspond to Heathcock and Denmark's proposed staggered antiperiplanar and synclinal arrangements between reactants (some computed geometries being eclipsed or in intermediate arrangements). Furthermore, steric interactions and dipole-dipole alignments were not necessarily minimized in the lowest energy transition state structures. Indeed, dipole-dipole minimization was not a deciding factor for establishing the favored pathway. As the simple models had been unsatisfactory, Lee *et al.* proposed that only computational models could quantitatively predict diastereoselectivity in the Mukaiyama aldol addition.

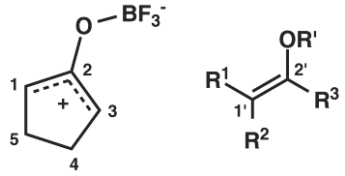
4.3 The Homologous Mukaiyama Aldol Addition / Project Objective

Recently, experimental results in the Burnell group[56c] and work done by Wu *et al.*[7a] has established that the interrupted Nazarov cyclizations with alkyl or silyl enol ethers, which are homologous Mukaiyama aldol additions,[7a] (SCHEME 4.11) proceed to form functionalized cyclopentenone derivatives with high levels of diastereoselectivity. However, the stereochemical outcomes were not really understood.

The aim of the work in this chapter is to rationalize the diastereoselectivity in the additions of silyl enol ethers and enols to cyclic oxyallyl cations, which are the immediate results of Nazarov reactions. The number of computational studies published on the Lewis acid-mediated Mukaiyama aldol addition is small, and these have focused on the addition of silyl enol ethers to aldehydes or ketones. No computational study has examined the Mukaiyama aldol additions of silyl enol ethers with oxyallyl cations. Hence, it was considered important to first study the reaction between a simple oxyallyl cation with boron trifluoride as the Lewis acid and a set of simple silyl enol ethers, or enols, (FIGURE 4.3) before undertaking a study involving the more elaborate oxyallyl cations produced by the Nazarov reactions of allenyl vinyl ketones.



SCHEME 4.11 Recent experimental results from Marx and Burnell[56c] (top) and from Wu *et al.*[7a] (bottom).



	R^1	R^2	R^3	R'
7	H	H	H	**a** H; **b** TMS
8	H	H	Me	
9	Me	H	Me	
10	H	Me	Me	

FIGURE 4.3 Systems of interest for the study of the homologous Mukaiyama aldol addition of (silyl) enol ethers with an oxyallyl cation.

4.4 Computational Methods

All following quantum mechanical calculations were performed using the Gaussian 09 software package.[57] All stationary points were fully optimized in their ground states at the B3LYP/6-31G(d) level of theory.[15,25] Minima and first-order saddle points were

characterized by their number of imaginary frequencies (0 for minima and 1 for first-order saddle points) following normal mode vibrational analysis. All first-order saddle points underwent intrinsic reaction coordinate calculations[36] in order to identify the minima on either side of the saddle point. All geometries and thermodynamic data were obtained from calculations done in the gas phase at 298.15 K and 1.0 atm unless otherwise indicated.

(Cartesian coordinates, energies and geometrical parameters for systems **7-10** presented in this chapter are given in Appendix 2.)

The reason for choosing B3LYP/6-31G(d) to perform these calculations lies partially in the fact, aside from a compromise between computational cost and accuracy, that the only computational studies[68b,86a] to date on similar systems also employed this level of theory to locate the structures of interest. In these studies, energies were presented in terms of single-point energy calculations at higher levels of theory on B3LYP/6-31G(d)-generated structures (e.g., MP2/6-311+G(d,p)//B3LYP/6-31G(d)[68b] or M06/6-311G(d)//B3LYP/6-31G(d)[86a]). However, as open-type transition states are not highly organized structures (as opposed to cyclic-type transition states), there can be much flexibility between the two approaching substrates. Although B3LYP/6-31G(d) geometries may be flawed, performing single-point calculations at higher levels of theory may not necessarily ameliorate energies given by the B3LYP/6-31G(d) level of theory. As such, for the purpose of these preliminary studies on the reaction between silyl enol ethers or enols with oxyallyl cations, results presented herein will be given at the B3LYP/6-31G(d) level of theory.

4.5 Preliminaries: Conformational Analysis of Silyl Enol Ethers and Oxyallyl Cation Precursors

The Lewis acid-mediated Mukaiyama aldol addition is thought to occur by open-type transition states, as discussed previously. There is probably little constraint in how the two reacting partners, the oxyallyl cation and the silyl enol ether, approach one another during the carbon-carbon bond forming event. It is therefore important to consider the minima and

first-order saddle points for the substrates before even considering how the two substrates orient themselves during the bond-forming event.

For the simple oxyallyl cation studied here, the global minimum places the boron trifluoride group oriented in an in-plane fashion with respect to the ring portion, i.e., with $D(C_3,C_2,O,B) = 0.0$ degrees. The transition state that involves rotation about the C-O bond is situated roughly 20 kJ mol^{-1} above the global minimum and has the boron trifluoride group oriented out of plane, i.e., $D(C_3,C_2,O,B) = \pm 87.0$ degrees (see Appendix 2, TABLE A2.1). In situations where there are unequivalent substituents on the ring, the minima and rotational isomerism saddle points would with no doubt be more numerous, and it would therefore be a more complicated task of considering all possible minima. While it may seem irrelevant to conduct these preliminary studies, one needs to consider all of the possible structures in order to study the subsequent bimolecular reactions that are governed by open-type transition states. As there is no predefined template for the mode of approach between the two entities, what could intuitively be the lowest pathway might not be the actual lowest energy pathway.

As for the silyl enol ether (or the enol and other analogues), there have been experimental[87] and computational[88] results that provide information about what minima exist for these types of structures as well as their associated stabilities. In general, the conformations of R' relative to the double-bond in $R'OCH=CH_2$ followed the order, in terms of increasing energy, *syn* < *gauche* << *anti* for bulky R' substituents (e.g. CH_3, SiH_3) and *syn* < *anti* for R' = H.[87,88] *Syn* conformations were said to be preferred over *anti* conformations because the former have smaller dipole moments than the latter.[70f] Opposing factors were postulated to stabilize *anti* and *gauche* conformations differently.[88a] For instance, electron delocalization from oxygen lone pairs to the π* orbital of the double-bond favors the *anti* conformer, whereas bond-bond repulsion between the vinyl C-H and O-R' favors the *gauche* conformer. Bond-bond repulsion dominates over the electron delocalization for large R', i.e., for CH_3 or SiH_3, and thus *gauche* conformers are preferred over the *anti* conformers. The opposite is true for R' = H.

The existence and relative energies of these minima could very well change with differing substitution patterns on the (silyl) enol ether. An exploration of the potential energy landscape for (silyl) enol ethers (with R' = H or TMS) of systems **7**-**10** yielded the results shown in FIGURES 4.4 and 4.5 (and TABLE A2.1 of Appendix 2).

As expected for R' = H (FIGURE 4.4), only the *syn* and *anti* conformations are minima for enols of systems **7**-**10a**, the former being lower in energy than the latter. It becomes more complicated with silyl enol ethers (R' = TMS) (FIGURE 4.5) depending on what the substituents R_1, R_2 and R_3 are (H or Me). For system **7b** (R_1, R_2 and R_3 = H), the *gauche* conformation is the lowest energy conformer, whereas the *syn* is more energetic. This goes against, to some extent, what was concluded from earlier studies with systems for R' = CH_3 or SiH_3 but should be expected by the greater size of TMS ($Si(CH_3)_3$), which would disfavor the *syn* arrangement of the TMS substituent relative the double-bond. Introducing a methyl group at the R_3 position (system **8b**), caused the silyl enol ether to adopt a *syn* conformation, and further introducing a methyl group at the R_1 position (system **9b**), caused the silyl enol ether to adopt a *gauche* conformation instead. This can be rationalized by assessing the steric interactions between the TMS and the two Me substituents, which restrict the existence of certain conformations as minima. For system **10b**, where R_2 and R_3 are methyls, the silyl enol ether was a minimum for both *gauche* and *syn* conformations, the *syn* being the lowest energy conformer. The methyl group at the R_3 position probably caused more steric strain relative to the hydrogen at the R_1 position, making the *syn* conformation more favored than the *gauche*.

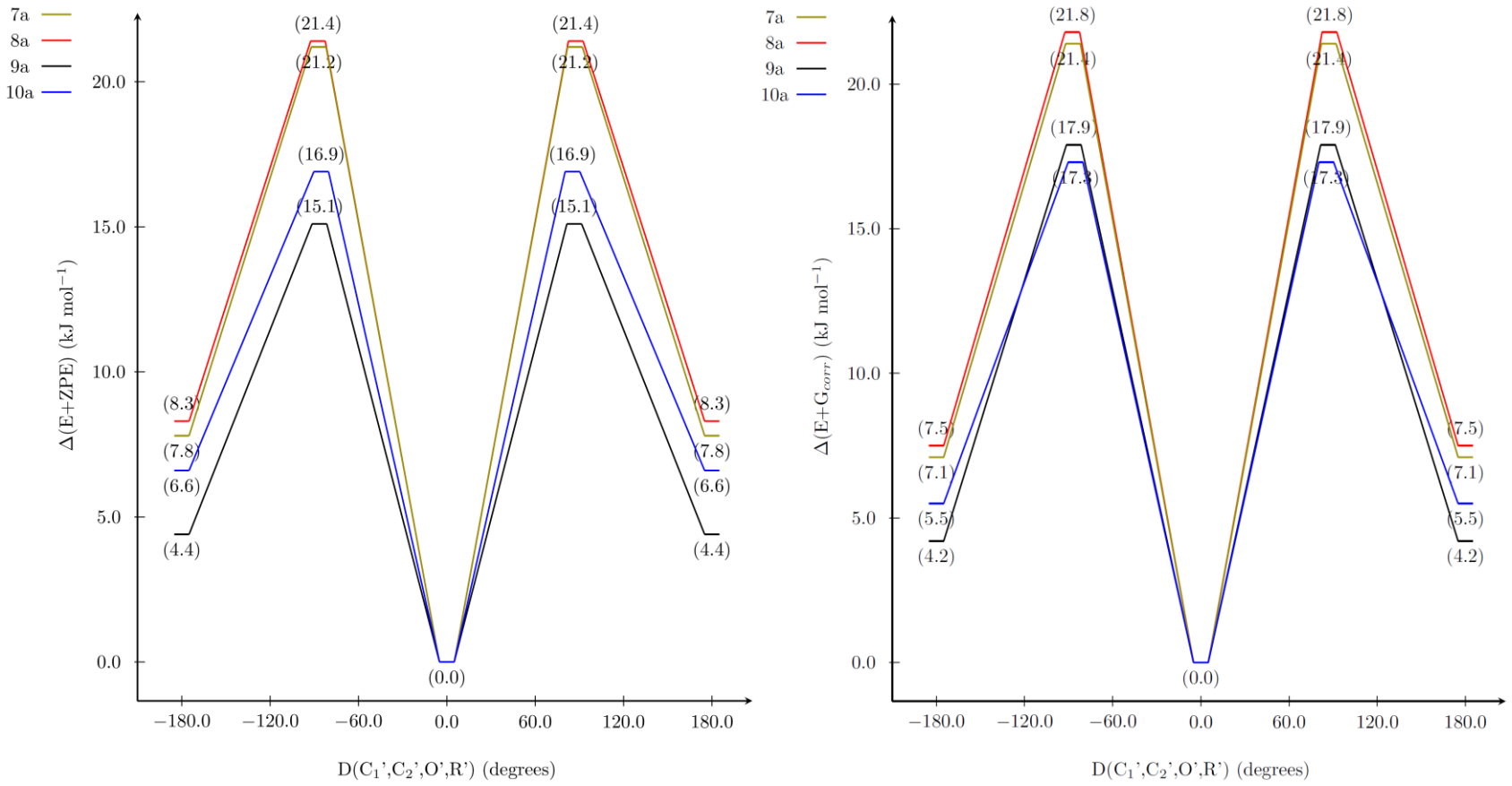


FIGURE 4.4 Stationary points found on the potential energy surface obtained by varying the D(C_1',C_2',O',R') dihedral angle for enols of systems **7-10a** (R' = H). Energies (zero-point, ZPE, or Gibbs, G_{corr}, corrected) are relative to that of global minimum. (Lines joining the points are to aid viewing.)

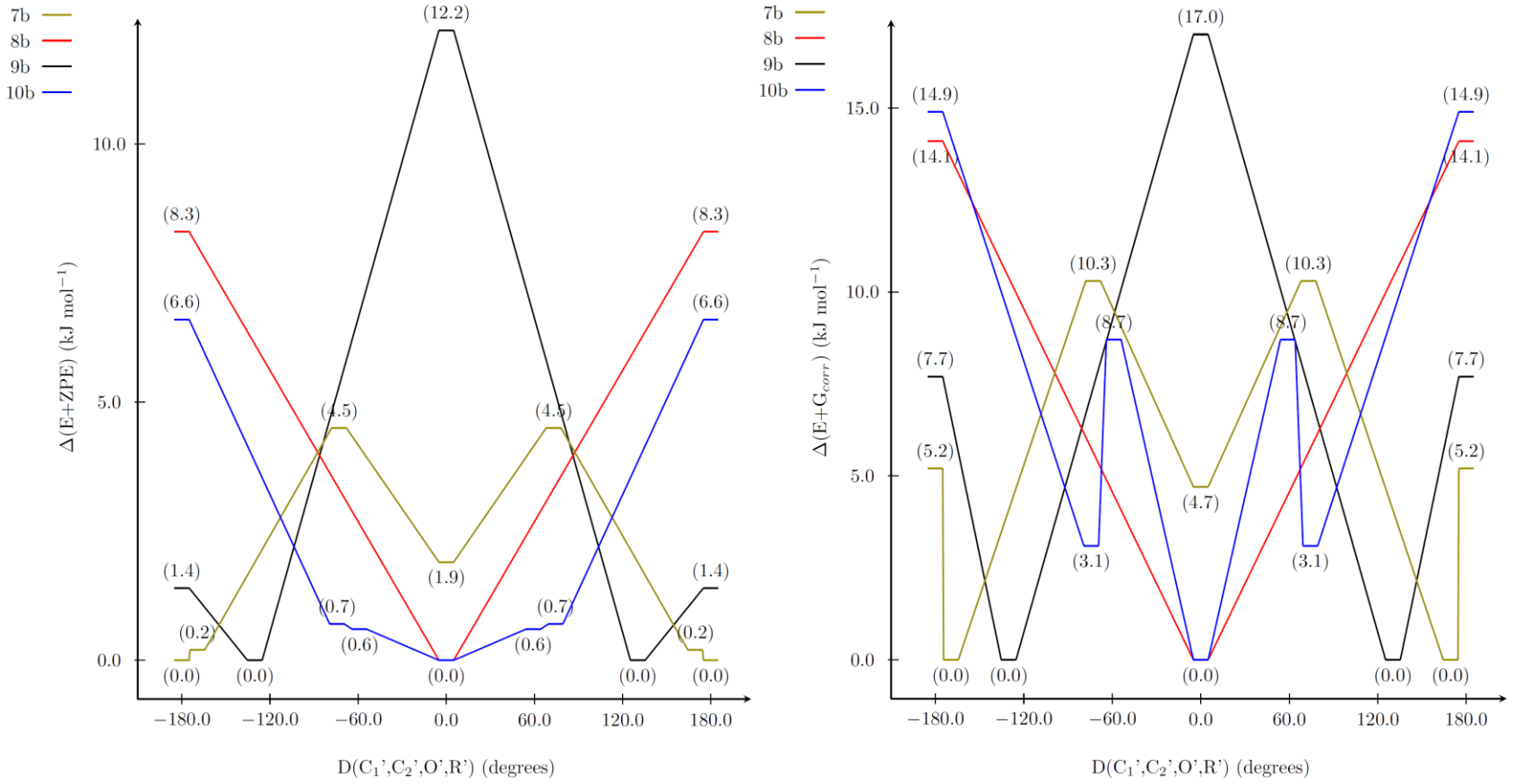


FIGURE 4.5 Stationary points found on the potential energy surface obtained by varying the D(C_1',C_2',O',R') dihedral angle for silyl enol ethers of systems **7**-**10b** (R' = TMS). Energies (zero-point, ZPE, or Gibbs, G_{corr}, corrected) are relative to that of global minimum. (Lines joining the points are to aid viewing.)

What remains to be considered is how both reactant structures approach one another during the carbon-carbon bond forming event (FIGURE 4.6). It is important to be reminded that FIGURE 4.6 depicts staggered conformations between the two reacting partners. The intention of the scheme is only to show the *approximate* orientation of the reacting pair in a representative manner. As Lee *et al.*[86a] showed, open-type transition states may not fit into strictly staggered transition state geometries and thus simple steric arguments based on these models may not lead to correct answers.

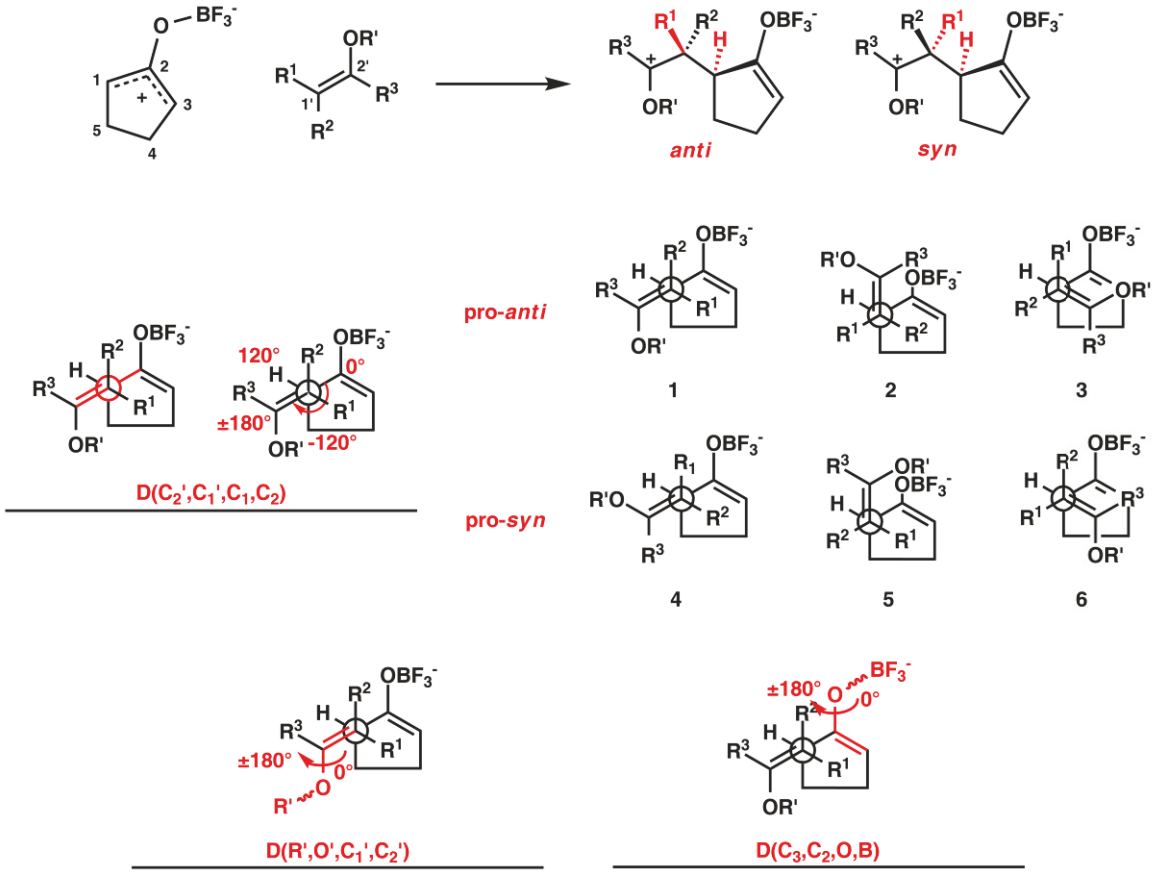


FIGURE 4.6 Modes of approach considered and key dihedral angles varied for the transition state model of the homologous Mukaiyama aldol addition between silyl enol ethers or enols and the oxyallyl cation.

Furthermore, from this same scheme, the boron trifluoride is placed *anti* to the silyl enol ether. This depiction does not mean that the silyl enol ether approaches the oxyallyl cation solely from this direction (attack on the C_1 carbon) or that these are the lower energy

pathways. The silyl enol ether could also approach the oxyallyl cation in a *syn* fashion to the boron trifluoride (attack on the C_3 carbon).

Altogether, four main questions were addressed when seeking the plausible pathways for the Lewis acid-mediated aldol addition of silyl enol ethers to the oxyallyl cation. (1) Which pathways are preferred in this reaction scheme, pro-*syn* or pro-*anti*? (2) How does the conformation of the silyl enol ether affect these pathways? (3) Is an attack on C_1 or C_3 more favorable than the other, i.e., when the boron trifluoride is considered to be *syn* or *anti* to the incoming silyl enol ether? (4) What factors overall control the diastereoselectivity in this reaction?

4.6 Results and Discussion

With all of this in mind, transition states for the homologous Mukaiyama aldol addition between silyl enol ethers or enols and the oxyallyl cation were located for systems **7**-**10**. Relative energies and key dihedral angles, defined earlier in FIGURE 4.6, are given in TABLE 4.1.

These are the results of extensive searches including scans of potential energy surfaces by varying various parameters, e.g. $D(C_2',C_1',C_1,C_2)$ and $R(C_1,C_2)$.

Values in parentheses in TABLE 4.1 refer to FIGURE 4.6 and categorize the transition states based on the value of the $D(C_2',C_1',C_1,C_2)$ dihedral angle. Transition states are also placed in order of increasing zero-point-corrected energies relative to that of the lowest lying transition state for that system. (Entry numbers are used to relate these transition states with their associated reactant and product complexes presented in TABLES A2.2-A2.5 of Appendix 2.)

TABLE 4.1 Transitions states for the homologous Mukaiyama aldol addition of silyl enol ethers to an oxyallyl cation located at the B3LYP/6-31G(d) level of theory.

Entry number (Type) [a]		$\Delta(E+ZPE)$ [a] (kJ mol^{-1})	$\Delta(E+G_{corr})$ [a] (kJ mol^{-1})	$R(C_1,C_1')$ (Å)	$D(C_2',C_1',C_1,C_2)$ (degrees)	$D(R',O',C_2',C_1')$ (degrees)	$D(C_3,C_2,O,B)$ (degrees)
7a							
1	(5)	-8.4	-0.4	2.545	30.4	155.3	153.8
2	(5)	7.1	13.2	2.472	-0.3	-7.4	166.6
4	(6)	15.3	21.3	2.152	-82.0	-9.0	-178.6
6	(3)	16.1	23.9	2.369	-64.8	-179.7	171.8
3	(6)	17.4	24.4	2.177	-72.8	-9.0	-44.3
5	(4)	21.9	26.9	2.355	-179.1	177.5	167.7
8	(3)	31.0	38.0	2.235	-65.5	-175.9	-3.7
7	(4)	31.6	36.9	2.179	160.2	176.4	-42.9
8a							
9	(6)	2.7	5.3	2.386	-86.9	-8.2	-41.3
10	(2)	5.9	8.7	2.434	105.8	6.9	-33.7
11	(3)	28.9	30.1	2.322	-70.5	-177.4	-3.6
9a							
14	(6)	3.9	8.4	2.389	-81.7	179.6	-41.3
13	(6)	5.1	10.2	2.367	-86.5	-7.3	-41.9
12	(1)	7.5	12.7	2.243	-176.6	8.1	-16.9
15	(2)	10.6	15.5	2.326	100.1	-177.4	-38.2
17	(2)	14.3	19.0	2.329	108.5	5.9	-41.5
16	(1)	16.3	20.8	2.182	177.2	-175.4	-18.4
19	(3)	38.6	43.2	2.287	-67.1	-172.7	-27.7
20	(4)	38.7	42.8	2.138	159.2	174.2	-17.6
18	(3)	42.9	48.5	2.175	-76.6	-174.6	134.7
10a							
21	(6)	10.1	15.8	2.311	-64.5	-11.0	-32.6
23	(4)	22.5	24.6	2.214	176.9	174.5	-16.7
22	(1)	30.9	33.0	2.119	158.8	-170.5	-16.3
7b							
24	(3)	6.8	32.2	2.308	-75.5	113.6	-35.1
25	(3)	8.1	34.5	2.344	-71.5	64.6	10.5
26	(6)	27.2	47.5	2.261	-76.2	-27.3	-43.3
8b							
27	(3)	2.1	5.8	2.411	-90.8	82.9	-38.2
28	(6)	11.3	9.4	2.405	-92.8	-30.5	-38.7
29	(2)	14.4	11.6	2.468	108.2	29.8	-32.9
9b							
30	(6)	2.1	8.7	2.411	-85.6	-159.1	-37.8
32	(2)	7.3	13.3	2.439	106.4	171.9	-38.7
31	(1)	10.0	14.9	2.272	178.6	160.4	-16.4
10b							
33	(3)	5.6	9.4	2.778	-92.0	87.4	-39.8

[a] See Discussion for more details on how the transition states are ordered.

4.6.1 Incipient Bond Length in the Transition States of the Homologous Mukaiyama Aldol Addition

The R(C_1,C_1') bond lengths for all transition states were found to be between roughly 2.1 and 2.6 Å, which are consistant with similar systems from previous studies.[68b,86a] No explanation can be provided to explain the different R(C_1,C_1') bond lengths for all of the transition states, other than they are probably the result of a combination of various steric and/or other electronic effects.

4.6.2 Site of Nucleophilic Attack of the Enols (or Silyl Enol Ethers) to the Oxyallyl Cation

Transition states for all systems containing R' = H were first located with the misconception that an attack on C_1 of the oxyallyl cation by the silyl enol ether would be more favored than that on the C_3 carbon. The rationale behind this was that the silyl enol ether would avoid the boron trifluoride for steric reasons and so would prefer to form a bond at the C_1 carbon. However, this turned out not to be true when an attempt to find transition states with the enol forming a bond at the C_3 carbon for system **7a** and **9a** was performed. For example, by comparing entries 3 and 4 for the value of the D(C_3,C_2,O,B) dihedral angle, one can see that the transition state placing the BF_3 *syn* to the attack of the enol (entry 4) is of lower energy than the converse (entry 3, BF_3 *anti* to the site of attack). The same is deduced from entries 5 and 7 or 6 and 8.

However, comparing the analogous transition states of entries 3 and 4 for system **9a** (entries 19 and 18, respectively), an attack on the C_1 carbon (entry 19) was found to be preferred over that on the C_3 carbon (entry 18). Here, though, the substituent on the enolate that lies closest to BF_3, R_1, is a methyl substituent in **9a**, whereas it is only a hydrogen atom in **7a**. Steric interactions between the methyl substituent and the boron trifluoride could be large enough to destabilize the transition state with the enolate attacking on the C_3 carbon, i.e., an attack *syn* to the BF_3.

On another matter, recall that transition states of type 2 and 5 were defined for values of $D(C_2',C_1',C_1,C_2)$ ranging from roughly 0-120 degrees, which places the silyl enol ether double-bond in between the oxyallyl cation carbonyl and the carbon alpha to it, C_1. It may be plausible to assume that a transition state of type 2 would only exist if the attack of the nucleophile took place at the C_1 carbon and that the dihedral angle $D(C_2',C_1',C_1,C_2)$ is closer to 120 degrees than it is to 0 degrees so as to minimize steric interactions between R^3, OR' and OBF_3^- as well as keeping the two oxygen atoms farther apart. Similarly, transition states of type 5 could only exist if the nucleophilic attack took place at the C_3 carbon and that the value of the dihedral angle is closer to 0 degrees than to 120 degrees. In fact, transition states of type 5 could only be found when the enolate added to the C_3 carbon (entries 1 and 2), whereas those of type 2 could only be found when the silyl enol ether added to the C_1 carbon (entries 10, 15, 17 and 32).

4.6.3 Conformation of the Silyl Enol Ethers in the Transition States of the Homologous Mukaiyama Aldol Additions

Consider now entries 13 and 14 (system **9a**). These have R' = H *syn* and *anti* to the double-bond of the enolate, respectively. The latter is lower in energy than the former, meaning that the enol in an *anti* conformation is preferred. The same can also be deduced from entries 1 and 2 or 15 and 17. However, comparing entries 12 and 16, one finds that the lowest energy transition state is the one incorporating the enol with the enol proton *syn* to the double-bond. By further inspection of all of these transition states, one finds that for the one of lowest energy in each pair (independent of if R' is *anti* or *syn* to the double-bond) places the OH and OBF_3 bond moments closer to an antiparallel manner than the other. This is analogous to the assumed dipole-dipole minimization of C=O dipoles within the models developed by Heathcock *et. al.*[84a] and by Denmark and Henke[84b] (*cf.* Section **4.2.2**).

Let us briefly discuss entries 24 and 25, which have R' = TMS, (FIGURE 4.7). These two transition states have the silyl enol ether adding to the C_1 carbon (*anti* to the Lewis acid) and have similar values of $D(C_2',C_1',C_1,C_2)$. Both have the TMS in a *gauche* conformation

to the double-bond, which is pointing away from the oxyallyl cation ring system. The lowest energy transition state should have the OTMS and OBF_3^- bond moments minimized. By looking through the O – BF_3 bond, one can observe how close the two bond moments (O – TMS and O – BF_3) are to an antiparallel arrangement. In this case, the closer the silicon atom lies behind the neighbouring oxygen, the more the two bond moments are antiparallel. Entry 24 is of lower energy and does in this case have the two bond moments closest to an antiparallel arrangement than entry 25.

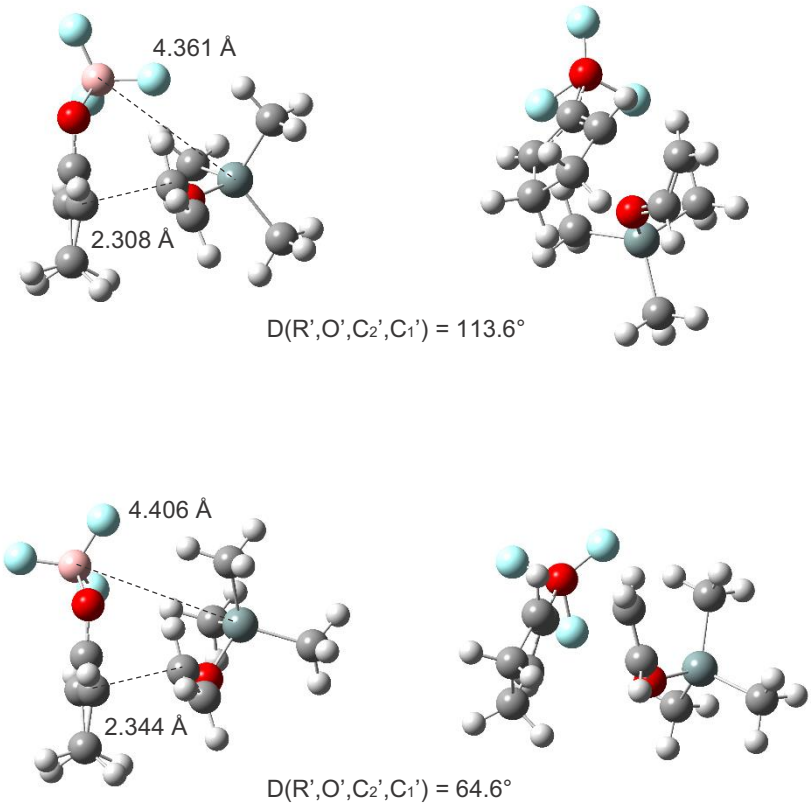


FIGURE 4.7 Side view (left) and view through the O – BF_3 bond (right) of the transition states of entries 24 (top) and 25 (bottom) in TABLE 4.1.

4.6.4 Mode of Approach of the Silyl Enol Ether to the Oxyallyl Cation

By using the arguments discussed regarding the site of nucleophilic attack (Section **4.6.2**) and bond moment minimization of OR' and OBF_3^- (Section **4.6.3**), one can explain the relative energies of transition states when the enol (and possibly the silyl enol ether) approaches the oxyallyl cation for a 'fixed' value of D(C_2',C_1',C_1,C_2) (FIGURE 4.8).

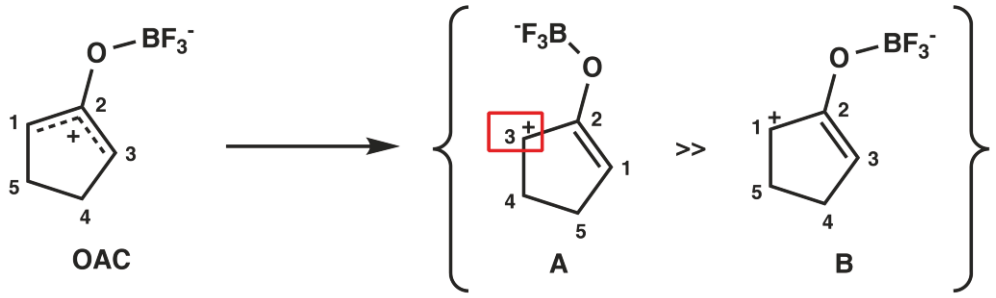
But what explains the relative ordering of these transition states when D(C_2',C_1',C_1,C_2) varies? The data presented in TABLE 4.1 seem to allude to the fact that the relative ordering of the transition states (excluding the effects just discussed) might be due to some extent to the bond moment minimization of the C-O bonds in the silyl enol ether and the oxyallyl cation.[84,86a] One would expect the transition states to be ordered as follows: 1, 6 < 2, 4 < 3, 5 (*cf.* FIGURE 4.6). Of course, there can easily be much variability in this ordering alone, especially when one considers that the silyl enol ether and oxyallyl cation are not necessarily in a co-planar arrangement. Dipoles (or bond moments) may not be as well-aligned as they are presented in Newman projections, substituents and their associated 'steric interactions' with groups or parts of the overall structure may not have as a considerable effect as one might think.

4.6.5 Diastereoselectivity in the Homologous Mukaiyama Aldol Addition of Silyl Enol Ethers to Oxyallyl Cations

Marx and Burnell[56c] and Wu *et al.*[7a] reported examples of high diastereoselectivity for the homologous Mukaiyama aldol additions of silyl enol ethers to oxyallyl cations produced from Nazarov cyclizations (*cf.* SCHEME 4.11). System **9** studied in this chapter can be considered as analogous to these two examples. One could therefore use this model to explain the selectivity. If a similar approach to assess the diastereoselectivity in work done by Lee *et al.*[86a] is taken, i.e., comparing the relative transition state energies to that of the lowest lying saddle point, the following conclusions can be made.

Preferred site of nucleophilic attack by the (silyl) enol ether

I. Inspection of the bond lengths in the oxyallyl cation (**OAC**) yields $R(C_1,C_2) < R(C_2,C_3)$. C_3 has a greater sp^3 character than C_1, and will therefore carry the positive charge more than C_1. The (silyl) enol ether should prefer to approach C_3 (**A**) over C_1 (**B**).



Thus, **C** and **E** are preferred over **D** and **F**, respectively, unless steric interactions between R^2 or R^1 with BF_3^- are too destabilizing (e.g., R_2 or R_1 = Me suffices); in which case the opposite is true (**D** and **F** preferred over **C** and **E**).

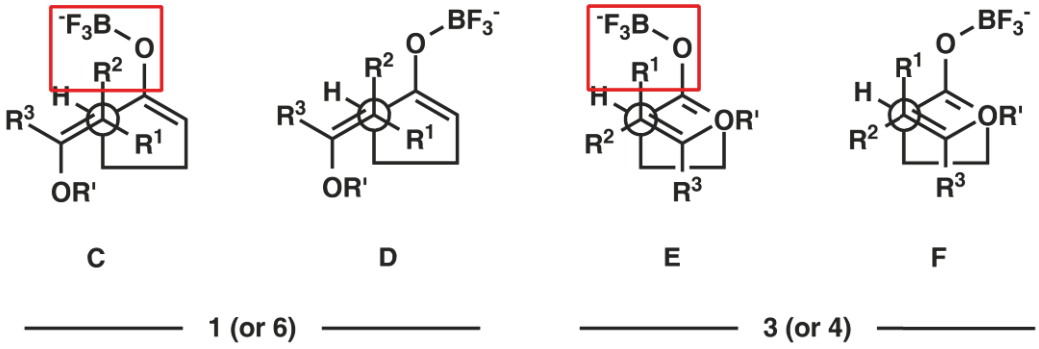
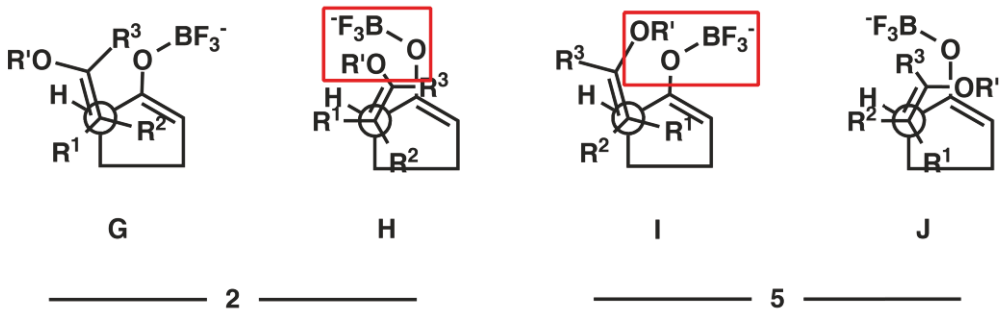


FIGURE 4.8 Preferred site of nucleophilic attack and bond moment minimization arguments for fixed values of $D(C_2',C_1',C_1,C_2)$ in the homologous Mukaiyama aldol additions of (silyl) enol ethers to oxyallyl cations.

II. For 2 and 5, **G** and **J** are preferred over **H** and **I**, respectively, to minimize interactions between R^3, OR' and OBF_3^- while keeping both oxygens further apart.



Minimization of the sum of OR' and OBF_3^- bond moments (R' = H or TMS)
OR' and OBF_3^- bond moments tend to be closest to an antiparallel arrangement so as to minimize the dipole moment. For instance, for 1, **K** is preferred over **L** and **M** is preferred over **N**.

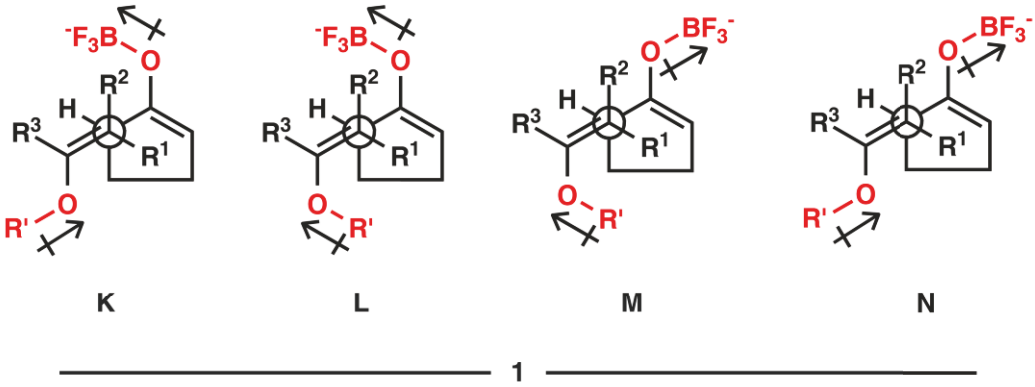


FIGURE 4.8 (continued) Preferred site of nucleophilic attack and bond moment minimization arguments for fixed values of $D(C_2',C_1',C_1,C_2)$ in the homologous Mukaiyama aldol additions of (silyl) enol ethers to oxyallyl cations.

System **9** (R' = OH or TMS) predicts an *syn:anti* selectivity of roughly >20:1 and thus disagrees with the selectivity observed by Marx and Burnell[56c] and Wu *et al.*[7a] for their analogous systems. However, there might be other low-lying transition states that were not located. For instance, **9b** has as its lowest transition state structure, one of type **6**. Perhaps there exists other low lying transition states, just as **7b** and **8b** both have transition states of type **3** that are lower in energy than the one of type **6** (which would be indicative of *anti*:*syn* selectivities of greater than 20:1 if $R^1 \neq R^2$). Furthermore, as some of the differences between the transition state energies are quite small (e.g., entries 3, 4 and 6 are within but

2 kJ mol^{-1} of one another), the relative ordering of these transition states might be incorrect if one thinks of the error brought on by the method by which the structures and energies were calculated.

On the other hand, recall that Wong and Wong[68b] had identified the possibility of separated reactants forming intermolecular complexes before attaining the transition states and then the respective products (*cf.* Section **4.2.2**). Maybe by taking these pre-transition state complexes into account as well as relative energy barriers between all pathways, a better agreement with the experimental results might be obtained.

Intermolecular reactant complexes were therefore located for each of the transition states presented earlier. (Data are presented in TABLES A2.2-A2.5 of Appendix 2.) All arguments made in the preceding sections in terms of relatives energies, etc. generally apply for the reactant complexes and so further discussion of these aspects will not be of concern here.

The approach taken by Wong and Wong[68b] with respect to the separated reactants assembling into reactant complexes before passing through the transition state can be debated. For instance, by comparing the relative zero-point corrected electronic energies between the separated reactants with the reactant complexes for the systems studied here (see TABLES A2.2-A2.5, Appendix 2), it was found that the fomer are generally higher in energy by at least 30 kJ mol^{-1}. This would mean that in order for two reactants to proceed to product formation, this amount of energy needs to be released to the surroundings. As such, it makes it unreasonable to assume that with all of this surplus energy, that other reacting molecules would be limited to passing through the lowest energy transition states to end up to the products. With this approach, one would thus predict that there would be no diastereoselectivity in the reaction between oxyallyl cations and silyl enol ethers. The fact that the energies of the separated reactants are larger than that of the reactant complexes and/or transition states should be of no great surprise, as the oxyallyl cation is afterall a reactive cationic species.

In either case, the fact that the differences in energies between transition states of competing pathways are small and within the error of the computational methods used or that in order for the reactants to proceed through with the reaction, large amounts of energy are introduced to the system, leads to the conclusion that diastereoselectivity in this reaction should be close to nil.

If the high levels of diastereoselectivity observed experimentally for the reaction of oxyallyl cations with silyl enol ethers cannot be attributed to the preference for a particular pathway in the bond forming event, then what accounts for the apparent diastereoselectivity? It is proposed that these levels of diastereoselectivity could be reached by an equilibration between product diastereomers to the more thermodynamically favored isomer after the bond has been formed and the system is brought back up to ambient temperature during the work-up and purification. After all, the reaction is performed in an acidic medium and so a mechanism involving enol/ tautomerism and thus equilibration between the *syn* and the *anti* isomers is possible.

Let us now turn our attention to the structure of the products, or rather the product complexes, that are associated with the transition states. FIGURE 4.9 shows the product intermediates that result from the various modes of approach of the silyl enol ether to the oxyallyl cation. Three distinct types of intermediates were found. Note that these will eventually lead to the dicarbonyl products shown in the top right of FIGURE 4.6 once the system has been subjected to work-up.

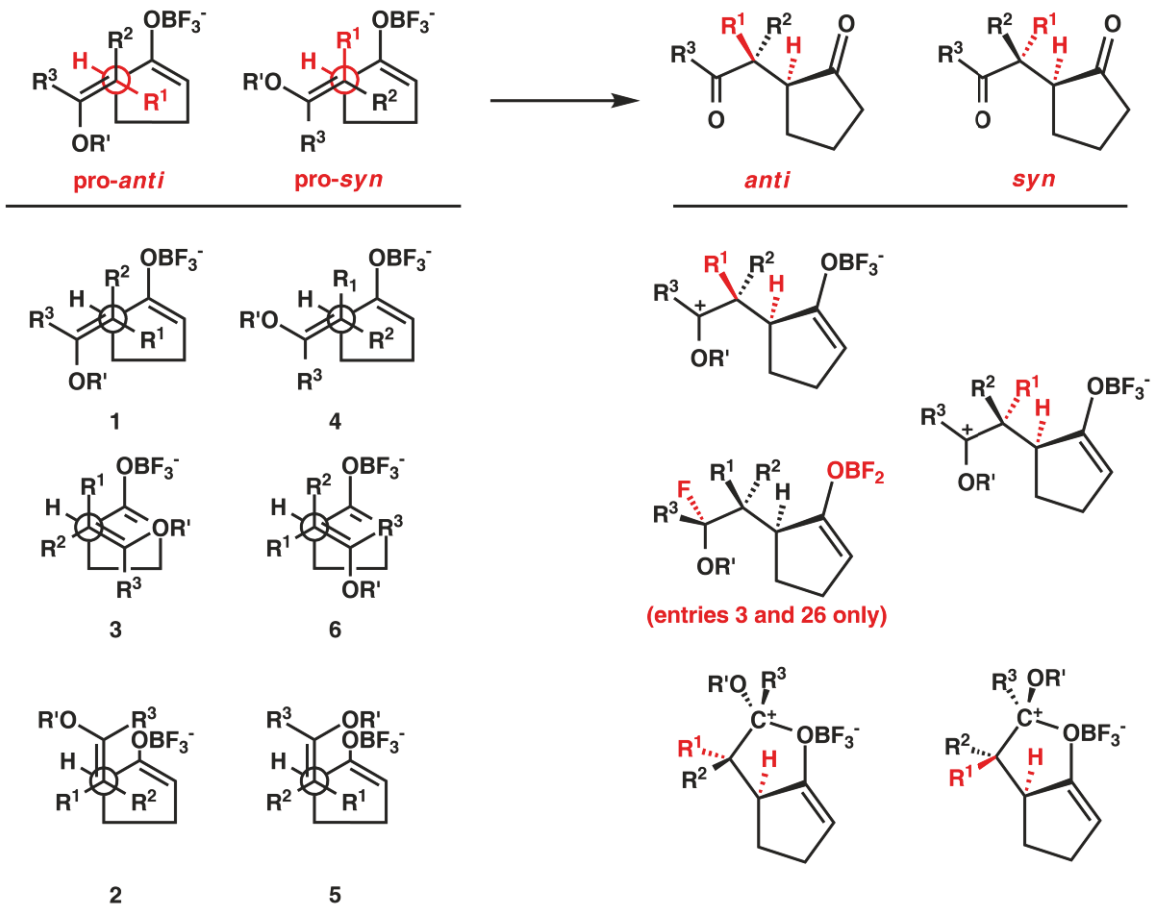


FIGURE 4.9 Product complexes formed in the pro-*anti* and pro-*syn* pathways.

Transition states of type 1 and 3 led to product intermediates of *anti* configuration, as expected. Similarly (with the exception of entries 3 and 26), transition states of type 4 and 6 led to intermediates of *syn* configuration.

Entries 3 and 26 differ from the other product complexes by the migration of one of the fluorine atoms of BF_3 to the C_2' carbon of the silyl enol ether. This has been documented previously[68b] in the study of stepwise pathways for Lewis acid-mediated aldol additions of silyl enol ethers to aldehydes (*cf.* SCHEME 4.10; Section **4.2.2**). A hypothesis to why a fluorine transfer is only observed for entries 3 and 26 can be formulated. This type of product was only observed for systems **7a** and **7b** where the mode of approach between the two reacting partners parallels **6** in either FIGURE 4.6 or FIGURE 4.9. This positions the

silyl enol ether in such a way that one of the fluorine atoms of the neighbouring boron trifluoride comes into close proximity of C_2'. This carbon atom develops a positive charge as the reaction progresses and allows for the transfer one of the fluorine atoms in the product complex. So then why does the same product intermediate not form for systems **8**, **9** or **10** in the same mode of approach as entries 3 and 26? This could possibly be due to the fact that these systems, in contrast to **7**, possess a methyl group at the R^3 position, which in turn, lessens the positive charge on C_2' and/or inhibits the approach of the BF_3 towards the silyl enol ether. Also, if the attack of the silyl enol ether takes place at the C_3 carbon instead of C_1 (as with entry 4), the boron trifluoride would unquestionably be too far away from the developing cationic charge on C_2' to allow for a fluorine transfer.

The third type of product intermediate found was analogous to that of an oxetane intermediate located by Wong and Wong[68b] or to that hypothesized by Wu and West for homologous aldol additions with alkynes.[7b] This was observed for pathways positioning the silyl enol ether as in **2** or **5** depicted in FIGURE 4.9. It should be expected that as C_2' is close to the oxygen of the oxyallyl cation, that latter could attack the electron-deficient center as the bond between C_1 and C_1' are being formed.

4.7 Conclusions and Future Work

The aim of the work presented in this chapter was to rationalize the high degrees of diastereoselectivity observed experimentally in the homologous Mukaiyama aldol additions of silyl enol ethers to oxyallyl cations.

However, as no previous studies had been conducted for silyl enol ethers reacting with oxyallyl cations, the elaboration of a preliminary model for the system of interest was initiated. Attention was placed on the various details of how the two reacting partners approach one another during the carbon-carbon bond forming event and hypotheses were presented to explain the relative ordering of the various transition state structures, in terms of the site of nucleophilic attack, bond moment minimization, etc. Although these hypotheses were based on the results obtained from the reaction of silyl enol ethers adding to a rather simple oxyallyl cation, they will prove useful for the continuing development of this and/or other models that are based on open-type transition states. More importantly, the results presented here should make one more mindful that when approaching similar problems it is important to consider all possible pathways, without discarding some of them too quickly.

In terms of the high levels of diastereoselectivity observed for examples in the literature on aldol additions of enol ethers to oxyallyl cations, it seems plausible that these are not linked to the kinetically-controlled bond-forming step of the reaction, which is likely to have little selectivity due to the high reactivity of the system. Rather, the apparent diastereoselectivity is probably the result of equilibration of the products to the thermodynamically preferred isomer when the system is brought up to ambient temperature during subsequent experimental procedures.

There is still much work to be done in the study of open-type transition states. A thorough benchmarking study should be considered in concert with further development of models for Lewis acid-mediated Mukaiyama aldol additions. As there are so few literature reports on this variant of the reaction, it would be the opportune moment to consider these types of

studies. Recall that relative energies between transition states or intermolecular complexes of competing pathways tend to be quite small. It would therefore be advantageous to be certain that the method that is being used to generate geometries and energies is adequate for the study of these complex reacting systems. Only then, should the results presented in this study be confirmed based on a more carefully chosen method that can reflect experimental results well.

CHAPTER 5 CONCLUSIONS

A computational study of stereochemical aspects of a Nazarov/homologous Mukaiyama sequence was undertaken in order to shed light on some recent experimental results.[7,56] In particular, these aspects were the torquoselectivity in the Nazarov reactions of terminally substituted allenyl vinyl ketones, and the diasteroselectivity of reactions that involved interception of the oxyallyl cation intermediate of the Nazarov reaction by the nucleophilic addition of silyl enol ethers.

In Chapter 3, the Nazarov cyclization of allenyl vinyl ketones was examined. The torquoselectivity giving rise to the kinetic product was found to be dictated by competing steric interactions between susbstituents at both termini and between those on the allene moiety. During inward rotation of the allene substituent, more strain is placed between substituents at the termini than during outward rotation. In order to alleviate these interactions, the allene must bend more before rotation about the termini occurs in an inward fashion. This makes the transition state for inward rotation higher in energy and thus unfavored over the transition state for outward rotation. The model presented was shown to apply to allenyl vinyl ketones bearing a variety of substituents. What remains to be addressed is if there are any substituents capable of reversing the torquoselectivity in allenyl vinyl ketones. This might include situations where substituents are capable of orbital overlap in a similar manner as theorized by Houk, or where inward rotation were stabilized via an attractive interaction between carefully chosen substituents on the termini of the allene and the vinyl group.

In Chapter 4, a study of silyl enol ethers and simple enols adding to a cyclic oxyallyl cation was carried out to assess the diastereoselectivity in the homologous Mukaiyama reaction. Based on the results of the calculations, factors influencing the relative ordering of the transition states located between the reacting substrates were inferred. However, because of the non-restrictive nature of the relative orientations of the substrates in the open-type transition states, an overall rationalization could not be made. Furthermore, the diastereoselectivity in the carbon-carbon bond forming event was predicted to be nil, and

so the high diastereomeric ratios observed in experiments appear to be the result of an equilibration reaction after the carbon-carbon bond has formed. However, the systems studied were simpler than the reactions that were examined experimentally. It would be interesting to ascertain whether a computational study similar to the one carried out here, but with the more complex substrates that were employed synthetically, would result in evidence for some significant kinetic control of the diastereoselectivity.

The results presented and interpretations made in this thesis should allow others to better elaborate synthetic approaches that include a Nazarov reaction in which stereochemistry develops. Indeed, work is underway to trap intramolecularly the oxyallyl cation intermediate of a torquoselective Nazarov reaction of an allenyl vinyl ketone. The key torquoselective step can now be predicted reliably based on the findings of this thesis. Also, the lack of stereoselectivity in the interrupted Nazarov reactions of silyloxy-substituted dienes can be rationalized by the study of the silyl enol ethers with the cyclic oxyallyl cation described in this thesis.

In a broader sense, these results presented in this thesis show that the use of simple steric and/or electronic arguments can sometimes be misleading and should make one more mindful of all the possibilities when investigating potential mechanisms, without rejecting some of them too quickly.

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APPENDIX 1 CARTESIAN COORDINATES, ENERGIES AND GEOMETRICAL PARAMETERS FOR COMPOUNDS **1-6** STUDIED IN CHAPTER 3

TABLE A1.1 Effects of exchanging H^+ and BF_3 on relative barrier heights and on differences in transition state energies, $\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$), between clockwise and counterclockwise modes of conrotations for system **1b**, R_3 = Me, at the B3LYP/6-31G(d) level of theory.

TABLE A1.2 Energies and geometrical parameters of system **1a**, R^3 = H, at different levels of theory/basis sets.

TABLE A1.3 Energies and geometrical parameters of system **6d**, R^3 = Ph, at different levels of theory/basis sets.

TABLES A1.4-A1.9 Energies and geometrical parameters of systems **1-6** at the B3LYP/6-31G(d) level of theory.

TABLES A1.10-A1.15 Energies and geometrical parameters of systems **1-6** at the ωB97X-D/6-31+G(d,p) level of theory.

TABLE A1.16 Differences in transition state energies, $\Delta(E+ZPE)^{\ddagger}$ / and in Gibbs energies of activation, $\Delta(E+G_{corr})^{\ddagger}$ (kJ mol^{-1}), between clockwise and counterclockwise modes of conrotation for systems **1-6** at the ***X***/6-31+G(d,p)//B3LYP/6-31G(d) level of theory where ***X*** = B3LYP, M06-2X or MP2.

TABLE A1.17 Energies and geometrical parameters of systems **1b**, **1b'** and **1b"** at the B3LYP/6-31G(d) level of theory.

Cartesian coordinates for systems **1-6**

TABLE A1.1 Effects of exchanging H^+ and BF_3 on relative barrier heights and on differences in transition state energies, $\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$), between clockwise and counterclockwise modes of conrotations for system **1b**, R_3 = Me, at the B3LYP/6-31G(d) level of theory.

Structure	Energies				
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})
syn-H^+					
cRT	-425.700474	0.197225	-425.503249	0.0	0.0
cTS	-425.680931	0.196003	-425.484928	51.3	48.1
cPT	-425.726543	0.198811	-425.527732	-68.4	-64.3
ccRT	-425.700361	0.197189	-425.503172	0.3	0.2
ccTS	-425.679192	0.195912	-425.483280	55.9	52.4
ccPT	-425.731071	0.198847	-425.532224	-80.3	-76.1
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-4.6	-4.3
anti-H^+					
cRT	-425.700703	0.197208	-425.503495	0.0	0.0
cTS	-425.682759	0.196116	-425.486643	47.1	44.2
cPT	-425.731040	0.199213	-425.531827	-79.6	-74.4
ccRT	-425.700555	0.197189	-425.503366	0.4	0.3
ccTS	-425.681001	0.196012	-425.484989	51.7	48.6
ccPT	-425.735476	0.199162	-425.536314	-91.3	-86.2
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-4.6	-4.3
syn-BF_3					
cRT	-749.910954	0.199288	-749.711666	0.0	0.0
cTS	-749.882820	0.198539	-749.684281	73.9	71.9
cPT	-749.923079	0.201682	-749.721397	-31.8	-25.5
ccRT	-749.910471	0.199238	-749.711233	1.3	1.1
ccTS	-749.880148	0.198591	-749.681557	80.9	79.1
ccPT	-749.927055	0.201650	-749.725405	-42.3	-36.1
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-7.0	-7.2
anti-BF_3					
cRT	-749.916799	0.199510	-749.717289	0.0	0.0
cTS	-749.887379	0.198480	-749.688899	77.2	74.5
cPT	-749.926547	0.201454	-749.725093	-25.6	-20.5
ccRT	-749.916652	0.199452	-749.717200	0.4	0.2
ccTS	-749.885274	0.198462	-749.686812	82.8	80.0
ccPT	-749.929935	0.201350	-749.728585	-34.5	-29.7
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-5.5	-5.5

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT.

TABLE A1.2 Energies and geometrical parameters of system **1a**, R^3 = H, at different levels of theory/basis sets.

Structure	Energies								Geometrical Parameters				
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	$\Delta(E+ZPE)$ [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	$\Delta(E+G_{corr})$ [a] (kJ mol^{-1})	$R(R^2,H^3)$ [b] (Å)	$R(H^2,H^3)$ (Å)	$R(R^1,R^2)$ [c] (Å)	$A(C_1,C_2,C_3)$ (degrees)	$D(C_2,C_3,C_5,C_6)$ (degrees)
B3LYP/6-31G(d)													
cRT	-710.593516	0.171237	-710.422279	0.0	0.0	0.128715	-710.464802	0.0	4.545	3.028	4.586	176.2	-45.1
cTS	-710.566312	0.170446	-710.395866	71.4	69.3	0.129424	-710.436888	73.3	4.389	2.798	4.011	153.0	-26.4
cPT	-710.612338	0.172863	-710.439475	-49.4	-45.1	0.131427	-710.480911	-42.3	4.296	2.718	3.332	131.1	0.0
cRTccRTTS	-710.589907	0.170862	-710.419045	9.5	9.5	0.128064	-710.461843	-1.7	3.326	3.048	4.563	174.5	-2.1
ccRT	-710.593480	0.171203	-710.422277	0.1	0.0	0.128729	-710.464751	0.1	2.781	4.014	4.674	176.2	44.6
ccTS	-710.565480	0.170353	-710.395127	73.6	71.3	0.129390	-710.436089	75.4	2.511	3.999	4.766	150.9	26.7
ccPT	-710.616809	0.172758	-710.444051	-61.2	-57.2	0.131372	-710.485437	-54.2	2.585	3.940	4.647	125.9	0.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-2.2	-1.9		$\Delta(E+G_{corr})^{\ddagger}$	-2.1					
B3LYP/6-311G(d)													
cRT	-710.782034	0.169768	-710.612266	0.0	0.0	0.126998	-710.655036	0.0	4.447	3.054	4.575	176.0	-46.3
cTS	-710.754245	0.169165	-710.585080	73.0	71.4	0.128075	-710.626170	75.8	4.381	2.793	4.007	153.1	-26.3
cPT	-710.799719	0.171711	-710.628008	-46.4	-41.3	0.130323	-710.669396	-37.7	4.290	2.715	3.329	131.1	0.0
ccRT	-710.781935	0.169731	-710.612204	0.3	0.2	0.126985	-710.654950	0.2	2.814	4.032	4.663	176.1	45.5
ccTS	-710.753255	0.169065	-710.584190	75.6	73.7	0.128033	-710.625222	78.3	2.528	3.994	4.761	151.0	26.7
ccPT	-710.804166	0.171565	-710.632601	-58.1	-53.4	0.130364	-710.673802	-49.3	4.534	3.935	4.640	125.9	0.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-2.6	-2.3		$\Delta(E+G_{corr})^{\ddagger}$	-2.5					
B3LYP/6-31+G(d,p)													
cRT	-710.650106	0.169851	-710.480255	0.0	0.0	0.127197	-710.522910	0.0	4.441	3.046	4.587	175.9	-45.7
cTS	-710.624199	0.169043	-710.455156	68.0	65.9	0.127811	-710.496388	69.6	4.381	2.789	4.023	153.3	-26.5
cPT	-710.671772	0.171584	-710.500188	-56.9	-52.3	0.130375	-710.541398	-48.5	4.299	2.720	3.335	131.0	0.0
ccRT	-710.650036	0.169814	-710.480222	0.2	0.1	0.127184	-710.522851	0.2	2.807	4.027	4.681	175.7	44.9
ccTS	-710.623273	0.168949	-710.454324	70.5	68.1	0.127794	-710.495478	72.0	2.521	3.991	4.773	151.2	26.8
ccPT	-710.676486	0.171488	-710.504998	-69.3	-65.0	0.130475	-710.546010	-60.6	2.595	3.942	4.644	125.7	0.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-2.4	-2.2		$\Delta(E+G_{corr})^{\ddagger}$	-2.4					
B3LYP/6-311+G(d,p)													
cRT	-710.813861	0.169080	-710.644781	0.0	0.0	0.126365	-710.687496	0.0	4.444	3.050	4.572	175.8	-46.1
cTS	-710.786981	0.168340	-710.618641	70.6	68.6	0.127111	-710.659870	72.5	4.366	2.778	4.007	153.3	-26.3
cPT	-710.833189	0.170830	-710.662359	-50.7	-46.2	0.129407	-710.703783	-42.8	4.291	2.716	3.327	131.0	0.0
ccRT	-710.813750	0.169037	-710.644713	0.3	0.2	0.126336	-710.687414	0.2	2.810	4.030	4.665	175.8	45.4
ccTS	-710.785920	0.168240	-710.617680	73.4	71.2	0.127078	-710.658841	75.2	2.517	3.978	4.763	151.1	26.5
ccPT	-710.837947	0.170802	-710.667145	-63.2	-58.7	0.129712	-710.708235	-54.5	2.594	3.935	4.635	125.7	0.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-2.8	-2.5		$\Delta(E+G_{corr})^{\ddagger}$	-2.7					
B3LYP/6-31G(d)/SCRF=(PCM, CH_2Cl_2, $\varepsilon = 8.93$)													
cRT	-710.607584	0.171056	-710.436528	0.1	0.0	0.128795	-710.478789	0.0	4.396	2.997	4.580	175.9	-44.3
cTS	-710.586433	0.170303	-710.416130	55.6	53.6	0.129197	-710.457236	56.6	4.349	2.739	4.063	155.5	-26.6
cPT	-710.638369	0.172637	-710.465732	12.9	12.8	0.130257	-710.508111	-77.0	4.296	2.723	3.317	130.6	0.0
ccRT	-710.607626	0.171088	-710.436538	0.0	0.0	0.128977	-710.478650	0.4	2.778	4.016	4.676	175.7	44.4
ccTS	-710.585578	0.170205	-710.415373	57.9	55.6	0.129189	-710.456389	58.8	2.471	3.965	4.768	153.2	27.0
ccPT	-710.643300	0.172700	-710.470600	-93.7	-89.4	0.130261	-710.513038	-89.9	2.599	3.943	4.626	125.3	0.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-2.2	-2.0		$\Delta(E+G_{corr})^{\ddagger}$	-2.2					

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers.

TABLE A1.2 (continued) Energies and geometrical parameters of system **1a**, R^3 = H, at different levels of theory/basis sets.

Structure	Energies								Geometrical Parameters				
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(R^2,H^3) [b] (Å)	R(H^2,H^3) (Å)	R(R^1,R^2) [c] (Å)	A(C_1,C_2,C_3) (degrees)	D(C_2,C_3,C_5,C_6) (degrees)
B3LYP/6-31G(d)/SCRF=(PCM, CH_3OH, ε = 32.6)													
cRT	-710.609673	0.170985	-710.438688	0.1	0.0	0.128679	-710.480994	0.0	4.392	2.991	4.579	175.9	-44.1
cTS	-710.589395	0.170263	-710.419132	53.4	51.4	0.129087	-710.460308	54.3	4.342	2.729	4.071	155.9	-26.6
cPT	-710.642154	0.172598	-710.469556	13.0	12.9	0.130334	-710.511821	-80.9	2.296	2.723	3.314	130.5	0.0
ccRT	-710.609718	0.171022	-710.438696	0.0	0.0	0.128904	-710.480815	0.5	2.776	4.010	4.676	175.7	44.2
ccTS	-710.588512	0.170121	-710.418391	55.7	53.3	0.128974	-710.459538	56.3	2.468	3.960	4.768	153.5	27.0
ccPT	-710.647124	0.172643	-710.474481	-98.2	-94.0	0.130149	-710.474481	17.1	2.599	3.943	4.623	125.3	0.0
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-2.3	-2.9		Δ(E+G_{corr})‡	-2.0					
M06-2X/6-31+G(d,p)													
cRT	-710.357670	0.172112	-710.185558	1.3	1.3	0.130012	-710.227659	1.1	4.377	2.975	4.589	176.8	-46.5
cTS	-710.329401	0.171252	-710.158149	75.5	73.3	0.130677	-710.198724	77.0	4.343	2.768	3.997	153.7	-27.2
cPT	-710.377254	0.173637	-710.203617	12.6	13.4	0.132256	-710.244998	-44.5	4.297	2.733	3.295	130.4	0.0
ccRT	-710.358174	0.172103	-710.186071	0.0	0.0	0.130114	-710.228060	0.0	2.650	3.932	4.678	177.8	45.6
ccTS	-710.328891	0.171185	-710.157706	76.9	74.5	0.130740	-710.198150	78.5	2.442	3.944	4.791	152.5	27.5
ccPT	-710.382071	0.173358	-710.208713	-62.7	-59.4	0.132553	-710.249518	-56.3	2.559	3.947	4.637	125.5	0.0
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-1.3	-1.2		Δ(E+G_{corr})‡	-1.5					
MP2/6-31+G(d,p)													
cRT	-708.674498	0.173003	-708.501495	0.7	0.8	0.130485	-708.544014	0.6	4.448	3.027	4.585	175.9	-48.7
cTS	-708.653728	0.172401	-708.481327	55.2	53.7	0.131342	-708.522386	57.4	4.388	2.840	4.054	154.1	-29.3
cPT	-708.697679	0.174435	-708.523244	11.6	13.2	0.133449	-708.564230	-52.5	4.323	2.765	3.237	129.9	-1.6
ccRT	-708.674769	0.172982	-708.501787	0.0	0.0	0.130534	-708.544236	0.0	2.687	4.017	4.687	176.7	48.0
ccTS	-708.653062	0.172302	-708.480760	57.0	55.2	0.131335	-708.521727	59.1	2.504	3.992	4.780	152.7	29.5
ccPT	-708.702079	0.173811	-708.528268	-71.7	-69.5	0.130399	-708.571680	-72.1	2.541	3.926	4.645	125.7	-180.0
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-1.7	-1.5		Δ(E+G_{corr})‡	-1.7					
ωB97X-D/6-31+G(d,p)													
cRT	-710.249572	0.171808	-710.249572	1.1	1.2	0.129356	-710.292025	0.8	4.427	3.017	4.584	176.6	-47.6
cTS	-710.222489	0.171031	-710.222489	74.2	72.3	0.130017	-710.263503	75.6	4.366	2.793	4.000	153.6	-27.9
cPT	-710.272196	0.173558	-710.272196	12.3	12.9	0.132235	-710.313520	-55.7	4.319	2.759	3.244	129.9	-1.1
ccRT	-710.250015	0.171777	-710.250015	0.0	0.0	0.129475	-710.292316	0.0	2.677	3.982	4.672	177.5	46.4
ccTS	-710.221966	0.170986	-710.221966	75.7	73.6	0.130137	-710.262815	77.5	2.484	3.968	4.777	152.3	28.3
ccPT	-710.277127	0.173301	-710.277127	-75.2	-71.2	0.132070	-710.318358	-68.4	2.571	3.934	4.634	125.6	0.0
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-1.5	-1.3		Δ(E+G_{corr})‡	-1.9					

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers.

TABLE A1.3 Energies and geometrical parameters of system **6d**, R^3 = Ph, at different levels of theory/basis sets.

Structure	Energies								Geometrical Parameters				
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(R^2,H^3) [b] (Å)	R(H^2,H^3) (Å)	R(R^1,R^2) [c] (Å)	A(C_1,C_2,C_3) (degrees)	D(C_2,C_3,C_5,C_6) (degrees)
B3LYP/6-31G(d)													
cRT	-1251.337879	0.391166	-1250.946713	1.1	0.6	0.330647	-1251.007232	0.0	4.551	3.033	5.818	177.3	-54.3
cTS	-1251.310614	0.390681	-1250.919933	72.6	70.9	0.334252	-1250.976363	81.0	4.344	2.763	5.070	152.3	-25.6
cPT	-1251.328479	0.393067	-1250.935412	25.7	30.3	0.337037	-1250.991442	41.5	4.355	2.791	4.565	134.6	-9.2
cRTccRTTS	-1251.332055	0.390934	-1250.941121	16.4	15.3	0.332357	-1250.999698	4.5	3.350	2.895	5.670	175.3	-4.7
ccRT	-1251.338283	0.391331	-1250.946952	0.0	0.0	0.331559	-1251.006724	1.3	2.490	3.970	5.886	177.3	47.7
ccTS	-1251.306232	0.390238	-1250.915994	84.1	81.3	0.333895	-1250.972337	91.6	2.325	3.959	5.943	146.9	20.7
ccPT	-1251.335626	0.393595	-1250.942031	7.0	12.9	0.336559	-1250.999067	21.4	2.061	3.963	6.119	126.4	1.3
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-11.5	-10.3		Δ(E+G_{corr})‡	-10.6					
B3LYP/6-31+G(d,p)													
cRT	-1251.428656	0.388878	-1251.039778	0.0	0.0	0.328383	-1251.100272	0.0	5.807	3.028	5.806	177.2	-54.3
cTS	-1251.402864	0.388471	-1251.014393	67.7	66.6	0.331844	-1251.071019	76.8	4.402	2.756	5.091	152.8	-25.6
cPT	-1251.421705	0.390584	-1251.031121	18.2	22.7	0.333902	-1251.087803	32.7	3.998	2.838	4.598	135.0	-11.4
ccRT	-1251.428627	0.389028	-1251.039599	0.1	0.5	0.329371	-1251.099257	2.7	3.260	3.960	5.898	176.3	47.5
ccTS	-1251.398418	0.388032	-1251.010386	79.4	77.2	0.331448	-1251.066970	87.4	3.055	3.959	5.954	147.1	20.8
ccPT	-1251.429104	0.391467	-1251.037637	-1.2	5.6	0.334575	-1251.094529	15.1	6.118	3.962	6.118	126.2	1.6
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-11.7	-10.5		Δ(E+G_{corr})‡	-10.6					
B3LYP/6-31G(d)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)													
cRT	-1251.353565	0.391007	-1250.962558	0.0	0.0	0.330573	-1251.022992	0.0	4.507	2.979	5.806	177.4	-53.1
cTS	-1251.331603	0.390475	-1250.941128	57.7	56.3	0.333738	-1250.997865	66.0	4.317	2.722	5.111	154.0	-25.5
cPT	-1251.352235	0.392672	-1250.959563	3.5	7.9	0.335727	-1251.016508	17.0	4.349	2.788	4.608	135.1	-10.5
ccRT	-1251.353391	0.391113	-1250.962278	0.5	0.7	0.331591	-1251.021800	3.1	2.482	4.013	5.892	176.4	49.1
ccTS	-1251.327643	0.390065	-1250.937578	68.1	65.6	0.333724	-1250.993919	76.3	2.320	3.952	5.942	148.4	21.3
ccPT	-1251.361050	0.393689	-1250.967361	-19.7	-12.6	0.336492	-1251.024557	-4.1	2.059	3.969	6.098	126.1	1.4
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-10.4	-9.3		Δ(E+G_{corr})‡	-10.4					
B3LYP/6-31+G(d,p)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)													
cRT	-1251.428656	0.388878	-1251.039778	0.0	0.0	0.328383	-1251.100272	0.0	4.532	3.028	5.806	177.2	-54.3
cTS	-1251.402864	0.388471	-1251.014393	67.7	66.6	0.331844	-1251.071019	76.8	4.338	2.756	5.091	152.8	-25.6
cPT	-1251.421705	0.390584	-1251.031121	18.2	22.7	0.333902	-1251.087803	32.7	4.379	2.838	4.598	135.0	-11.4
ccRT	-1251.428627	0.389028	-1251.039599	0.1	0.5	0.329371	-1251.099257	2.7	2.559	3.960	5.898	176.3	47.5
ccTS	-1251.398418	0.388032	-1251.010386	79.4	77.2	0.331448	-1251.066970	87.4	2.348	3.959	5.954	147.1	20.8
ccPT	-1251.429104	0.391467	-1251.037637	-1.2	5.6	0.334575	-1251.094529	15.1	2.078	3.962	6.118	126.2	1.6
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-11.7	-10.5		Δ(E+G_{corr})‡	-10.6					
M06-2X/6-31G(d)													
cRT	-1250.827531	0.395314	-1250.432217	12.2	11.1	0.334545	-1250.492986	3.3	4.479	2.969	5.715	176.8	-53.3
cTS	-1250.803352	0.394686	-1250.408666	75.7	73.0	0.338654	-1250.464698	77.6	4.321	2.766	4.969	153.6	-27.1
cPT	-1250.826260	0.397426	-1250.428834	13.2	12.5	0.342545	-1250.483715	27.6	4.386	2.919	4.211	131.7	-9.2
ccRT	-1250.832166	0.395712	-1250.436454	0.0	0.0	0.337928	-1250.494238	0.0	2.528	3.779	5.784	178.3	46.7
ccTS	-1250.802777	0.394348	-1250.408429	77.2	73.6	0.339541	-1250.463236	81.4	2.463	3.936	5.988	149.9	23.7
ccPT	-1250.831282	0.397698	-1250.433584	2.3	7.5	0.341495	-1250.489787	11.7	2.091	3.997	6.112	126.6	3.1
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-1.5	-0.6		Δ(E+G_{corr})‡	-3.8					

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers.

TABLE A1.3 (continued) Energies and geometrical parameters of system **6d**, R^3 = Ph, at different levels of theory/basis sets.

Structure	Energies								Geometrical Parameters				
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(R^2,H^3) [b] (Å)	R(H^2,H^3) (Å)	R(R^1,R^2) [c] (Å)	A(C_1,C_2,C_3) (degrees)	D(C_2,C_3,C_5,C_6) (degrees)
M06-2X/6-31+G(d,p)													
cRT	-1250.899834	0.392968	-1250.506866	11.3	10.6	0.332626	-1250.567208	4.4	4.468	2.968	5.715	176.6	-53.1
cTS	-1250.876921	0.392395	-1250.484526	71.5	69.2	0.336257	-1250.540665	74.1	4.316	2.759	4.988	154.1	-27.1
cPT	-1250.900503	0.394694	-1250.505809	14.9	13.2	0.338547	-1250.561957	18.2	4.411	2.974	4.250	132.1	-11.5
ccRT	-1250.904142	0.393242	-1250.510900	0.0	0.0	0.335252	-1250.568889	0.0	2.556	3.779	5.801	178.3	46.4
ccTS	-1250.876366	0.392023	-1250.484343	72.9	69.7	0.337100	-1250.539265	77.8	2.473	3.932	5.992	150.3	23.7
ccPT	-1250.906183	0.395356	-1250.510827	-5.4	0.2	0.338889	-1250.567294	4.2	2.120	3.995	6.114	126.3	3.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-1.5	-0.5		$\Delta(E+G_{corr})^{\ddagger}$	-3.7					
M06-2X/6-31G(d)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)													
cRT	-1250.843615	0.395118	-1250.448497	9.9	9.9	0.335452	-1250.508164	5.1	4.437	2.916	5.713	176.9	-51.8
cTS	-1250.824544	0.394439	-1250.430105	60.0	58.2	0.338447	-1250.486097	63.0	4.293	2.719	5.023	155.6	-27.0
cPT	-1250.850083	0.396750	-1250.453333	19.9	17.6	0.340713	-1250.509370	1.9	4.388	2.930	4.235	131.9	-10.6
ccRT	-1250.847404	0.395130	-1250.452274	0.0	0.0	0.337309	-1250.510094	0.0	2.559	3.769	5.786	178.6	45.7
ccTS	-1250.824262	0.394149	-1250.430113	60.8	58.2	0.339444	-1250.484818	66.4	2.412	3.911	5.975	152.0	23.8
ccPT	-1250.857659	0.397635	-1250.460024	-26.9	-20.3	0.341621	-1250.516038	-15.6	2.071	3.998	6.090	126.1	2.8
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-0.7	0.0		$\Delta(E+G_{corr})^{\ddagger}$	-3.4					
M06-2X/6-31+G(d,p)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)													
cRT	-1250.918271	0.392601	-1250.525670	8.7	8.3	0.332912	-1250.585358	2.8	4.426	2.906	5.716	176.9	-51.3
cTS	-1250.900780	0.391975	-1250.508805	54.6	52.6	0.335632	-1250.565148	55.9	4.287	2.709	5.051	156.4	-27.2
cPT	-1250.927768	0.394236	-1250.533532	20.6	18.4	0.338125	-1250.589643	-8.5	4.387	2.292	4.262	132.1	-10.5
ccRT	-1250.921578	0.392740	-1250.528838	0.0	0.0	0.335154	-1250.586424	0.0	2.578	3.773	5.804	178.6	45.4
ccTS	-1250.900633	0.391635	-1250.508998	55.0	52.1	0.336632	-1250.564001	58.9	2.434	3.912	5.983	152.6	24.1
ccPT	-1250.935613	0.395080	-1250.540533	-36.8	-30.7	0.338565	-1250.597049	-27.9	2.096	3.996	6.091	125.9	3.1
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-0.4	0.5		$\Delta(E+G_{corr})^{\ddagger}$	-3.0					
ωB97X-D/6-31G(d)													
cRT	-1250.946395	0.395505	-1250.550890	13.2	11.9	0.334518	-1250.611876	5.5	4.545	3.038	5.720	176.2	-55.2
cTS	-1250.922977	0.395139	-1250.527838	74.6	72.4	0.338775	-1250.584202	78.2	4.343	2.794	4.983	153.9	-28.1
cPT	-1250.949530	0.397914	-1250.551616	12.4	12.4	0.342795	-1250.606735	19.0	4.391	2.915	4.271	132.1	-9.4
ccRT	-1250.951409	0.395977	-1250.555432	0.0	0.0	0.337432	-1250.613977	0.0	2.590	3.854	5.781	178.3	48.8
ccTS	-1250.922418	0.394801	-1250.527617	76.1	73.0	0.339659	-1250.582758	82.0	2.511	3.951	5.974	150.2	24.9
ccPT	-1250.954247	0.397911	-1250.556336	-7.5	-2.4	0.340581	-1250.613666	0.8	2.153	3.985	6.120	127.2	2.8
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-1.5	-0.6		$\Delta(E+G_{corr})^{\ddagger}$	-3.8					
ωB97X-D/6-31+G(d,p)													
cRT	-1251.022240	0.393359	-1250.628881	12.4	11.1	0.332785	-3283684.8	4.7	5.515	3.024	5.699	175.9	-54.6
cTS	-1251.000421	0.392812	-1250.607609	69.7	66.9	0.336044	-3283619.0	70.6	4.333	2.781	5.005	154.5	-28.1
cPT	-1251.027936	0.395347	-1250.632589	14.6	13.3	0.338966	-3283683.6	6.0	4.413	2.967	4.304	132.5	-11.7
cRTccRTTS	-1251.017195	0.393171	-1250.624024	25.7	23.8	0.334251	-784815.4	-3.8	3.260	2.830	5.715	176.6	-10.1
ccRT	-1251.026972	0.393875	-1250.633097	0.0	0.0	0.335714	-3283689.6	0.0	2.606	3.852	5.799	178.4	48.7
ccTS	-1250.999777	0.392709	-1250.607068	71.4	68.3	0.337291	-3283614.0	75.5	2.513	3.942	5.977	150.6	24.7
ccPT	-1251.033501	0.395860	-1250.637641	-17.1	-11.9	0.338719	-3283698.8	-9.3	2.155	3.986	6.117	126.7	3.2
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-1.7	-1.4		$\Delta(E+G_{corr})^{\ddagger}$	-5.0					

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers.

TABLE A1.3 (continued) Energies and geometrical parameters of system **6d**, R^3 = Ph, at different levels of theory/basis sets.

Structure	Energies								Geometrical Parameters				
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(R^2,H^3) [b] (Å)	R(H^2,H^3) (Å)	R(R^1,R^2) [c] (Å)	A(C_1,C_2,C_3) (degrees)	D(C_2,C_3,C_5,C_6) (degrees)
ωB97X-D/6-31G(d)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)													
cRT	-1250.962708	0.395226	-1250.567482	11.1	10.4	0.335149	-1250.627560	5.0	4.482	2.966	5.708	176.3	-53.2
cTS	-1250.944418	0.394736	-1250.549682	59.1	57.1	0.338186	-1250.606232	61.0	4.314	2.745	5.034	155.8	-28.0
cPT	-1250.974051	0.397649	-1250.576402	18.4	16.7	0.342083	-1250.631967	-6.6	4.391	2.932	4.299	132.3	-11.0
ccRT	-1250.966924	0.395497	-1250.571427	0.0	0.0	0.337477	-1250.629447	0.0	2.609	3.842	5.786	178.8	47.7
ccTS	-1250.944197	0.394305	-1250.549892	59.7	56.5	0.338413	-1250.605784	62.1	2.467	3.933	5.966	152.0	25.1
ccPT	-1250.981044	0.398270	-1250.582774	-37.1	-29.8	0.342058	-1250.638986	-25.0	2.114	3.992	6.091	126.2	2.9
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-0.6	0.6		Δ(E+G_{corr})‡	-1.2					
ωB97X-D/6-31+G(d,p)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)													
cRT	-1251.041192	0.392897	-1250.648295	9.8	8.9	0.332715	-1250.708477	3.1	4.460	2.951	5.696	176.1	-52.4
cTS	-1251.024803	0.392649	-1250.632154	52.8	51.3	0.336250	-1250.688554	55.4	4.305	2.732	5.059	156.5	-28.0
cPT	-1251.055918	0.394969	-1250.660949	20.2	17.8	0.338948	-1250.716971	-19.2	4.387	2.911	4.315	132.6	-10.6
ccRT	-1251.044927	0.393246	-1250.651681	0.0	0.0	0.332715	-1250.709671	0.0	2.616	3.841	5.799	178.9	47.4
ccTS	-1251.024634	0.392085	-1250.632549	53.3	50.2	0.336250	-1250.688198	56.4	2.475	3.927	5.970	152.6	25.2
ccPT	-1251.063613	0.395902	-1250.667711	-49.1	-42.1	0.338948	-1250.724106	-37.9	2.114	3.988	6.089	126.0	3.0
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-0.4	1.0		Δ(E+G_{corr})‡	-0.9					

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers.

TABLE A1.4 Energies and geometrical parameters of system **1** at the B3LYP/6-31G(d) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(R^2,H^3) [b] (Å)	R(H^2,H^3) (Å)	R(R^1,R^5) [c] (Å)	A(C_1,C_2,C_3) (degrees)	D(C_2,C_3,C_5,C_6) (degrees)	D(R^3,C_6,C_5,C_4) [d] (degrees)	D(R^2,C_2,C_3,C_4) (degrees)
1a, R^3 = H															
cRT	-710.593516	0.171237	-710.422279	0.0	0.0	0.128715	-710.464802	0.0	4.545	3.028	4.586	176.2	-45.1	-176.6	-92.1
cTS	-710.566312	0.170446	-710.395866	71.4	69.3	0.129424	-710.436888	73.3	4.389	2.798	4.011	153.0	-26.4	156.0	-132.5
cPT	-710.612338	0.172863	-710.439475	-49.4	-45.1	0.131427	-710.480911	-42.3	4.296	2.718	3.332	131.1	0.0	120.8	-180.0
ccRT	-710.593480	0.171203	-710.422277	0.1	0.0	0.128729	-710.464751	0.1	2.781	4.014	4.674	176.2	44.6	176.7	-98.1
ccTS	-710.565480	0.170353	-710.395127	73.6	71.3	0.129390	-710.436089	75.4	2.511	3.999	4.766	150.9	26.7	-156.7	-136.0
ccPT	-710.616809	0.172758	-710.444051	-61.2	-57.2	0.131372	-710.485437	-54.2	2.585	3.940	4.647	125.9	0.0	-120.8	180.0
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-2.2	-1.9		Δ(E+G_{corr})‡	-2.1							
1b, R^3 = Me															
cRT	-749.916799	0.199510	-749.717289	0.0	0.0	0.154868	-749.761931	0.0	4.547	3.006	4.582	176.2	-45.1	-176.8	-91.7
cTS	-749.887379	0.198480	-749.688899	77.2	74.5	0.155414	-749.731965	78.7	4.417	2.858	3.954	150.6	-26.1	157.8	-134.3
cPT	-749.926547	0.201454	-749.725093	-25.6	-20.5	0.158192	-749.768355	-16.9	4.278	2.744	3.319	130.4	0.3	124.1	179.0
ccRT	-749.916652	0.199452	-749.717200	0.4	0.2	0.154819	-749.761833	0.3	2.763	3.987	4.671	176.1	44.4	176.7	-98.9
ccTS	-749.885274	0.198462	-749.686812	82.8	80.0	0.155494	-749.729780	84.4	2.609	4.015	4.711	147.1	24.3	-157.3	-145.7
ccPT	-749.929935	0.201350	-749.728585	-34.5	-29.7	0.158268	-749.771667	-25.6	2.565	3.919	4.627	124.7	-2.4	-119.5	-170.5
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-5.5	-5.5		Δ(E+G_{corr})‡	-5.7							
1c, R^3 = ^{i}Pr															
c/s RT	-828.544933	0.256512	-828.288421	0.0	0.0	0.207644	-828.337290	0.0	4.410	3.016	4.583	176.2	-45.5	-176.0 / -4.8	-91.8
c/s TS	-828.512016	0.255750	-828.256266	86.4	84.4	0.209078	-828.302938	90.2	4.444	2.912	3.828	146.5	-24.6	162.1 / -39.2	-138.2
c/s PT	-828.551425	0.258871	-828.292554	-17.0	-10.9	0.213379	-828.338046	-2.0	4.235	2.631	3.304	129.6	8.7	106.1 / -72.5	166.9
cc/s RT	-828.544825	0.256474	-828.288351	0.3	0.2	0.207716	-828.337108	0.5	2.781	3.997	4.671	176.1	44.6	175.9 / 4.5	-98.8
cc/s TS	-828.506277	0.255811	-828.250466	101.5	99.7	0.209336	-828.296941	105.9	2.737	4.057	4.568	140.1	21.2	-160.9 / 35.5	-152.6
cc/s PT	-828.552918	0.258860	-828.294058	-21.0	-14.8	0.213475	-828.339443	-5.7	2.455	3.912	4.617	123.4	-9.8	-103.2 / 69.1	-156.7
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-15.1	-15.2		Δ(E+G_{corr})‡	-15.7							
c/d RT	-828.544254	0.256695	-828.287559	0.0	0.0	0.208189	-828.336064	0.0	4.408	3.017	4.584	176.2	-45.8	-175.4 / -124.6	-91.7
c/d TS	-828.514954	0.255582	-828.259372	76.9	74.0	0.208906	-828.306048	78.8	4.422	2.866	3.951	150.6	-26.1	158.6 / -156.3	-134.5
c/d PT	-828.554914	0.258646	-828.296268	-28.0	-22.9	0.213184	-828.341731	-14.9	4.230	2.390	3.321	130.4	4.3	115.1 / -173.4	174.1
cc/u RT	-828.544108	0.256665	-828.287443	0.4	0.3	0.208203	-828.335879	0.5	2.768	4.002	4.672	176.1	45.2	175.3 / 124.7	-98.6
cc/u TS	-828.512630	0.255589	-828.257041	83.0	80.1	0.208844	-828.303538	85.4	2.633	4.022	4.705	146.7	24.2	-158.9 / 161.9	-146.7
cc/u PT	-828.558003	0.258523	-828.299480	-36.1	-31.3	0.213787	-828.339275	-8.4	2.521	3.897	4.631	124.6	-4.8	-112.1 / 172.8	-171.6
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-6.1	-6.1		Δ(E+G_{corr})‡	-6.6							
c/u RT	-828.544083	0.256708	-828.287375	0.0	0.0	0.208211	-828.335897	0.0	4.407	3.017	4.583	176.2	-45.9	-176.3 / 120.5	-91.7
c/u TS	-828.512382	0.255394	-828.256988	83.2	79.8	0.209117	-828.303512	85.0	4.433	2.900	3.891	148.6	-25.2	159.4 / 55.8	-135.5
c/u PT	-828.553063	0.258949	-828.294114	-23.6	-17.7	0.212857	-828.345146	-24.3	4.226	2.648	3.302	129.6	5.8	114.4 / 59.5	170.2
cc/d RT	-828.543959	0.256699	-828.287260	0.3	0.3	0.208349	-828.335610	0.8	2.793	3.999	4.668	175.9	45.1	176.1 / -120.4	-99.2
cc/d TS	-828.508183	0.255418	-828.252765	94.3	90.9	0.208966	-828.299218	96.3	2.709	4.039	4.651	143.0	22.8	-158.9 / -38.9	-153.5
cc/d PT	-828.554212	0.258878	-828.295334	-26.6	-20.9	0.213763	-828.340449	-12.0	2.508	3.903	4.602	122.9	-7.0	-112.1 / -58.4	-158.6
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-11.0	-11.1		Δ(E+G_{corr})‡	-11.3							
1d, R^3 = Ph															
cRT	-941.659348	0.253047	-941.406301	0.0	0.0	0.202903	-941.456444	0.0	4.530	2.974	4.583	176.3	-44.7	-177.6	-90.9
cTS	-941.629948	0.251856	-941.378092	77.2	74.1	0.203911	-941.426037	79.8	4.416	2.849	3.943	150.5	-25.1	155.0	-135.0
cPT	-941.662778	0.254618	-941.408160	-9.0	-4.9	0.207148	-941.455630	2.1	4.267	2.746	3.320	130.6	1.5	119.0	-179.3
ccRT	-941.659150	0.252994	-941.406156	0.5	0.4	0.202861	-941.456290	0.4	2.748	3.955	4.675	176.2	43.9	177.6	-98.7
ccTS	-941.627411	0.251665	-941.375746	83.9	80.2	0.203750	-941.423661	86.1	2.676	4.050	4.732	146.1	24.4	-155.8	-152.4
ccPT	-941.665745	0.253996	-941.411749	-16.8	-14.3	0.205165	-941.460579	-10.9	2.685	3.916	4.627	125.0	-0.3	-124.3	-176.3
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-6.7	-6.2		Δ(E+G_{corr})‡	-6.2							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] D(R^3(H),R^3, C_5,C_4) is also indicated for systems with R^3 = ^{i}Pr after D(R^3,C_6, C_5,C_4).

TABLE A1.5 Energies and geometrical parameters of system **2** at the B3LYP/6-31G(d) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	$\Delta(E+G_{corr})$ [a] (kJ mol^{-1})	$R(R^2,H^3)$ [b] (Å)	$R(H^2,H^3)$ (Å)	$R(R^1,R^2)$ [c] (Å)	$A(C_1,C_2,C_3)$ (degrees)	$D(C_2,C_3,C_5,C_6)$ (degrees)	$D(R^3,C_6,C_5,C_4)$ [d] (degrees)	$D(R^2,C_2,C_3,C_4)$ (degrees)
2a, R^3 = H															
cRT	-828.530490	0.256102	-828.274388	0.0	0.0	0.208710	-828.321780	0.0	4.588	3.071	4.632	176.7	-54.2	-176.2	-88.5
cTS	-828.504186	0.255831	-828.248355	69.1	68.3	0.211028	-828.293158	75.1	4.361	2.747	4.106	154.6	-27.3	155.1	-128.9
cPT	-828.535806	0.258416	-828.277390	-14.0	-7.9	0.212806	-828.323000	-3.2	4.406	2.785	3.725	135.1	-9.1	130.2	-150.5
ccRT	-828.530421	0.256072	-828.274349	0.2	0.1	0.208740	-828.321681	0.3	2.711	4.185	4.721	176.5	54.2	176.1	-96.6
ccTS	-828.503448	0.255725	-828.247723	71.0	70.0	0.210939	-828.292509	76.9	2.484	3.982	4.806	152.0	27.8	-156.5	-134.7
ccPT	-828.548760	0.258796	-828.289964	-48.0	-40.9	0.213635	-828.335124	-35.0	2.441	3.883	4.801	129.6	0.0	-120.8	180.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-1.9	-1.7		$\Delta(E+G_{cor})^{\ddagger}$	-1.7							
2b, R^3 = Me															
cRT	-867.853964	0.284349	-867.569615	0.0	0.0	0.234580	-867.619384	0.0	4.572	3.054	4.640	176.8	-54.3	-176.7	-88.1
cTS	-867.825068	0.283932	-867.541136	75.9	74.8	0.237196	-867.587872	82.7	4.407	2.830	4.056	152.0	-27.2	157.4	-130.3
cPT	-867.849729	0.286868	-867.562861	11.1	17.7	0.239712	-867.610016	24.6	4.447	2.920	3.672	133.3	-10.6	135.5	-147.3
ccRT	-867.853731	0.284308	-867.569423	0.6	0.5	0.234600	-867.619131	0.7	2.700	4.172	4.722	176.5	54.4	176.4	-96.8
ccTS	-867.822765	0.283898	-867.538867	81.9	80.7	0.237158	-867.585608	88.7	2.582	3.997	4.750	148.1	24.9	-157.1	-145.8
ccPT	-867.861264	0.287428	-867.573836	-19.2	-11.1	0.240616	-867.620648	-3.3	2.362	3.850	4.787	128.2	-4.1	-117.5	-164.1
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-6.0	-6.0		$\Delta(E+G_{cor})^{\ddagger}$	-5.9							
2c, R^3 = ^{i}Pr															
c/s RT	-946.482089	0.341354	-946.140735	0.0	0.0	0.287386	-946.194703	0.0	4.588	3.065	4.639	176.8	-54.7	-176.1 / -3.8	-88.2
c/s TS	-946.448716	0.341296	-946.107420	87.6	87.5	0.290928	-946.157787	96.9	4.434	2.882	3.966	147.9	-25.6	161.6 / -44.0	-132.9
c/s PT	-946.471690	0.344148	-946.127542	27.3	34.6	0.294441	-946.177249	45.8	4.444	2.923	3.636	131.9	-8.0	127.8 / -95.0	-147.3
cc/s RT	-946.481825	0.341301	-946.140524	0.7	0.6	0.287427	-946.194398	0.8	2.732	4.186	4.717	176.3	54.6	175.4 / 3.6	-97.6
cc/s TS	-946.442180	0.341439	-946.100741	104.8	105.0	0.291288	-946.150892	115.0	2.619	4.008	4.619	141.9	20.7	-160.0 / 35.7	-149.7
cc/s PT	-946.484833	0.344829	-946.140004	-7.2	1.9	0.296127	-946.188706	15.7	2.282	3.841	4.783	126.7	-12.0	-101.1 / 68.1	-148.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-17.2	-17.5		$\Delta(E+G_{cor})^{\ddagger}$	-18.1							
c/d RT	-946.481372	0.341714	-946.139658	0.0	0.0	0.289251	-946.192122	3.0	4.579	3.065	4.638	176.8	-54.8	-175.5 / -124.3	-88.2
c/d TS	-946.452614	0.341008	-946.111606	75.5	73.7	0.290770	-946.161844	82.5	4.411	2.836	4.049	151.8	-27.1	158.2 / -158.5	-130.8
c/d PT	-946.476821	0.344025	-946.132796	11.9	18.1	0.294398	-946.182423	28.4	4.392	2.820	3.660	133.1	-7.0	126.5 / -174.0	-150.3
cc/u RT	-946.481143	0.341468	-946.139675	0.6	0.0	0.287957	-946.193253	0.0	2.715	4.181	4.721	176.5	55.0	175.0 / 124.7	-96.7
cc/u TS	-946.450054	0.341020	-946.109034	82.2	80.4	0.290695	-946.158946	90.1	2.607	4.003	4.743	147.6	24.7	-158.0 / 164.1	-147.1
cc/u PT	-946.489655	0.344682	-946.144973	-21.7	-13.9	0.294323	-946.179135	37.1	2.338	3.823	4.794	128.1	-6.3	-111.8 / 173.3	-166.3
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-6.7	-6.8		$\Delta(E+G_{cor})^{\ddagger}$	-7.6							
c/u RT	-946.481210	0.341529	-946.139681	0.0	0.0	0.287995	-946.193148	0.0	4.582	3.068	4.637	176.8	-55.1	-176.5 / 120.6	-88.2
c/u TS	-946.449640	0.340853	-946.108787	82.9	81.1	0.290882	-946.159172	89.2	4.415	2.857	4.010	150.0	-26.1	159.1 / 54.3	-131.2
c/u PT	-946.473457	0.344107	-946.129350	20.4	27.1	0.295646	-946.194009	-2.3	4.390	2.802	3.642	132.4	-6.2	126.4 / 53.4	-151.0
cc/d RT	-946.480941	0.341529	-946.139412	0.7	0.7	0.288172	-946.192770	1.0	2.753	4.190	4.716	176.3	55.2	175.5 / -120.4	-98.0
cc/d TS	-946.444928	0.340995	-946.103933	95.3	93.9	0.291026	-946.153901	103.0	2.653	4.011	4.697	144.2	23.1	-158.6 / -38.0	-153.2
cc/d PT	-946.485344	0.344942	-946.140402	-10.9	-1.9	0.296372	-946.188972	11.0	2.313	3.827	4.771	126.0	-9.3	-110.0 / -58.6	-149.3
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-12.4	-12.7		$\Delta(E+G_{cor})^{\ddagger}$	-13.8							
2d, R^3 = Ph															
cRT	-1059.596846	0.337933	-1059.258913	0.0	0.0	0.282684	-1059.314163	0.0	4.561	3.030	4.657	177.0	-53.9	-178.0	-87.3
cTS	-1059.567613	0.337288	-1059.230325	76.8	75.1	0.285676	-1059.281937	84.6	4.409	2.827	4.041	151.4	-26.1	154.5	-131.1
cPT	-1059.587457	0.339994	-1059.247463	24.7	30.1	0.288880	-1059.298577	40.9	4.418	2.881	3.669	133.5	-8.9	128.5	-147.0
ccRT	-1059.596508	0.337853	-1059.258655	0.9	0.7	0.282444	-1059.314064	0.3	2.687	4.173	4.735	176.6	54.4	177.6	-95.7
ccTS	-1059.564900	0.337075	-1059.227825	83.9	81.6	0.285463	-1059.279438	91.2	2.667	4.038	4.776	146.9	25.3	-155.7	-154.2
ccPT	-1059.596852	0.340018	-1059.256834	0.0	5.5	0.287506	-1059.309346	12.6	2.503	3.854	4.786	128.5	-1.4	-122.9	-171.9
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-7.1	-6.6		$\Delta(E+G_{cor})^{\ddagger}$	-6.6							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] $D(R^3(H),R^3, C_5,C_4)$ is also indicated for systems with R^3 = ^{i}Pr after $D(R^3,C_6, C_5,C_4)$.

TABLE A1.6 Energies and geometrical parameters of system **3** at the B3LYP/6-31G(d) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	$\Delta(E+G_{corr})$ [a] (kJ mol^{-1})	$R(R^2,H^3)$ [b] (Å)	$R(H^2,H^3)$ (Å)	$R(R^1,R^2)$ [c] (Å)	$A(C_1,C_2,C_3)$ (degrees)	$D(C_2,C_3,C_5,C_6)$ (degrees)	$D(R^3,C_6,C_5,C_4)$ [d] (degrees)	$D(R^2,C_2,C_3,C_4)$ (degrees)
3a, R^3 = H															
cRT	-828.536066	0.256045	-828.280021	0.0	0.0	0.208208	-828.327857	0.0	4.142	3.015	4.633	176.4	-44.7	-176.5	-92.0
cTS	-828.507720	0.255486	-828.252234	74.4	73.0	0.209397	-828.298323	77.5	4.387	2.734	4.145	154.2	-26.0	155.2	-132.7
cPT	-828.543818	0.257957	-828.285861	-20.4	-15.3	0.212122	-828.331696	-10.1	4.247	2.554	3.685	135.3	1.6	118.4	175.9
ccRT	-828.534794	0.255952	-828.278842	3.3	3.1	0.208312	-828.326482	3.6	2.214	4.053	4.697	174.3	43.9	176.4	-105.3
ccTS	-828.503673	0.255368	-828.248305	85.0	83.3	0.209198	-828.294475	87.6	2.308	4.058	4.755	146.9	26.7	-157.0	-160.4
ccPT	-828.553584	0.258109	-828.295475	-46.0	-40.6	0.211251	-828.342334	-38.0	2.280	3.973	4.614	123.3	0.0	-121.1	180.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-10.6	-10.3		$\Delta(E+G_{corr})^{\ddagger}$	-10.1							
3b, R^3 = Me															
cRT	-867.859266	0.284293	-867.574973	0.0	0.0	0.234246	-867.625020	0.0	4.180	2.993	4.629	176.4	-44.9	-176.7	-91.7
cTS	-867.828450	0.283573	-867.544877	80.9	79.0	0.235613	-867.592837	84.5	4.422	2.794	4.096	151.8	-25.7	157.4	-134.9
cPT	-867.857690	0.286573	-867.571117	4.1	10.1	0.239017	-867.618673	16.7	4.220	2.568	3.672	134.5	2.8	120.2	172.9
ccRT	-867.857799	0.284218	-867.573581	3.9	3.7	0.234442	-867.623357	4.4	2.207	4.011	4.691	174.0	43.1	176.4	-106.6
ccTS	-867.820877	0.283442	-867.537435	100.8	98.6	0.235677	-867.585200	104.5	2.340	4.071	4.634	141.7	22.9	-157.4	-161.3
ccPT	-867.864171	0.286700	-867.577471	-12.9	-6.6	0.239033	-867.625138	-0.3	2.335	3.958	4.596	122.1	-3.7	-117.4	-167.7
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-19.9	-19.5		$\Delta(E+G_{corr})^{\ddagger}$	-20.1							
3c, R^3 = ^{i}Pr															
c/s RT	-946.487401	0.341277	-946.146124	0.0	0.0	0.287137	-946.200264	0.0	4.230	3.020	4.627	176.4	-46.0	-175.3 / -6.0	-91.8
c/s TS	-946.452317	0.340912	-946.111405	92.1	91.2	0.289580	-946.162737	98.5	4.448	2.835	3.989	147.5	-24.0	161.5 / -43.0	-139.3
c/s PT	-946.481597	0.343920	-946.137677	15.2	22.2	0.293702	-946.187895	32.5	4.189	2.456	3.661	134.0	9.8	103.8 / -72.0	165.4
cc/s RT	-946.485533	0.341292	-946.144241	4.9	4.9	0.287559	-946.197975	6.0	2.221	4.107	4.663	172.6	44.6	173.2 / 7.5	-111.9
cc/s TS	-946.439595	0.340686	-946.098909	125.5	124.0	0.290100	-946.149496	133.3	2.643	4.061	4.464	135.8	18.4	-157.5 / -7.2	-158.1
cc/s PT	-946.484591	0.344282	-946.140309	7.4	15.3	0.294825	-946.189766	27.6	2.341	3.976	4.565	120.3	-12.1	-99.5 / 69.3	-150.2
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-33.4	-32.8		$\Delta(E+G_{corr})^{\ddagger}$	-34.8							
c/d RT	-946.486715	0.341473	-946.145242	0.0	0.0	0.287570	-946.199144	0.0	4.190	3.004	4.632	176.5	-45.5	-175.3 / -124.6	-91.5
c/d TS	-946.455956	0.340684	-946.115272	80.8	78.7	0.289401	-946.166556	85.6	4.426	2.799	4.081	151.4	-25.5	158.4 / -157.2	-136.0
c/d PT	-946.485624	0.343580	-946.142044	2.9	8.4	0.292864	-946.192760	-76.2	4.203	2.522	3.675	134.6	4.4	114.3 / -173.9	175.0
cc/u RT	-946.485272	0.341401	-946.143871	3.8	3.6	0.287664	-946.198871	0.7	2.208	4.039	4.694	174.0	44.4	175.0 / 125.3	-106.5
cc/u TS	-946.448125	0.340577	-946.107548	101.3	99.0	0.289079	-946.163746	92.9	2.346	4.069	4.617	141.1	22.2	-157.9 / 164.8	-160.7
cc/u PT	-946.492261	0.343892	-946.148369	-14.6	-8.2	0.293172	-946.189962	24.1	2.343	3.941	4.599	122.0	-5.8	-112.6 / 172.0	-168.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-20.6	-20.3		$\Delta(E+G_{corr})^{\ddagger}$	-7.4							
c/u RT	-946.486535	0.341472	-946.145063	0.0	0.0	0.287814	-946.197458	0.0	4.231	3.021	4.626	176.3	-46.3	-175.9 / 120.0	-91.9
c/u TS	-946.452825	0.340511	-946.112314	88.5	86.0	0.289731	-946.158394	102.6	4.443	2.834	4.018	149.2	-24.8	159.9 / 56.9	-137.9
c/u PT	-946.483134	0.343887	-946.139247	8.9	15.3	0.293823	-946.198438	-2.6	4.198	2.483	3.657	133.8	6.1	113.3 / 58.2	170.9
cc/d RT	-946.484559	0.341535	-946.143024	5.2	5.4	0.288274	-946.196286	3.1	2.227	4.145	4.666	172.3	46.5	173.2 / -118.9	-112.9
cc/d TS	-946.440498	0.340541	-946.099957	120.9	118.4	0.290143	-946.150354	123.7	2.335	4.081	4.497	137.1	18.9	-155.9 / -40.2	-158.7
cc/d PT	-946.484761	0.344231	-946.140530	4.7	11.9	0.294673	-946.190089	19.3	2.400	3.964	4.544	119.5	-9.5	-108.7 / -56.4	-150.7
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-32.4	-32.4		$\Delta(E+G_{corr})^{\ddagger}$	-21.1							
3d, R^3 = Ph															
cRT	-1059.601790	0.337828	-1059.263962	0.0	0.0	0.282283	-1059.319507	0.0	4.165	2.962	4.629	176.6	-44.3	-177.5	-90.9
cTS	-1059.570876	0.336928	-1059.233948	81.2	78.8	0.284113	-1059.286763	86.0	4.420	2.784	4.088	151.4	-24.5	154.5	-135.6
cPT	-1059.593644	0.339568	-1059.254076	21.4	26.0	0.287266	-1059.306378	34.5	4.265	2.615	3.670	134.6	0.4	120.2	-176.2
ccRT	-1059.600333	0.337834	-1059.262499	3.8	3.8	0.283109	-1059.317224	6.0	2.204	4.025	4.699	173.7	44.0	177.3	-107.6
ccTS	-1059.562695	0.336703	-1059.225992	102.6	99.7	0.284423	-1059.278272	108.3	2.417	4.113	4.637	139.9	22.8	-156.0	-167.2
ccPT	-1059.600138	0.339376	-1059.260762	4.3	8.4	0.286238	-1059.313899	14.7	2.436	3.954	4.593	122.2	-1.9	-122.1	-172.5
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-21.5	-20.9		$\Delta(E+G_{corr})^{\ddagger}$	-22.3							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] $D(R^3(H),R^3, C_5,C_4)$ is also indicated for systems with R^3 = ^{i}Pr after $D(R^3,C_6, C_5,C_4)$.

TABLE A1.7 Energies and geometrical parameters of system **4** at the B3LYP/6-31G(d) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	$\Delta(E+G_{corr})$ [a] (kJ mol^{-1})	$R(R^2,H^3)$ [b] (Å)	$R(H^2,H^3)$ (Å)	$R(R^1,R^2)$ [c] (Å)	$A(C_1,C_2,C_3)$ (degrees)	$D(C_2,C_3,C_5,C_6)$ (degrees)	$D(R^3,C_6,C_5,C_4)$ [d] (degrees)	$D(R^2,C_2,C_3,C_4)$ (degrees)
4a, R^3 = H															
cRT	-946.472808	0.340871	-946.131937	0.0	0.0	0.288280	-946.184527	0.0	4.471	3.051	4.698	177.4	-54.3	-176.0	-87.4
cTS	-946.443000	0.340920	-946.102080	78.3	78.4	0.291704	-946.151297	87.2	4.341	2.658	4.340	156.4	-26.6	153.4	-126.2
cPT	-946.463532	0.343360	-946.120172	24.4	30.9	0.293282	-946.170249	37.5	3.971	2.715	4.106	139.2	-12.2	134.9	-141.9
ccRT	-946.471055	0.340825	-946.130230	4.6	4.5	0.288110	-946.182946	4.2	2.181	4.366	4.796	173.5	58.6	175.1	-103.1
ccTS	-946.440952	0.340788	-946.100164	83.6	83.4	0.291069	-946.149883	91.0	2.283	4.038	4.812	148.3	27.8	-156.7	-161.6
ccPT	-946.483177	0.344196	-946.138981	-27.2	-18.5	0.293205	-946.189972	-14.3	2.207	3.919	4.783	126.8	0.0	-121.1	180.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-5.4	-5.0		$\Delta(E+G_{corr})^{\ddagger}$	-3.7							
4b, R^3 = Me															
cRT	-985.796220	0.369102	-985.427118	0.0	0.0	0.314100	-985.482120	0.0	4.518	3.034	4.704	177.4	-54.4	-176.5	-87.1
cTS	-985.763022	0.369034	-985.393988	87.2	87.0	0.317995	-985.445027	97.4	4.404	2.753	4.299	153.3	-26.4	156.3	-127.9
cPT	-985.777565	0.371908	-985.405657	49.0	56.3	0.321218	-985.456347	67.7	4.486	2.860	4.076	137.2	-13.7	139.9	-139.6
ccRT	-985.794179	0.369079	-985.425100	5.4	5.3	0.314011	-985.480168	5.1	2.181	4.359	4.797	173.1	59.1	175.3	-104.2
ccTS	-985.756969	0.368982	-985.387987	103.1	102.7	0.317816	-985.439153	112.8	2.317	4.046	4.705	143.2	23.5	-156.8	-163.3
ccPT	-985.793409	0.372832	-985.420577	7.4	17.2	0.321453	-985.471956	26.7	2.356	3.893	4.770	125.1	-5.7	-116.0	-160.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-15.9	-15.8		$\Delta(E+G_{corr})^{\ddagger}$	-15.4							
4c, R^3 = ^{i}Pr															
c/s RT	-1064.424359	0.426086	-1063.998273	0.0	0.0	0.366972	-1064.057388	0.0	4.595	3.048	4.704	177.4	-55.0	-175.9 / -4.8	-87.2
c/s TS	-1064.386955	0.426246	-1063.960709	98.2	98.6	0.371734	-1064.015222	110.7	4.422	2.795	4.267	151.1	-25.9	156.7 / -90.6	-129.0
c/s PT	-1064.398660	0.428822	-1063.969838	67.5	74.7	0.374822	-1064.023839	88.1	4.540	2.975	4.053	135.6	-15.0	143.4 / -92.4	-137.0
cc/s RT	-1064.421832	0.426226	-1063.995606	6.6	7.0	0.367488	-1064.055994	3.7	2.264	4.475	4.783	172.4	61.7	172.0 / 5.5	-108.4
cc/s TS	-1064.372550	0.426563	-1063.945987	136.0	137.3	0.372481	-1064.000069	150.5	2.426	4.024	4.612	137.9	18.0	-157.3 / -5.2	-160.1
cc/s PT	-1064.414967	0.430158	-1063.984809	24.7	35.3	0.377096	-1064.037870	51.2	2.226	3.914	4.751	122.9	-14.5	-98.1 / 67.9	-141.4
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-37.8	-38.7		$\Delta(E+G_{corr})^{\ddagger}$	-39.8							
c/d RT	-1064.423624	0.426286	-1063.997338	0.0	0.0	0.367526	-1064.056097	0.0	4.517	3.042	4.704	177.5	-54.8	-175.3 / -124.1	-87.1
c/d TS	-1064.390033	0.426221	-1063.963812	88.2	88.0	0.372055	-1064.017978	100.1	4.413	2.759	4.279	152.2	-26.1	158.0 / -159.1	-130.4
c/d PT	-1064.402999	0.428706	-1063.974293	54.2	60.5	0.374491	-1064.028509	72.4	4.413	2.715	4.078	137.3	-9.8	132.0 / -173.2	-144.2
cc/u RT	-1064.421648	0.426257	-1063.995391	5.2	5.1	0.367488	-1064.055994	0.3	2.193	4.373	4.796	173.2	59.8	173.8 / 125.5	-103.9
cc/u TS	-1064.383949	0.426136	-1063.957813	104.2	103.8	0.371811	-1064.014129	110.2	2.337	4.040	4.686	142.5	22.5	-157.5 / 166.1	-162.2
cc/u PT	-1064.421721	0.430083	-1063.991638	5.0	15.0	0.375109	-1064.024011	84.2	2.267	3.869	4.777	125.2	-7.5	-110.8 / 172.3	-163.3
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-16.0	-15.6		$\Delta(E+G_{corr})^{\ddagger}$	-10.1							
c/u RT	-1064.423482	0.426273	-1063.997209	0.0	0.0	0.367539	-1064.054109	0.0	4.534	3.051	4.704	177.5	-55.4	-176.3 / 120.4	-87.0
c/u TS	-1064.385940	0.426136	-1063.959804	98.6	98.2	0.371954	-1064.011995	110.6	4.439	2.804	4.246	150.5	-26.0	160.3 / 57.0	-130.9
c/u PT	-1064.399120	0.428916	-1063.970204	64.0	70.9	0.376539	-1064.045182	23.4	4.409	2.702	4.059	136.6	-8.9	131.3 / 52.6	-144.8
cc/d RT	-1064.420850	0.426358	-1063.994492	6.9	7.1	0.368041	-1064.052809	3.4	2.275	4.468	4.779	172.4	62.2	171.5 / -119.7	-108.8
cc/d TS	-1064.374715	0.426302	-1063.948413	128.0	128.1	0.372612	-1064.002104	136.5	2.298	4.045	4.605	139.1	19.0	-155.5 / -39.2	-160.5
cc/d PT	-1064.414191	0.430102	-1063.984089	24.4	34.4	0.376771	-1064.037421	43.8	2.297	3.905	4.736	121.7	-11.9	-108.8 / -57.2	-139.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-29.5	-29.9		$\Delta(E+G_{corr})^{\ddagger}$	-26.0							
4d, R^3 = Ph															
cRT	-1177.539058	0.422683	-1177.116375	0.0	0.0	0.362166	-1177.176892	0.0	4.553	3.008	4.719	177.7	-54.1	-177.8	-86.3
cTS	-1177.505054	0.422398	-1177.082656	89.3	88.5	0.366575	-1177.138479	100.9	4.413	2.754	4.278	151.9	-25.1	153.7	-129.5
cPT	-1177.514761	0.424541	-1177.090220	63.8	68.7	0.368498	-1177.146263	80.4	4.478	2.850	4.089	138.0	-14.3	140.3	-139.3
ccRT	-1177.536947	0.422655	-1177.114292	5.5	5.5	0.361099	-1177.175848	2.7	2.212	4.394	4.817	172.9	60.2	176.8	-103.0
ccTS	-1177.498480	0.422244	-1177.076236	106.5	105.4	0.366573	-1177.131908	118.1	2.406	4.087	4.705	141.2	23.3	-155.7	-169.2
ccPT	-1177.528928	0.425512	-1177.103416	26.6	34.0	0.368926	-1177.160002	44.3	2.332	3.894	4.767	125.4	-3.2	-121.3	-166.9
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-17.3	-16.9		$\Delta(E+G_{corr})^{\ddagger}$	-17.3							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] $D(R^3(H),R^3, C_5,C_4)$ is also indicated for systems with R^3 = ^{i}Pr after $D(R^3,C_6, C_5,C_4)$.

TABLE A1.8 Energies and geometrical parameters of system **5** at the B3LYP/6-31G(d) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	$\Delta(E+G_{corr})$ [a] (kJ mol^{-1})	$R(R^2,H^3)$ [b] (Å)	$R(H^2,H^3)$ (Å)	$R(R^1,R^2)$ [c] (Å)	$A(C_1,C_2,C_3)$ (degrees)	$D(C_2,C_3,C_5,C_6)$ (degrees)	$D(R^3,C_6,C_5,C_4)$ [d] (degrees)	$D(R^2,C_2,C_3,C_4)$ (degrees)
5a, R^3 = H															
cRT	-902.334100	0.224463	-902.109637	1.5	1.3	0.176366	-902.157734	0.1	4.374	3.007	5.739	176.1	-44.6	-176.9	-93.0
cTS	-902.309760	0.223916	-902.085844	65.4	63.8	0.177763	-902.131998	67.7	4.337	2.763	4.994	153.6	-26.1	156.2	-133.1
cPT	-902.352755	0.226610	-902.126145	-47.4	-42.1	0.181083	-902.171673	-36.5	4.281	2.647	4.231	132.7	-3.7	127.5	-171.7
ccRT	-902.334684	0.224556	-902.110128	0.0	0.0	0.176919	-902.157765	0.0	2.626	3.893	5.843	176.7	41.0	177.2	-97.5
ccTS	-902.307498	0.223607	-902.083891	71.4	68.9	0.177607	-902.129891	73.2	2.245	3.951	5.996	150.6	24.3	-154.8	-139.7
ccPT	-902.358984	0.226668	-902.132316	-63.8	-58.3	0.179902	-902.179083	-56.0	2.242	3.964	5.965	123.5	0.0	-120.7	-180.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-5.9	-5.1		$\Delta(E+G_{corr})^{\ddagger}$	-5.5							
5b, R^3 = Me															
cRT	-941.657561	0.252725	-941.404836	1.6	1.3	0.202483	-941.455077	0.1	4.334	2.981	5.735	176.1	-44.3	-177.1	-92.5
cTS	-941.631013	0.251957	-941.379056	71.3	69.0	0.203860	-941.427153	73.4	4.360	2.807	4.923	151.3	-25.6	157.7	-135.2
cPT	-941.666852	0.255019	-941.411833	-22.8	-17.0	0.207758	-941.459095	-10.4	4.279	2.684	4.198	131.8	-3.8	131.3	-172.3
ccRT	-941.658154	0.252810	-941.405344	0.0	0.0	0.203038	-941.455116	0.0	2.598	3.875	5.846	176.7	41.2	177.5	-97.5
ccTS	-941.628806	0.251732	-941.377074	77.1	74.2	0.203871	-941.424935	79.2	2.267	3.979	5.961	147.2	22.6	-155.5	-147.1
ccPT	-941.672474	0.255141	-941.417333	-37.6	-31.5	0.207295	-941.465180	-26.4	2.085	3.988	5.953	122.9	-1.5	-121.2	-175.8
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-5.8	-5.2		$\Delta(E+G_{corr})^{\ddagger}$	-5.8							
5c, R^3 = ^{i}Pr															
c/s RT	-1020.285727	0.309727	-1019.976000	1.7	1.4	0.255283	-1020.030444	0.4	4.365	2.995	5.736	176.2	-45.0	-176.4 / -4.8	-92.4
c/s TS	-1020.256121	0.309266	-1019.946855	79.4	77.9	0.257297	-1020.001318	76.8	4.384	2.849	4.787	147.3	-24.0	161.5 / -37.6	-139.2
c/s PT	-1020.289918	0.311941	-1019.977977	-9.3	-3.8	0.260329	-1020.029589	2.6	4.236	2.576	4.125	129.9	1.5	121.8 / -63.2	179.4
cc/s RT	-1020.286359	0.309834	-1019.976525	0.0	0.0	0.255780	-1020.030578	0.0	2.605	3.868	5.844	176.7	40.9	177.3 / 1.5	-97.4
cc/s TS	-1020.249607	0.308880	-1019.940727	96.5	94.0	0.257571	-1019.992036	101.2	2.276	3.994	5.774	141.1	18.4	-157.9 / 33.9	-147.6
cc/s PT	-1020.293024	0.312260	-1019.980764	-17.5	-11.1	0.261567	-1020.031456	-2.3	2.026	3.998	5.926	121.5	-9.4	104.2 / 70.8	-147.8
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-17.1	-16.1		$\Delta(E+G_{corr})^{\ddagger}$	-24.4							
c/d RT	-1020.285024	0.309905	-1019.975119	1.5	1.2	0.255803	-1020.029221	0.0	4.364	2.995	5.736	176.2	-45.2	-175.8 / -124.5	-92.5
c/d TS	-1020.258615	0.309031	-1019.949584	70.9	68.3	0.257297	-1020.001318	73.3	4.366	2.816	4.926	151.4	-25.7	158.4 / -156.5	-135.0
c/d PT	-1020.293839	0.311706	-1019.982133	-21.6	-17.2	0.261018	-1020.032821	-9.5	4.253	2.645	4.191	131.6	-2.4	129.4 / -174.8	-174.3
cc/u RT	-1020.285602	0.310009	-1019.975593	0.0	0.0	0.255904	-1020.028974	0.6	2.588	3.869	5.844	176.9	41.4	176.5 / 123.4	-97.1
cc/u TS	-1020.256109	0.308768	-1019.947341	77.4	74.2	0.257265	-1019.999041	79.2	2.343	3.980	5.950	143.1	19.6	-155.8 / 157.6	-149.8
cc/u PT	-1020.299748	0.312259	-1019.987489	-37.1	-31.2	0.262265	-1020.029785	-1.5	2.063	3.966	5.917	122.6	-3.9	-115.5 / 171.5	-176.9
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-6.6	-5.9		$\Delta(E+G_{corr})^{\ddagger}$	-6.0							
c/u RT	-1020.284879	0.309938	-1019.974941	1.8	1.6	0.256389	-1020.029212	0.0	4.364	2.996	5.735	176.2	-45.4	-176.8 / 120.3	-92.4
c/u TS	-1020.256306	0.308903	-1019.947403	76.8	73.9	0.257258	-1019.998852	79.7	4.377	2.847	4.856	149.3	-24.7	158.9 / 56.5	-136.3
c/u PT	-1020.292051	0.312262	-1019.979789	-17.1	-11.2	0.261785	-1020.037963	-23.0	4.230	2.576	4.154	130.8	1.3	120.6 / 58.2	-177.5
cc/d RT	-1020.285551	0.310019	-1019.975532	0.0	0.0	0.256362	-1020.029188	0.1	2.597	3.885	5.845	176.6	41.9	177.2 / -121.7	-97.9
cc/d TS	-1020.250805	0.308707	-1019.942098	91.2	87.8	0.257151	-1019.993654	93.4	2.273	3.986	5.851	146.8	22.5	-156.3 / -32.0	-147.6
cc/d PT	-1020.294180	0.312287	-1019.981893	-22.7	-16.7	0.262169	-1020.032010	-7.3	2.057	3.985	5.910	121.4	-6.8	-112.8 / -59.4	-161.8
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-14.4	-13.9		$\Delta(E+G_{corr})^{\ddagger}$	-13.6							
5d, R^3 = Ph															
cRT	-1133.400062	0.306262	-1133.093800	3.0	2.5	0.250496	-1133.149565	0.0	4.336	2.961	5.730	176.2	-44.4	-177.7	-91.8
cTS	-1133.373549	0.305322	-1133.068227	72.6	69.6	0.252372	-1133.121176	74.6	4.363	2.802	4.905	151.2	-24.8	155.1	-135.6
cPT	-1133.402576	0.307676	-1133.094900	-3.6	-0.4	0.254663	-1133.147913	4.4	4.282	2.710	4.215	132.3	-5.1	133.5	-170.0
ccRT	-1133.401197	0.306443	-1133.094754	0.0	0.0	0.251613	-1133.149583	0.0	2.568	3.820	5.845	177.0	40.0	178.2	-97.0
ccTS	-1133.369004	0.304943	-1133.064061	84.5	80.6	0.252335	-1133.116668	86.4	2.326	3.990	5.915	145.7	20.3	-152.1	-147.8
ccPT	-1133.406365	0.307711	-1133.098654	-13.6	-10.2	0.253713	-1133.152653	-8.1	2.179	3.967	5.937	122.5	-0.5	-124.2	-176.9
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-11.9	-10.9		$\Delta(E+G_{corr})^{\ddagger}$	-11.8							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] $D(R^3(H),R^3, C_5,C_4)$ is also indicated for systems with R^3 = ^{i}Pr after $D(R^3,C_6, C_5,C_4)$.

TABLE A1.9 Energies and geometrical parameters of system **6** at the B3LYP/6-31G(d) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	$\Delta(E+G_{corr})$ [a] (kJ mol^{-1})	$R(R^2,H^3)$ [b] (Å)	$R(H^2,H^3)$ (Å)	$R(R^1,R^2)$ [c] (Å)	$A(C_1,C_2,C_3)$ (degrees)	$D(C_2,C_3,C_5,C_6)$ (degrees)	$D(R^3,C_6,C_5,C_4)$ [d] (degrees)	$D(R^2,C_2,C_3,C_4)$ (degrees)
6a, R^3 = H															
cRT	-1020.271248	0.309328	-1019.961920	0.5	0.3	0.256326	-1020.014922	0.0	4.559	3.056	5.789	176.9	-54.2	-176.4	-89.1
cTS	-1020.247276	0.309254	-1019.938022	63.4	63.1	0.259470	-1019.987806	71.2	4.294	2.694	5.156	155.8	-26.9	155.1	-128.7
cPT	-1020.278091	0.311892	-1019.966199	-17.5	-10.9	0.262569	-1020.015522	-1.6	4.350	2.743	4.626	135.5	-9.7	131.9	-148.9
ccRT	-1020.271420	0.309378	-1019.962042	0.0	0.0	0.256900	-1020.014520	1.1	2.500	4.050	5.887	176.8	49.9	176.7	-97.1
ccTS	-1020.245263	0.308860	-1019.936403	68.7	67.3	0.258933	-1019.986330	75.1	2.243	3.924	6.026	151.9	25.0	-154.5	-138.0
ccPT	-1020.288801	0.312678	-1019.976123	-45.6	-37.0	0.261752	-1020.027049	-31.8	2.092	3.948	6.142	127.1	1.8	-124.1	174.5
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-5.3	-4.3		$\Delta(E+G_{cor})^{\ddagger}$	-3.9							
6b, R^3 = Me															
cRT	-1059.594912	0.337553	-1059.257359	0.4	0.3	0.281925	-1059.312987	0.0	4.545	3.039	5.802	177.1	-54.2	-177.2	-88.3
cTS	-1059.568206	0.337326	-1059.230880	70.5	69.8	0.285688	-1059.282519	80.0	4.333	2.758	5.097	153.1	-26.4	157.2	-130.6
cPT	-1059.591760	0.340027	-1059.251733	8.7	15.1	0.288475	-1059.303284	25.5	4.379	2.829	4.578	134.4	-10.7	137.9	-148.4
ccRT	-1059.595072	0.337604	-1059.257468	0.0	0.0	0.282801	-1059.312272	1.9	2.471	4.045	5.899	176.9	50.5	177.5	-96.1
ccTS	-1059.566265	0.337032	-1059.229233	75.6	74.1	0.285389	-1059.280875	84.3	2.263	3.951	5.981	148.2	22.9	-155.3	-146.0
ccPT	-1059.601993	0.341080	-1059.260913	-18.2	-9.0	0.289438	-1059.312555	1.1	2.008	3.952	6.128	126.3	-0.8	-123.0	-175.2
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-5.1	-4.3		$\Delta(E+G_{cor})^{\ddagger}$	-2.3							
6c, R^3 = ^{i}Pr															
c/s RT	-1138.223082	0.394556	-1137.828526	0.5	0.2	0.334838	-1137.888243	0.0	4.557	3.048	5.802	177.1	-54.6	-176.7 / -3.3	-88.4
c/s TS	-1138.192271	0.394725	-1137.797546	81.4	81.5	0.339695	-1137.852576	93.6	4.347	2.788	5.002	149.1	-24.5	160.8 / -41.2	-133.9
c/s PT	-1138.213094	0.396918	-1137.816176	26.7	32.6	0.341734	-1137.871360	44.3	4.410	2.902	4.508	132.7	-10.3	137.1 / -94.9	-146.9
cc/s RT	-1138.223266	0.394663	-1137.828603	0.0	0.0	0.335736	-1137.887530	1.9	3.234	4.073	5.897	176.6	51.1	176.5 / 2.3	-96.9
cc/s TS	-1138.185835	0.394343	-1137.791492	98.3	97.4	0.339514	-1137.846321	110.1	2.226	3.937	5.801	142.9	18.0	-157.3 / 34.2	-144.7
cc/s PT	-1138.222988	0.398155	-1137.824833	0.7	9.9	0.344094	-1137.878893	24.5	1.978	3.927	6.138	125.3	-11.3	-102.6 / 70.5	-154.3
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-16.9	-15.9		$\Delta(E+G_{cor})^{\ddagger}$	-16.4							
c/d RT	-1138.222320	0.394697	-1137.827623	0.3	0.2	0.335219	-1137.887100	0.0	4.552	3.052	5.799	177.1	-54.7	-176.0 / -124.3	-88.4
c/d TS	-1138.195825	0.394444	-1137.801381	69.9	69.1	0.339435	-1137.856390	80.6	4.338	2.767	5.093	152.9	-26.4	157.9 / -160.1	-130.6
c/d PT	-1138.218329	0.397023	-1137.821306	10.8	16.8	0.342673	-1137.875656	30.0	4.332	2.739	4.561	134.0	-7.5	130.1 / -173.7	-150.6
cc/u RT	-1138.222453	0.394766	-1137.827687	0.0	0.0	0.335517	-1137.886686	1.1	2.475	4.039	5.891	176.9	50.6	176.5 / 123.5	-95.9
cc/u TS	-1138.193510	0.394085	-1137.799425	76.0	74.2	0.339253	-1137.853827	87.4	2.272	3.956	5.869	147.9	22.7	-156.1 / 159.2	-146.4
cc/u PT	-1138.229325	0.398277	-1137.831048	-18.0	-8.8	0.343473	-1137.872143	39.3	1.977	3.917	6.127	125.9	-3.8	-115.4 / 172.1	-177.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-6.1	-5.1		$\Delta(E+G_{cor})^{\ddagger}$	-6.7							
c/u RT	-1138.222419	0.394851	-1137.827568	0.0	0.0	0.336061	-1137.886392	0.0	4.556	3.054	5.800	177.1	-55.1	-177.1 / 120.5	-88.3
c/u TS	-1138.193080	0.394285	-1137.798795	77.0	75.5	0.338817	-1137.854694	83.2	4.340	2.784	5.048	151.1	-25.3	158.5 / 53.8	-131.5
c/u PT	-1138.215616	0.397316	-1137.818300	17.9	24.3	0.344139	-1137.885187	3.2	4.316	2.700	4.533	133.3	-5.9	127.9 / 54.7	-152.2
cc/d RT	-1138.222203	0.394755	-1137.827448	0.6	0.3	0.336415	-1137.886004	1.0	2.509	4.072	5.896	176.5	51.4	176.4 / -121.6	-97.8
cc/d TS	-1138.187603	0.394044	-1137.793559	91.4	89.3	0.339050	-1137.848553	99.3	2.328	3.928	5.970	145.1	19.4	-155.0 / -35.5	-146.1
cc/d PT	-1138.223609	0.398128	-1137.825481	-3.1	5.5	0.344224	-1137.879385	18.4	3.091	3.915	6.132	125.1	-8.4	-111.6 / -59.4	-155.1
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-14.4	-13.7		$\Delta(E+G_{cor})^{\ddagger}$	-16.1							
6d, R^3 = Ph															
cRT	-1251.337879	0.391166	-1250.946713	1.1	0.6	0.330647	-1251.007232	0.0	4.551	3.033	5.818	177.3	-54.3	-178.2	-87.4
cTS	-1251.310614	0.390681	-1250.919933	72.6	70.9	0.334252	-1250.976363	81.0	4.344	2.763	5.070	152.3	-25.6	154.6	-131.3
cPT	-1251.328479	0.393067	-1250.935412	25.7	30.3	0.337037	-1250.991442	41.5	4.355	2.791	4.565	134.6	-9.2	131.3	-147.9
ccRT	-1251.338283	0.391331	-1250.946952	0.0	0.0	0.331559	-1251.006724	1.3	2.490	3.970	5.886	177.3	47.7	178.6	-96.0
ccTS	-1251.306232	0.390238	-1250.915994	84.1	81.3	0.333895	-1250.972337	91.6	2.325	3.959	5.943	146.9	20.7	-151.9	-146.7
ccPT	-1251.335626	0.393595	-1250.942031	7.0	12.9	0.336559	-1250.999067	21.4	2.061	3.963	6.119	126.4	1.3	-126.8	180.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-11.5	-10.3		$\Delta(E+G_{cor})^{\ddagger}$	-10.6							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] $D(R^3(H),R^3, C_5,C_4)$ is also indicated for systems with R^3 = ^{i}Pr after $D(R^3,C_6, C_5,C_4)$.

TABLE A1.10 Energies and geometrical parameters of system **1** at the ωB97X-D/6-31+G(d,p) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(R^2,H^3) [b] (Å)	R(H^2,H^3) (Å)	R(R^1,R^2) [c] (Å)	A(C_1,C_2,C_3) (degrees)	D(C_2,C_3,C_5,C_6) (degrees)	D(R^3,C_6,C_5,C_4) [d] (degrees)	D(R^2,C_2,C_3,C_4) (degrees)
1a, R^3 = H															
cRT	-710.421380	0.171808	-710.249572	1.1	1.2	0.129356	-710.292025	0.8	4.427	3.017	4.584	176.6	-47.6	-176.0	-90.3
cTS	-710.393520	0.171031	-710.222489	74.2	72.3	0.130017	-710.263503	75.6	4.366	2.793	4.000	153.6	-27.9	156.9	-130.0
cPT	-710.445754	0.173558	-710.272196	-62.9	-58.2	0.132235	-710.313520	-55.7	4.292	2.737	3.244	129.9	1.1	118.9	177.0
ccRT	-710.421792	0.171777	-710.250015	0.0	0.0	0.129475	-710.292316	0.0	2.677	3.982	4.672	177.5	46.4	176.2	-94.9
ccTS	-710.392952	0.170986	-710.221966	75.7	73.6	0.130137	-710.262815	77.5	2.484	3.968	4.777	152.3	28.3	-157.4	-132.7
ccPT	-710.450427	0.173301	-710.277126	-75.2	-71.2	0.132070	-710.318357	-68.4	2.571	3.934	4.634	125.6	0.0	-120.5	180.0
			ΔE‡ (or Δ(E+ZPE)‡)	-1.5	-1.4		Δ(E+G_{corr})‡	-1.8							
1b, R^3 = Me															
cRT	-749.736246	0.199899	-749.536347	1.1	0.4	0.155225	-749.581021	0.0	4.399	2.984	4.583	176.7	-47.5	-176.3	-89.9
cTS	-749.708067	0.198879	-749.509188	75.1	71.7	0.155603	-749.552465	75.0	4.394	2.849	3.969	152.1	-28.0	158.4	-130.7
cPT	-749.753727	0.202371	-749.551356	-44.8	-39.1	0.159612	-749.594114	-34.4	4.312	2.805	3.225	129.3	-1.6	126.4	-176.3
ccRT	-749.736658	0.200176	-749.536482	0.0	0.0	0.155782	-749.580875	0.4	2.635	3.956	4.676	177.7	46.5	176.5	-94.6
ccTS	-749.706585	0.199105	-749.507480	79.0	76.1	0.155766	-749.550818	79.3	2.573	3.983	4.717	149.0	25.9	-157.6	-142.7
ccPT	-749.757734	0.201951	-749.555783	-55.3	-50.7	0.159086	-749.598648	-46.3	2.522	3.915	4.619	124.7	-2.1	-119.5	-171.4
			ΔE‡ (or Δ(E+ZPE)‡)	-3.9	-4.5		Δ(E+G_{corr})‡	-4.3							
1c, R^3 = ^{i}Pr															
c/s RT	-828.350763	0.257353	-828.093410	2.5	2.2	0.208614	-828.142150	0.8	4.380	2.957	4.596	177.2	-47.3	-176.9 / -4.2	-89.2
c/s TS	-828.319933	0.256655	-828.063278	83.4	81.3	0.210244	-828.109689	86.1	4.403	2.878	3.848	148.1	-26.1	163.1 / -35.3	-135.4
c/s PT	-828.366058	0.259556	-828.106502	-37.7	-32.2	0.213289	-828.152769	-27.1	4.234	2.647	3.222	128.4	7.6	110.6 / -63.8	165.6
cc/s RT	-828.351698	0.257469	-828.094229	0.0	0.0	0.209232	-828.142466	0.0	2.607	3.974	4.689	178.0	47.5	176.6 / 6.0	-92.9
cc/s TS	-828.314644	0.257095	-828.057549	97.3	96.3	0.210985	-828.103659	101.9	2.632	4.818	4.560	142.1	22.2	-161.4 / 33.4	-148.8
cc/s PT	-828.369018	0.259539	-828.109479	-45.5	-40.0	0.213944	-828.155073	-33.1	2.415	3.896	4.599	122.9	-8.7	-107.2 / 61.9	-152.5
			ΔE‡ (or Δ(E+ZPE)‡)	-13.9	-15.0		Δ(E+G_{corr})‡	-15.8							
c/d RT	-828.350475	0.257483	-828.092992	1.4	1.2	0.209153	-828.141321	0.7	4.407	2.989	4.588	176.9	-48.1	-174.4 / -125.3	-89.7
c/d TS	-828.323286	0.256362	-828.066924	72.8	69.7	0.209725	-828.113561	73.6	4.398	2.850	4.000	153.0	-28.3	158.3 / -159.5	-129.2
c/d PT	-828.369871	0.259569	-828.110302	-49.5	-44.2	0.213467	-828.156405	-38.9	4.252	2.719	3.237	129.4	3.5	117.9 / -175.1	174.3
cc/u RT	-828.351001	0.257548	-828.093453	0.0	0.0	0.209425	-828.141575	0.0	2.621	3.955	4.679	178.0	46.9	174.9 / 124.8	-93.5
cc/u TS	-828.322036	0.256607	-828.065429	76.0	73.6	0.210567	-828.111468	79.0	2.614	3.996	4.735	149.5	26.6	-158.2 / 168.7	-143.2
cc/u PT	-828.368198	0.259780	-828.108418	-45.2	-39.3	0.214273	-828.153924	-32.4	4.242	2.674	3.212	128.5	5.6	115.4 / 173.9	-170.9
			ΔE‡ (or Δ(E+ZPE)‡)	-3.3	-3.9		Δ(E+G_{corr})‡	-5.5							
c/u RT	-828.350688	0.257284	-828.093404	46.0	39.4	0.208830	-828.141858	31.7	4.369	2.952	4.596	177.2	-47.4	178.1 / 121.7	-89.0
c/u TS	-828.321335	0.256074	-828.065261	79.4	75.2	0.209402	-828.111933	78.6	4.393	2.865	3.936	150.7	-26.9	158.8 / 54.1	-130.8
c/u PT	-828.373847	0.259271	-828.114576	-58.5	-54.3	0.213165	-828.160682	-49.4	2.485	3.899	4.622	124.6	-3.8	116.4 / 58.7	169.2
cc/d RT	-828.351576	0.257685	-828.093891	0.0	0.0	0.210065	-828.141511	0.9	2.625	3.984	4.686	177.7	47.9	177.5 / -119.4	-94.0
cc/d TS	-828.317924	0.256501	-828.061423	88.4	85.2	0.210769	-828.107155	91.1	2.618	3.991	4.656	145.5	24.1	-158.5 / -40.4	-149.0
cc/d PT	-828.370601	0.260101	-828.110500	-50.0	-43.6	0.214863	-828.155739	-36.4	2.453	3.896	4.594	122.8	-7.0	-112.4 / -57.6	-155.2
			ΔE‡ (or Δ(E+ZPE)‡)	-9.0	-10.1		Δ(E+G_{corr})‡	-12.5							
1d, R^3 = Ph															
cRT	-941.418974	0.254299	-941.164675	2.0	2.2	0.203634	-941.215340	0.4	3.738	2.930	4.591	177.0	-46.9	-177.3	-88.5
cTS	-941.393202	0.253193	-941.140009	69.6	67.0	0.205259	-941.187943	72.3	4.382	2.819	4.003	153.2	-27.3	154.6	-129.7
cPT	-941.433536	0.255460	-941.178076	-36.2	-33.0	0.206290	-941.227246	-30.9	4.318	2.824	3.286	130.2	-2.8	127.5	-172.8
ccRT	-941.419730	0.254221	-941.165509	0.0	0.0	0.204235	-941.215495	0.0	2.577	3.895	4.689	178.3	45.9	177.7	-92.5
ccTS	-941.392345	0.253470	-941.138875	71.9	69.9	0.206192	-941.186153	77.0	2.634	4.010	4.762	150.0	26.7	-154.8	-143.6
ccPT	-941.437965	0.255531	-941.182434	-47.9	-44.4	0.206931	-941.231034	-40.8	2.648	3.922	4.620	125.0	0.2	-123.9	179.4
			ΔE‡ (or Δ(E+ZPE)‡)	-2.3	-3.0		Δ(E+G_{corr})‡	-4.7							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] D(R^3(H),R^3, C_5,C_4) is also indicated for systems with R^3 = ^{i}Pr after D(R^3,C_6, C_5,C_4).

TABLE A1.11 Energies and geometrical parameters of system **2** at the ωB97X-D/6-31+G(d,p) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	$R(R^2,H^3)$ [b] (Å)	$R(H^2,H^3)$ (Å)	$R(R^1,R^2)$ [c] (Å)	$A(C_1,C_2,C_3)$ (degrees)	$D(C_2,C_3,C_5,C_6)$ (degrees)	$D(R^3,C_6,C_5,C_4)$ [d] (degrees)	$D(R^2,C_2,C_3,C_4)$ (degrees)
2a, R^3 = H															
cRT	-828.341511	0.257230	-828.084281	1.1	1.5	0.210430	-828.131081	1.4	4.588	3.067	4.603	176.4	-55.2	-175.8	-89.0
cTS	-828.315311	0.256917	-828.058394	69.9	69.4	0.212399	-828.102912	75.4	4.349	2.763	4.060	154.7	-28.8	156.2	-127.3
cPT	-828.353281	0.259597	-828.093684	-29.8	-23.2	0.214672	-828.138609	-18.3	4.436	2.877	3.648	133.4	-9.9	130.1	-147.1
ccRT	-828.341929	0.257092	-828.084837	0.0	0.0	0.210302	-828.131627	0.0	2.627	4.143	4.685	177.6	54.8	175.8	-95.5
ccTS	-828.313978	0.256559	-828.057419	73.4	72.0	0.211706	-828.102272	77.1	2.467	3.955	4.800	153.0	29.2	-157.2	-131.8
ccPT	-828.364777	0.259830	-828.104947	-60.0	-52.8	0.214914	-828.149863	-47.9	2.437	3.880	4.787	129.3	0.0	-120.5	180.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-3.5	-2.6		$\Delta(E+G_{corr})^{\ddagger}$	-1.7							
2b, R^3 = Me															
cRT	-867.656600	0.285109	-867.371491	1.1	1.7	0.235788	-867.420812	1.9	4.564	3.042	4.610	176.6	-55.2	-176.4	-88.5
cTS	-867.629930	0.284786	-867.345144	71.1	70.9	0.237931	-867.391998	77.6	4.390	2.839	4.032	153.0	-29.1	157.9	-127.7
cPT	-867.661530	0.288018	-867.373512	-11.9	-3.6	0.241450	-867.420081	3.8	4.466	2.997	3.617	132.0	-11.4	135.4	-144.5
ccRT	-867.657014	0.284882	-867.372132	0.0	0.0	0.235471	-867.421543	0.0	2.582	4.114	4.688	177.8	54.7	176.4	-94.9
ccTS	-867.627386	0.284685	-867.342701	77.8	77.3	0.237470	-867.389916	83.0	2.557	3.969	4.746	150.1	26.9	-157.1	-142.1
ccPT	-867.671667	0.288260	-867.383407	-38.5	-29.6	0.241417	-867.430250	-22.9	2.332	3.848	4.776	128.1	-4.0	-117.3	-164.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-6.7	-6.4		$\Delta(E+G_{corr})^{\ddagger}$	-5.5							
2c, R^3 = ^{i}Pr															
c/s RT	-946.271139	0.342175	-945.928964	2.6	1.7	0.288442	-945.982696	0.0	4.543	3.008	4.618	177.0	-54.8	-176.9 / -3.5	-88.5
c/s TS	-946.241130	0.342665	-945.898465	81.4	81.8	0.292708	-945.948422	90.0	4.396	2.858	3.953	149.3	-27.1	162.6 / -38.5	-130.9
c/s PT	-946.271380	0.345356	-945.926024	2.0	9.4	0.295781	-945.975598	18.6	4.506	3.100	3.583	130.3	-12.2	137.7 / -89.3	-142.0
cc/s RT	-946.272135	0.342519	-945.929616	0.0	0.0	0.289790	-945.982344	0.9	2.561	4.103	4.687	178.0	54.4	176.6 / 3.7	-94.3
cc/s TS	-946.234361	0.342852	-945.891509	99.2	100.0	0.293072	-945.941289	108.7	2.533	3.957	4.586	143.6	21.9	-160.4 / 32.4	-146.2
cc/s PT	-946.283771	0.345882	-945.937889	-30.6	-21.7	0.296631	-945.987140	-11.7	2.260	3.837	4.761	125.9	-11.5	-104.7 / 169.5	169.5
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-17.8	-18.3		$\Delta(E+G_{corr})^{\ddagger}$	-18.7							
c/d RT	-946.270820	0.343082	-945.927738	1.5	3.0	0.290330	-945.980490	3.7	4.570	3.045	4.614	176.8	-55.8	-174.6 / -124.9	-88.6
c/d TS	-946.245309	0.342069	-945.903240	68.5	67.3	0.291795	-945.953514	74.5	4.392	2.837	4.049	153.6	-29.2	158.0 / -160.3	-126.8
c/d PT	-946.276511	0.345354	-945.931157	-13.4	-6.0	0.295470	-945.981040	2.3	4.445	2.955	3.609	131.8	-10.0	133.0 / -175.1	-145.9
cc/u RT	-946.271406	0.342533	-945.928873	0.0	0.0	0.289502	-945.981903	0.0	2.568	4.111	4.689	178.1	55.1	174.8 / 124.7	-93.8
cc/u TS	-946.242954	0.342197	-945.900757	74.7	73.8	0.292349	-945.950605	82.2	2.594	3.980	4.750	149.9	27.1	-158.0 / 169.2	-143.8
cc/u PT	-946.288495	0.345332	-945.943163	-44.9	-37.5	0.295224	-945.993270	-29.8	2.296	3.826	4.780	128.1	-7.0	-112.2 / 174.3	-162.7
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-6.2	-6.5		$\Delta(E+G_{corr})^{\ddagger}$	-7.6							
c/u RT	-946.271003	0.342757	-945.928246	2.6	2.2	0.289855	-945.981148	0.0	4.533	3.007	4.618	177.0	-54.9	-178.0 / 122.0	-88.2
c/u TS	-946.243101	0.342086	-945.901015	75.9	73.7	0.292244	-945.950857	79.5	4.381	2.842	4.006	151.6	-27.8	158.6 / 53.7	-127.8
c/u PT	-946.273041	0.344866	-945.928175	-2.7	2.4	0.294331	-945.978710	6.4	4.451	2.960	3.591	131.1	-9.7	133.8 / 47.2	-145.7
cc/d RT	-946.272010	0.342932	-945.929078	0.0	0.0	0.290892	-945.981117	0.1	2.591	4.115	4.687	177.8	55.1	177.2 / -120.6	-95.0
cc/d TS	-946.238321	0.342345	-945.895976	88.5	86.9	0.292691	-945.945631	93.2	2.574	3.969	4.681	146.4	24.5	158.1 / -40.4	-148.8
cc/d PT	-946.285586	0.346112	-945.939474	-35.6	-27.3	0.297463	-945.988123	-18.3	2.276	3.835	4.578	125.7	-10.2	-109.5 / -57.0	-144.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-12.5	-13.2		$\Delta(E+G_{corr})^{\ddagger}$	-13.7							
2d, R^3 = Ph															
cRT	-1059.339520	0.339450	-1059.000070	1.9	2.0	0.284326	-1059.055194	1.5	4.519	2.990	4.623	177.0	-54.7	-177.3	-87.5
cTS	-1059.315215	0.338931	-1058.976284	65.7	64.4	0.287253	-1059.027963	73.0	4.380	2.812	4.051	153.8	-28.4	154.2	-127.3
cPT	-1059.342624	0.341548	-1059.001076	-6.2	-0.6	0.289552	-1059.053072	7.0	4.455	2.977	3.632	132.7	-11.5	133.9	-144.0
ccRT	-1059.340256	0.339425	-1059.000831	0.0	0.0	0.284501	-1059.055755	0.0	2.525	4.033	4.695	178.5	53.2	177.9	-92.8
ccTS	-1059.313282	0.338985	-1058.974297	70.8	69.7	0.287770	-1059.025512	79.4	2.626	4.000	4.780	150.1	27.4	-154.6	-144.6
ccPT	-1059.351976	0.341607	-1059.010369	-30.8	-25.0	0.288521	-1059.063455	-20.2	2.448	3.883	4.777	128.8	0.2	-123.2	177.4
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-5.1	-5.2		$\Delta(E+G_{corr})^{\ddagger}$	-6.4							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] $D(R^3(H),R^3, C_5,C_4)$ is also indicated for systems with R^3 = ^{i}Pr after $D(R^3,C_6, C_5,C_4)$.

TABLE A1.12 Energies and geometrical parameters of system **3** at the ωB97X-D/6-31+G(d,p) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	$R(R^2,H^3)$ [b] (Å)	$R(H^2,H^3)$ (Å)	$R(R^1,R^2)$ [c] (Å)	$A(C_1,C_2,C_3)$ (degrees)	$D(C_2,C_3,C_5,C_6)$ (degrees)	$D(R^3,C_6,C_5,C_4)$ [d] (degrees)	$D(R^2,C_2,C_3,C_4)$ (degrees)
3a, R^3 = H															
cRT	-828.345474	0.256926	-828.088548	0.0	0.0	0.209214	-828.136261	0.0	4.125	3.016	4.606	176.4	-46.9	-176.2	-88.4
cTS	-828.317422	0.256492	-828.060930	73.7	72.5	0.210536	-828.106886	77.1	4.370	2.752	4.108	154.7	-27.6	156.1	-129.1
cPT	-828.359440	0.259284	-828.100156	-36.7	-30.5	0.214048	-828.145391	-24.0	4.248	2.566	3.643	134.6	1.4	118.7	176.0
ccRT	-828.344867	0.256782	-828.088085	1.6	1.2	0.209543	-828.135325	2.5	2.413	3.998	4.677	175.9	45.2	176.1	-101.4
ccTS	-828.312926	0.256205	-828.056721	85.5	83.6	0.210349	-828.102578	88.4	2.263	4.024	4.770	148.4	28.3	-157.7	-159.4
ccPT	-828.368995	0.258742	-828.110253	-61.8	-57.0	0.211651	-828.157344	-55.4	2.259	3.968	4.598	122.9	0.0	-120.8	180.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-11.8	-11.1		$\Delta(E+G_{corr})^{\ddagger}$	-11.3							
3b, R^3 = Me															
cRT	-867.660457	0.285221	-867.375236	0.0	0.0	0.235319	-867.425139	0.0	4.086	2.970	4.613	176.6	-46.3	-176.8	-86.9
cTS	-867.632172	0.284529	-867.347643	74.3	72.4	0.236617	-867.395556	77.7	4.400	2.806	4.093	153.2	-27.5	157.5	-129.3
cPT	-867.667148	0.287574	-867.379574	-17.6	-11.4	0.240352	-867.426796	-4.4	4.229	2.585	3.362	134.0	2.1	121.3	174.2
ccRT	-867.660017	0.285211	-867.374806	1.2	1.1	0.236134	-867.423883	3.3	2.133	3.934	4.674	175.9	44.0	176.0	-101.7
ccTS	-867.624488	0.284446	-867.340042	94.4	92.4	0.237108	-867.387379	99.1	2.261	4.032	4.651	144.0	24.7	-157.2	-160.4
ccPT	-867.674865	0.287776	-867.387089	-37.8	-31.1	0.240840	-867.434024	-23.3	2.291	3.952	4.585	122.0	-3.4	-117.5	-168.8
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-20.2	-20.0		$\Delta(E+G_{corr})^{\ddagger}$	-21.5							
3c, R^3 = ^{i}Pr															
c/s RT	-946.275433	0.342456	-945.932977	0.0	0.0	0.288826	-945.986607	0.0	4.118	2.949	4.627	176.9	-47.2	-177.2 / -4.7	-86.1
c/s TS	-946.243992	0.342359	-945.901633	82.5	82.3	0.291585	-945.952408	89.8	4.395	2.799	3.997	149.4	-25.0	161.8 / -36.8	-135.3
c/s PT	-946.279694	0.344954	-945.934740	-11.2	-4.6	0.294693	-945.985002	4.2	4.172	2.465	3.636	133.2	9.8	107.2 / -63.3	160.8
cc/s RT	-946.274463	0.342651	-945.931812	2.5	3.1	0.290020	-945.984443	5.7	2.083	4.126	4.668	173.3	49.0	173.1 / 6.8	-109.6
cc/s TS	-946.231669	0.341946	-945.889723	114.9	113.6	0.291570	-945.940098	122.1	2.375	4.017	4.455	137.8	20.1	-157.8 / -7.2	-156.5
cc/s PT	-946.283433	0.345226	-945.938207	-21.0	-13.7	0.295344	-945.988090	-3.9	2.286	3.966	4.544	119.8	-11.2	-102.6 / 62.7	-146.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-32.4	-31.3		$\Delta(E+G_{corr})^{\ddagger}$	-32.3							
c/d RT	-946.274812	0.342612	-945.932200	0.0	0.0	0.288965	-945.985847	0.0	4.060	2.970	4.625	176.8	-46.7	175.5 / -125.3	-85.8
c/d TS	-946.247860	0.342035	-945.905825	70.8	69.2	0.290938	-945.956922	75.9	3.671	2.815	4.097	153.7	-28.1	158.1 / -159.0	-129.3
c/d PT	-946.283752	0.344920	-945.938832	-23.5	-17.4	0.294696	-945.989056	-106.8	4.165	2.534	3.640	134.1	5.4	115.0 -176.1	170.0
cc/u RT	-946.274814	0.342688	-945.932126	0.0	0.2	0.289713	-945.985101	2.0	2.111	3.860	4.667	176.3	42.0	175.3 / 120.7	-100.6
cc/u TS	-946.240524	0.342103	-945.898421	90.0	88.7	0.292141	-945.948383	98.4	2.278	4.034	4.638	143.9	24.3	-157.7 / 167.9	-159.8
cc/u PT	-946.291701	0.345208	-945.946493	-44.3	-37.5	0.295049	-945.996651	-28.4	2.290	3.939	4.591	122.1	-4.8	-115.0 / 173.4	-169.2
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-19.3	-19.4		$\Delta(E+G_{corr})^{\ddagger}$	-22.4							
c/u RT	-946.275458	0.342618	-945.932840	0.0	0.0	0.289507	-945.985950	0.0	4.106	2.949	4.628	176.8	-47.4	-178.3 / 120.9	-85.5
c/u TS	-946.245706	0.341716	-945.903990	78.1	75.7	0.290499	-945.955208	80.7	4.415	2.836	4.039	151.5	-27.2	159.6 / 53.9	-131.6
c/u PT	-946.281866	0.345099	-945.936767	-16.8	-10.3	0.295136	-945.986730	-2.0	4.185	2.485	3.632	133.3	7.6	112.4 / 58.1	165.0
cc/d RT	-946.274193	0.342981	-945.931212	3.3	4.3	0.291076	-945.983117	7.4	2.106	4.167	4.666	173.1	50.5	173.7 / -117.8	-110.4
cc/d TS	-946.232996	0.341803	-945.891193	111.5	109.3	0.291731	-945.941265	117.3	2.238	4.032	4.503	139.8	20.5	-155.5 / -40.1	-157.0
cc/d PT	-946.284144	0.345547	-945.938597	-22.8	-15.1	0.295865	-945.988279	-6.1	2.344	3.963	4.534	119.3	-9.6	-108.5 / -53.2	-148.4
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-33.4	-33.6		$\Delta(E+G_{corr})^{\ddagger}$	-36.6							
3d, R^3 = Ph															
cRT	-1059.343436	0.339303	-1059.004133	1.0	0.0	0.283612	-1059.059825	0.0	4.249	2.889	4.634	177.0	-44.6	-178.6	-84.2
cTS	-1059.318239	0.338649	-1058.979590	67.1	64.4	0.285852	-1059.032387	72.0	4.381	2.769	4.132	154.4	-26.5	152.7	-127.1
cPT	-1059.347620	0.341035	-1059.006585	-10.0	-6.4	0.288333	-1059.059288	1.4	4.330	2.706	3.641	134.3	-4.0	129.7	-169.6
ccRT	-1059.343806	0.339869	-1059.003937	0.0	0.5	0.286042	-1059.057764	5.4	2.056	3.997	4.716	175.6	47.3	177.3	-100.4
ccTS	-1059.311483	0.338564	-1058.972919	84.9	82.0	0.287364	-1059.024119	93.7	2.290	4.064	4.654	143.5	24.6	-154.4	-162.9
ccPT	-1059.356744	0.341275	-1059.015469	-34.0	-29.8	0.289187	-1059.067558	-20.3	2.306	3.956	4.591	122.5	-1.3	-121.3	-175.7
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-17.7	-17.5		$\Delta(E+G_{corr})^{\ddagger}$	-21.7							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] $D(R^3(H),R^3, C_5,C_4)$ is also indicated for systems with R^3 = ^{i}Pr after $D(R^3,C_6, C_5,C_4)$.

TABLE A1.13 Energies and geometrical parameters of system **4** at the ωB97X-D/6-31+G(d,p) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	$R(R^2,H^3)$ [b] (Å)	$R(H^2,H^3)$ (Å)	$R(R^1,R^2)$ [c] (Å)	$A(C_1,C_2,C_3)$ (degrees)	$D(C_2,C_3,C_5,C_6)$ (degrees)	$D(R^3,C_6,C_5,C_4)$ [d] (degrees)	$D(R^2,C_2,C_3,C_4)$ (degrees)
4a, R^3 = H															
cRT	-946.266426	0.342221	-945.924205	0.0	0.0	0.290216	-945.976211	0.0	4.573	3.058	4.613	175.7	-54.1	-175.9	-88.9
cTS	-946.237967	0.342271	-945.895696	74.7	74.9	0.293434	-945.944532	83.2	4.327	2.670	4.290	156.7	-28.0	154.5	-123.6
cPT	-946.264382	0.344771	-945.919611	5.4	12.1	0.295547	-945.968835	19.4	4.462	2.804	4.039	137.5	-12.7	134.5	-139.2
ccRT	-946.265129	0.342238	-945.922891	3.4	3.4	0.291028	-945.974102	5.5	2.129	4.250	4.742	175.3	57.1	175.3	-100.8
ccTS	-946.234160	0.342041	-945.892119	84.7	84.2	0.292320	-945.941840	90.2	2.262	4.008	4.784	149.2	29.3	-157.3	-159.1
ccPT	-946.281490	0.345388	-945.936102	-39.6	-31.2	0.294005	-945.987486	-29.6	2.203	3.867	4.769	126.6	-2.2	-118.3	-170.1
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-10.0	-9.4		$\Delta(E+G_{corr})^{\ddagger}$	-7.1							
4b, R^3 = Me															
cRT	-985.581542	0.370102	-985.211440	0.0	0.0	0.315364	-985.266178	0.0	4.450	3.017	4.621	176.0	-53.4	-176.7	-88.1
cTS	-985.552621	0.370200	-985.182421	75.9	76.2	0.319224	-985.233397	86.1	4.376	2.758	4.271	154.8	-28.1	156.4	-123.9
cPT	-985.572968	0.373256	-985.199712	22.5	30.8	0.322621	-985.250347	41.6	4.508	2.930	4.017	135.9	-14.3	140.0	-136.7
ccRT	-985.580492	0.370599	-985.209893	2.8	4.1	0.316919	-985.263572	6.8	2.098	4.278	4.755	175.0	59.2	174.5	-100.0
ccTS	-985.545404	0.370549	-985.174855	94.9	96.1	0.319859	-985.225545	106.7	2.260	4.003	4.664	145.0	25.1	-156.2	-160.0
ccPT	-985.587256	0.374010	-985.213246	-15.0	-4.7	0.322821	-985.264434	4.6	2.230	3.888	4.750	124.8	-6.0	-115.7	-160.3
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-18.9	-19.9		$\Delta(E+G_{corr})^{\ddagger}$	-20.6							
4c, R^3 = ^{i}Pr															
c/s RT	-1064.196541	0.427595	-1063.768946	0.0	0.0	0.369299	-1063.827242	0.0	4.330	2.944	4.638	176.5	-51.7	-178.9 / -1.6	-86.5
c/s TS	-1064.165054	0.427640	-1063.737414	82.7	82.8	0.373393	-1063.791660	93.4	4.369	2.768	4.251	153.1	-27.3	153.2 / -89.0	-124.9
c/s PT	-1064.182862	0.430811	-1063.752051	35.9	44.4	0.377268	-1063.805594	56.8	4.554	3.035	3.994	134.3	-15.2	142.8 / -90.0	-134.2
cc/s RT	-1064.195311	0.427900	-1063.767411	3.2	4.0	0.370718	-1063.824593	7.0	2.108	4.312	4.694	173.0	58.0	173.9 / -0.5	-111.4
cc/s TS	-1064.150009	0.428216	-1063.721793	122.2	123.8	0.374580	-1063.775428	136.0	2.394	4.000	4.584	139.1	20.7	-158.0 / -7.2	-162.4
cc/s PT	-1064.197722	0.431554	-1063.766168	-3.1	7.3	0.377874	-1063.819847	19.4	2.206	3.917	4.718	121.8	-14.1	-101.3 / 62.6	-137.4
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-39.5	-41.0		$\Delta(E+G_{corr})^{\ddagger}$	-42.6							
c/d RT	-1064.195866	0.428013	-1063.767853	0.0	0.0	0.369872	-1063.825995	0.0	4.436	3.023	4.628	176.1	-54.0	-175.1 / -124.8	-87.3
c/d TS	-1064.168242	0.427772	-1063.740470	72.5	71.9	0.373872	-1063.794370	83.0	4.392	2.769	4.262	154.5	-28.5	157.7 / -159.3	-125.8
c/d PT	-1064.188000	0.430507	-1063.757493	20.7	27.2	0.376715	-1063.811285	38.6	4.478	2.873	4.011	135.9	-12.8	137.9 / -173.9	-139.2
cc/u RT	-1064.195247	0.427742	-1063.767505	1.6	0.9	0.369688	-1063.825558	1.1	2.081	4.325	4.767	175.1	61.5	173.0 / 127.7	-97.8
cc/u TS	-1064.161455	0.427659	-1063.733796	90.3	89.4	0.373812	-1063.787643	100.7	2.278	4.008	4.655	144.8	24.8	-157.1 / 168.4	-160.2
cc/u PT	-1064.204995	0.431694	-1063.773301	-24.0	-14.3	0.377951	-1063.827043	-2.8	2.222	3.873	4.755	125.0	-8.1	-111.8 / 173.8	176.7
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-17.8	-17.5		$\Delta(E+G_{corr})^{\ddagger}$	-17.7							
c/u RT	-1064.196530	0.427873	-1063.768657	0.0	0.0	0.369919	-1063.826611	0.0	4.439	2.943	4.640	176.5	-51.7	-179.9 / 122.8	-86.0
c/u TS	-1064.165289	0.427615	-1063.737674	82.0	81.3	0.373665	-1063.791623	91.9	4.415	2.817	4.228	152.5	-28.5	160.1 / 54.6	-126.5
c/u PT	-1064.184478	0.430287	-1063.754191	31.6	38.0	0.375620	-1063.808858	46.6	4.460	2.835	4.000	135.5	-11.7	137.3 / 51.5	-141.0
cc/d RT	-1064.194970	0.428239	-1063.766731	4.1	5.1	0.371315	-1063.823656	7.8	2.118	4.348	4.704	173.0	59.8	173.1 / -122.3	-110.6
cc/d TS	-1064.152866	0.428056	-1063.724810	114.6	115.1	0.374937	-1063.777930	127.8	2.232	4.008	4.566	141.1	21.2	-155.1 / -39.7	-160.0
cc/d PT	-1064.198687	0.431731	-1063.766956	-5.7	4.5	0.378611	-1063.820076	17.2	2.255	3.910	4.705	121.2	-12.7	-107.5 / -54.5	-137.2
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-32.6	-33.8		$\Delta(E+G_{corr})^{\ddagger}$	-36.0							
4d, R^3 = Ph															
cRT	-1177.264614	0.424383	-1176.840231	0.5	0.1	0.363959	-1176.900655	0.0	4.381	2.949	4.640	176.4	-52.5	-178.1	-86.2
cTS	-1177.238873	0.424523	-1176.814350	68.1	68.1	0.369022	-1176.869852	80.9	4.364	2.729	4.277	154.9	-26.9	152.2	-124.0
cPT	-1177.255189	0.426834	-1176.828355	25.2	31.3	0.370928	-1176.884261	43.0	4.488	2.884	4.032	137.0	-14.1	138.4	-136.6
ccRT	-1177.264802	0.424528	-1176.840274	0.0	0.0	0.365730	-1176.899073	4.2	2.070	4.762	4.210	175.3	57.7	177.1	-98.7
ccTS	-1177.232274	0.424311	-1176.807963	85.4	84.8	0.369276	-1176.862997	98.9	2.292	4.042	4.669	144.3	25.2	-154.0	-163.0
ccPT	-1177.269053	0.427912	-1176.841141	-11.2	-2.3	0.372014	-1176.897039	9.5	2.237	3.990	4.756	125.6	-3.1	-119.6	-170.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-17.3	-16.8		$\Delta(E+G_{corr})^{\ddagger}$	-18.0							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] $D(R^3(H),R^3, C_5,C_4)$ is also indicated for systems with R^3 = ^{i}Pr after $D(R^3,C_6, C_5,C_4)$.

TABLE A1.14 Energies and geometrical parameters of system **5** at the ωB97X-D/6-31+G(d,p) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	$E+G_{corr}$ (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(R^2,H^3) [b] (Å)	R(H^2,H^3) (Å)	R(R^1,R^2) [c] (Å)	A(C_1,C_2,C_3) (degrees)	D(C_2,C_3,C_5,C_6) (degrees)	D(R^3,C_6,C_5,C_4) [d] (degrees)	D(R^2,C_2,C_3,C_4) (degrees)
5a, R^3 = H															
cRT	-902.103005	0.225846	-901.877159	4.1	4.0	0.177696	-901.925310	2.0	4.383	3.010	5.694	176.3	-47.0	-176.5	-90.0
cTS	-902.077676	0.225101	-901.852575	70.6	68.6	0.178892	-901.898785	71.6	4.332	2.786	4.911	153.7	-27.7	157.0	-129.7
cPT	-902.127478	0.227836	-901.899642	-60.1	-55.0	0.182438	-901.945040	-49.8	4.304	2.720	4.020	131.0	-3.7	126.5	-170.9
ccRT	-902.104577	0.225883	-901.878694	0.0	0.0	0.178520	-901.926058	0.0	2.551	3.868	5.802	178.5	43.5	176.7	-93.6
ccTS	-902.076057	0.224754	-901.851303	74.9	71.9	0.178687	-901.897370	75.3	2.295	3.920	6.011	152.3	26.1	-155.6	-133.2
ccPT	-902.131811	0.227719	-901.904092	-71.5	-66.7	0.178146	-901.953665	-72.5	2.228	3.958	5.952	123.1	0.0	120.4	180.0
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-4.3	-3.3		$\Delta(E+G_{corr})^{\ddagger}$	-3.7							
5b, R^3 = Me															
cRT	-941.418173	0.253812	-941.164361	5.3	4.8	0.203359	-941.214815	2.7	4.344	2.978	5.697	176.4	-46.6	-176.9	-88.9
cTS	-941.392536	0.253042	-941.139494	72.6	70.0	0.204663	-941.187872	73.5	4.355	2.829	4.876	152.3	-27.6	158.2	-130.4
cPT	-941.435544	0.256403	-941.179141	-40.3	-34.0	0.209239	-941.226304	-27.4	4.306	2.772	3.992	130.3	-4.2	130.8	-170.1
ccRT	-941.420192	0.254019	-941.166173	0.0	0.0	0.204341	-941.215850	0.0	2.505	3.859	5.825	179.2	44.8	177.6	-91.1
ccTS	-941.392161	0.253147	-941.139014	73.6	71.3	0.205692	-941.186469	77.1	2.312	3.940	5.969	149.3	24.3	-156.3	-140.6
ccPT	-941.440463	0.256372	-941.184091	-53.2	-47.0	0.208566	-941.231897	-42.1	2.088	3.990	5.956	122.9	-0.7	-122.1	-179.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-1.0	-1.3		$\Delta(E+G_{corr})^{\ddagger}$	-3.7							
5c, R^3 = ^{i}Pr															
c/s RT	-1020.032949	0.311346	-1019.721603	10.9	10.4	0.256843	-1019.776106	4.5	4.292	2.926	5.725	177.2	-45.6	-178.7 / -2.9	-87.3
c/s TS	-1020.005089	0.310701	-1019.694388	84.1	81.9	0.259106	-1019.745983	83.6	4.359	2.844	4.750	148.6	-25.5	162.3 / -33.7	-135.1
c/s PT	-1020.047033	0.313554	-1019.733479	-26.0	-20.8	0.262513	-1019.784521	-17.6	4.248	2.622	3.928	128.7	1.9	119.8 / -62.2	179.5
cc/s RT	-1020.037112	0.311545	-1019.725567	0.0	0.0	0.259303	-1019.777809	0.0	2.461	3.895	5.859	178.5	47.2	178.0 / 3.1	-86.4
cc/s TS	-1020.000998	0.310904	-1019.690094	94.8	93.1	0.260314	-1019.740684	97.5	2.232	3.931	5.797	143.3	19.8	-159.9 / 26.4	-142.4
cc/s PT	-1020.050523	0.313532	-1019.736991	-35.2	-30.0	0.262587	-1019.787935	-26.6	2.071	3.976	5.937	121.7	-7.9	-109.5 / 64.0	-158.6
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-10.7	-11.3		$\Delta(E+G_{corr})^{\ddagger}$	-13.9							
c/d RT	-1020.032467	0.311256	-1019.721211	6.8	6.5	0.257128	-1019.775339	5.5	4.346	2.977	5.705	176.7	-47.1	-175.5 / -125.0	-88.6
c/d TS	-1020.008040	0.310650	-1019.697390	71.0	69.1	0.259019	-1019.749021	74.6	4.357	2.831	4.937	153.6	-27.9	157.7 / -160.8	-127.6
c/d PT	-1020.051385	0.313141	-1019.738244	-42.8	-38.2	0.262156	-1019.789229	-30.9	4.285	2.727	3.978	130.1	-2.4	127.7 / -175.7	-172.0
cc/u RT	-1020.035065	0.311363	-1019.723702	0.0	0.0	0.257614	-1019.777451	0.0	2.456	3.819	5.830	179.5	44.3	177.4 / 120.5	-88.4
cc/u TS	-1020.008057	0.310367	-1019.697690	70.9	68.3	0.259227	-1019.748830	75.1	2.370	3.951	5.985	150.3	24.9	156.7 / 164.6	-138.9
cc/u PT	-1020.056503	0.313351	-1019.743152	-56.3	-51.1	0.261979	-1019.794524	-44.8	2.060	3.975	5.955	122.8	-2.1	-119.8 / 172.2	-178.9
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	0.0	0.8		$\Delta(E+G_{corr})^{\ddagger}$	-0.5							
c/u RT	-1020.032923	0.311523	-1019.721400	10.4	9.6	0.257460	-1019.775463	4.0	4.281	2.926	5.731	177.3	-45.8	179.9 / 122.3	-86.5
c/u TS	-1020.006463	0.310336	-1019.696127	79.8	75.9	0.258608	-1019.747854	76.4	4.347	2.836	4.867	151.4	-26.3	157.9 / 54.2	-129.8
c/u PT	-1020.049749	0.313749	-1019.736000	-33.8	-28.8	0.263285	-1019.786464	-24.9	4.266	2.665	3.948	129.2	-0.1	124.0 / 56.0	-176.1
cc/d RT	-1020.036874	0.311828	-1019.725046	0.0	0.0	0.259905	-1019.776969	0.0	2.517	3.910	5.850	178.7	47.7	178.2 / -119.0	-87.7
cc/d TS	-1020.004374	0.310337	-1019.694037	85.3	81.4	0.260181	-1019.744193	86.1	2.384	3.918	5.866	146.8	21.3	-155.8 / -38.8	-141.3
cc/d PT	-1020.052272	0.313194	-1019.739078	-40.4	-36.8	0.262169	-1019.790103	-34.5	2.119	3.973	5.940	122.0	-6.0	-114.7 / -56.2	-161.4
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	-5.5	-5.5		$\Delta(E+G_{corr})^{\ddagger}$	-9.6							
5d, R^3 = Ph															
cRT	-1133.100811	0.308398	-1132.792413	13.3	13.8	0.252461	-1132.848350	8.4	4.299	2.923	5.707	176.8	-46.1	-177.7	-87.9
cTS	-1133.077810	0.307375	-1132.770435	73.6	71.5	0.254283	-1132.823527	73.6	4.346	2.802	4.933	153.8	-27.2	154.4	-128.6
cPT	-1133.115546	0.309933	-1132.805613	-25.4	-20.9	0.257218	-1132.858328	-17.8	4.313	2.796	4.011	130.9	-5.3	131.8	-167.4
ccRT	-1133.105860	0.308200	-1132.797660	0.0	0.0	0.254300	-1132.851560	0.0	2.614	3.769	5.825	178.2	44.3	-179.8	-85.6
ccTS	-1133.078376	0.307107	-1132.771269	72.2	69.3	0.255670	-1132.822706	75.8	2.525	3.952	5.986	150.4	24.0	-152.0	-137.1
ccPT	-1133.120129	0.310038	-1132.810091	-37.5	-32.6	0.257242	-1132.862887	-29.7	2.161	3.996	5.955	123.2	1.7	-127.0	172.3
			$\Delta E^{\ddagger}$ (or $\Delta(E+ZPE)^{\ddagger}$)	1.5	2.2		$\Delta(E+G_{corr})^{\ddagger}$	-2.2							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] D(R^3(H),R^3, C_5,C_4) is also indicated for systems with R^3 = ^{i}Pr after D(R^3,C_6, C_5,C_4).

TABLE A1.16 Energies and geometrical parameters of system **6** at the ωB97X-D/6-31+G(d,p) level of theory.

Structure	Energies								Geometrical Parameters						
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(R^2,H^3) [b] (Å)	R(H^2,H^3) (Å)	R(R^1,R^2) [c] (Å)	A(C_1,C_2,C_3) (degrees)	D(C_2,C_3,C_5,C_6) (degrees)	D(R^3,C_6,C_5,C_4) [d] (degrees)	D(R^2,C_2,C_3,C_4) (degrees)
6a, R^3 = H															
cRT	-1020.023949	0.311098	-1019.712851	3.6	3.6	0.258697	-1019.765252	2.2	4.572	3.086	5.678	175.4	-54.9	-176.3	-89.7
cTS	-1020.000119	0.310764	-1019.689355	66.1	65.3	0.260950	-1019.739168	70.7	4.305	2.743	5.000	155.2	-28.5	156.4	-126.8
cPT	-1020.038640	0.313500	-1019.725140	-35.0	-28.7	0.264458	-1019.774183	-21.2	4.399	2.881	4.320	132.9	-10.3	131.9	-146.6
ccRT	-1020.025302	0.311094	-1019.714208	0.0	0.0	0.259204	-1019.766097	0.0	2.479	4.007	5.787	178.5	50.8	176.5	-95.5
ccTS	-1019.997391	0.310416	-1019.686975	73.3	71.5	0.260474	-1019.736917	76.6	2.230	3.905	6.007	153.0	26.9	-155.3	-132.3
ccPT	-1020.044891	0.313864	-1019.731027	-51.4	-44.2	0.263379	-1019.781512	-40.5	2.093	3.990	6.132	126.9	3.8	-126.8	165.1
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-7.2	-6.2		Δ(E+G_{cor})‡	-5.9							
6b, R^3 = Me															
cRT	-1059.339288	0.339276	-1059.000012	5.3	4.5	0.284238	-1059.055050	1.5	4.539	3.061	5.682	175.5	-54.5	-177.0	-89.0
cTS	-1059.315025	0.338769	-1058.976256	69.0	66.9	0.286814	-1059.028211	72.0	4.338	2.802	4.969	153.5	-28.5	157.8	-127.4
cPT	-1059.347074	0.342045	-1059.005029	-15.1	-8.7	0.291563	-1059.055511	0.3	4.421	2.981	4.287	131.7	-11.5	136.9	-145.0
ccRT	-1059.341308	0.339577	-1059.001731	0.0	0.0	0.285685	-1059.055624	0.0	2.423	3.997	5.823	179.0	52.4	178.3	-90.8
ccTS	-1059.313411	0.338733	-1058.974678	73.2	71.0	0.287287	-1059.026124	77.5	2.316	3.926	5.961	149.9	24.9	-156.1	-140.3
ccPT	-1059.353287	0.343083	-1059.010204	-31.5	-22.2	0.291762	-1059.061524	-15.5	2.082	3.960	6.126	126.7	0.1	-123.5	-179.7
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-4.2	-4.1		Δ(E+G_{cor})‡	-5.5							
6c, R^3 = ^{i}Pr															
c/s RT	-1137.954002	0.396578	-1137.557424	11.7	10.3	0.337750	-1137.616251	3.5	4.488	3.002	5.811	176.2	-53.3	-178.3 / -2.4	-88.3
c/s TS	-1137.926888	0.396690	-1137.530198	82.9	81.8	0.341930	-1137.584958	85.6	4.336	2.809	4.879	150.0	-26.3	162.0 / -36.6	-131.0
c/s PT	-1137.956997	0.399147	-1137.557850	3.9	9.2	0.345389	-1137.611608	15.7	4.459	3.080	4.244	130.1	-12.1	139.2 / -90.1	-142.8
cc/s RT	-1137.958467	0.397130	-1137.561337	0.0	0.0	0.340897	-1137.617570	0.0	2.431	3.977	5.819	179.0	51.8	178.7 / -0.9	-89.4
cc/s TS	-1137.921532	0.396355	-1137.525177	97.0	94.9	0.341706	-1137.579827	99.1	2.195	3.893	5.779	144.4	19.9	-159.4 / 29.1	-140.7
cc/s PT	-1137.964225	0.399753	-1137.564472	-15.1	-8.2	0.345130	-1137.619096	-4.0	2.055	3.904	6.128	125.1	-10.8	-107.3 / 63.1	-148.3
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-14.1	-13.2		Δ(E+G_{cor})‡	-13.5							
c/d RT	-1137.953561	0.396665	-1137.556896	7.2	6.9	0.337900	-1137.615661	4.2	4.543	3.065	5.691	175.8	-55.1	-175.3 / -124.7	-88.9
c/d TS	-1137.930742	0.396247	-1137.534495	67.1	65.7	0.340931	-1137.589812	72.1	2.372	2.803	5.002	154.4	-28.6	157.5 / -161.7	-125.6
c/d PT	-1137.962457	0.399303	-1137.563154	-16.2	-9.6	0.345420	-1137.617038	0.6	4.403	2.942	4.283	131.5	-10.2	135.0 / -175.9	-146.1
cc/u RT	-1137.956295	0.396782	-1137.559513	0.0	0.0	0.339030	-1137.617265	0.0	2.397	3.961	5.824	178.5	52.0	178.5 / 120.1	-87.7
cc/u TS	-1137.929536	0.395901	-1137.533635	70.3	67.9	0.340884	-1137.588652	75.1	2.365	3.935	5.976	150.6	25.5	156.7 / 166.1	-139.0
cc/u PT	-1137.969634	0.399627	-1137.570007	-35.0	-27.6	0.344195	-1137.625439	-21.5	2.057	3.930	6.141	126.9	-2.7	-118.7 / 173.8	-177.3
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-3.2	-2.3		Δ(E+G_{cor})‡	-3.0							
c/u RT	-1137.953911	0.396561	-1137.557350	11.1	9.7	0.337887	-1137.616024	4.0	4.475	2.999	5.700	176.0	-53.3	-179.4 / 122.5	-88.1
c/u TS	-1137.928851	0.395939	-1137.532912	76.9	73.9	0.340626	-1137.588226	77.0	4.323	2.798	4.952	152.4	-26.9	157.7 / 53.6	-127.2
c/u PT	-1137.959586	0.399257	-1137.560329	-3.8	1.9	0.344784	-1137.614802	7.2	4.395	2.915	4.270	130.9	-9.1	134.2 / 48.7	-147.0
cc/d RT	-1137.958137	0.397090	-1137.561047	0.0	0.0	0.340582	-1137.617555	0.0	2.498	3.991	5.810	179.2	52.4	178.4 / -121.5	-90.5
cc/d TS	-1137.925524	0.396222	-1137.529302	85.6	83.3	0.342466	-1137.583058	90.6	2.351	3.892	5.853	147.5	21.7	-155.6 / -37.9	-140.7
cc/d PT	-1137.966322	0.399628	-1137.566694	-21.5	-14.8	0.345171	-1137.621150	-9.4	2.091	3.898	6.134	125.4	-9.6	-111.3 / -58.0	-149.4
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-8.7	-9.5		Δ(E+G_{cor})‡	-13.6							
6d, R^3 = Ph															
cRT	-1251.022239	0.393359	-1250.628880	12.4	11.1	0.332788	-1250.689452	4.7	4.515	3.024	5.699	175.9	-54.6	-178.0	-87.9
cTS	-1251.000422	0.392815	-1250.607607	69.7	66.9	0.336048	-1250.664373	70.6	4.333	2.781	5.005	154.5	-28.1	154.1	-126.5
cPT	-1251.027936	0.395349	-1250.632587	-2.5	1.3	0.338970	-1250.688966	6.0	4.413	2.967	4.304	132.5	-11.7	136.2	-144.6
ccRT	-1251.026972	0.393875	-1250.633097	0.0	0.0	0.335714	-1250.691258	0.0	2.606	3.852	5.799	178.4	48.7	-180.0	-88.2
ccTS	-1250.999777	0.392709	-1250.607068	71.4	68.3	0.337291	-1250.662485	75.5	3.984	3.942	5.977	150.6	24.7	-152.1	-138.0
ccPT	-1251.033501	0.395860	-1250.637641	-17.1	-11.9	0.338719	-1250.694782	-9.3	2.155	3.986	6.117	126.7	3.2	-127.8	168.7
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-1.7	-1.4		Δ(E+G_{cor})‡	-5.0							

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers. [d] D(R^3(H),R^3, C_5,C_4) is also indicated for systems with R^3 = ^{i}Pr after D(R^3,C_6, C_5,C_4).

TABLE A1.17 Differences in transition state energies, $\Delta(E+ZPE)^{\ddagger}$ / and in Gibbs energies of activation, $\Delta(E+G_{corr})^{\ddagger}$ (kJ mol^{-1}),[a] between clockwise and counterclockwise modes of conrotation for systems **1-6** at the ***X***/6-31+G(d,p)//B3LYP/6-31G(d) level of theory where ***X*** = B3LYP, M06-2X or MP2.

B3LYP/6-31+G(d,p)//B3LYP/6-31G(d)

R^1,R^2 =	**1** Me,Me	**2** ^{t}Bu,Me	**3** Me,^{t}Bu	**4** ^{t}Bu,^{t}Bu	**5** Me,Ph	**6** ^{t}Bu,Ph
R^3 =						
a H	-2.2 / -2.4	-2.0 / -2.1	-10.5 / -10.3	-5.5 / -4.1	-5.3 / -5.7	-3.9 / -3.5
b Me	-5.7 / -5.9	-6.3 / -6.3	-19.8 / 20.3	-16.1 / -15.8	-5.5 / -6.1	-4.3 / -4.3
c ^{i}Pr ~ Me [a]	-6.4 / -6.2	-7.3 / -7.0	-20.2 / -21.4	-16.0 / -16.0	-6.0 / -6.6	-4.6 / -3.9
c ^{i}Pr [a]	-11.1 / -10.6	-13.0 / -13.0	-32.7 / -24.7	-30.5 / -32.2	-14.7 / -14.9	-14.4 / -14.5
c ^{i}Pr ~ ^{t}Bu [a]	-15.4 / -15.9	-17.7 / -18.3	-32.5 / -35.2	-39.2 / -40.3	-16.6 / -17.1	-16.0 / -16.5
d Ph	-6.9 / -6.9	-7.3 / -7.3	-22.2 / -23.6	-18.1 / -18.5	-11.6 / -12.5	-10.5 / -10.7

M06-2X/6-31+G(d,p)//B3LYP/6-31G(d)

R^1,R^2 =	**1** Me,Me	**2** ^{t}Bu,Me	**3** Me,^{t}Bu	**4** ^{t}Bu,^{t}Bu	**5** Me,Ph	**6** ^{t}Bu,Ph
R^3 =						
a H	-1.2 / -1.4	-2.9 / 3.0	-11.6 / -11.4	-7.7 / -6.4	-4.2 / -4.6	-5.4 / -5.0
b Me	-4.3 / -4.6	-6.8 / -6.8	-21.6 / -22.1	-18.6 / -18.3	-1.8 / -2.5	-3.6 / -3.6
c ^{i}Pr ~ Me [a]	-4.6 / -4.5	-7.8 / -7.5	-21.2 / -22.3	-17.2 / -17.1	-2.3 / -2.9	-4.0 / -3.4
c ^{i}Pr [a]	-10.3 / -9.9	-14.4 / -16.4	-35.4 / -30.8	-33.2 / -34.9	-9.8 / -10.1	-10.5 / -17.9
c ^{i}Pr ~ ^{t}Bu [a]	-14.6 / -15.1	-18.4 / -19.0	-34.5 / -30.5	-41.2 / -42.3	-13.0 / -13.5	-14.5 / -15.0
d Ph	-3.5 / -3.6	-5.8 / -5.8	-20.1 / -18.8	-17.2 / -17.6	-5.8 / -6.7	-6.6 / -6.8

MP2/6-31+G(d,p)//B3LYP/6-31G(d)

R^1,R^2 =	**1** Me,Me	**2** ^{t}Bu,Me	**3** Me,^{t}Bu	**4** ^{t}Bu,^{t}Bu	**5** Me,Ph	**6** ^{t}Bu,Ph
R^3 =						
a H	-1.6 / -1.8	-3.2 / -3.3	-11.4 / -11.2	-9.0 / -7.6	-2.0 / -2.4	-5.3 -4.9
b Me	-4.7 / -5.0	-7.3 / -7.3	-20.8 / -21.4	-18.7 / -18.4	1.5 / 0.8	-2.3 / 2.3
c ^{i}Pr ~ Me [a]	-4.5/ -4.3	-7.3 / -7.1	-19.4 / -20.6	-17.9 / -17.9	3.2 / 2.6	-0.3 / 0.4
c ^{i}Pr [a]	-9.3 / -10.0	-13.2 / -13.2	-33.3 / -36.0	-33.0 / -34.7	-2.9 / -3.1	-6.8 / -6.9
c ^{i}Pr ~ ^{t}Bu [a]	-14.4 / -15.0	-18.9 / -19.4	-33.2 / -35.2	-43.1 / -44.2	-6.8 / -7.3	-10.0 / -10.5
d Ph	-2.6 / -2.7	-5.3 / -5.3	-16.9 -18.3	-16.1 / -16.5	4.7 / 3.8	0.3 / 0.1

[a] Zero-point energy (ZPE) corrections (or thermal corrections to Gibbs energies, G_{corr}) from the B3LYP/6-31G(d) level of theory were included. [b] *cf.* Section **3.6.2**. The **c/d**,**cc/u** and **c/s**,**cc/s** pairs are approximated as having R^3 = Me and R^3 = ^{t}Bu, respectively instead of R^3 = ^{i}Pr.

TABLE A1.18 Energies and geometrical parameters of systems **1b**, **1b'** and **1b"** at the B3LYP/6-31G(d) level of theory.

Structure	Energies								Geometrical Parameters					
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	ΔE [a] (kJ mol^{-1})	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(R^2, H^3) [b] (Å)	R(H^2, H^3) (Å)	R(R^1,R^2) [c] (Å)	A(C_1,C_2,C_3) (degrees)	D(C_2,C_3,C_5,C_6) (degrees)	D(R^3,C_6, C_5,C_4) (degrees)
1b, R^2 = Me, R^3 = Me														
cRT	-749.916799	0.199510	-749.717289	0.0	0.0	0.154868	-749.761931	0.0	4.547	3.006	4.582	176.2	-45.1	-176.8
cTS	-749.887379	0.198480	-749.688899	77.2	74.5	0.155414	-749.731965	78.7	4.417	2.858	3.954	150.6	-26.1	157.8
cPT	-749.926547	0.201454	-749.725093	-25.6	-20.5	0.158192	-749.768355	-16.9	4.278	2.744	3.319	130.4	0.3	124.1
ccRT	-749.916652	0.199452	-749.717200	0.4	0.2	0.154819	-749.761833	0.3	2.763	3.987	4.671	176.1	44.4	176.7
ccTS	-749.885274	0.198462	-749.686812	82.8	80.0	0.155494	-749.729780	84.4	2.609	4.015	4.711	147.1	24.3	-157.3
ccPT	-749.929935	0.201350	-749.728585	-34.5	-29.7	0.158268	-749.771667	-25.6	2.565	3.919	4.627	124.7	-2.4	-119.5
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-5.5	-5.5		Δ(E+G_{corr})‡	-5.7						
1b', R^2 = Me, H^3 ↬ R^3 = Me														
cRT	-749.916652	0.199452	-749.717200	0.4	0.2	0.154819	-749.761833	0.3	2.763	3.987	4.671	176.1	44.4	176.7
cTS	-749.885274	0.198462	-749.686812	82.8	80.0	0.155494	-749.729780	84.4	2.609	4.015	4.711	147.1	24.3	-157.3
cPT	-749.929935	0.201350	-749.728585	-34.5	-29.7	0.158268	-749.771667	-25.6	2.565	3.919	4.627	124.7	-2.4	-119.5
ccRT	-749.916799	0.199510	-749.717289	0.0	0.0	0.154868	-749.761931	0.0	4.547	3.006	4.582	176.2	-45.1	-176.8
ccTS	-749.887379	0.198480	-749.688899	77.2	74.5	0.155414	-749.731965	78.7	4.417	2.858	3.954	150.6	-26.1	157.8
ccPT	-749.926547	0.201454	-749.725093	-25.6	-20.5	0.158192	-749.768355	-16.9	4.278	2.744	3.319	130.4	0.3	124.1
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	5.5	5.5		Δ(E+G_{corr})‡	5.7						
1b", H^2 ↬ R^2 = Me, R^3 = Me														
cRT	-749.910660	0.199645	-749.711015	0.0	0.0	0.155275	-749.755385	0.0	2.775	4.633	4.621	177.6	-50.4	-2.2
cTS	-749.879008	0.198798	-749.680210	83.1	80.9	0.156091	-749.722917	85.2	2.459	2.980	4.046	153.7	-29.0	-61.9
cPT	-749.926547	0.201454	-749.725093	-41.7	-37.0	0.158192	-749.768355	-34.1	2.395	2.744	3.319	130.4	-0.3	-124.1
ccRT	-749.909650	0.199605	-749.710045	2.7	2.5	0.155213	-749.754437	2.5	4.410	5.164	4.677	175.9	54.5	2.5
ccTS	-749.876200	0.198677	-749.677523	90.5	87.9	0.155962	-749.720238	92.3	4.385	4.109	4.800	149.8	32.6	60.1
ccPT	-749.929935	0.201350	-749.728585	-50.6	-46.1	0.158268	-749.771667	-42.7	4.176	3.919	4.627	124.7	2.4	119.5
			$\Delta E^{\ddagger}$ (or Δ(E+ZPE)‡)	-7.4	-7.1		Δ(E+G_{corr})‡	-7.0						

[a] Energies relative to that of the lowest lying reactant pentadienyl cation, cRT or ccRT. [b] Distance between closest atom of R^2 substituent and H^3. [c] Distance between R^1 and R^2 centers.

Cartesian coordinates for systems **1-6**

RB3LYP/6-31G(d)

1a

cRT

C 3.5913680000 -0.1605970000 -0.0848590000
C 2.3804740000 0.2873960000 -0.2711780000
C 1.1762990000 0.8190260000 -0.4247320000
C -0.0410300000 0.0218120000 -0.1792290000
C -0.0553900000 -1.4486370000 -0.1675900000
C 0.7186090000 -2.2054310000 -0.9552900000
H -0.8137170000 -1.8908400000 0.4693090000
C 0.9783360000 2.2909150000 -0.7379710000
O -1.0892650000 0.6788320000 0.0383130000
H 1.9394530000 2.7773930000 -0.9164270000
H 0.4709850000 2.7906640000 0.0932760000
H 0.3438240000 2.4146470000 -1.6219970000
B -2.6248230000 0.0337940000 0.2746680000
F -3.3725030000 1.1511380000 0.4232830000
F -2.4869760000 -0.7332760000 1.4048270000
F -2.8456370000 -0.6849710000 -0.8648670000
C 4.3312480000 -0.1388690000 1.2327120000
H 4.1174200000 -0.5952500000 -0.9372470000
H 3.7304940000 0.3170610000 2.0232400000
H 5.2662500000 0.4254300000 1.1333860000
H 4.5954110000 -1.1582080000 1.5387940000
H 1.4273260000 -1.7825210000 -1.6592140000
H 0.6273580000 -3.2877140000 -0.9433430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171237 (Hartree/Particle)
Thermal correction to Energy= 0.185937
Thermal correction to Enthalpy= 0.186881
Thermal correction to Gibbs (Free) Energy= 0.128715
Sum of electronic and zero-point Energies= -710.422279
Sum of electronic and thermal Energies= -710.407580
Sum of electronic and thermal Enthalpies= -710.406636
Sum of electronic and thermal (Free) Energies= -710.464802

cTS

C -3.4308880000 -0.6691320000 -0.5300490000
C -2.1997260000 -0.3091250000 -0.1908380000
C -1.1847590000 0.5926780000 -0.0886210000
C 0.1430220000 0.0176410000 -0.1166720000
C 0.0847290000 -1.4153900000 -0.0896310000
C -1.0700030000 -1.9744640000 0.4260530000
C -1.3651830000 2.0708830000 0.1178820000
O 1.1754080000 0.7523230000 -0.2284240000
H -0.8538950000 2.6072950000 -0.6905060000
H -0.8910810000 2.3934280000 1.0517620000
H -2.4186760000 2.3569550000 0.1277190000
H 0.8412400000 -1.9876700000 -0.6154640000
B 2.6324690000 0.0740370000 -0.1137580000
F 2.5894310000 -0.6530680000 1.0590620000
F 3.4907490000 1.1276850000 -0.1026690000
F 2.7340820000 -0.7410590000 -1.2274400000
H -3.9297430000 -1.4480610000 0.0453010000
C -4.1783560000 -0.1207350000 -1.7180550000
H -3.6170750000 0.6696790000 -2.2220780000
H -5.1479290000 0.2821500000 -1.3984170000
H -4.3856220000 -0.9161620000 -2.4453910000
H -1.3589410000 -2.9838060000 0.1339950000
H -1.4808580000 -1.6607720000 1.3822410000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170446 (Hartree/Particle)
Thermal correction to Energy= 0.184102
Thermal correction to Enthalpy= 0.185046
Thermal correction to Gibbs (Free) Energy= 0.129424
Sum of electronic and zero-point Energies= -710.395866
Sum of electronic and thermal Energies= -710.382210
Sum of electronic and thermal Enthalpies= -710.381266
Sum of electronic and thermal (Free) Energies= -710.436888

cPT

C -3.4249680000 -0.5562230000 0.0000000000
C -2.0653920000 -0.5471190000 0.0000000000
C -1.1311330000 0.5395930000 0.0000000000
C 0.2120400000 0.0355130000 0.0000000000
C 0.1389160000 -1.3690230000 0.0000010000
C -1.2606670000 -1.8352390000 0.0000000000
C -1.3822030000 2.0067570000 0.0000010000
O 1.2466210000 0.8053190000 0.0000000000
H -1.9569490000 2.3122730000 -0.8833490000
H -0.4268950000 2.5356830000 0.0000020000
H -1.9569500000 2.3122720000 0.8833500000
H 1.0078220000 -2.0133110000 0.0000010000
B 2.6643500000 0.1292070000 0.0000000000
F 2.7090010000 -0.6615010000 1.1437990000
F 3.5565330000 1.1605830000 0.0000000000
F 2.7090010000 -0.6615010000 -1.1438000000
H -3.8902450000 -1.5430870000 0.0000000000
C -4.3929060000 0.5790820000 -0.0000010000
H -3.9267610000 1.5629240000 -0.0000030000
H -5.0513320000 0.5050320000 0.8768460000
H -5.0513340000 0.5050290000 -0.8768460000
H -1.4875030000 -2.4618410000 -0.8776420000
H -1.4875040000 -2.4618410000 0.8776430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172863 (Hartree/Particle)
Thermal correction to Energy= 0.186335
Thermal correction to Enthalpy= 0.187279
Thermal correction to Gibbs (Free) Energy= 0.131427
Sum of electronic and zero-point Energies= -710.439475
Sum of electronic and thermal Energies= -710.426003
Sum of electronic and thermal Enthalpies= -710.425059
Sum of electronic and thermal (Free) Energies= -710.480911

cRTccRT TS

C 3.6528450000 0.0467650000 -0.3732040000
C 2.3912050000 0.3764920000 -0.3087950000
C 1.1508360000 0.8322100000 -0.2391510000
C -0.0525690000 -0.0280310000 -0.1511280000
C -0.0999970000 -1.5006820000 -0.1899150000
C 0.9298500000 -2.3508700000 -0.2983860000
H -1.1059600000 -1.8964510000 -0.1311310000
C 0.8912080000 2.3311250000 -0.2280510000
O -1.1272510000 0.6138110000 -0.0382990000
H 1.8331590000 2.8785260000 -0.3023150000
H 0.3751490000 2.6249530000 0.6913260000
H 0.2434330000 2.6149580000 -1.0635480000
B -2.7047490000 0.0267460000 0.1484660000
F -3.4089750000 1.1785450000 0.2127150000
F -2.6343750000 -0.6949130000 1.3060770000
F -2.9050430000 -0.7291230000 -0.9734490000
C 4.5585390000 -0.1744470000 0.8166260000
H 4.0937180000 -0.0977770000 -1.3622690000
H 4.0322500000 -0.0064150000 1.7593090000
H 5.4163360000 0.5070540000 0.7691320000
H 4.9555160000 -1.1968980000 0.8145620000
H 1.9632260000 -2.0378210000 -0.3687110000
H 0.7389670000 -3.4202910000 -0.3183510000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170862 (Hartree/Particle)
Thermal correction to Energy= 0.184986
Thermal correction to Enthalpy= 0.185930
Thermal correction to Gibbs (Free) Energy= 0.128064
Sum of electronic and zero-point Energies= -710.419045
Sum of electronic and thermal Energies= -710.404921
Sum of electronic and thermal Enthalpies= -710.403977
Sum of electronic and thermal (Free) Energies= -710.461843

ccRT

C -3.5116810000 0.1255760000 0.6998830000
C -2.3219570000 0.4935020000 0.3120500000
C -1.1292470000 0.9460930000 -0.0471670000
C 0.0633430000 0.0810950000 0.0303310000
C -0.0056570000 -1.3861150000 0.1071010000
C -0.9380730000 -2.1216590000 -0.5106460000
H 0.8191140000 -1.8519040000 0.6354900000
C -0.8993450000 2.3952800000 -0.4346680000

O 1.1696190000 0.6758350000 0.0442970000
H -1.8470280000 2.9360630000 -0.4757240000
H -0.4060120000 2.4600010000 -1.4102560000
H -0.2394450000 2.8811940000 0.2910420000
B 2.6827880000 -0.0592210000 0.0515960000
F 3.5087500000 1.0114890000 0.0220800000
F 2.6654610000 -0.8307520000 -1.0747600000
F 2.6933090000 -0.7751760000 1.2227650000
C -4.5786200000 -0.4759920000 -0.1836080000
H -3.7596100000 0.2483290000 1.7563950000
H -4.8372430000 -1.4845110000 0.1616860000
H -4.2554810000 -0.5355280000 -1.2261440000
H -5.4929720000 0.1274790000 -0.1395650000
H -1.7248510000 -1.6821570000 -1.1145020000
H -0.9076220000 -3.2062680000 -0.4612080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171203 (Hartree/Particle)
Thermal correction to Energy= 0.185903
Thermal correction to Enthalpy= 0.186847
Thermal correction to Gibbs (Free) Energy= 0.128729
Sum of electronic and zero-point Energies= -710.422277
Sum of electronic and thermal Energies= -710.407577
Sum of electronic and thermal Enthalpies= -710.406633
Sum of electronic and thermal (Free) Energies= -710.464751

ccTS

C 3.1174550000 -0.6988770000 -0.3221570000
C 1.8743420000 -0.3018250000 -0.0807610000
C 0.8987570000 0.6506700000 -0.1161250000
C -0.4488190000 0.1371850000 -0.2126170000
C -0.4620640000 -1.2928980000 -0.0989410000
C 0.6150180000 -1.8691970000 0.5496640000
H -1.1981810000 -1.8634670000 -0.6549110000
C 1.1390620000 2.1297870000 -0.0028390000
O -1.4338950000 0.9070890000 -0.4485590000
H 2.2031130000 2.3676490000 0.0486100000
H 0.6302470000 2.5414680000 0.8763480000
H 0.6993890000 2.6272600000 -0.8757470000
B -2.9232800000 0.2961090000 -0.4105310000
F -3.7334830000 1.3819230000 -0.5163940000
F -2.9982970000 -0.3692900000 0.7976360000
F -2.9793120000 -0.5732670000 -1.4857010000
C 3.9194260000 -1.7165540000 0.4375490000
H 3.5980210000 -0.2682540000 -1.2044110000
H 4.2042890000 -2.5538500000 -0.2119920000
H 3.3775810000 -2.1119810000 1.3002140000
H 4.8519660000 -1.2645310000 0.7986820000
H 0.9493720000 -1.5130040000 1.5202740000
H 0.8709990000 -2.9091180000 0.3505970000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170353 (Hartree/Particle)
Thermal correction to Energy= 0.183988
Thermal correction to Enthalpy= 0.184933
Thermal correction to Gibbs (Free) Energy= 0.129390
Sum of electronic and zero-point Energies= -710.395127
Sum of electronic and thermal Energies= -710.381491
Sum of electronic and thermal Enthalpies= -710.380547
Sum of electronic and thermal (Free) Energies= -710.436089

ccPT

C 3.4105970000 0.3139260000 0.0000010000
C 2.0965900000 -0.0240970000 0.0000000000
C 0.9948790000 0.8893360000 -0.0000010000
C -0.2464070000 0.1749110000 -0.0000020000
C 0.0612200000 -1.1942020000 -0.0000020000
C 1.5253020000 -1.4285590000 -0.0000010000
C 1.0172610000 2.3703020000 -0.0000010000
O -1.3890350000 0.7754340000 -0.0000020000
H 2.0201700000 2.8011920000 0.0000010000
H 0.4590580000 2.7381110000 0.8712390000
H 0.4590610000 2.7381110000 -0.8712420000
H -0.6860790000 -1.9763570000 -0.0000040000
B -2.6792920000 -0.1179880000 0.0000010000
F -3.7259080000 0.7571690000 0.0000020000
F -2.5981230000 -0.9059130000 1.1439830000
F -2.5981280000 -0.9059150000 -1.1439810000
C 4.5635740000 -0.6322030000 0.0000020000
H 3.6665370000 1.3725390000 0.0000010000
H 4.2556980000 -1.6805020000 0.0000010000
H 5.2007700000 -0.4556430000 0.8775800000
H 5.2007710000 -0.4556430000 -0.8775760000
H 1.8470480000 -2.0099430000 0.8779960000
H 1.8470500000 -2.0099430000 -0.8779980000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172758 (Hartree/Particle)
Thermal correction to Energy= 0.186283
Thermal correction to Enthalpy= 0.187227
Thermal correction to Gibbs (Free) Energy= 0.131372
Sum of electronic and zero-point Energies= -710.444051
Sum of electronic and thermal Energies= -710.430526
Sum of electronic and thermal Enthalpies= -710.429582
Sum of electronic and thermal (Free) Energies= -710.485437

1b

cRT *syn*-H^+ (u)

C 0.7541870000 0.8944840000 -0.2768630000
C -0.5663130000 1.1685920000 0.2496470000
C -1.6769640000 0.2729260000 0.3822890000
C -1.8591050000 -0.8486850000 -0.3586020000
H -2.4525610000 0.6072020000 1.0672020000
C 1.2069220000 -0.3618460000 -0.3222950000
H -1.1241270000 -1.1082800000 -1.1167580000
C -3.0359620000 -1.7466030000 -0.2425840000
C 1.7616630000 -1.5374720000 -0.3526780000
C 1.6433250000 2.0721420000 -0.6621840000
H 1.6420330000 -2.1284610000 -1.2642300000
C 2.5606560000 -2.1632450000 0.7685040000
O -0.8355930000 2.3816400000 0.6809830000
H -0.0646240000 2.9787180000 0.6283470000
H 1.1272890000 2.7614540000 -1.3410280000
H 2.5378830000 1.7115960000 -1.1721290000
H 1.9890210000 2.6313530000 0.2190590000
H -3.7367040000 -1.4288380000 0.5327100000
H -2.7014260000 -2.7709790000 -0.0258670000
H -3.5621790000 -1.8025500000 -1.2054800000
H 2.6316000000 -1.5065630000 1.6375900000
H 3.5704960000 -2.3909170000 0.4098090000
H 2.0975840000 -3.1086090000 1.0715040000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197225 (Hartree/Particle)
Thermal correction to Energy= 0.209355
Thermal correction to Enthalpy= 0.210300
Thermal correction to Gibbs (Free) Energy= 0.159103
Sum of electronic and zero-point Energies= -425.503249
Sum of electronic and thermal Energies= -425.491118
Sum of electronic and thermal Enthalpies= -425.490174
Sum of electronic and thermal (Free) Energies= -425.541370

cTS *syn*-H^+

C 0.6454840000 -0.8396440000 -0.2038270000
C 1.5334800000 0.2046180000 0.2001150000
C 0.9526950000 1.4799890000 0.2565470000
C -0.2453430000 1.6654760000 -0.4382100000
H 1.3631020000 2.2444770000 0.9116040000
C -0.6648590000 -0.4548200000 -0.2505300000
H -0.2982400000 1.3020740000 -1.4651100000
C -1.2293570000 2.7403360000 -0.0960400000
C -1.9700410000 -0.6625070000 -0.1964330000
C 1.1472590000 -2.2009780000 -0.6210230000
H -2.6266260000 -0.0262080000 -0.7900690000
C -2.6397980000 -1.6789940000 0.6883520000
O 2.8078060000 0.0307870000 0.5278870000
H 3.0382850000 -0.9099560000 0.6258490000
H 1.9740310000 -2.1239920000 -1.3365210000
H 0.3516900000 -2.7929780000 -1.0759700000
H 1.5050820000 -2.7595580000 0.2556990000
H -1.2221920000 2.9953070000 0.9660260000
H -2.2447790000 2.4566650000 -0.3901240000
H -0.9839080000 3.6421270000 -0.6749440000
H -1.9224450000 -2.2931600000 1.2360500000
H -3.2764580000 -2.3269860000 0.0732720000

H -3.2971180000 -1.1749720000 1.4074220000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.196003 (Hartree/Particle)
Thermal correction to Energy= 0.207384
Thermal correction to Enthalpy= 0.208328
Thermal correction to Gibbs (Free) Energy= 0.159349
Sum of electronic and zero-point Energies= -425.484928
Sum of electronic and thermal Energies= -425.473548
Sum of electronic and thermal Enthalpies= -425.472603
Sum of electronic and thermal (Free) Energies= -425.521583

cPT *syn*-H^+

C 0.2747820000 -0.8514690000 0.0148390000
C 1.6015950000 -0.3238720000 -0.0682280000
C 1.5424100000 1.0347170000 -0.3091420000
C 0.1432610000 1.5065810000 -0.3909590000
H 2.4141600000 1.6721260000 -0.4163540000
C -0.6518250000 0.2241130000 -0.1723130000
H -0.0427340000 1.8770550000 -1.4146160000
C -0.1717110000 2.6694180000 0.5857260000
C -2.0190730000 0.2101210000 -0.1953130000
C -0.0155690000 -2.2958340000 0.2425370000
H -2.4872890000 1.1788850000 -0.3736130000
C -2.9906300000 -0.8971980000 -0.0167890000
O 2.7630240000 -0.9776240000 0.0481190000
H 2.6412230000 -1.9225080000 0.2354900000
H 0.8932520000 -2.8981300000 0.3297770000
H -0.6039640000 -2.7131560000 -0.5828460000
H -0.5932540000 -2.4403280000 1.1632300000
H -0.0298990000 2.3588470000 1.6245580000
H -1.2021340000 3.0111550000 0.4582570000
H 0.4871370000 3.5175600000 0.3803400000
H -2.5564310000 -1.8738050000 0.1840470000
H -3.6224820000 -0.9665830000 -0.9146720000
H -3.6812130000 -0.6395910000 0.7992990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198811 (Hartree/Particle)
Thermal correction to Energy= 0.209980
Thermal correction to Enthalpy= 0.210925
Thermal correction to Gibbs (Free) Energy= 0.162051
Sum of electronic and zero-point Energies= -425.527732
Sum of electronic and thermal Energies= -425.516563
Sum of electronic and thermal Enthalpies= -425.515618
Sum of electronic and thermal (Free) Energies= -425.564492

ccRT *syn*-H^+ (u)

C -1.5361370000 1.7087610000 -0.6384030000
C -1.2130460000 0.5015240000 -0.2799650000
C -1.0016100000 -0.7753160000 0.0523220000
C 0.3129310000 -1.3570780000 -0.1178630000
C 1.5766650000 -0.6898030000 -0.2263960000
C 1.8422660000 0.5509740000 0.2525650000
H 2.3765930000 -1.2962210000 -0.6444330000
H 1.0573640000 1.1002150000 0.7674580000
C 3.1680080000 1.2146640000 0.1668490000
C -2.1467650000 -1.6795990000 0.4951000000
H -1.8476200000 1.8467800000 -1.6773700000
C -1.5168500000 2.9386070000 0.2391410000
O 0.4198350000 -2.6655460000 -0.1969060000
H -3.0314500000 -1.0799120000 0.7140040000
H -1.8908070000 -2.2401780000 1.4020680000
H -2.4369620000 -2.3889520000 -0.2932100000
H -1.2079920000 2.7123170000 1.2621040000
H -2.5189280000 3.3804590000 0.2662890000
H -0.8409490000 3.6893030000 -0.1854840000
H 3.9122270000 0.6078770000 -0.3537660000
H 3.5354620000 1.4526530000 1.1745360000
H 3.0678180000 2.1794520000 -0.3501570000
H -0.4462140000 -3.1158360000 -0.1668810000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197189 (Hartree/Particle)
Thermal correction to Energy= 0.209314
Thermal correction to Enthalpy= 0.210258
Thermal correction to Gibbs (Free) Energy= 0.159114
Sum of electronic and zero-point Energies= -425.503172
Sum of electronic and thermal Energies= -425.491047
Sum of electronic and thermal Enthalpies= -425.490103
Sum of electronic and thermal (Free) Energies= -425.541247

cTS *syn*-H^+

C -1.5106110000 -1.4061290000 -0.4744240000
C -0.3924530000 -0.7751760000 -0.1421820000
C 0.9672420000 -0.7593920000 0.0038590000
C 1.5387890000 0.5484570000 -0.0516310000
C 0.6067880000 1.5937330000 -0.0475200000
C -0.6890350000 1.2983050000 0.3889310000
H 0.8565510000 2.5555720000 -0.4885290000
H -0.7991370000 0.7695550000 1.3365430000
C -1.8729010000 2.1131890000 -0.0354240000
C 1.8047860000 -1.9837440000 0.2814200000
H -1.4315250000 -2.0788530000 -1.3340790000
C -2.8718920000 -1.2847350000 0.1376650000
O 2.8385020000 0.8046060000 -0.1347230000
H 1.1794130000 -2.8588770000 0.4623990000
H 2.4570840000 -1.8390120000 1.1504910000
H 2.4390160000 -2.2128480000 -0.5871590000
H -2.8859870000 -0.6537220000 1.0282510000
H -3.2199180000 -2.2859460000 0.4207130000
H -3.5936030000 -0.9027340000 -0.5953760000
H -1.7446270000 2.5476070000 -1.0293910000
H -2.0179230000 2.9291710000 0.6870860000
H -2.7926870000 1.5226330000 -0.0211250000
H 3.3610510000 0.0035640000 -0.3162010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.195912 (Hartree/Particle)
Thermal correction to Energy= 0.207247
Thermal correction to Enthalpy= 0.208191
Thermal correction to Gibbs (Free) Energy= 0.159390
Sum of electronic and zero-point Energies= -425.483280
Sum of electronic and thermal Energies= -425.471946
Sum of electronic and thermal Enthalpies= -425.471002
Sum of electronic and thermal (Free) Energies= -425.519803

cPT *syn*-H^+

C 1.6532430000 -1.1697710000 -0.0417400000
C 0.5761110000 -0.3306330000 -0.0788670000
C -0.7782540000 -0.7627770000 0.0646470000
C -1.6406590000 0.3577930000 -0.1420950000
C -0.8764980000 1.4764290000 -0.3938930000
C 0.5769980000 1.1689700000 -0.3373340000
H -1.2827440000 2.4660000000 -0.5765660000
H 1.0390050000 1.3896580000 -1.3127410000
C 1.2958390000 2.0266790000 0.7417950000
C -1.2931840000 -2.1283640000 0.3501600000
H 1.4662430000 -2.2208130000 0.1740470000
C 3.0738690000 -0.8216630000 -0.2848740000
O -2.9797270000 0.3749930000 -0.1108710000
H -0.5069570000 -2.8633250000 0.5248440000
H -1.9096690000 -2.4856900000 -0.4874030000
H -1.9393350000 -2.1110140000 1.2393910000
H 3.2361280000 0.2183730000 -0.5690360000
H 3.4779190000 -1.4723020000 -1.0733930000
H 3.6692970000 -1.0497680000 0.6118520000
H 0.8826710000 1.8276590000 1.7346000000
H 1.1681980000 3.0894260000 0.5180400000
H 2.3666460000 1.8131230000 0.7610620000
H -3.3543770000 -0.5012460000 0.0754680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198847 (Hartree/Particle)
Thermal correction to Energy= 0.209989
Thermal correction to Enthalpy= 0.210933
Thermal correction to Gibbs (Free) Energy= 0.162748
Sum of electronic and zero-point Energies= -425.532224
Sum of electronic and thermal Energies= -425.521082
Sum of electronic and thermal Enthalpies= -425.520138
Sum of electronic and thermal (Free) Energies= -425.568323

P *syn*-H^+ (s-a)

C -3.0422290000 0.0485350000 0.4019230000
C -1.7616520000 0.2744340000 0.3011710000

C -0.4534570000 0.5265720000 0.2030890000
C 0.4105730000 -0.6496710000 0.1388850000
C 1.8335690000 -0.7329230000 0.0039790000
C 2.7265360000 0.2815030000 -0.1465610000
H 2.2035500000 -1.7553580000 0.0175960000
H 2.3937710000 1.3129370000 -0.1738240000
C 4.1885340000 0.0692830000 -0.2882630000
C 0.0524480000 1.9575630000 0.1744130000
H -3.4544380000 -0.0378350000 1.4114390000
C -4.0159170000 -0.0749540000 -0.7477910000
H -0.7901580000 2.6404750000 0.2951910000
H 0.5363760000 2.1952510000 -0.7789630000
H 0.7570530000 2.1510500000 0.9898970000
H -3.5211740000 0.0072030000 -1.7173400000
H -4.7690070000 0.7166460000 -0.6640450000
H -4.5421900000 -1.0337780000 -0.6893690000
H 4.4712740000 -0.9850950000 -0.2542290000
H 4.7216200000 0.6135750000 0.5042480000
H 4.5380850000 0.5080510000 -1.2336840000
O -0.1332720000 -1.8446070000 0.2165610000
H -1.1090220000 -1.7783220000 0.3155370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197717 (Hartree/Particle)
Thermal correction to Energy= 0.209699
Thermal correction to Enthalpy= 0.210643
Thermal correction to Gibbs (Free) Energy= 0.159208
Sum of electronic and zero-point Energies= -425.504219
Sum of electronic and thermal Energies= -425.492238
Sum of electronic and thermal Enthalpies= -425.491293
Sum of electronic and thermal (Free) Energies= -425.542728

P *syn*-H^+ (s-v)

C -2.3410560000 -1.2078150000 0.5264160000
C -1.5971630000 -0.1635910000 0.3168360000
C -0.8842030000 0.9479550000 0.1066760000
C 0.5525060000 0.8425700000 -0.0174310000
C 1.2843740000 -0.3826990000 0.0737730000
C 2.6363770000 -0.4386230000 -0.0470430000
H 0.7052540000 -1.2823620000 0.2486750000
H 3.1826820000 0.4871900000 -0.2215690000
C 3.4410230000 -1.6813040000 0.0419740000
C -1.5408090000 2.3163180000 -0.0009850000
H -2.5271280000 -1.4834860000 1.5680820000
C -2.9757480000 -2.0742000000 -0.5381630000
H -2.6213920000 2.2248330000 0.1173060000
H -1.3626010000 2.7768550000 -0.9821350000
H -1.1882350000 2.9986980000 0.7841790000
H -2.7321430000 -1.7316230000 -1.5455790000
H -4.0638560000 -2.0633170000 -0.4114360000
H -2.6409010000 -3.1103720000 -0.4196210000
H 2.8333250000 -2.5720300000 0.2173620000
H 4.1841090000 -1.5863660000 0.8463250000
H 4.0220140000 -1.8155090000 -0.8813720000
O 1.2573450000 1.9341990000 -0.2268920000
H 0.6983070000 2.7322300000 -0.2774000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197276 (Hartree/Particle)
Thermal correction to Energy= 0.209418
Thermal correction to Enthalpy= 0.210363
Thermal correction to Gibbs (Free) Energy= 0.159098
Sum of electronic and zero-point Energies= -425.510393
Sum of electronic and thermal Energies= -425.498250
Sum of electronic and thermal Enthalpies= -425.497306
Sum of electronic and thermal (Free) Energies= -425.548571

P *syn*-H^+ (w)

C -3.0482990000 -0.2883220000 0.4428330000
C -1.8598970000 0.2253720000 0.2871770000
C -0.6463580000 0.7607660000 0.1316700000
C 0.4750130000 -0.1652920000 0.1228750000
C 1.8253000000 0.2629150000 -0.0498280000
C 2.8752110000 -0.6048740000 -0.0507010000
H 1.9962230000 1.3246500000 -0.1830800000
H 2.6710970000 -1.6658530000 0.0870330000
C 4.2927840000 -0.2140790000 -0.2260860000
C -0.4284090000 2.2555250000 -0.0256610000
H -3.4171040000 -0.3893270000 1.4676170000
C -3.9790170000 -0.7261410000 -0.6651590000
H -1.3865680000 2.7757430000 0.0163000000
H 0.0408740000 2.4895270000 -0.9872670000
H 0.2055780000 2.6505890000 0.7752620000
H -3.5286780000 -0.6067810000 -1.6523630000
H -4.8960310000 -0.1281090000 -0.6181280000
H -4.2646090000 -1.7737030000 -0.5209340000
H 4.4284790000 0.8615070000 -0.3591740000
H 4.7188990000 -0.7444740000 -1.0898790000
H 4.8795490000 -0.5506000000 0.6407980000
O 0.2746470000 -1.4547950000 0.2782780000
H -0.6828530000 -1.6400270000 0.3948740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197441 (Hartree/Particle)
Thermal correction to Energy= 0.209526
Thermal correction to Enthalpy= 0.210470
Thermal correction to Gibbs (Free) Energy= 0.159308
Sum of electronic and zero-point Energies= -425.511242
Sum of electronic and thermal Energies= -425.499157
Sum of electronic and thermal Enthalpies= -425.498213
Sum of electronic and thermal (Free) Energies= -425.549375

cRT *anti*-H^+ (u)

C 0.7402910000 0.9251560000 -0.2698050000
C -0.5855840000 1.1614830000 0.2405220000
C -1.6593590000 0.2172500000 0.3904930000
C -1.8263630000 -0.8888790000 -0.3751890000
H -2.4221690000 0.4725550000 1.1266390000
C 1.2112800000 -0.3275930000 -0.3183630000
H -1.1120440000 -1.0887700000 -1.1702130000
C -2.9555560000 -1.8443620000 -0.2415000000
C 1.7970510000 -1.4875230000 -0.3529280000
C 1.6061860000 2.1224560000 -0.6328790000
H 1.6959650000 -2.0786110000 -1.2666660000
C 2.6126380000 -2.0938750000 0.7678170000
O -0.7898420000 2.4086860000 0.6108500000
H 1.8218910000 2.7264340000 0.2544640000
H 1.0979410000 2.7657140000 -1.3581250000
H 2.5497960000 1.7834330000 -1.0624330000
H -3.6384830000 -1.5856720000 0.5710650000
H -2.5638970000 -2.8568100000 -0.0697320000
H -3.5175540000 -1.8979750000 -1.1838280000
H 2.6651960000 -1.4363410000 1.6375520000
H 3.6286740000 -2.2912580000 0.4087880000
H 2.1767800000 -3.0526010000 1.0692320000
H -1.7068650000 2.5657370000 0.9074440000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197208 (Hartree/Particle)
Thermal correction to Energy= 0.209388
Thermal correction to Enthalpy= 0.210333
Thermal correction to Gibbs (Free) Energy= 0.159016
Sum of electronic and zero-point Energies= -425.503495
Sum of electronic and thermal Energies= -425.491314
Sum of electronic and thermal Enthalpies= -425.490370
Sum of electronic and thermal (Free) Energies= -425.541687

cTS *anti*-H^+

C 0.6204080000 -0.8674600000 -0.2092630000
C 1.5344800000 0.1554740000 0.1958830000
C 0.9919440000 1.4462690000 0.2554670000
C -0.1981280000 1.6704220000 -0.4456400000
H 1.3991920000 2.2012280000 0.9256950000
C -0.6785620000 -0.4532480000 -0.2593310000
H -0.2571500000 1.3149740000 -1.4740360000
C -1.1538660000 2.7683630000 -0.0980620000
C -1.9897970000 -0.6176780000 -0.2061990000
C 1.0952210000 -2.2396160000 -0.6088160000
H -2.6237140000 0.0235160000 -0.8192640000
C -2.6937230000 -1.5913500000 0.6996590000
O 2.7696970000 -0.2073910000 0.5235870000
H 1.6143660000 -2.7015800000 0.2396830000
H 1.8154230000 -2.1827230000 -1.4323160000
H 0.2635550000 -2.8805410000 -0.9037990000
H -1.1408550000 3.0186880000 0.9651420000
H -2.1760300000 2.5104030000 -0.3924610000

H -0.8881770000 3.6663920000 -0.6741100000
H -1.9969720000 -2.2143290000 1.2635780000
H -3.3481390000 -2.2331030000 0.0967650000
H -3.3377570000 -1.0505340000 1.4039980000
H 3.3508130000 0.5596830000 0.6702300000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.196116 (Hartree/Particle)
Thermal correction to Energy= 0.207484
Thermal correction to Enthalpy= 0.208429
Thermal correction to Gibbs (Free) Energy= 0.159421
Sum of electronic and zero-point Energies= -425.486643
Sum of electronic and thermal Energies= -425.475274
Sum of electronic and thermal Enthalpies= -425.474330
Sum of electronic and thermal (Free) Energies= -425.523337

cPT *anti*-H^+

C 0.2636780000 -0.8461480000 0.0174270000
C 1.5931440000 -0.3187210000 -0.0735520000
C 1.5421060000 1.0348770000 -0.3160550000
C 0.1374320000 1.5125670000 -0.3929690000
H 2.4019820000 1.6886300000 -0.4305020000
C -0.6578400000 0.2288470000 -0.1733370000
H -0.0535270000 1.8876110000 -1.4131860000
C -0.1738280000 2.6653070000 0.5942360000
C -2.0259120000 0.2075080000 -0.1977150000
C 0.0149090000 -2.2916220000 0.2601850000
H -2.5030730000 1.1726190000 -0.3732000000
C -2.9823350000 -0.9122560000 -0.0255320000
O 2.6437910000 -1.1376810000 0.0718050000
H -0.5858090000 -2.4385530000 1.1662040000
H 0.9555780000 -2.8324480000 0.3726710000
H -0.5453760000 -2.7354320000 -0.5725580000
H -0.0255880000 2.3468700000 1.6300050000
H -1.2057780000 3.0067440000 0.4767100000
H 0.4808060000 3.5179800000 0.3929460000
H -2.5326340000 -1.8857980000 0.1543420000
H -3.6241620000 -0.9734690000 -0.9169340000
H -3.6666980000 -0.6743280000 0.8021490000
H 3.4858270000 -0.6611420000 -0.0192230000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199213 (Hartree/Particle)
Thermal correction to Energy= 0.210213
Thermal correction to Enthalpy= 0.211157
Thermal correction to Gibbs (Free) Energy= 0.163041
Sum of electronic and zero-point Energies= -425.531827
Sum of electronic and thermal Energies= -425.520828
Sum of electronic and thermal Enthalpies= -425.519884
Sum of electronic and thermal (Free) Energies= -425.568000

ccRT *anti*-H^+ (u)

C -0.3519780000 -1.2313230000 0.0427760000
C 1.0453990000 -0.9193450000 -0.1115970000
C 1.6569250000 0.3754740000 -0.2429560000
C 1.1515900000 1.5251540000 0.2668950000
H 2.6342360000 0.3954510000 -0.7261030000
C -1.2689550000 -0.3114250000 -0.2835180000
C 1.8043770000 2.8548150000 0.1551880000
H 0.2219330000 1.4855900000 0.8297820000
C -2.2448060000 0.4720520000 -0.6343810000
C -0.7429730000 -2.6413300000 0.4592720000
C -2.9604950000 1.4647290000 0.2525700000
H -2.5777980000 0.4071240000 -1.6739460000
O 1.8190400000 -1.9845230000 -0.1434730000
H -0.4419510000 -3.3663600000 -0.3039300000
H -1.8236700000 -2.7043450000 0.5931790000
H -0.2526690000 -2.9216490000 1.3968680000
H -2.5770510000 1.4566160000 1.2753620000
H -4.0284300000 1.2219930000 0.2790260000
H -2.8654640000 2.4745120000 -0.1620610000
H 2.0042620000 3.2623200000 1.1554860000
H 1.1165860000 3.5648870000 -0.3250010000
H 2.7362200000 2.8247290000 -0.4143180000
H 2.7669690000 -1.7574810000 -0.2020610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197168 (Hartree/Particle)
Thermal correction to Energy= 0.209347
Thermal correction to Enthalpy= 0.210291
Thermal correction to Gibbs (Free) Energy= 0.159009
Sum of electronic and zero-point Energies= -425.503366
Sum of electronic and thermal Energies= -425.491187
Sum of electronic and thermal Enthalpies= -425.490243
Sum of electronic and thermal (Free) Energies= -425.541526

ccTS *anti*-H^+

C 0.9552990000 -0.7819320000 0.0032030000
C 1.5431700000 0.5203200000 -0.0494780000
C 0.6300930000 1.5809680000 -0.0493830000
C -0.6713410000 1.3096560000 0.3920750000
H 0.8747890000 2.5373050000 -0.5082810000
C -0.4022530000 -0.7832140000 -0.1442790000
C -1.8434790000 2.1371130000 -0.0381450000
H -0.7894640000 0.7865070000 1.3407440000
C -1.5336810000 -1.3870690000 -0.4804390000
C 1.7836910000 -2.0101040000 0.2705040000
C -2.8858630000 -1.2552510000 0.1493280000
H -1.4745960000 -2.0421420000 -1.3552750000
O 2.8649210000 0.6035420000 -0.1556590000
H 2.5715770000 -2.0833990000 -0.4887200000
H 1.1775270000 -2.9160790000 0.2405480000
H 2.2832030000 -1.9447050000 1.2436510000
H -2.8805070000 -0.6368850000 1.0489750000
H -3.2439360000 -2.2557570000 0.4224870000
H -3.6112780000 -0.8535680000 -0.5694090000
H -1.9896610000 2.9510330000 0.6865880000
H -2.7677810000 1.5530660000 -0.0327170000
H -1.7055130000 2.5733390000 -1.0300980000
H 3.1824460000 1.5200240000 -0.0735360000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.196012 (Hartree/Particle)
Thermal correction to Energy= 0.207338
Thermal correction to Enthalpy= 0.208282
Thermal correction to Gibbs (Free) Energy= 0.159455
Sum of electronic and zero-point Energies= -425.484989
Sum of electronic and thermal Energies= -425.473664
Sum of electronic and thermal Enthalpies= -425.472720
Sum of electronic and thermal (Free) Energies= -425.521546

ccPT *anti*-H^+

C -0.7669250000 -0.7713950000 0.0662440000
C -1.6393110000 0.3462380000 -0.1411260000
C -0.8907300000 1.4697140000 -0.3940480000
C 0.5715650000 1.1742350000 -0.3386780000
H -1.2861240000 2.4642360000 -0.5792790000
C 0.5806610000 -0.3261480000 -0.0782260000
C 1.2855590000 2.0338660000 0.7389030000
H 1.0300330000 1.3949150000 -1.3153110000
C 1.6612970000 -1.1617810000 -0.0412740000
C -1.2884700000 -2.1267210000 0.3515820000
C 3.0800800000 -0.8105310000 -0.2855150000
H 1.4746010000 -2.2126610000 0.1756290000
O -2.9658030000 0.1653070000 -0.0705520000
H -1.9442910000 -2.0854000000 1.2318570000
H -0.5125080000 -2.8743930000 0.5169300000
H -1.9342200000 -2.4525270000 -0.4757770000
H 3.2400750000 0.2295320000 -0.5708550000
H 3.4854920000 -1.4626220000 -1.0722140000
H 3.6756080000 -1.0367270000 0.6117770000
H 1.1533570000 3.0967060000 0.5169920000
H 2.3579830000 1.8275580000 0.7586640000
H 0.8746450000 1.8321970000 1.7323250000
H -3.4505770000 0.9918640000 -0.2334850000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199162 (Hartree/Particle)
Thermal correction to Energy= 0.210146
Thermal correction to Enthalpy= 0.211090
Thermal correction to Gibbs (Free) Energy= 0.163281
Sum of electronic and zero-point Energies= -425.536314
Sum of electronic and thermal Energies= -425.525331
Sum of electronic and thermal Enthalpies= -425.524387
Sum of electronic and thermal (Free) Energies= -425.572195

cRT *anti*-H^+ (s-a)

C 3.0105260000 -0.1378610000 0.5626000000
C 1.7506400000 -0.3005170000 0.3039660000
C 0.4502880000 -0.5137350000 0.0480500000
C -0.3943270000 0.6550650000 -0.0130480000
C -1.8255840000 0.7177520000 -0.1452820000
C -2.7194610000 -0.2760310000 0.0922820000
H -2.2215720000 1.6974810000 -0.4156440000
H -2.3721870000 -1.2560640000 0.4022040000
C -4.1913750000 -0.1094740000 -0.0112290000
C -0.0556610000 -1.9281130000 -0.1890060000
H 3.3122740000 -0.1838570000 1.6124790000
C 4.0987330000 0.1170850000 -0.4568870000
H 0.7925590000 -2.5811680000 -0.4018810000
H -0.7399450000 -1.9753610000 -1.0418890000
H -0.5624830000 -2.3350820000 0.6933950000
H 3.7067950000 0.1468290000 -1.4751720000
H 4.8553690000 -0.6718490000 -0.3877660000
H 4.5904720000 1.0702840000 -0.2348300000
H -4.4867160000 0.8931290000 -0.3291690000
H -4.6611780000 -0.3340580000 0.9566000000
H -4.5992060000 -0.8469040000 -0.7166700000
O 0.2503100000 1.8078220000 0.0203580000
H -0.3593420000 2.5690210000 0.0268090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197435 (Hartree/Particle)
Thermal correction to Energy= 0.209531
Thermal correction to Enthalpy= 0.210476
Thermal correction to Gibbs (Free) Energy= 0.159002
Sum of electronic and zero-point Energies= -425.500000
Sum of electronic and thermal Energies= -425.487903
Sum of electronic and thermal Enthalpies= -425.486959
Sum of electronic and thermal (Free) Energies= -425.538433

ccRT *anti*-H^+ (s-a)

C -3.0634450000 -0.0310970000 -0.3128720000
C -1.7821420000 -0.2278340000 -0.3042450000
C -0.4627420000 -0.4749440000 -0.2983470000
C 0.4076550000 0.6736490000 -0.2159890000
C 1.8408460000 0.7038180000 -0.0930630000
C 2.6598720000 -0.3084220000 0.2913680000
H 2.2990120000 1.6746350000 -0.2865250000
H 2.2456470000 -1.2818480000 0.5314760000
C 4.1305190000 -0.1712200000 0.4445990000
C 0.0419790000 -1.9045820000 -0.4150000000
H -3.5298900000 0.1415000000 -1.2867000000
C -3.9693680000 -0.0113070000 0.8982760000
H -0.7734150000 -2.5452690000 -0.7554100000
H 0.3824780000 -2.2993840000 0.5489960000
H 0.8591730000 -1.9870160000 -1.1385370000
H -3.4194850000 -0.1906720000 1.8240160000
H -4.7426490000 -0.7791270000 0.7877420000
H -4.4719060000 0.9597480000 0.9628450000
H 4.4957940000 0.8260580000 0.1885970000
H 4.6396050000 -0.9147140000 -0.1845750000
H 4.4218010000 -0.4080410000 1.4775060000
O -0.2048180000 1.8409210000 -0.3043340000
H 0.4133350000 2.5883910000 -0.2031190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197432 (Hartree/Particle)
Thermal correction to Energy= 0.209528
Thermal correction to Enthalpy= 0.210472
Thermal correction to Gibbs (Free) Energy= 0.158927
Sum of electronic and zero-point Energies= -425.499956
Sum of electronic and thermal Energies= -425.487860
Sum of electronic and thermal Enthalpies= -425.486916
Sum of electronic and thermal (Free) Energies= -425.538461

P *anti*-H^+ (s-v)

C -2.3166090000 -1.2200340000 0.5246750000
C -1.5783580000 -0.1720360000 0.3162710000
C -0.8918670000 0.9603370000 0.1067900000
C 0.5390480000 0.8814220000 -0.0178390000
C 1.2864690000 -0.3457840000 0.0755870000
C 2.6308070000 -0.4467170000 -0.0505770000
H 0.6977940000 -1.2375170000 0.2606100000
H 3.2417210000 0.4398320000 -0.2402970000
C 3.3994640000 -1.7151780000 0.0476580000
C -1.5721660000 2.3136390000 0.0011230000
H -2.5020100000 -1.4976810000 1.5660920000
C -2.9476030000 -2.0884870000 -0.5412920000
H -2.6506120000 2.2017850000 0.1199090000
H -1.3708150000 2.7743450000 -0.9714860000
H -1.2017620000 2.9950110000 0.7739720000
H -2.7063110000 -1.7424830000 -1.5480840000
H -4.0356350000 -2.0808300000 -0.4139250000
H -2.6092420000 -3.1237380000 -0.4249590000
H 2.7584640000 -2.5792230000 0.2364830000
H 4.1469040000 -1.6394930000 0.8493780000
H 3.9669530000 -1.8828640000 -0.8780380000
O 1.1110460000 2.0472740000 -0.2251790000
H 2.0810780000 1.9916910000 -0.3026010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197014 (Hartree/Particle)
Thermal correction to Energy= 0.209362
Thermal correction to Enthalpy= 0.210306
Thermal correction to Gibbs (Free) Energy= 0.158028
Sum of electronic and zero-point Energies= -425.507218
Sum of electronic and thermal Energies= -425.494870
Sum of electronic and thermal Enthalpies= -425.493926
Sum of electronic and thermal (Free) Energies= -425.546204

cRT *anti*-H^+ (w)

C -3.0913580000 -0.2155380000 0.4393400000
C -1.8827410000 0.2257910000 0.2837870000
C -0.6434030000 0.7198590000 0.1308570000
C 0.4542480000 -0.2068830000 0.1739320000
C 1.8236290000 0.2325640000 0.0946540000
C 2.8813590000 -0.5827140000 -0.1426380000
H 1.9919620000 1.2987820000 0.1954150000
H 2.7261660000 -1.6514300000 -0.3106700000
C 4.2940550000 -0.1343780000 -0.2380630000
C -0.4025680000 2.2068850000 -0.0830130000
H -3.4794080000 -0.2488830000 1.4611140000
C -4.0112250000 -0.6927550000 -0.6630950000
H -1.3595290000 2.7275140000 -0.1432930000
H 0.1433340000 2.3957520000 -1.0132290000
H 0.1623740000 2.6465750000 0.7467360000
H -3.5417630000 -0.6240190000 -1.6460710000
H -4.9255220000 -0.0896810000 -0.6605950000
H -4.2976440000 -1.7329750000 -0.4746080000
H 4.4065440000 0.9392650000 -0.0720910000
H 4.7042680000 -0.3933250000 -1.2239280000
H 4.9078350000 -0.6784740000 0.4934380000
O 0.1385680000 -1.4822010000 0.2829240000
H 0.9208550000 -2.0484830000 0.4098200000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197051 (Hartree/Particle)
Thermal correction to Energy= 0.209349
Thermal correction to Enthalpy= 0.210293
Thermal correction to Gibbs (Free) Energy= 0.158359
Sum of electronic and zero-point Energies= -425.503475
Sum of electronic and thermal Energies= -425.491177
Sum of electronic and thermal Enthalpies= -425.490232
Sum of electronic and thermal (Free) Energies= -425.542167

ccRT *anti*-H^+ (w)

C 3.0807690000 -0.2592850000 -0.4590610000
C 1.8771530000 0.1941040000 -0.2995180000
C 0.6437900000 0.6993980000 -0.1354730000
C -0.4530270000 -0.2268270000 -0.0660900000
C -1.8049530000 0.2123360000 0.1665680000
C -2.9074030000 -0.5544850000 -0.0240430000
H -1.9276470000 1.2440030000 0.4762180000
H -2.8094960000 -1.5771220000 -0.3970500000
C -4.3044700000 -0.1030830000 0.2001860000
C 0.4072190000 2.1993340000 -0.0389890000
H 3.4259110000 -0.3945850000 -1.4878450000
C 4.0486430000 -0.6220950000 0.6457300000
H 1.3526730000 2.7278710000 -0.1702500000
H 0.0020560000 2.4814380000 0.9393680000

H -0.2834730000 2.5472840000 -0.8141670000
H 3.6204470000 -0.4558720000 1.6358990000
H 4.9583830000 -0.0206280000 0.5443510000
H 4.3335170000 -1.6753590000 0.5504420000
H -4.3607080000 0.9246790000 0.5654990000
H -4.8004520000 -0.7692700000 0.9199260000
H -4.8803420000 -0.1880430000 -0.7317180000
O -0.1547370000 -1.4996550000 -0.2354470000
H -0.9192880000 -2.0835420000 -0.0829590000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197053 (Hartree/Particle)
Thermal correction to Energy= 0.209352
Thermal correction to Enthalpy= 0.210296
Thermal correction to Gibbs (Free) Energy= 0.158354
Sum of electronic and zero-point Energies= -425.503460
Sum of electronic and thermal Energies= -425.491162
Sum of electronic and thermal Enthalpies= -425.490217
Sum of electronic and thermal (Free) Energies= -425.542159

1b

cRT *syn*-BF_3 (u)

C 2.4556770000 -1.9513920000 -0.0318730000
C 1.4487500000 -1.2275320000 0.3778460000
C 0.3685270000 -0.5709440000 0.7679710000
C 0.0292900000 0.6891480000 0.0608840000
C 1.0561760000 1.6673840000 -0.3057860000
C 2.2774410000 1.7582600000 0.2507990000
H 0.7217610000 2.4070730000 -1.0298730000
H 2.5590890000 1.0463820000 1.0234950000
C 3.2918890000 2.7979830000 -0.0991420000
C -0.5453120000 -1.1067910000 1.8604150000
H 3.4300930000 -1.8036390000 0.4382950000
C 2.3776780000 -2.9927620000 -1.1244210000
O -1.1445760000 1.0123230000 -0.2445630000
H 0.0287050000 -1.7525860000 2.5295550000
H -1.3653160000 -1.6789520000 1.4237560000
H -0.9860920000 -0.2896830000 2.4368700000
H 1.3658990000 -3.0703820000 -1.5293490000
H 2.6761300000 -3.9744770000 -0.7367320000
H 3.0641320000 -2.7428840000 -1.9426800000
H 2.9334460000 3.4796660000 -0.8754830000
H 4.2183910000 2.3239220000 -0.4504600000
H 3.5628540000 3.3861320000 0.7876630000
F -3.2461210000 0.8199730000 -1.2790560000
F -3.0951810000 0.2459800000 0.9418380000
F -2.1844730000 -1.1237360000 -0.6715190000
B -2.5762410000 0.1421550000 -0.3160140000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199288 (Hartree/Particle)
Thermal correction to Energy= 0.215654
Thermal correction to Enthalpy= 0.216598
Thermal correction to Gibbs (Free) Energy= 0.154519
Sum of electronic and zero-point Energies= -749.711666
Sum of electronic and thermal Energies= -749.695301
Sum of electronic and thermal Enthalpies= -749.694357
Sum of electronic and thermal (Free) Energies= -749.756436

cTS *syn*-BF_3

C -2.8176250000 1.1898930000 -0.0414800000
C -1.7159970000 0.5277030000 0.2854250000
C -0.3715310000 0.4966220000 0.5328880000
C 0.2369980000 -0.7848960000 0.2051760000
C -0.7703300000 -1.7671830000 -0.0350870000
C -2.0588140000 -1.5241000000 0.4344930000
H -0.5485120000 -2.5978920000 -0.7003610000
H -2.1932200000 -1.2268180000 1.4731620000
C -3.2668450000 -2.1876300000 -0.1714970000
C 0.3462290000 1.6387150000 1.2012400000
H -3.7825730000 0.8182480000 0.3030480000
C -2.8426980000 2.4008180000 -0.9379740000
O 1.4755280000 -1.0660170000 0.0948960000
H -0.3553880000 2.2438770000 1.7812440000
H 0.8154130000 2.2646040000 0.4355870000
H 1.1560730000 1.2749410000 1.8357930000
H -1.8360060000 2.7142430000 -1.2238250000
H -3.3417500000 3.2347950000 -0.4278520000
H -3.4149550000 2.1947830000 -1.8516870000
H -3.1124850000 -2.4418360000 -1.2235370000
H -4.1488290000 -1.5427570000 -0.0966630000
H -3.5017280000 -3.1075950000 0.3798570000
F 3.5528690000 -0.8120620000 -0.9361700000
F 3.1298890000 0.4240690000 0.9553910000
F 2.0664880000 0.9439970000 -1.0227490000
B 2.6560370000 -0.0488270000 -0.2502540000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198539 (Hartree/Particle)
Thermal correction to Energy= 0.213742
Thermal correction to Enthalpy= 0.214686
Thermal correction to Gibbs (Free) Energy= 0.155723
Sum of electronic and zero-point Energies= -749.684281
Sum of electronic and thermal Energies= -749.669079
Sum of electronic and thermal Enthalpies= -749.668135
Sum of electronic and thermal (Free) Energies= -749.727098

cPT *syn*-BF_3

C 2.9398050000 0.8766940000 0.0499180000
C 1.8628510000 0.0896040000 -0.2111010000
C 0.4788320000 0.4489840000 -0.3493610000
C -0.3197450000 -0.7550340000 -0.4675410000
C 0.5718850000 -1.8234990000 -0.5520030000
C 1.9905390000 -1.4191720000 -0.4147280000
H 0.2464780000 -2.8497490000 -0.6918160000
H 2.5234560000 -1.5910070000 -1.3665370000
C 2.7406370000 -2.1958920000 0.6887630000
C -0.0806340000 1.8169100000 -0.4735110000
H 3.9049340000 0.3692510000 0.0594430000
C 3.0060800000 2.3353840000 0.3672430000
O -1.6024950000 -0.8695490000 -0.5659520000
H 0.6108090000 2.4938380000 -0.9807970000
H -0.3024680000 2.2124890000 0.5275830000
H -1.0456010000 1.7863780000 -0.9847770000
H 2.0564630000 2.7540670000 0.6996660000
H 3.3401090000 2.9027710000 -0.5148740000
H 3.7581410000 2.5098910000 1.1454230000
H 2.2814430000 -2.0234360000 1.6668990000
H 3.7918620000 -1.8956720000 0.7388890000
H 2.7131540000 -3.2700670000 0.4791270000
F -3.6324200000 -0.7992190000 0.5822060000
F -3.0287590000 1.0351690000 -0.6636230000
F -1.9075790000 0.5587090000 1.2921480000
B -2.6163010000 0.0323670000 0.2053460000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201682 (Hartree/Particle)
Thermal correction to Energy= 0.216273
Thermal correction to Enthalpy= 0.217218
Thermal correction to Gibbs (Free) Energy= 0.159981
Sum of electronic and zero-point Energies= -749.721397
Sum of electronic and thermal Energies= -749.706806
Sum of electronic and thermal Enthalpies= -749.705862
Sum of electronic and thermal (Free) Energies= -749.763098

ccRT *syn*-BF_3 (u)

C -0.3060690000 -0.7951340000 0.4227280000
C 0.1102950000 0.5827000000 0.0631880000
C -0.8660520000 1.6569640000 -0.1397940000
C -2.1196440000 1.6743720000 0.3470150000
H -0.4619600000 2.5256430000 -0.6550000000
C -1.3784630000 -1.2929800000 -0.1718860000
C -3.0767130000 2.8099360000 0.1791500000
H -2.4739190000 0.8224310000 0.9229860000
C -2.3773320000 -1.8602710000 -0.7929650000
C 0.5254980000 -1.6220150000 1.3921140000
C -3.8142100000 -1.8782030000 -0.3297300000
H -2.1610200000 -2.3671480000 -1.7358640000
O 1.3096990000 0.9281540000 -0.0679290000
B 2.7399250000 0.0639950000 -0.2334900000
H 1.3545070000 -2.1004960000 0.8683030000
H -0.1041880000 -2.3899070000 1.8481960000
H 0.9532630000 -0.9920410000 2.1757450000
H -3.9385670000 -1.3691980000 0.6299480000
H -4.1658260000 -2.9108980000 -0.2175390000

H -4.4640050000 -1.3942950000 -1.0696170000
H -3.3873430000 3.2001720000 1.1574320000
H -3.9920230000 2.4677660000 -0.3222680000
H -2.6462780000 3.6291210000 -0.4035700000
F 3.4913100000 0.9391600000 -0.9437410000
F 2.3724940000 -1.0661210000 -0.9178450000
F 3.1502270000 -0.1528800000 1.0497200000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199238 (Hartree/Particle)
Thermal correction to Energy= 0.215619
Thermal correction to Enthalpy= 0.216563
Thermal correction to Gibbs (Free) Energy= 0.154529
Sum of electronic and zero-point Energies= -749.711233
Sum of electronic and thermal Energies= -749.694852
Sum of electronic and thermal Enthalpies= -749.693908
Sum of electronic and thermal (Free) Energies= -749.755943

ccTS *syn*-BF_3

C 0.2696910000 -0.6889620000 -0.2585180000
C -0.3202570000 0.6404680000 -0.2738560000
C 0.6969010000 1.6342390000 -0.1810100000
C 2.0130390000 1.2789890000 -0.4746940000
H 0.4526370000 2.5940880000 0.2673960000
C 1.6007180000 -0.6899280000 0.0613280000
C 3.1641330000 2.0720500000 0.0919060000
H 2.2269820000 0.7880930000 -1.4226870000
C 2.6215400000 -1.3663190000 0.5797500000
C -0.4472740000 -1.9469310000 -0.6701220000
C 4.0733640000 -1.2910650000 0.2067590000
H 2.3753450000 -2.0447100000 1.4008660000
O -1.5542520000 0.9578570000 -0.3201020000
B -2.7860090000 0.0751500000 0.1819760000
H -0.8896040000 -2.4151460000 0.2155800000
H 0.2511670000 -2.6492510000 -1.1325910000
H -1.2735380000 -1.7249720000 -1.3467640000
H 4.2476240000 -0.6813660000 -0.6828380000
H 4.4473640000 -2.3016970000 -0.0001250000
H 4.6804360000 -0.8965980000 1.0325930000
H 3.4177620000 2.8922060000 -0.5932970000
H 4.0631400000 1.4598530000 0.1993840000
H 2.9200830000 2.5009900000 1.0674810000
F -3.6858210000 0.9968690000 0.6275400000
F -2.2694870000 -0.7292510000 1.1887850000
F -3.2209670000 -0.6471000000 -0.9100260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198591 (Hartree/Particle)
Thermal correction to Energy= 0.213695
Thermal correction to Enthalpy= 0.214639
Thermal correction to Gibbs (Free) Energy= 0.156029
Sum of electronic and zero-point Energies= -749.681557
Sum of electronic and thermal Energies= -749.666453
Sum of electronic and thermal Enthalpies= -749.665509
Sum of electronic and thermal (Free) Energies= -749.724120

ccPT *syn*-BF_3

C 0.3745600000 -0.5890610000 -0.0805360000
C -0.3457010000 0.6441300000 -0.3527100000
C 0.6215400000 1.6275880000 -0.5564410000
C 2.0148980000 1.1514710000 -0.3710220000
H 0.3647570000 2.6559310000 -0.7912150000
C 1.7900950000 -0.3303090000 -0.1137270000
C 2.7272300000 1.9119690000 0.7770930000
H 2.6014460000 1.2949300000 -1.2929200000
C 2.7474890000 -1.2854330000 0.0059230000
C -0.2628090000 -1.8979960000 0.1569710000
C 4.2230640000 -1.1014780000 -0.1129720000
H 2.4251060000 -2.3075390000 0.1944640000
O -1.6121100000 0.8737260000 -0.4573290000
B -2.7863670000 0.0065260000 0.0693750000
H -0.8525410000 -1.8299520000 1.0810900000
H 0.4437210000 -2.7270670000 0.2135680000
H -1.0260720000 -2.0813340000 -0.6083460000
H 4.5148320000 -0.0871750000 -0.3901570000
H 4.6249860000 -1.7940300000 -0.8647070000
H 4.7168710000 -1.3637410000 0.8337570000
H 2.7477960000 2.9848900000 0.5606540000
H 3.7595490000 1.5742600000 0.9030700000
H 2.1955870000 1.7628020000 1.7217490000
F -3.8715740000 0.8346230000 0.0596430000
F -2.4276870000 -0.4079740000 1.3570850000
F -2.9262420000 -1.0810590000 -0.7905870000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201650 (Hartree/Particle)
Thermal correction to Energy= 0.216245
Thermal correction to Enthalpy= 0.217189
Thermal correction to Gibbs (Free) Energy= 0.159209
Sum of electronic and zero-point Energies= -749.725405
Sum of electronic and thermal Energies= -749.710810
Sum of electronic and thermal Enthalpies= -749.709866
Sum of electronic and thermal (Free) Energies= -749.767847

cRT *syn*-BF_3 (s-a)

C -1.5942310000 2.0902090000 0.8616410000
C -0.5792380000 1.5761670000 0.2269070000
C 0.4677010000 1.0595590000 -0.3933800000
C 0.8628400000 -0.3246310000 -0.0378270000
C 2.2714400000 -0.7172370000 0.0991680000
C 3.2880100000 0.1255040000 0.3497240000
H 2.4358090000 -1.7924900000 0.0846800000
H 3.0897510000 1.1934870000 0.4161130000
C 4.7030710000 -0.2966130000 0.5815980000
C 1.2444290000 1.8418260000 -1.4484290000
H -1.4009760000 2.6212540000 1.7961120000
C -3.0325310000 1.9615170000 0.4217000000
O 0.0410760000 -1.2492690000 0.1772230000
H 0.5490410000 2.4537080000 -2.0289520000
H 1.7603840000 1.1682120000 -2.1385520000
H 1.9922790000 2.5157180000 -1.0142660000
H -3.1045520000 1.4152490000 -0.5189550000
H -3.4921740000 2.9514780000 0.3162200000
H -3.5913830000 1.4027790000 1.1805210000
H 4.8267090000 -1.3801160000 0.4995880000
H 5.0410700000 0.0196740000 1.5773920000
H 5.3722820000 0.1890390000 -0.1412040000
F -1.6740790000 -2.7542130000 -0.3640940000
F -1.8599690000 -0.6302720000 -1.2089180000
F -2.1979860000 -1.0101850000 1.0375560000
B -1.6014960000 -1.4219260000 -0.1187960000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198991 (Hartree/Particle)
Thermal correction to Energy= 0.215483
Thermal correction to Enthalpy= 0.216427
Thermal correction to Gibbs (Free) Energy= 0.154047
Sum of electronic and zero-point Energies= -749.708459
Sum of electronic and thermal Energies= -749.691967
Sum of electronic and thermal Enthalpies= -749.691023
Sum of electronic and thermal (Free) Energies= -749.753403

ccRT *syn*-BF_3 (s-a)

C -1.8448920000 1.9844230000 -0.0648570000
C -0.7114680000 1.4717470000 0.3158200000
C 0.4363290000 0.9225800000 0.6795700000
C 0.7859410000 -0.3831680000 0.0741660000
C 2.1769560000 -0.7741070000 -0.1997920000
C 3.2049750000 0.0701400000 -0.3893670000
H 2.3084340000 -1.8427370000 -0.3555920000
H 3.0440090000 1.1412360000 -0.2871850000
C 4.5873490000 -0.3517540000 -0.7727950000
C 1.3447490000 1.5879720000 1.7084390000
H -2.7269910000 1.6725740000 0.4960630000
C -2.0523830000 2.9061110000 -1.2394840000
O -0.0639520000 -1.2481400000 -0.2515710000
H 0.7312090000 2.1084580000 2.4485450000
H 2.0200700000 2.3288120000 1.2644290000
H 1.9565610000 0.8489040000 2.2333320000
H -1.1076780000 3.1665660000 -1.7237840000
H -2.5511860000 3.8297320000 -0.9224720000
H -2.6992910000 2.4175600000 -1.9776740000
H 4.6758810000 -1.4386660000 -0.8556140000
H 5.3174630000 0.0047030000 -0.0338910000
H 4.8746690000 0.0962360000 -1.7333470000
F -1.7552230000 -2.8366370000 0.1027320000

F -2.3168180000 -0.9272090000 -1.0454070000
F -1.9668230000 -0.8517910000 1.2296500000
B -1.7094180000 -1.4822390000 0.0413590000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198931 (Hartree/Particle)
Thermal correction to Energy= 0.215415
Thermal correction to Enthalpy= 0.216359
Thermal correction to Gibbs (Free) Energy= 0.153951
Sum of electronic and zero-point Energies= -749.706774
Sum of electronic and thermal Energies= -749.690289
Sum of electronic and thermal Enthalpies= -749.689345
Sum of electronic and thermal (Free) Energies= -749.751753

P *syn*-BF_3 (s-v)

C 3.4001350000 -1.0972110000 0.3203050000
C 2.0985200000 -1.0151460000 0.3623700000
C 0.7725270000 -0.9948400000 0.4019610000
C 0.0833960000 0.3055150000 0.2411530000
C 0.8739090000 1.5440320000 0.2387560000
C 0.2935710000 2.7438540000 0.0581940000
H 1.9450530000 1.4578000000 0.3855960000
H -0.7855550000 2.7684710000 -0.0873160000
C 1.0154150000 4.0502730000 0.0422700000
C -0.0172650000 -2.2730560000 0.6067890000
H 3.9502390000 -0.9979830000 1.2588370000
C 4.2193230000 -1.3188350000 -0.9306640000
O -1.1600810000 0.4165660000 0.1304410000
H -0.7560700000 -2.1455880000 1.4013520000
H 0.6594090000 -3.0908060000 0.8639060000
H -0.5702510000 -2.5286700000 -0.2996420000
H 3.5845270000 -1.4044840000 -1.8158460000
H 4.8130550000 -2.2360860000 -0.8368800000
H 4.9215080000 -0.4900860000 -1.0819280000
H 2.0926060000 3.9333020000 0.1942370000
H 0.6212590000 4.7147920000 0.8229480000
H 0.8494140000 4.5677350000 -0.9121620000
F -3.4081540000 0.5154340000 -0.5403040000
F -2.8331860000 -1.1438530000 0.9364280000
F -2.1735910000 -1.2753270000 -1.2710640000
B -2.5494700000 -0.4829450000 -0.2217940000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199278 (Hartree/Particle)
Thermal correction to Energy= 0.215710
Thermal correction to Enthalpy= 0.216655
Thermal correction to Gibbs (Free) Energy= 0.153414
Sum of electronic and zero-point Energies= -749.716342
Sum of electronic and thermal Energies= -749.699910
Sum of electronic and thermal Enthalpies= -749.698965
Sum of electronic and thermal (Free) Energies= -749.762206

P *syn*-BF_3 (w)

C -2.5191190000 1.3245810000 0.7998870000
C -1.3116850000 1.4319970000 0.3284210000
C -0.0620690000 1.5440090000 -0.1019920000
C 0.8536160000 0.4091870000 0.1041490000
C 2.2971040000 0.6694040000 0.1460400000
C 3.1914380000 -0.3360450000 0.1972510000
H 2.6308760000 1.7018670000 0.1291460000
H 2.8055430000 -1.3544470000 0.1968680000
C 4.6725220000 -0.1653030000 0.2499940000
C 0.4468900000 2.8313460000 -0.7339940000
H -2.6859530000 1.6251480000 1.8364620000
C -3.6948780000 0.7474030000 0.0506160000
O 0.4781260000 -0.7814190000 0.2722540000
H -0.3973410000 3.4826050000 -0.9713510000
H 0.9941140000 2.6325490000 -1.6620540000
H 1.1139630000 3.3855670000 -0.0619120000
H -3.4209860000 0.4872370000 -0.9717660000
H -4.5341830000 1.4525180000 0.0463920000
H -4.0150370000 -0.1697770000 0.5571090000
H 4.9725000000 0.8867960000 0.2461150000
H 5.1461640000 -0.6699950000 -0.6027560000
H 5.0789980000 -0.6431520000 1.1516470000
F -0.3138630000 -2.8415160000 -0.4890940000
F -1.3841360000 -0.9629640000 -1.2575290000
F -1.6805730000 -1.6518480000 0.9215570000
B -0.8698870000 -1.6396160000 -0.1777130000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199221 (Hartree/Particle)
Thermal correction to Energy= 0.215506
Thermal correction to Enthalpy= 0.216450
Thermal correction to Gibbs (Free) Energy= 0.154913
Sum of electronic and zero-point Energies= -749.714109
Sum of electronic and thermal Energies= -749.697823
Sum of electronic and thermal Enthalpies= -749.696879
Sum of electronic and thermal (Free) Energies= -749.758416

cRT *anti*-BF_3 (u)

C -1.0674880000 -1.0835820000 -0.5334840000
C 0.1076430000 -0.2688330000 -0.1559750000
C 0.0504680000 1.1733170000 0.0731010000
C -0.7937650000 2.0017330000 -0.5668850000
H 0.8144310000 1.5628570000 0.7377770000
C -2.2970700000 -0.6672310000 -0.2719040000
H -1.4942690000 1.5952020000 -1.2931270000
C -0.8113490000 3.4855320000 -0.3896090000
C -3.5282270000 -0.3386480000 0.0103700000
H -4.1027690000 0.2075640000 -0.7406390000
C -4.2315670000 -0.6480770000 1.3117470000
O 1.1846430000 -0.9076670000 -0.0243520000
B 2.6804770000 -0.2441600000 0.2954320000
C -0.7889160000 -2.4603600000 -1.1086960000
H -0.2398410000 -3.0694450000 -0.3838220000
H -0.1624430000 -2.3846950000 -2.0039120000
H -1.7226540000 -2.9641250000 -1.3671670000
H -0.0828640000 3.8178830000 0.3548740000
H -1.8101900000 3.8230450000 -0.0811630000
H -0.5933370000 3.9889030000 -1.3408590000
H -3.5822160000 -1.1970180000 1.9979060000
H -5.1303110000 -1.2481340000 1.1247570000
H -4.5538900000 0.2781900000 1.8025700000
F 2.8772900000 0.6272760000 -0.7398250000
F 2.5265460000 0.3677830000 1.5169200000
F 3.4786580000 -1.3385260000 0.3005130000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199510 (Hartree/Particle)
Thermal correction to Energy= 0.215778
Thermal correction to Enthalpy= 0.216722
Thermal correction to Gibbs (Free) Energy= 0.154868
Sum of electronic and zero-point Energies= -749.717289
Sum of electronic and thermal Energies= -749.701021
Sum of electronic and thermal Enthalpies= -749.700076
Sum of electronic and thermal (Free) Energies= -749.761931

cTS *anti*-BF_3

C -0.9054680000 -1.0316230000 -0.3313500000
C 0.3185370000 -0.3055680000 -0.0911030000
C 0.0665340000 1.0970790000 0.0130540000
C -1.1069070000 1.5718250000 -0.5690570000
H 0.6951700000 1.7070330000 0.6537280000
C -2.0327710000 -0.2647380000 -0.2519820000
H -1.3216040000 1.2930330000 -1.6001390000
C -1.7423520000 2.8678010000 -0.1403780000
C -3.3324830000 -0.1394680000 -0.0126100000
H -3.8880190000 0.6495730000 -0.5192200000
C -4.1000280000 -0.9655230000 0.9867150000
O 1.4299060000 -0.9125890000 0.0647370000
B 2.7726660000 -0.0488030000 0.1783320000
C -0.8694570000 -2.4835040000 -0.7144130000
H -0.3740120000 -3.0487000000 0.0844860000
H -0.2658190000 -2.6332050000 -1.6169440000
H -1.8697660000 -2.8905090000 -0.8745770000
H -1.5544250000 3.0876990000 0.9139410000
H -2.8247600000 2.8513410000 -0.3059510000
H -1.3414830000 3.6928560000 -0.7434330000
H -3.4770940000 -1.7433150000 1.4349290000
H -4.9622090000 -1.4397630000 0.5002570000
H -4.4954020000 -0.3324700000 1.7916830000
F 2.7535610000 0.7885560000 -0.9219350000
F 2.6526420000 0.6581830000 1.3646080000
F 3.7719320000 -0.9719080000 0.1727060000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198480 (Hartree/Particle)
Thermal correction to Energy= 0.213782
Thermal correction to Enthalpy= 0.214726
Thermal correction to Gibbs (Free) Energy= 0.155414
Sum of electronic and zero-point Energies= -749.688899
Sum of electronic and thermal Energies= -749.673597
Sum of electronic and thermal Enthalpies= -749.672653
Sum of electronic and thermal (Free) Energies= -749.731965

cPT *anti*-BF_3

C -0.9474980000 -0.8399100000 0.0332690000
C 0.3530170000 -0.2422100000 -0.0416000000
C 0.1724280000 1.1263810000 -0.2993240000
C -1.2583930000 1.4929280000 -0.3917540000
H 0.9905590000 1.8264140000 -0.4092820000
C -1.9602680000 0.1551170000 -0.1707610000
H -1.4768060000 1.8522750000 -1.4129480000
C -1.6640280000 2.6180190000 0.5896630000
C -3.3141850000 0.0405750000 -0.2067610000
H -3.8626120000 0.9655600000 -0.3889850000
C -4.1861350000 -1.1583510000 -0.0344030000
O 1.4428020000 -0.9168400000 0.1084100000
B 2.8027200000 -0.1415920000 0.0021150000
C -1.0862860000 -2.3017320000 0.2780600000
H -1.6719300000 -2.5009000000 1.1841520000
H -0.0941260000 -2.7430560000 0.3931040000
H -1.5993760000 -2.7971900000 -0.5558990000
H -1.5039670000 2.3053720000 1.6258890000
H -2.7168720000 2.8885100000 0.4635740000
H -1.0632980000 3.5133820000 0.4031100000
H -3.6441860000 -2.0831720000 0.1549130000
H -4.8068050000 -1.2963430000 -0.9309530000
H -4.8888510000 -0.9899810000 0.7936600000
F 2.8173660000 0.4330450000 -1.2652440000
F 2.7584950000 0.8431270000 0.9846460000
F 3.7719550000 -1.0809600000 0.1987610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201454 (Hartree/Particle)
Thermal correction to Energy= 0.216401
Thermal correction to Enthalpy= 0.217345
Thermal correction to Gibbs (Free) Energy= 0.158192
Sum of electronic and zero-point Energies= -749.725093
Sum of electronic and thermal Energies= -749.710146
Sum of electronic and thermal Enthalpies= -749.709201
Sum of electronic and thermal (Free) Energies= -749.768355

ccRT *anti*-BF_3 (u)

C 3.3865900000 -0.7325440000 0.7365390000
C 2.1782950000 -0.9663110000 0.3024800000
C 0.9608150000 -1.2887120000 -0.1068830000
C -0.1662350000 -0.3424950000 0.0366710000
C 0.0032900000 1.1009630000 0.1921430000
C 1.0102600000 1.8045010000 -0.3548040000
H -0.8069530000 1.6030540000 0.7105110000
H 1.7650790000 1.2888790000 -0.9447340000
C 1.1480550000 3.2895480000 -0.2560570000
C 0.6259440000 -2.6782370000 -0.6175400000
H 3.6034020000 -0.9657750000 1.7812290000
C 4.5183100000 -0.1524200000 -0.0781900000
O -1.3110360000 -0.8666700000 0.0359160000
B -2.7616730000 -0.0452190000 0.0790070000
H 1.5304150000 -3.2843100000 -0.7013610000
H 0.1387950000 -2.6224950000 -1.5968670000
H -0.0760540000 -3.1717650000 0.0618980000
H 4.2195410000 0.0312840000 -1.1135980000
H 5.3736210000 -0.8386260000 -0.0833990000
H 4.8632750000 0.7920380000 0.3604830000
H 2.1188150000 3.5570840000 0.1828140000
H 0.3544800000 3.7347450000 0.3501070000
H 1.1220210000 3.7452760000 -1.2547800000
F -3.6600020000 -1.0571080000 0.0186690000
F -2.7082680000 0.7652280000 -1.0211720000
F -2.7319210000 0.6345820000 1.2735240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199452 (Hartree/Particle)
Thermal correction to Energy= 0.215732
Thermal correction to Enthalpy= 0.216676
Thermal correction to Gibbs (Free) Energy= 0.154819
Sum of electronic and zero-point Energies= -749.717200
Sum of electronic and thermal Energies= -749.700920
Sum of electronic and thermal Enthalpies= -749.699976
Sum of electronic and thermal (Free) Energies= -749.761833

ccTS *anti*-BF_3

C 3.2324920000 0.7321810000 -0.4757310000
C 1.9519360000 0.6388770000 -0.1245150000
C 0.7454210000 1.2701460000 -0.0081730000
C -0.3961550000 0.3890330000 -0.0433120000
C 0.0180810000 -0.9755570000 -0.0662190000
C 1.3002390000 -1.2621640000 0.4032610000
H -0.5929140000 -1.7084030000 -0.5834450000
H 1.5800490000 -0.9019150000 1.3927220000
C 2.0130840000 -2.5185010000 -0.0303350000
C 0.5619680000 2.7428450000 0.2200770000
H 3.4547290000 1.3780120000 -1.3291520000
C 4.4078090000 0.0237840000 0.1322060000
O -1.5852560000 0.8455120000 -0.1223570000
B -2.8124200000 -0.1757210000 -0.0138540000
H 1.5061690000 3.2875530000 0.1623860000
H 0.0929480000 2.9318540000 1.1929720000
H -0.1305830000 3.1326940000 -0.5354980000
H 4.1379310000 -0.5429350000 1.0263130000
H 5.1696170000 0.7603710000 0.4178600000
H 4.8836960000 -0.6547910000 -0.5882360000
H 3.0984780000 -2.4168800000 0.0490800000
H 1.7633860000 -2.7910250000 -1.0593020000
H 1.7198930000 -3.3492030000 0.6253690000
F -3.9145800000 0.6205160000 0.0308430000
F -2.5752880000 -0.8991810000 1.1406730000
F -2.7266300000 -0.9718560000 -1.1455720000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198462 (Hartree/Particle)
Thermal correction to Energy= 0.213707
Thermal correction to Enthalpy= 0.214651
Thermal correction to Gibbs (Free) Energy= 0.155494
Sum of electronic and zero-point Energies= -749.686812
Sum of electronic and thermal Energies= -749.671568
Sum of electronic and thermal Enthalpies= -749.670623
Sum of electronic and thermal (Free) Energies= -749.729780

ccPT *anti*-BF_3

C -3.2101490000 0.7435090000 -0.1077330000
C -1.9328790000 0.2849830000 -0.0775520000
C -0.7757400000 1.1080860000 0.1149160000
C 0.4182770000 0.3316820000 -0.0237290000
C 0.0233430000 -0.9859090000 -0.2906370000
C -1.4553530000 -1.1457800000 -0.2946830000
H 0.7195540000 -1.8006410000 -0.4429060000
H -1.7937100000 -1.5181530000 -1.2752230000
C -1.9172000000 -2.1556680000 0.7876310000
C -0.7024210000 2.5622740000 0.3882720000
H -3.3699690000 1.8048560000 0.0777220000
C -4.4446250000 -0.0441090000 -0.3930310000
O 1.5966670000 0.8482110000 0.0898780000
B 2.8261800000 -0.1134870000 -0.0561480000
H -1.6735420000 3.0430510000 0.5187460000
H -0.1562260000 3.0553810000 -0.4273510000
H -0.0862950000 2.7262160000 1.2819540000
H -4.2436340000 -1.0854390000 -0.6503860000
H -4.9975100000 0.4152950000 -1.2235490000
H -5.1226640000 -0.0197150000 0.4720850000
H -3.0013330000 -2.2969900000 0.7671250000
H -1.6303130000 -1.8063550000 1.7840270000
H -1.4450400000 -3.1280740000 0.6173550000
F 3.9268140000 0.6771430000 0.1041810000
F 2.7188290000 -0.6852360000 -1.3208530000
F 2.6740170000 -1.0810270000 0.9323830000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201350 (Hartree/Particle)
Thermal correction to Energy= 0.216343
Thermal correction to Enthalpy= 0.217287

Thermal correction to Gibbs (Free) Energy= 0.158268
Sum of electronic and zero-point Energies= -749.728585
Sum of electronic and thermal Energies= -749.713592
Sum of electronic and thermal Enthalpies= -749.712648
Sum of electronic and thermal (Free) Energies= -749.771667

cRT *anti*-BF_3 (s-a)

C 3.4028710000 -0.3114220000 -0.1389190000
C 2.3114450000 0.3670800000 -0.3478300000
C 1.1984770000 1.0602400000 -0.5433270000
C -0.0792990000 0.3307480000 -0.3412270000
C -1.3646950000 1.0026170000 -0.1362350000
C -1.5179860000 2.1927200000 0.4704140000
H -2.2319360000 0.4147830000 -0.4187110000
H -0.6448480000 2.7459620000 0.8097710000
C -2.8430460000 2.8139210000 0.7750920000
C 1.2524490000 2.5071920000 -1.0127810000
H 3.8114980000 -0.8807930000 -0.9763290000
C 4.1411290000 -0.4015930000 1.1757470000
O -0.0265610000 -0.9261560000 -0.3858410000
H 2.1795170000 2.6784380000 -1.5656750000
H 1.2344770000 3.2192490000 -0.1795010000
H 0.4104640000 2.7417950000 -1.6703830000
H 3.6588250000 0.1994670000 1.9504080000
H 5.1763390000 -0.0592350000 1.0583650000
H 4.1754320000 -1.4433830000 1.5153750000
H -3.6728330000 2.2113540000 0.3960420000
H -2.9069120000 3.8203920000 0.3401020000
H -2.9683520000 2.9353260000 1.8593590000
F -0.6573860000 -3.1800850000 -0.1533250000
F -2.2184590000 -1.7127680000 -0.9941310000
F -1.6460630000 -1.6267370000 1.2307330000
B -1.2640140000 -1.9733610000 -0.0374370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199524 (Hartree/Particle)
Thermal correction to Energy= 0.215792
Thermal correction to Enthalpy= 0.216736
Thermal correction to Gibbs (Free) Energy= 0.154491
Sum of electronic and zero-point Energies= -749.710542
Sum of electronic and thermal Energies= -749.694273
Sum of electronic and thermal Enthalpies= -749.693329
Sum of electronic and thermal (Free) Energies= -749.755574

ccRT *anti*-BF_3 (s-a)

C -3.2944610000 -0.5089750000 -0.7269840000
C -2.1475770000 -0.9324210000 -0.2786730000
C -0.9729640000 -1.3630250000 0.1592920000
C 0.1317710000 -0.3705170000 0.1720430000
C 1.5467280000 -0.7447650000 0.2250510000
C 2.0589950000 -1.8679480000 -0.3079030000
H 2.2010140000 0.0137010000 0.6422040000
H 1.4007050000 -2.5927220000 -0.7824180000
C 3.5188070000 -2.1865080000 -0.3498120000
C -0.8028380000 -2.7849680000 0.6750600000
H -3.5081610000 -0.6374770000 -1.7900790000
C -4.3514000000 0.1769750000 0.1065150000
O -0.1993480000 0.8440450000 0.1694460000
H -1.7588560000 -3.1542310000 1.0547800000
H -0.0700030000 -2.8272610000 1.4859590000
H -0.4749240000 -3.4779400000 -0.1085170000
H -4.0463390000 0.2595420000 1.1521590000
H -5.2980050000 -0.3743960000 0.0558600000
H -4.5348680000 1.1859230000 -0.2809280000
H 4.1175560000 -1.4234210000 0.1546770000
H 3.8628240000 -2.2672470000 -1.3896250000
H 3.7152870000 -3.1600460000 0.1191160000
F -0.0387800000 3.1840560000 -0.0024070000
F 1.5047630000 1.9034260000 -1.1357490000
F 1.6161950000 2.0788480000 1.1536560000
B 0.8253170000 2.1398310000 0.0288390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199504 (Hartree/Particle)
Thermal correction to Energy= 0.215794
Thermal correction to Enthalpy= 0.216738
Thermal correction to Gibbs (Free) Energy= 0.154468
Sum of electronic and zero-point Energies= -749.710706
Sum of electronic and thermal Energies= -749.694416
Sum of electronic and thermal Enthalpies= -749.693472
Sum of electronic and thermal (Free) Energies= -749.755741

cRT *anti*-BF_3 (s-v)

C 3.7689910000 0.0658350000 0.3339030000
C 2.5775150000 -0.4667620000 0.3297170000
C 1.3882440000 -1.0491630000 0.3232330000
C 0.1509130000 -0.2439850000 0.1929620000
C 0.2466700000 1.2050730000 0.0797730000
C -0.7735830000 2.0587150000 0.2981630000
H 1.2373320000 1.5927660000 -0.1387940000
H -1.7461820000 1.6686440000 0.5808930000
C -0.6492770000 3.5423210000 0.2043140000
C 1.2245170000 -2.5509850000 0.4461610000
H 4.1929920000 0.3627220000 1.2957680000
C 4.6201730000 0.3116280000 -0.8906330000
O -0.9151120000 -0.9143930000 0.2046230000
H 2.1984440000 -3.0392960000 0.5209770000
H 0.6862500000 -2.9487450000 -0.4201710000
H 0.6295800000 -2.7998800000 1.3310950000
H 4.1140890000 -0.0118140000 -1.8034970000
H 5.5698540000 -0.2304990000 -0.8073980000
H 4.8613830000 1.3775450000 -0.9827330000
H 0.3609120000 3.8650350000 -0.0654110000
H -0.9306600000 4.0135190000 1.1555970000
H -1.3538290000 3.9259100000 -0.5460830000
F -2.9637100000 -1.8544870000 -0.4316770000
F -2.3883910000 0.1688200000 -1.3596840000
F -3.0254430000 0.0539040000 0.8478530000
B -2.4852720000 -0.6021920000 -0.2342440000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199525 (Hartree/Particle)
Thermal correction to Energy= 0.215797
Thermal correction to Enthalpy= 0.216741
Thermal correction to Gibbs (Free) Energy= 0.154935
Sum of electronic and zero-point Energies= -749.719092
Sum of electronic and thermal Energies= -749.702820
Sum of electronic and thermal Enthalpies= -749.701876
Sum of electronic and thermal (Free) Energies= -749.763682

ccRT *anti*-BF_3 (s-v)

C -3.7461670000 -0.0685450000 -0.5059820000
C -2.5560560000 -0.5651780000 -0.3051710000
C -1.3663940000 -1.1102500000 -0.1024630000
C -0.1481970000 -0.2683850000 -0.0418760000
C -0.2621250000 1.1722200000 -0.2252870000
C 0.6780900000 2.0670100000 0.1388750000
H -1.2068720000 1.5179860000 -0.6344950000
H 1.5938700000 1.7202100000 0.6070240000
C 0.5324860000 3.5414270000 -0.0352020000
C -1.1828300000 -2.6039990000 0.0773470000
H -4.0945020000 0.0254480000 -1.5370060000
C -4.6926020000 0.3942850000 0.5775600000
O 0.9168450000 -0.9019890000 0.1820180000
H -2.1410900000 -3.1216900000 -0.0021550000
H -0.7376120000 -2.8204980000 1.0539770000
H -0.4959160000 -2.9977090000 -0.6787720000
H -4.2587210000 0.2649930000 1.5720600000
H -5.6305730000 -0.1719660000 0.5294330000
H -4.9442370000 1.4528830000 0.4403940000
H -0.4208720000 3.8201060000 -0.4943630000
H 1.3499990000 3.9222800000 -0.6623010000
H 0.6251030000 4.0547570000 0.9312690000
F 3.0724380000 -1.7903080000 -0.0414090000
F 2.8480940000 0.1581750000 1.1568100000
F 2.6166880000 0.1817240000 -1.1319980000
B 2.5308910000 -0.5497420000 0.0202710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199532 (Hartree/Particle)
Thermal correction to Energy= 0.215802
Thermal correction to Enthalpy= 0.216746
Thermal correction to Gibbs (Free) Energy= 0.154944
Sum of electronic and zero-point Energies= -749.719098
Sum of electronic and thermal Energies= -749.702828
Sum of electronic and thermal Enthalpies= -749.701884

Sum of electronic and thermal (Free) Energies= -749.763686

cRT *anti*-BF_3 (w)

C 3.4705220000 -0.1474790000 -0.3825370000
C 2.4044820000 0.5924690000 -0.2805670000
C 1.3138460000 1.3402220000 -0.1849800000
C 0.0097100000 0.6419080000 -0.0717380000
C -1.2061950000 1.4451450000 -0.1160160000
C -2.4031020000 1.0399290000 0.3573800000
H -1.1064060000 2.4491710000 -0.5177210000
H -2.4886250000 0.0585820000 0.8143160000
C -3.6391310000 1.8726110000 0.3201830000
C 1.3953050000 2.8572100000 -0.1869810000
H 3.8004670000 -0.4303160000 -1.3842630000
C 4.2776990000 -0.6775700000 0.7792150000
O 0.0444240000 -0.6093850000 0.0726060000
H 2.4403070000 3.1743500000 -0.1635780000
H 0.8885550000 3.2873750000 0.6843160000
H 0.9371170000 3.2876580000 -1.0860060000
H 3.8734550000 -0.3397420000 1.7363400000
H 5.3218520000 -0.3513370000 0.7019760000
H 4.2718840000 -1.7737430000 0.7677600000
H -3.4754500000 2.8533410000 -0.1365740000
H -4.0403390000 2.0133740000 1.3327480000
H -4.4190870000 1.3454900000 -0.2460010000
F -0.2756280000 -2.8864970000 -0.3489920000
F -1.8462860000 -1.4235450000 -1.1722360000
F -1.7418850000 -1.8506210000 1.0862500000
B -1.0647490000 -1.8079650000 -0.1146210000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199583 (Hartree/Particle)
Thermal correction to Energy= 0.215765
Thermal correction to Enthalpy= 0.216709
Thermal correction to Gibbs (Free) Energy= 0.155043
Sum of electronic and zero-point Energies= -749.713566
Sum of electronic and thermal Energies= -749.697385
Sum of electronic and thermal Enthalpies= -749.696440
Sum of electronic and thermal (Free) Energies= -749.758106

ccRT *anti*-BF_3 (w)

C 3.4615020000 -0.1026230000 -0.4795660000
C 2.3927300000 0.6243150000 -0.3261350000
C 1.3006720000 1.3585060000 -0.1640250000
C -0.0004920000 0.6488950000 -0.0952010000
C -1.1955230000 1.4304860000 0.1989240000
C -2.4527910000 1.0324450000 -0.0870310000
H -1.0352940000 2.4135460000 0.6315280000
H -2.6083250000 0.0750320000 -0.5752330000
C -3.6698640000 1.8431770000 0.2026300000
C 1.3774480000 2.8723070000 -0.0612930000
H 3.7816380000 -0.3266230000 -1.4992550000
C 4.2842480000 -0.6927830000 0.6415720000
O 0.0150070000 -0.5920750000 -0.3131160000
H 2.4029910000 3.2058600000 -0.2348880000
H 1.0744060000 3.2289620000 0.9308360000
H 0.7316070000 3.3575510000 -0.8019330000
H 3.8901490000 -0.4103380000 1.6206380000
H 5.3261340000 -0.3580050000 0.5704410000
H 4.2825060000 -1.7866450000 0.5696580000
H -3.4374570000 2.8010870000 0.6776560000
H -4.3398190000 1.2754190000 0.8626050000
H -4.2370930000 2.0305710000 -0.7188920000
F -0.2118710000 -2.8917860000 0.0403460000
F -1.9106300000 -1.8101580000 -1.0678720000
F -1.6277970000 -1.4958460000 1.1937540000
B -1.0372800000 -1.8156130000 -0.0007090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199596 (Hartree/Particle)
Thermal correction to Energy= 0.215771
Thermal correction to Enthalpy= 0.216715
Thermal correction to Gibbs (Free) Energy= 0.155059
Sum of electronic and zero-point Energies= -749.713569
Sum of electronic and thermal Energies= -749.697394
Sum of electronic and thermal Enthalpies= -749.696450
Sum of electronic and thermal (Free) Energies= -749.758106

1b'

cRT

C 3.3865890000 -0.7325450000 -0.7365400000
C 2.1782940000 -0.9663110000 -0.3024800000
C 0.9608150000 -1.2887120000 0.1068840000
C -0.1662360000 -0.3424950000 -0.0366700000
C 0.0032900000 1.1009630000 -0.1921430000
C 1.0102600000 1.8045000000 0.3548060000
H -0.8069520000 1.6030540000 -0.7105130000
C 0.6259440000 -2.6782360000 0.6175440000
O -1.3110370000 -0.8666700000 -0.0359160000
H 1.5304150000 -3.2843090000 0.7013640000
H -0.0760550000 -3.1717650000 -0.0618920000
H 0.1387970000 -2.6224920000 1.5968720000
B -2.7616720000 -0.0452190000 -0.0790080000
F -2.7082670000 0.7652290000 1.0211710000
F -3.6600020000 -1.0571080000 -0.0186700000
F -2.7319200000 0.6345810000 -1.2735250000
C 4.5183090000 -0.1524190000 0.0781860000
C 1.1480550000 3.2895480000 0.2560600000
H 4.8632750000 0.7920380000 -0.3604890000
H 5.3736210000 -0.8386260000 0.0833970000
H 4.2195420000 0.0312870000 1.1135950000
H 3.6034010000 -0.9657780000 -1.7812300000
H 0.3544830000 3.7347450000 -0.3501080000
H 2.1188180000 3.5570830000 -0.1828080000
H 1.1220170000 3.7452750000 1.2547830000
H 1.7650770000 1.2888770000 0.9447370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199452 (Hartree/Particle)
Thermal correction to Energy= 0.215732
Thermal correction to Enthalpy= 0.216676
Thermal correction to Gibbs (Free) Energy= 0.154819
Sum of electronic and zero-point Energies= -749.717200
Sum of electronic and thermal Energies= -749.700920
Sum of electronic and thermal Enthalpies= -749.699976
Sum of electronic and thermal (Free) Energies= -749.761833

cTS

C 3.2324920000 -0.7321800000 -0.4757310000
C 1.9519360000 -0.6388770000 -0.1245150000
C 4.4078090000 -0.0237840000 0.1322070000
H 3.4547300000 -1.3780120000 -1.3291510000
C 0.7454210000 -1.2701460000 -0.0081730000
H 5.1696160000 -0.7603720000 0.4178620000
H 4.1379300000 0.5429350000 1.0263130000
H 4.8836960000 0.6547900000 -0.5882350000
C -0.3961560000 -0.3890340000 -0.0433130000
C 0.5619680000 -2.7428450000 0.2200770000
C 0.0180810000 0.9755570000 -0.0662200000
O -1.5852560000 -0.8455120000 -0.1223570000
H 1.5061690000 -3.2875520000 0.1623880000
H -0.1305810000 -3.1326950000 -0.5355000000
H 0.0929470000 -2.9318540000 1.1929710000
C 1.3002390000 1.2621630000 0.4032600000
H -0.5929140000 1.7084020000 -0.5834460000
B -2.8124200000 0.1757210000 -0.0138530000
C 2.0130840000 2.5185010000 -0.0303350000
H 1.5800480000 0.9019150000 1.3927210000
F -2.5752880000 0.8991810000 1.1406730000
F -3.9145800000 -0.6205150000 0.0308440000
F -2.7266310000 0.9718560000 -1.1455720000
H 1.7633860000 2.7910250000 -1.0593020000
H 3.0984780000 2.4168800000 0.0490800000
H 1.7198930000 3.3492030000 0.6253690000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198462 (Hartree/Particle)
Thermal correction to Energy= 0.213707
Thermal correction to Enthalpy= 0.214651
Thermal correction to Gibbs (Free) Energy= 0.155494
Sum of electronic and zero-point Energies= -749.686812
Sum of electronic and thermal Energies= -749.671568
Sum of electronic and thermal Enthalpies= -749.670623
Sum of electronic and thermal (Free) Energies= -749.729780

cPT

C -3.2101490000 0.7435090000 0.1077330000
C -1.9328790000 0.2849830000 0.0775520000
C -0.7757410000 1.1080860000 -0.1149160000
C 0.4182770000 0.3316820000 0.0237300000
C 0.0233430000 -0.9859090000 0.2906380000
C -1.4553530000 -1.1457800000 0.2946840000
C -0.7024210000 2.5622740000 -0.3882710000
O 1.5966670000 0.8482110000 -0.0898770000
H -1.6735420000 3.0430500000 -0.5187480000
H -0.0862930000 2.7262160000 -1.2819520000
H -0.1562290000 3.0553810000 0.4273530000
B 2.8261800000 -0.1134870000 0.0561480000
F 2.7188300000 -0.6852370000 1.3208520000
F 3.9268130000 0.6771430000 -0.1041810000
F 2.6740170000 -1.0810270000 -0.9323830000
C -4.4446260000 -0.0441090000 0.3930300000
H 0.7195540000 -1.8006410000 0.4429070000
C -1.9172000000 -2.1556680000 -0.7876310000
H -1.7937100000 -1.5181530000 1.2752230000
H -1.6303120000 -1.8063550000 -1.7840260000
H -3.0013320000 -2.2969900000 -0.7671250000
H -1.4450400000 -3.1280740000 -0.6173540000
H -4.9975110000 0.4152950000 1.2235480000
H -4.2436340000 -1.0854390000 0.6503860000
H -5.1226630000 -0.0197160000 -0.4720870000
H -3.3699690000 1.8048560000 -0.0777230000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201350 (Hartree/Particle)
Thermal correction to Energy= 0.216343
Thermal correction to Enthalpy= 0.217287
Thermal correction to Gibbs (Free) Energy= 0.158268
Sum of electronic and zero-point Energies= -749.728585
Sum of electronic and thermal Energies= -749.713592
Sum of electronic and thermal Enthalpies= -749.712648
Sum of electronic and thermal (Free) Energies= -749.771667

ccRT

C 3.5282270000 -0.3386470000 0.0103710000
C 2.2970700000 -0.6672300000 -0.2719030000
C 4.2315670000 -0.6480780000 1.3117480000
C 1.0674880000 -1.0835810000 -0.5334850000
C -0.1076440000 -0.2688330000 -0.1559760000
C 0.7889170000 -2.4603590000 -1.1086980000
C -0.0504690000 1.1733170000 0.0731020000
O -1.1846430000 -0.9076670000 -0.0243520000
H 0.1624430000 -2.3846930000 -2.0039140000
H 1.7226550000 -2.9641220000 -1.3671710000
H 0.2398440000 -3.0694450000 -0.3838250000
H -0.8144320000 1.5628570000 0.7377770000
C 0.7937640000 2.0017330000 -0.5668850000
B -2.6804770000 -0.2441610000 0.2954320000
C 0.8113480000 3.4855320000 -0.3896090000
F -2.8772900000 0.6272750000 -0.7398250000
F -3.4786580000 -1.3385270000 0.3005130000
F -2.5265460000 0.3677820000 1.5169200000
H 5.1303110000 -1.2481350000 1.1247570000
H 3.5822150000 -1.1970210000 1.9979050000
H 4.5538890000 0.2781870000 1.8025730000
H 4.1027690000 0.2075660000 -0.7406370000
H 0.5933380000 3.9889040000 -1.3408590000
H 1.8101890000 3.8230440000 -0.0811620000
H 0.0828630000 3.8178840000 0.3548730000
H 1.4942680000 1.5952020000 -1.2931270000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199510 (Hartree/Particle)
Thermal correction to Energy= 0.215778
Thermal correction to Enthalpy= 0.216722
Thermal correction to Gibbs (Free) Energy= 0.154868
Sum of electronic and zero-point Energies= -749.717289
Sum of electronic and thermal Energies= -749.701021
Sum of electronic and thermal Enthalpies= -749.700076
Sum of electronic and thermal (Free) Energies= -749.761931

ccTS

C 3.3324830000 -0.1394680000 -0.0126090000
C 2.0327710000 -0.2647380000 -0.2519820000
C 4.1000280000 -0.9655230000 0.9867160000
H 3.8880180000 0.6495730000 -0.5192190000
C 0.9054680000 -1.0316230000 -0.3313500000
H 3.4770940000 -1.7433140000 1.4349300000
H 4.4954020000 -0.3324700000 1.7916830000
H 4.9622090000 -1.4397630000 0.5002570000
C -0.3185370000 -0.3055690000 -0.0911030000
C 0.8694580000 -2.4835040000 -0.7144130000
C -0.0665340000 1.0970790000 0.0130540000
O -1.4299060000 -0.9125890000 0.0647370000
H 0.3740120000 -3.0487000000 0.0844850000
H 1.8697660000 -2.8905090000 -0.8745770000
H 0.2658200000 -2.6332040000 -1.6169450000
C 1.1069070000 1.5718250000 -0.5690570000
H -0.6951700000 1.7070330000 0.6537280000
B -2.7726660000 -0.0488030000 0.1783320000
C 1.7423520000 2.8678010000 -0.1403790000
H 1.3216040000 1.2930330000 -1.6001390000
F -3.7719320000 -0.9719080000 0.1727060000
F -2.7535610000 0.7885560000 -0.9219350000
F -2.6526420000 0.6581820000 1.3646090000
H 1.5544250000 3.0876990000 0.9139410000
H 1.3414820000 3.6928560000 -0.7434330000
H 2.8247600000 2.8513420000 -0.3059510000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198480 (Hartree/Particle)
Thermal correction to Energy= 0.213782
Thermal correction to Enthalpy= 0.214726
Thermal correction to Gibbs (Free) Energy= 0.155414
Sum of electronic and zero-point Energies= -749.688899
Sum of electronic and thermal Energies= -749.673597
Sum of electronic and thermal Enthalpies= -749.672653
Sum of electronic and thermal (Free) Energies= -749.73196

ccPT

C -3.3141850000 0.0405760000 0.2067600000
C -1.9602680000 0.1551170000 0.1707610000
C -0.9474980000 -0.8399100000 -0.0332690000
C 0.3530170000 -0.2422100000 0.0416010000
C 0.1724280000 1.1263810000 0.2993260000
C -1.2583930000 1.4929280000 0.3917550000
C -1.0862860000 -2.3017320000 -0.2780590000
O 1.4428020000 -0.9168400000 -0.1084090000
H -1.6719300000 -2.5009000000 -1.1841520000
H -1.5993770000 -2.7971900000 0.5558990000
H -0.0941270000 -2.7430560000 -0.3931040000
B 2.8027190000 -0.1415920000 -0.0021150000
F 3.7719540000 -1.0809600000 -0.1987610000
F 2.8173670000 0.4330460000 1.2652430000
F 2.7584940000 0.8431250000 -0.9846470000
C -1.6640270000 2.6180190000 -0.5896640000
C -4.1861350000 -1.1583510000 0.0344020000
H 0.9905590000 1.8264140000 0.4092850000
H -3.6441850000 -2.0831720000 -0.1549130000
H -4.8888500000 -0.9899810000 -0.7936620000
H -4.8068060000 -1.2963430000 0.9309520000
H -3.8626120000 0.9655600000 0.3889830000
H -2.7168710000 2.8885100000 -0.4635740000
H -1.5039660000 2.3053720000 -1.6258890000
H -1.0632970000 3.5133820000 -0.4031100000
H -1.4768060000 1.8522760000 1.4129480000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201454 (Hartree/Particle)
Thermal correction to Energy= 0.216401
Thermal correction to Enthalpy= 0.217345
Thermal correction to Gibbs (Free) Energy= 0.158192
Sum of electronic and zero-point Energies= -749.725093
Sum of electronic and thermal Energies= -749.710146
Sum of electronic and thermal Enthalpies= -749.709201
Sum of electronic and thermal (Free) Energies= -749.768355

1b"

cRT

C 3.4579730000 -0.2789110000 -0.1768070000
C 2.2437590000 -0.5762850000 0.1934830000
C 1.0246980000 -0.9324190000 0.5701580000
C -0.1441500000 -0.1624140000 0.1046640000
C -0.0592220000 1.1797750000 -0.4869810000
C 0.6378300000 2.2410370000 -0.0423000000
H -0.7412450000 1.3154460000 -1.3207710000
C 0.7526330000 -2.1984550000 1.3601610000
O -1.2465890000 -0.7644360000 0.1713910000
H 1.6896160000 -2.6739320000 1.6577550000
H 0.1668520000 -2.9023180000 0.7605520000
H 0.1637130000 -1.9742420000 2.2558720000
B -2.7376410000 -0.1453850000 -0.2771270000
F -3.5678180000 -1.1645140000 0.0489800000
F -2.6042170000 0.0871390000 -1.6244330000
F -2.8647380000 0.9856960000 0.4771800000
C 4.1211250000 -0.7481550000 -1.4508540000
C 1.4849780000 2.4012570000 1.1819470000
H 3.4571260000 -1.3880670000 -2.0367770000
H 5.0343320000 -1.3094420000 -1.2194340000
H 4.4124380000 0.1102350000 -2.0679180000
H 4.0470510000 0.3679430000 0.4772810000
H 2.5191420000 2.6451100000 0.9030300000
H 1.4976760000 1.5176250000 1.8216040000
H 1.1140430000 3.2508680000 1.7694010000
H 0.5133740000 3.1557080000 -0.6224560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199645 (Hartree/Particle)
Thermal correction to Energy= 0.215801
Thermal correction to Enthalpy= 0.216745
Thermal correction to Gibbs (Free) Energy= 0.155275
Sum of electronic and zero-point Energies= -749.711015
Sum of electronic and thermal Energies= -749.694859
Sum of electronic and thermal Enthalpies= -749.693915
Sum of electronic and thermal (Free) Energies= -749.755385

cTS

C 3.2676460000 0.2193780000 -0.4541530000
C 3.9771640000 -0.2129440000 -1.7121750000
C 2.0214150000 -0.1084960000 -0.1446040000
H 3.8137810000 0.8919490000 0.2076380000
H 4.2151250000 0.6543750000 -2.3413950000
H 3.3729030000 -0.9083950000 -2.2997730000
H 4.9292830000 -0.6972830000 -1.4602550000
C 0.9552150000 -0.9499880000 -0.1151060000
C -0.3347100000 -0.2843790000 -0.0929550000
C 1.0377690000 -2.4497420000 -0.0611760000
C -0.1703210000 1.1270760000 0.0554320000
O -1.4090810000 -0.9330210000 -0.3040180000
H 0.5550730000 -2.8339600000 0.8447650000
H 0.4799710000 -2.8657840000 -0.9087660000
H 2.0694050000 -2.8045410000 -0.1010100000
H -0.8352760000 1.7884720000 -0.4909710000
C 0.9916840000 1.5779750000 0.6774660000
B -2.8175980000 -0.1680000000 -0.1628520000
H 1.3472880000 2.5585240000 0.3472920000
C 1.4092790000 1.2721790000 2.1055080000
F -2.8316570000 0.7483300000 -1.1998980000
F -3.7460780000 -1.1558160000 -0.2686920000
F -2.7646240000 0.4464100000 1.0728210000
H 2.4954440000 1.3158590000 2.2399520000
H 0.9747540000 2.0522160000 2.7451710000
H 1.0371450000 0.3056060000 2.4497540000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198798 (Hartree/Particle)
Thermal correction to Energy= 0.213897
Thermal correction to Enthalpy= 0.214841
Thermal correction to Gibbs (Free) Energy= 0.156091
Sum of electronic and zero-point Energies= -749.680210
Sum of electronic and thermal Energies= -749.665111
Sum of electronic and thermal Enthalpies= -749.664166
Sum of electronic and thermal (Free) Energies= -749.722917

cPT

C -3.3141850000 0.0405760000 0.2067600000
C -1.9602680000 0.1551170000 0.1707610000
C -0.9474980000 -0.8399100000 -0.0332690000
C 0.3530170000 -0.2422100000 0.0416010000
C 0.1724280000 1.1263810000 0.2993250000
C -1.2583930000 1.4929280000 0.3917540000
C -1.0862860000 -2.3017320000 -0.2780610000
O 1.4428020000 -0.9168400000 -0.1084090000
H -1.5993760000 -2.7971900000 0.5558980000
H -0.0941270000 -2.7430560000 -0.3931060000
H -1.6719310000 -2.5008990000 -1.1841520000
B 2.8027190000 -0.1415920000 -0.0021150000
F 2.7584940000 0.8431250000 -0.9846470000
F 3.7719550000 -1.0809600000 -0.1987600000
F 2.8173660000 0.4330470000 1.2652430000
C -4.1861350000 -1.1583510000 0.0344030000
H -3.6441850000 -2.0831720000 -0.1549110000
H -4.8888510000 -0.9899810000 -0.7936610000
H -4.8068060000 -1.2963420000 0.9309530000
C -1.6640260000 2.6180190000 -0.5896640000
H -3.8626120000 0.9655600000 0.3889840000
H 0.9905590000 1.8264130000 0.4092850000
H -2.7168710000 2.8885100000 -0.4635750000
H -1.5039650000 2.3053710000 -1.6258890000
H -1.0632970000 3.5133820000 -0.4031100000
H -1.4768060000 1.8522760000 1.4129480000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201454 (Hartree/Particle)
Thermal correction to Energy= 0.216401
Thermal correction to Enthalpy= 0.217345
Thermal correction to Gibbs (Free) Energy= 0.158192
Sum of electronic and zero-point Energies= -749.725093
Sum of electronic and thermal Energies= -749.710146
Sum of electronic and thermal Enthalpies= -749.709201
Sum of electronic and thermal (Free) Energies= -749.768355

ccRT

C 3.3116600000 -0.6624070000 0.8860680000
C 4.5005450000 -0.0048040000 0.2266150000
C 2.1398500000 -0.8542310000 0.3463280000
H 3.4521870000 -1.0086130000 1.9125810000
H 4.8003970000 0.8923750000 0.7818220000
H 4.2875460000 0.2780550000 -0.8067440000
H 5.3573860000 -0.6890320000 0.2293860000
C 0.9550230000 -1.1392550000 -0.1744280000
C -0.1908160000 -0.2393380000 0.0564800000
C 0.6722670000 -2.4561140000 -0.8731550000
C -0.0633420000 1.1439390000 0.5389160000
O -1.3241680000 -0.7600020000 -0.1022460000
H 0.2283650000 -2.2818590000 -1.8590610000
H 1.5920880000 -3.0325930000 -0.9919280000
H -0.0488220000 -3.0447230000 -0.2972670000
H -0.7982220000 1.3959880000 1.2976430000
C 0.7315590000 2.1136960000 0.0549180000
B -2.8007410000 0.0094940000 0.1072290000
H 0.6272450000 3.0883110000 0.5320850000
C 1.6627370000 2.0961800000 -1.1179940000
F -2.7403090000 1.0746400000 -0.7444440000
F -3.6706380000 -0.9692540000 -0.2378860000
F -2.8047220000 0.3489430000 1.4378140000
H 2.6788420000 2.3737100000 -0.8094940000
H 1.3411490000 2.8548410000 -1.8435830000
H 1.7030090000 1.1311350000 -1.6254560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199605 (Hartree/Particle)
Thermal correction to Energy= 0.215769
Thermal correction to Enthalpy= 0.216713
Thermal correction to Gibbs (Free) Energy= 0.155213
Sum of electronic and zero-point Energies= -749.710045
Sum of electronic and thermal Energies= -749.693881
Sum of electronic and thermal Enthalpies= -749.692937
Sum of electronic and thermal (Free) Energies= -749.754437

ccTS

C 3.1324500000 -0.5890980000 -0.4305130000
C 4.0311430000 -1.6159660000 0.1983300000
C 1.9077950000 -0.2238550000 -0.0775620000
H 3.5187190000 -0.1193020000 -1.3394120000

H 4.2230660000 -2.4412670000 -0.4993250000
H 3.6155840000 -2.0341140000 1.1169930000
H 5.0050620000 -1.1688500000 0.4340080000
C 0.9102500000 0.7074130000 -0.0735020000
C -0.4239210000 0.1523770000 -0.1755620000
C 1.1130320000 2.1916230000 0.0326440000
C -0.3800770000 -1.2735330000 -0.0625440000
O -1.4263000000 0.8874490000 -0.4502450000
H 0.6156040000 2.5930020000 0.9234060000
H 2.1712000000 2.4582550000 0.0564960000
H 0.6370310000 2.6744380000 -0.8296520000
H -1.0308400000 -1.8708170000 -0.6933860000
C 0.6640000000 -1.8181730000 0.6814070000
B -2.8891040000 0.2195500000 -0.4509510000
H 0.9678310000 -2.8299450000 0.4008850000
C 0.9053850000 -1.5208080000 2.1537150000
F -2.9701110000 -0.4529380000 0.7541480000
F -3.7396560000 1.2730580000 -0.5727060000
F -2.8861130000 -0.6473610000 -1.5293050000
H 1.9473410000 -1.6626770000 2.4525410000
H 0.3009370000 -2.2346570000 2.7296500000
H 0.5856900000 -0.5138040000 2.4274420000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198677 (Hartree/Particle)
Thermal correction to Energy= 0.213803
Thermal correction to Enthalpy= 0.214747
Thermal correction to Gibbs (Free) Energy= 0.155962
Sum of electronic and zero-point Energies= -749.677523
Sum of electronic and thermal Energies= -749.662397
Sum of electronic and thermal Enthalpies= -749.661453
Sum of electronic and thermal (Free) Energies= -749.720238

ccPT

C -3.2101490000 0.7435090000 0.1077330000
C -1.9328790000 0.2849820000 0.0775520000
C -0.7757410000 1.1080860000 -0.1149160000
C 0.4182770000 0.3316820000 0.0237300000
C 0.0233430000 -0.9859090000 0.2906380000
C -1.4553530000 -1.1457800000 0.2946840000
C -0.7024220000 2.5622740000 -0.3882710000
O 1.5966670000 0.8482110000 -0.0898770000
H -1.6735420000 3.0430510000 -0.5187450000
H -0.0862960000 2.7262160000 -1.2819550000
H -0.1562260000 3.0553810000 0.4273510000
B 2.8261800000 -0.1134870000 0.0561480000
F 3.9268130000 0.6771430000 -0.1041810000
F 2.6740170000 -1.0810270000 -0.9323830000
F 2.7188290000 -0.6852370000 1.3208520000
C -4.4446260000 -0.0441090000 0.3930300000
H -4.2436340000 -1.0854390000 0.6503850000
H -5.1226640000 -0.0197150000 -0.4720860000
H -4.9975100000 0.4152940000 1.2235490000
C -1.9172000000 -2.1556680000 -0.7876310000
H -3.0013320000 -2.2969900000 -0.7671260000
H -1.4450400000 -3.1280740000 -0.6173550000
H -1.6303110000 -1.8063550000 -1.7840270000
H -1.7937110000 -1.5181530000 1.2752230000
H -3.3699690000 1.8048560000 -0.0777220000
H 0.7195540000 -1.8006400000 0.4429080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201350 (Hartree/Particle)
Thermal correction to Energy= 0.216343
Thermal correction to Enthalpy= 0.217287
Thermal correction to Gibbs (Free) Energy= 0.158268
Sum of electronic and zero-point Energies= -749.728585
Sum of electronic and thermal Energies= -749.713592
Sum of electronic and thermal Enthalpies= -749.712648
Sum of electronic and thermal (Free) Energies= -749.771667

1c

c/s RT

C -2.7310910000 -2.1411070000 -0.0420550000
C -1.4805790000 -1.9209390000 -0.3438040000
H -3.5000580000 -1.7711770000 -0.7233550000
C -3.2100910000 -2.8669230000 1.1939570000
C -0.1965970000 -1.7833220000 -0.6369870000
H -2.3735420000 -3.2013600000 1.8121680000
H -3.8093840000 -3.7414590000 0.9131880000
H -3.8505120000 -2.2128830000 1.7980220000
C 0.5775470000 -0.6276500000 -0.1350540000
C 0.5776770000 -2.8528650000 -1.3856550000
C -0.0327470000 0.6319790000 0.2835960000
O 1.8236720000 -0.8008770000 -0.0744050000
H 1.3487260000 -3.2842140000 -0.7396230000
H 1.0899260000 -2.4223480000 -2.2527660000
H -0.0926470000 -3.6458750000 -1.7237150000
C -1.1508210000 1.1434660000 -0.2615610000
H 0.5398420000 1.1988110000 1.0105100000
B 2.9460690000 0.3532180000 0.3495190000
H -1.6629730000 0.5977670000 -1.0534370000
C -1.7413940000 2.4767710000 0.0974300000
F 2.7373430000 1.3592090000 -0.5539650000
F 4.1123130000 -0.3227150000 0.2131710000
F 2.6183740000 0.6897200000 1.6418500000
C -3.2012880000 2.3073160000 0.5629050000
C -1.6512370000 3.4378800000 -1.1057010000
H -1.1580780000 2.9021110000 0.9240190000
H -3.2691940000 1.6512580000 1.4372510000
H -3.6290330000 3.2795180000 0.8320130000
H -3.8222150000 1.8786260000 -0.2338520000
H -0.6122610000 3.5871460000 -1.4158990000
H -2.2109860000 3.0479040000 -1.9650080000
H -2.0758840000 4.4135500000 -0.8438130000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256512 (Hartree/Particle)
Thermal correction to Energy= 0.275530
Thermal correction to Enthalpy= 0.276474
Thermal correction to Gibbs (Free) Energy= 0.207644
Sum of electronic and zero-point Energies= -828.288421
Sum of electronic and thermal Energies= -828.269403
Sum of electronic and thermal Enthalpies= -828.268459
Sum of electronic and thermal (Free) Energies= -828.337290

c/s TS

C -2.8144610000 -1.4733680000 0.0121920000
C -1.5427130000 -1.1435670000 -0.2012670000
H -3.6014570000 -0.8557680000 -0.4130270000
C -3.2564340000 -2.6243180000 0.8777210000
C -0.2585830000 -1.5898690000 -0.3578380000
H -2.4092860000 -3.2121440000 1.2392170000
H -3.9299900000 -3.2820120000 0.3129350000
H -3.8207800000 -2.2628050000 1.7473920000
C 0.7491810000 -0.6057270000 -0.0627130000
C 0.1287640000 -2.9429410000 -0.8817710000
C 0.1567540000 0.6674640000 0.1761620000
O 1.9863260000 -0.9178900000 0.0123080000
H 0.7891130000 -3.4288490000 -0.1530630000
H 0.7093950000 -2.8498270000 -1.8068880000
H -0.7395530000 -3.5797480000 -1.0613600000
C -1.1322520000 0.8862030000 -0.3184440000
H 0.6512720000 1.3663930000 0.8429200000
B 3.0635420000 0.2478160000 0.1728340000
H -1.3250400000 0.6845810000 -1.3738440000
C -1.9613820000 2.0343040000 0.2398920000
F 2.7793170000 1.1448980000 -0.8425170000
F 4.2664440000 -0.3778760000 0.0551080000
F 2.8272670000 0.8007550000 1.4229840000
C -3.4721260000 1.8941370000 -0.0000920000
C -1.4413660000 3.3442270000 -0.3970500000
H -1.7865490000 2.0890140000 1.3218620000
H -3.9049520000 1.0792100000 0.5863730000
H -3.9839620000 2.8176220000 0.2909380000
H -3.6942300000 1.7168420000 -1.0605590000
H -0.3723640000 3.4888110000 -0.2131730000
H -1.5984220000 3.3412680000 -1.4825670000
H -1.9810650000 4.2021980000 0.0192790000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255750 (Hartree/Particle)
Thermal correction to Energy= 0.273614
Thermal correction to Enthalpy= 0.274558
Thermal correction to Gibbs (Free) Energy= 0.209078
Sum of electronic and zero-point Energies= -828.256266

Sum of electronic and thermal Energies= -828.238401
Sum of electronic and thermal Enthalpies= -828.237457
Sum of electronic and thermal (Free) Energies= -828.302938

c/s PT

C -3.0233070000 -0.9340170000 -0.3556640000
C -1.7151220000 -0.5848660000 -0.2483920000
H -3.7064450000 -0.1458610000 -0.6675800000
C -3.6750570000 -2.2646990000 -0.1577560000
C -0.5798930000 -1.3860970000 0.1256690000
H -2.9758550000 -3.0835320000 0.0057000000
H -4.2926000000 -2.5072830000 -1.0324650000
H -4.3652610000 -2.2229720000 0.6974530000
C 0.6284360000 -0.6826770000 -0.1670800000
C -0.5301830000 -2.7437140000 0.7331290000
C 0.2660740000 0.5328130000 -0.7662650000
O 1.8103280000 -1.1452910000 0.0818160000
H -1.2999850000 -2.8839330000 1.4975970000
H 0.4605260000 -2.9042190000 1.1665560000
H -0.6792380000 -3.5174760000 -0.0339870000
C -1.1826300000 0.7933960000 -0.6507570000
H 0.9846300000 1.2022520000 -1.2187680000
B 2.9844920000 -0.1136150000 0.0061250000
H -1.6103250000 1.1381330000 -1.6043780000
C -1.4551840000 1.9226880000 0.4286250000
F 3.1147410000 0.2483670000 -1.3306900000
F 4.0734020000 -0.7521330000 0.5200320000
F 2.5682260000 0.9871720000 0.7664270000
C -2.9087650000 2.4117120000 0.3929510000
C -0.4775180000 3.0990190000 0.2696650000
H -1.2629820000 1.4544900000 1.4029670000
H -3.6232000000 1.6163560000 0.6256680000
H -3.0519390000 3.2061990000 1.1338420000
H -3.1646470000 2.8288310000 -0.5894080000
H 0.5558620000 2.7937750000 0.4624200000
H -0.5300650000 3.5310620000 -0.7382260000
H -0.7319920000 3.8925840000 0.9807770000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258871 (Hartree/Particle)
Thermal correction to Energy= 0.276237
Thermal correction to Enthalpy= 0.277182
Thermal correction to Gibbs (Free) Energy= 0.213379
Sum of electronic and zero-point Energies= -828.292554
Sum of electronic and thermal Energies= -828.275187
Sum of electronic and thermal Enthalpies= -828.274243
Sum of electronic and thermal (Free) Energies= -828.338046

cc/s RT

C -2.5326260000 2.3053060000 0.6575450000
C -1.3248000000 2.0754100000 0.2202400000
C -3.8089790000 2.0591200000 -0.1113910000
H -2.6381800000 2.6996930000 1.6705210000
C -0.0783370000 1.9281280000 -0.2021510000
H -4.3940410000 2.9837020000 -0.1835060000
H -4.4323770000 1.3194040000 0.4061310000
H -3.6083720000 1.6995320000 -1.1240510000
C 0.6678930000 0.6773530000 0.0508640000
C 0.6923910000 3.0664280000 -0.8454760000
C 0.0277080000 -0.6003660000 0.3561560000
O 1.9223240000 0.7817650000 0.0049590000
H 1.5341750000 3.3597480000 -0.2103430000
H 0.0423850000 3.9299710000 -1.0011720000
H 1.1109500000 2.7536100000 -1.8079960000
C -1.1648120000 -0.9846180000 -0.1323270000
H 0.6352230000 -1.2867340000 0.9370930000
B 3.0090560000 -0.4721080000 0.1436880000
H -1.7207180000 -0.3152850000 -0.7882770000
C -1.7890400000 -2.3297940000 0.1064540000
F 4.1948430000 0.1617440000 -0.0223140000
F 2.6506160000 -1.3273320000 -0.8623630000
F 2.7914850000 -0.9749430000 1.4047670000
C -3.1813140000 -2.1690530000 0.7489490000
C -1.8772450000 -3.1163610000 -1.2174360000
H -1.1479000000 -2.8897640000 0.7990780000
H -3.8572940000 -1.6095110000 0.0899620000
H -3.6311550000 -3.1515050000 0.9307060000
H -3.1218880000 -1.6391260000 1.7055910000
H -2.5005010000 -2.5879310000 -1.9497060000
H -0.8858260000 -3.2629280000 -1.6574090000
H -2.3258730000 -4.1009940000 -1.0440880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256474 (Hartree/Particle)
Thermal correction to Energy= 0.275482
Thermal correction to Enthalpy= 0.276427
Thermal correction to Gibbs (Free) Energy= 0.207716
Sum of electronic and zero-point Energies= -828.288351
Sum of electronic and thermal Energies= -828.269342
Sum of electronic and thermal Enthalpies= -828.268398
Sum of electronic and thermal (Free) Energies= -828.337108

cc/s TS

C -2.6215060000 1.8681300000 0.3781010000
C -1.4188680000 1.3422910000 0.1259600000
C -3.9428960000 1.5534800000 -0.2539900000
H -2.6419320000 2.6566260000 1.1359670000
C -0.1075760000 1.7261670000 -0.0009590000
H -4.3368070000 2.4720840000 -0.7100610000
H -4.6858100000 1.2295440000 0.4849800000
H -3.8657840000 0.7943020000 -1.0335400000
C 0.8475780000 0.6555400000 0.0749490000
C 0.3460300000 3.1246400000 -0.3049280000
C 0.1857060000 -0.5967090000 0.1835970000
O 2.1066580000 0.8771830000 0.1070670000
H 1.2239660000 3.3509840000 0.3100710000
H -0.4369590000 3.8624190000 -0.1177610000
H 0.6708150000 3.2112240000 -1.3495130000
C -1.1526400000 -0.6816340000 -0.2224680000
H 0.6760890000 -1.4046500000 0.7170800000
B 3.1038410000 -0.3638400000 0.0262060000
H -1.4070220000 -0.3889290000 -1.2430610000
C -1.9548860000 -1.8693000000 0.3071060000
F 4.3384980000 0.1942550000 -0.1023100000
F 2.6850170000 -1.0938570000 -1.0737850000
F 2.9156960000 -1.0688480000 1.2062110000
C -3.4758460000 -1.6850280000 0.3386220000
C -1.5873100000 -3.1034070000 -0.5488840000
H -1.6200700000 -2.0575660000 1.3351720000
H -3.8799850000 -1.4846800000 -0.6607380000
H -3.9480520000 -2.6039650000 0.7026440000
H -3.7735490000 -0.8714860000 1.0048410000
H -1.8994080000 -2.9634330000 -1.5912290000
H -0.5102740000 -3.2969410000 -0.5442250000
H -2.0972900000 -3.9927680000 -0.1618650000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255811 (Hartree/Particle)
Thermal correction to Energy= 0.273510
Thermal correction to Enthalpy= 0.274454
Thermal correction to Gibbs (Free) Energy= 0.209336
Sum of electronic and zero-point Energies= -828.250466
Sum of electronic and thermal Energies= -828.232767
Sum of electronic and thermal Enthalpies= -828.231823
Sum of electronic and thermal (Free) Energies= -828.296941

cc/s PT

C 2.7825220000 1.5682430000 0.1788760000
C 1.5991840000 0.9081120000 0.1137750000
C 4.0847630000 1.0790770000 0.7209780000
H 2.7856610000 2.6092100000 -0.1424660000
C 0.3604090000 1.5355550000 -0.2659970000
H 4.4177280000 1.7437990000 1.5299480000
H 4.8674250000 1.1240540000 -0.0491910000
H 4.0372780000 0.0611480000 1.1095490000
C -0.7424180000 0.7054960000 0.0961200000
C 0.1434470000 2.8612700000 -0.8926130000
C -0.2095170000 -0.4165070000 0.7419530000
O -1.9779900000 1.0170350000 -0.1314150000
H -0.4862050000 2.7326170000 -1.7826990000
H 1.0633250000 3.3798980000 -1.1682620000
H -0.4456090000 3.4944880000 -0.2153470000
C 1.2624600000 -0.5101330000 0.5714170000
H -0.8207140000 -1.1508680000 1.2480090000
B -3.0245860000 -0.1254240000 0.0770980000
H 1.7692700000 -0.7903920000 1.5050480000

C 1.5826280000 -1.6196100000 -0.5170180000
F -4.2053520000 0.3604630000 -0.4012680000
F -3.0385080000 -0.4132240000 1.4386950000
F -2.5364630000 -1.2228830000 -0.6435550000
C 3.0811370000 -1.9167430000 -0.6375250000
C 0.7860940000 -2.9081350000 -0.2507800000
H 1.2336400000 -1.2015690000 -1.4705980000
H 3.4955050000 -2.2859620000 0.3094120000
H 3.2424040000 -2.6969430000 -1.3898550000
H 3.6551380000 -1.0391280000 -0.9479280000
H 0.9819890000 -3.3006790000 0.7556290000
H -0.2912330000 -2.7460230000 -0.3568510000
H 1.0798940000 -3.6817650000 -0.9685400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258860 (Hartree/Particle)
Thermal correction to Energy= 0.276202
Thermal correction to Enthalpy= 0.277146
Thermal correction to Gibbs (Free) Energy= 0.213475
Sum of electronic and zero-point Energies= -828.294058
Sum of electronic and thermal Energies= -828.276716
Sum of electronic and thermal Enthalpies= -828.275772
Sum of electronic and thermal (Free) Energies= -828.339443

c/d RT

C -3.3993540000 -1.2359070000 0.0715010000
C -2.1500390000 -1.4160630000 -0.2602100000
H -4.0416370000 -0.6808070000 -0.6153480000
C -4.0373200000 -1.7305360000 1.3491400000
C -0.8930860000 -1.6836840000 -0.5796540000
H -3.3217260000 -2.2746930000 1.9701650000
H -4.8793560000 -2.3952520000 1.1212330000
H -4.4338400000 -0.8890040000 1.9299920000
C 0.2057660000 -0.7939030000 -0.1467600000
C -0.4973940000 -2.9669020000 -1.2871470000
C 0.0149480000 0.6059180000 0.2238270000
O 1.3447580000 -1.3305650000 -0.1000870000
H 0.1283590000 -3.5823420000 -0.6332270000
H 0.0938500000 -2.7470490000 -2.1825310000
H -1.3841920000 -3.5354800000 -1.5749170000
C -0.9128130000 1.4045780000 -0.3341560000
H 0.7516860000 0.9952830000 0.9164130000
B 2.7693860000 -0.5513370000 0.2573400000
H -1.5763350000 0.9922770000 -1.0925830000
C -1.0936950000 2.8742820000 -0.0668770000
F 2.8434850000 0.4460760000 -0.6769800000
F 3.6791450000 -1.5464220000 0.1227390000
F 2.5953870000 -0.0946270000 1.5429800000
C -0.9311890000 3.6618710000 -1.3864130000
C -0.1911420000 3.4351000000 1.0373720000
H -2.1438430000 2.9948020000 0.2494030000
H -1.6022200000 3.2857450000 -2.1672950000
H -1.1590610000 4.7212350000 -1.2265990000
H 0.0968530000 3.5852860000 -1.7572370000
H -0.3314010000 2.9030490000 1.9844380000
H 0.8667320000 3.3620220000 0.7606620000
H -0.4191160000 4.4923640000 1.2090420000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256695 (Hartree/Particle)
Thermal correction to Energy= 0.275574
Thermal correction to Enthalpy= 0.276519
Thermal correction to Gibbs (Free) Energy= 0.208189
Sum of electronic and zero-point Energies= -828.287559
Sum of electronic and thermal Energies= -828.268679
Sum of electronic and thermal Enthalpies= -828.267735
Sum of electronic and thermal (Free) Energies= -828.336064

c/d TS

C -2.8996630000 -1.3831200000 -0.0800560000
C -1.6063350000 -1.1815500000 -0.3017480000
H -3.6262190000 -0.7507750000 -0.5900330000
C -3.4519060000 -2.3854190000 0.9004680000
C -0.3239110000 -1.6463320000 -0.3680190000
H -2.6610250000 -2.9856320000 1.3567550000
H -4.1575730000 -3.0570810000 0.3945750000
H -4.0089500000 -1.8810190000 1.7005680000
C 0.6797140000 -0.6427440000 -0.1088270000
C 0.0736980000 -3.0412480000 -0.7587810000
C 0.0909930000 0.6543740000 -0.0043990000
O 1.9053550000 -0.9585740000 0.0591390000
H 0.6794910000 -3.4758230000 0.0457980000
H 0.7102050000 -3.0292960000 -1.6509700000
H -0.7934200000 -3.6796040000 -0.9393800000
C -1.1559050000 0.8318150000 -0.6015720000
H 0.5525530000 1.3918220000 0.6429990000
B 2.9921910000 0.2060100000 0.1871280000
H -1.2748530000 0.5095820000 -1.6364540000
C -2.1151590000 1.9377390000 -0.2093680000
F 2.7850110000 1.0148000000 -0.9155880000
F 4.1880480000 -0.4431200000 0.1983540000
F 2.6883700000 0.8641360000 1.3697890000
C -1.8111810000 3.2011870000 -1.0451630000
C -2.1235470000 2.2396200000 1.2948650000
H -3.1205610000 1.5972760000 -0.4968940000
H -1.8421200000 2.9921310000 -2.1203220000
H -2.5494820000 3.9816100000 -0.8305160000
H -0.8177420000 3.5973370000 -0.8080180000
H -2.3209920000 1.3357100000 1.8814500000
H -1.1661190000 2.6554080000 1.6277510000
H -2.8998220000 2.9754400000 1.5305680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255582 (Hartree/Particle)
Thermal correction to Energy= 0.273532
Thermal correction to Enthalpy= 0.274477
Thermal correction to Gibbs (Free) Energy= 0.208906
Sum of electronic and zero-point Energies= -828.259372
Sum of electronic and thermal Energies= -828.241422
Sum of electronic and thermal Enthalpies= -828.240477
Sum of electronic and thermal (Free) Energies= -828.306048

c/d PT

C -3.1610620000 -0.6427510000 -0.2976460000
C -1.8177740000 -0.4434600000 -0.3251800000
H -3.7746430000 0.2317790000 -0.5181170000
C -3.9417970000 -1.8866620000 -0.0269650000
C -0.7371820000 -1.3455000000 -0.0424420000
H -3.3300040000 -2.7809590000 0.0826140000
H -4.6610420000 -2.0560660000 -0.8393770000
H -4.5422750000 -1.7620030000 0.8858860000
C 0.5119760000 -0.7013190000 -0.3065910000
C -0.7713870000 -2.7420070000 0.4715690000
C 0.2295500000 0.5747350000 -0.8178860000
O 1.6613750000 -1.2525280000 -0.0862650000
H -1.4473810000 -2.8450000000 1.3269770000
H 0.2378930000 -3.0407800000 0.7644070000
H -1.1188790000 -3.4368440000 -0.3057920000
C -1.2095500000 0.8929870000 -0.7456420000
H 0.9986100000 1.2396430000 -1.1891540000
B 2.8844440000 -0.2828120000 0.0129850000
H -1.5935330000 1.1887440000 -1.7357970000
C -1.5188440000 2.0942700000 0.2264600000
F 3.0785930000 0.2569720000 -1.2554820000
F 3.9252060000 -1.0423310000 0.4579700000
F 2.4937550000 0.7182970000 0.9107370000
C -1.0070450000 3.4123190000 -0.3711950000
C -0.9552830000 1.8621120000 1.6350300000
H -2.6139580000 2.1587490000 0.2905470000
H -1.4052810000 3.5843270000 -1.3783870000
H -1.3136590000 4.2552480000 0.2578080000
H 0.0871730000 3.4287810000 -0.4295040000
H -1.3532020000 0.9462190000 2.0863650000
H 0.1375350000 1.7800270000 1.6216150000
H -1.2281640000 2.6976370000 2.2890120000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258646 (Hartree/Particle)
Thermal correction to Energy= 0.276079
Thermal correction to Enthalpy= 0.277023
Thermal correction to Gibbs (Free) Energy= 0.213184
Sum of electronic and zero-point Energies= -828.296268
Sum of electronic and thermal Energies= -828.278836
Sum of electronic and thermal Enthalpies= -828.277892
Sum of electronic and thermal (Free) Energies= -828.341731

cc/d RT

C 2.7832020000 -2.0130100000 0.7388960000
C 1.5488300000 -1.9398750000 0.3218380000
C 4.0137600000 -1.7987280000 -0.1100130000
H 2.9485640000 -2.2386470000 1.7946180000
C 0.2827780000 -1.9514680000 -0.0663420000
H 4.6635430000 -2.6809820000 -0.0673310000
H 4.5959320000 -0.9479280000 0.2652530000
H 3.7563800000 -1.6119450000 -1.1559210000
C -0.5534470000 -0.7361610000 0.0276630000
C -0.4130150000 -3.2291190000 -0.4991900000
C -0.0140520000 0.6194080000 0.1091660000
O -1.7963860000 -0.9410380000 0.0515790000
H -1.2095960000 -3.4840450000 0.2068390000
H 0.2992450000 -4.0552770000 -0.5502810000
H -0.8833100000 -3.0992100000 -1.4797300000
C 1.1240860000 1.0120510000 -0.4904250000
H -0.6628660000 1.3314360000 0.6049190000
B -2.9744090000 0.2338870000 0.0619250000
H 1.7058010000 0.2817430000 -1.0507030000
C 1.6789550000 2.4114020000 -0.5054990000
F -4.1105120000 -0.5034210000 0.0286840000
F -2.7159420000 0.9707600000 -1.0621340000
F -2.7611140000 0.9194210000 1.2348580000
C 0.8112020000 3.4466190000 0.2182590000
C 3.1245300000 2.4001440000 0.0408610000
H 1.7434310000 2.6987110000 -1.5679110000
H 0.7300280000 3.2200460000 1.2879270000
H 1.2555560000 4.4428890000 0.1223040000
H -0.2006370000 3.4865800000 -0.1978090000
H 3.1363920000 2.1255780000 1.1019280000
H 3.7566240000 1.6879960000 -0.5023800000
H 3.5751710000 3.3935150000 -0.0579370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256699 (Hartree/Particle)
Thermal correction to Energy= 0.275556
Thermal correction to Enthalpy= 0.276500
Thermal correction to Gibbs (Free) Energy= 0.208349
Sum of electronic and zero-point Energies= -828.287260
Sum of electronic and thermal Energies= -828.268404
Sum of electronic and thermal Enthalpies= -828.267459
Sum of electronic and thermal (Free) Energies= -828.335610

cc/d TS

C 2.5498260000 1.7697310000 -0.4161870000
C 1.3389530000 1.3140830000 -0.0925950000
C 3.8723990000 1.4323670000 0.2027120000
H 2.5858840000 2.4698240000 -1.2554400000
C 0.0187230000 1.6729410000 -0.0152600000
H 4.3920380000 2.3609350000 0.4717400000
H 4.5259750000 0.9016900000 -0.5022710000
H 3.7661630000 0.8287450000 1.1057240000
C -0.9061730000 0.5719730000 -0.0375610000
C -0.4779070000 3.0769940000 0.1730570000
C -0.2134090000 -0.6708380000 -0.0143630000
O -2.1671510000 0.7605810000 -0.1294650000
H -0.9302950000 3.2013560000 1.1645650000
H -1.2761960000 3.2674550000 -0.5537020000
H 0.3164160000 3.8152550000 0.0474180000
C 1.1070360000 -0.6791680000 0.4510340000
H -0.6704930000 -1.5397200000 -0.4765140000
B -3.1464620000 -0.4906500000 0.0158500000
H 1.3060910000 -0.2562050000 1.4361190000
C 2.0147830000 -1.8398960000 0.0442680000
F -4.3949440000 0.0510100000 0.0276000000
F -2.7735530000 -1.1051500000 1.1983560000
F -2.8842690000 -1.2960670000 -1.0832000000
C 2.5261500000 -1.7233300000 -1.4040500000
C 3.1489250000 -2.1133050000 1.0415680000
H 1.3519010000 -2.7182630000 0.0683630000
H 3.2380710000 -0.8990400000 -1.5133560000
H 3.0333640000 -2.6480670000 -1.6997760000
H 1.7008120000 -1.5520190000 -2.1030990000
H 3.9051300000 -1.3217260000 1.0324410000
H 2.7670990000 -2.2086830000 2.0646190000
H 3.6566220000 -3.0503800000 0.7891060000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255418 (Hartree/Particle)
Thermal correction to Energy= 0.273326
Thermal correction to Enthalpy= 0.274270
Thermal correction to Gibbs (Free) Energy= 0.208966
Sum of electronic and zero-point Energies= -828.252765
Sum of electronic and thermal Energies= -828.234857
Sum of electronic and thermal Enthalpies= -828.233913
Sum of electronic and thermal (Free) Energies= -828.299218

cc/d PT

C -2.7722350000 1.4765420000 -0.0970810000
C -1.5810770000 0.8276090000 -0.1562580000
C -4.0952190000 1.0438380000 -0.6342240000
H -2.7684680000 2.4700860000 0.3499090000
C -0.3389810000 1.4376560000 0.2361680000
H -4.4779970000 1.8101800000 -1.3220940000
H -4.8351160000 0.9670460000 0.1748190000
H -4.0584120000 0.0911920000 -1.1625240000
C 0.7625020000 0.6505450000 -0.2153510000
C -0.1145630000 2.7077800000 0.9667770000
C 0.2279580000 -0.4374490000 -0.9142350000
O 1.9973780000 0.9604990000 0.0243780000
H 0.6083430000 2.5266950000 1.7720790000
H -1.0226200000 3.1523740000 1.3780020000
H 0.3740070000 3.4326820000 0.3008610000
C -1.2479050000 -0.5256250000 -0.7809910000
H 0.8401250000 -1.1758040000 -1.4176630000
B 3.0394090000 -0.1922910000 -0.1160220000
H -1.7365620000 -0.6475580000 -1.7586120000
C -1.5893380000 -1.8200040000 0.0702860000
F 4.2223700000 0.3181120000 0.3314610000
F 3.0582120000 -0.5665880000 -1.4578350000
F 2.5455050000 -1.2388280000 0.6727080000
C -0.9318170000 -1.8094210000 1.4582040000
C -3.0926080000 -2.1028050000 0.1668240000
H -1.1411060000 -2.6416200000 -0.5048330000
H -1.2935130000 -0.9700200000 2.0656190000
H -1.1876530000 -2.7313070000 1.9920310000
H 0.1589830000 -1.7449870000 1.3996470000
H -3.6067960000 -1.3568220000 0.7826060000
H -3.5720850000 -2.1310340000 -0.8188390000
H -3.2522750000 -3.0798830000 0.6363680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258878 (Hartree/Particle)
Thermal correction to Energy= 0.276180
Thermal correction to Enthalpy= 0.277124
Thermal correction to Gibbs (Free) Energy= 0.213763
Sum of electronic and zero-point Energies= -828.295334
Sum of electronic and thermal Energies= -828.278032
Sum of electronic and thermal Enthalpies= -828.277088
Sum of electronic and thermal (Free) Energies= -828.340449

c/u RT

C -2.9531190000 -1.8776520000 0.0411540000
C -1.6799210000 -1.8220260000 -0.2402390000
H -3.6658510000 -1.5646270000 -0.7245930000
C -3.5304740000 -2.3363650000 1.3603100000
C -0.3813750000 -1.8491850000 -0.4980340000
H -2.7454990000 -2.6315840000 2.0606800000
H -4.2008510000 -3.1904610000 1.2056680000
H -4.1231220000 -1.5351850000 1.8182100000
C 0.4834500000 -0.6971440000 -0.1639680000
C 0.3093840000 -3.0944940000 -1.0234430000
C -0.0128840000 0.6656570000 0.0105810000
O 1.7058050000 -0.9669690000 -0.0213200000
H 1.0189560000 -3.4751920000 -0.2821620000
H 0.8828790000 -2.8647910000 -1.9278570000
H -0.4228320000 -3.8717020000 -1.2521440000
C -1.0590540000 1.1711880000 -0.6673460000
H 0.5957420000 1.2888150000 0.6546870000
B 2.9159000000 0.1379900000 0.2653450000
H -1.5933050000 0.5312160000 -1.3676620000
C -1.5669580000 2.5856920000 -0.5879310000
F 2.8249290000 1.0083790000 -0.7869130000
F 4.0197250000 -0.6474940000 0.2801840000
F 2.5852540000 0.6975770000 1.4773510000
C -0.7623130000 3.4989340000 0.3430880000

C -3.0669090000 2.5731510000 -0.2161250000
H -1.4968320000 2.9893390000 -1.6114300000
H 0.2925350000 3.5419160000 0.0532590000
H -1.1634890000 4.5173590000 0.3100870000
H -0.8152150000 3.1539480000 1.3824840000
H -3.6491630000 1.9477440000 -0.9029020000
H -3.2118180000 2.1880530000 0.7997650000
H -3.4762130000 3.5882600000 -0.2561360000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256708 (Hartree/Particle)
Thermal correction to Energy= 0.275590
Thermal correction to Enthalpy= 0.276534
Thermal correction to Gibbs (Free) Energy= 0.208203
Sum of electronic and zero-point Energies= -828.287375
Sum of electronic and thermal Energies= -828.268493
Sum of electronic and thermal Enthalpies= -828.267549
Sum of electronic and thermal (Free) Energies= -828.335879

c/u TS

C 2.7396630000 1.4034200000 -0.0195060000
C 1.4614950000 1.1224460000 -0.2548190000
H 3.5115620000 0.8402280000 -0.5395690000
C 3.2117960000 2.4185850000 0.9890450000
C 0.1663110000 1.5519240000 -0.3189960000
H 2.3780120000 2.9589260000 1.4437050000
H 3.8829450000 3.1419390000 0.5080600000
H 3.7863740000 1.9342800000 1.7894070000
C -0.8141190000 0.5178720000 -0.0990040000
C -0.2648650000 2.9454230000 -0.6778030000
C -0.1977080000 -0.7657580000 -0.0308880000
O -2.0498940000 0.7998730000 0.0599660000
H 0.5854240000 3.6149690000 -0.8212730000
H -0.9014700000 3.3364960000 0.1252430000
H -0.8818490000 2.9405330000 -1.5837720000
C 1.0694670000 -0.9010050000 -0.6010090000
H -0.6603230000 -1.5456890000 0.5650080000
B -3.1120440000 -0.3906580000 0.1329720000
H 1.2106620000 -0.5521580000 -1.6241640000
C 1.9910610000 -2.0429300000 -0.1936600000
F -2.8777840000 -1.1525550000 -0.9973410000
F -4.3217390000 0.2323830000 0.1568530000
F -2.8061560000 -1.0874400000 1.2930550000
C 2.3401300000 -2.0276360000 1.3049820000
C 3.2451380000 -2.1392820000 -1.0752950000
H 1.3964880000 -2.9521330000 -0.3793360000
H 1.4403090000 -2.0003010000 1.9278140000
H 2.9063330000 -2.9260710000 1.5729680000
H 2.9513090000 -1.1539750000 1.5567650000
H 2.9876490000 -2.1586340000 -2.1405880000
H 3.9268570000 -1.2978510000 -0.9057990000
H 3.7999860000 -3.0561050000 -0.8504250000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255394 (Hartree/Particle)
Thermal correction to Energy= 0.273376
Thermal correction to Enthalpy= 0.274320
Thermal correction to Gibbs (Free) Energy= 0.208844
Sum of electronic and zero-point Energies= -828.256988
Sum of electronic and thermal Energies= -828.239006
Sum of electronic and thermal Enthalpies= -828.238062
Sum of electronic and thermal (Free) Energies= -828.303538

c/u PT

C 2.9748760000 0.8986290000 -0.3623560000
C 1.6628840000 0.5433570000 -0.3364520000
H 3.6688380000 0.1375890000 -0.7147480000
C 3.6231400000 2.1981960000 -0.0113050000
C 0.5125160000 1.3136670000 0.0517860000
H 2.9234940000 3.0013450000 0.2143220000
H 4.2687640000 2.5226890000 -0.8381290000
H 4.2876580000 2.0641240000 0.8546680000
C -0.6830840000 0.6076080000 -0.2878940000
C 0.4333470000 2.6408680000 0.7205560000
C -0.3002510000 -0.5791890000 -0.9297820000
O -1.8707970000 1.0445730000 -0.0171800000
H 0.6503630000 3.4498560000 0.0083940000
H 1.1466110000 2.7292060000 1.5458760000
H -0.5834010000 2.7917710000 1.0918150000
C 1.1581970000 -0.7977790000 -0.8690170000
H -1.0113170000 -1.2732580000 -1.3610930000
B -3.0149510000 -0.0196950000 -0.0080750000
H 1.5732140000 -0.9962100000 -1.8699370000
C 1.4695940000 -2.0808380000 0.0030680000
F -3.1639690000 -0.4691970000 -1.3174500000
F -4.1129200000 0.6191900000 0.4866020000
F -2.5511020000 -1.0566720000 0.8110230000
C 0.9039910000 -1.9835800000 1.4268200000
C 2.9608520000 -2.4428820000 0.0099030000
H 0.9390580000 -2.8917700000 -0.5144050000
H -0.1803560000 -1.8343900000 1.4300250000
H 1.1216560000 -2.9073090000 1.9743900000
H 1.3646200000 -1.1577690000 1.9833130000
H 3.3847820000 -2.4660110000 -1.0016540000
H 3.5441320000 -1.7384860000 0.6135600000
H 3.0985640000 -3.4377070000 0.4478860000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258949 (Hartree/Particle)
Thermal correction to Energy= 0.276251
Thermal correction to Enthalpy= 0.277195
Thermal correction to Gibbs (Free) Energy= 0.213787
Sum of electronic and zero-point Energies= -828.294114
Sum of electronic and thermal Energies= -828.276811
Sum of electronic and thermal Enthalpies= -828.275867
Sum of electronic and thermal (Free) Energies= -828.339275

cc/u RT

C -2.9689310000 -1.9326880000 -0.7997600000
C -1.7567150000 -1.8979670000 -0.3178140000
C -4.2210190000 -1.5172080000 -0.0644260000
H -3.0960750000 -2.2823860000 -1.8265640000
C -0.5177050000 -1.9485000000 0.1469750000
H -4.9320480000 -2.3509890000 -0.0225640000
H -4.7190270000 -0.6924050000 -0.5889420000
H -4.0032120000 -1.1999700000 0.9587810000
C 0.4128140000 -0.8161540000 -0.0464410000
C 0.0535060000 -3.2039410000 0.7802560000
C -0.0201600000 0.5501420000 -0.3291630000
O 1.6362440000 -1.1071650000 0.0311570000
H 0.8645810000 -3.6033580000 0.1632810000
H -0.7218500000 -3.9649940000 0.8902490000
H 0.4795500000 -2.9804110000 1.7641460000
C -1.1565970000 1.0890000000 0.1479240000
H 0.7005940000 1.1475930000 -0.8747610000
B 2.8972660000 -0.0257550000 -0.0469290000
H -1.8101520000 0.4786060000 0.7692000000
C -1.6024200000 2.5156440000 -0.0283870000
F 3.9723190000 -0.8290720000 0.1393440000
F 2.6376530000 0.8568510000 0.9664720000
F 2.7964590000 0.5266730000 -1.3024240000
C -1.7726000000 3.1771970000 1.3576660000
C -0.7034290000 3.3533580000 -0.9441610000
H -2.6064100000 2.4633830000 -0.4827270000
H -0.8056820000 3.2625180000 1.8656320000
H -2.1918640000 4.1832710000 1.2491920000
H -2.4444010000 2.5987980000 2.0024520000
H 0.3033900000 3.4580260000 -0.5242190000
H -0.6108440000 2.9065540000 -1.9398730000
H -1.1211880000 4.3584760000 -1.0644340000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256665 (Hartree/Particle)
Thermal correction to Energy= 0.275542
Thermal correction to Enthalpy= 0.276486
Thermal correction to Gibbs (Free) Energy= 0.208211
Sum of electronic and zero-point Energies= -828.287443
Sum of electronic and thermal Energies= -828.268566
Sum of electronic and thermal Enthalpies= -828.267622
Sum of electronic and thermal (Free) Energies= -828.335897

cc/u TS

C -3.3161190000 -0.0096690000 0.8790030000
C -2.1183280000 0.1175060000 0.3114090000
C -4.5564230000 -0.6150850000 0.2889990000
H -3.4027060000 0.3429810000 1.9101250000

C -0.9820480000 0.8684620000 0.1975140000
H -5.3881420000 0.0946630000 0.3835930000
H -4.8562180000 -1.5230360000 0.8290370000
H -4.4403290000 -0.8571600000 -0.7697850000
C 0.1839670000 0.1291280000 -0.2181740000
C -0.9092780000 2.3554520000 0.3938520000
C -0.1557830000 -1.2177780000 -0.5375790000
O 1.3465400000 0.6574660000 -0.2011180000
H -0.1062630000 2.5777440000 1.1067390000
H -1.8494860000 2.7664540000 0.7662890000
H -0.6381350000 2.8601430000 -0.5410470000
C -1.4881830000 -1.4840240000 -0.8577570000
H 0.5801890000 -1.9970870000 -0.3725040000
B 2.5747550000 -0.1620900000 -0.8107460000
H -1.9537680000 -0.8800160000 -1.6372340000
C -2.0730920000 -2.8803200000 -0.7361030000
F 3.6154580000 0.7142750000 -0.7874980000
F 2.1647170000 -0.5373590000 -2.0774320000
F 2.7343420000 -1.2602530000 0.0219910000
C -1.7149570000 -3.6923090000 -2.0013570000
C -1.6478220000 -3.6112660000 0.5452060000
H -3.1647200000 -2.7739170000 -0.7209280000
H -0.6322510000 -3.8400400000 -2.0791750000
H -2.1914780000 -4.6781490000 -1.9630920000
H -2.0514380000 -3.1884800000 -2.9143510000
H -0.5716970000 -3.8160640000 0.5566350000
H -1.8880380000 -3.0227590000 1.4374520000
H -2.1651030000 -4.5737480000 0.6218730000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255589 (Hartree/Particle)
Thermal correction to Energy= 0.273467
Thermal correction to Enthalpy= 0.274411
Thermal correction to Gibbs (Free) Energy= 0.209117
Sum of electronic and zero-point Energies= -828.257041
Sum of electronic and thermal Energies= -828.239163
Sum of electronic and thermal Enthalpies= -828.238219
Sum of electronic and thermal (Free) Energies= -828.303512

cc/u PT

C 2.9186070000 -1.4408760000 -0.1073070000
C 1.6869570000 -0.8797170000 -0.2030570000
C 4.2297700000 -0.7999090000 -0.4194750000
H 2.9760300000 -2.4805440000 0.2128020000
C 0.4549770000 -1.5664290000 0.0614860000
H 4.7752180000 -1.4016870000 -1.1590330000
H 4.8650740000 -0.7729280000 0.4773310000
H 4.1326780000 0.2159020000 -0.8068770000
C -0.6539250000 -0.7268780000 -0.2624320000
C 0.2460410000 -2.9378770000 0.5833720000
C -0.1323620000 0.4599580000 -0.7923680000
O -1.8859330000 -1.0754240000 -0.0709370000
H -0.4262980000 -2.8891700000 1.4496710000
H 1.1667080000 -3.4544530000 0.8607220000
H -0.2935780000 -3.5345650000 -0.1645950000
C 1.3435230000 0.5307630000 -0.6673150000
H -0.7574440000 1.2454900000 -1.1965510000
B -2.9361560000 0.0814130000 -0.0633390000
H 1.8125310000 0.7443870000 -1.6402010000
C 1.7854950000 1.6839370000 0.3161530000
F -4.1114040000 -0.4861920000 0.3318940000
F -2.9688650000 0.6101270000 -1.3514240000
F -2.4394750000 1.0308970000 0.8377210000
C 1.5221810000 3.0574190000 -0.3175710000
C 1.1160220000 1.5664040000 1.6929640000
H 2.8700170000 1.5783970000 0.4480170000
H 0.4497140000 3.2468270000 -0.4381280000
H 1.9236450000 3.8504950000 0.3227720000
H 1.9976280000 3.1497150000 -1.3015990000
H 0.0266400000 1.6625000000 1.6226200000
H 1.3364880000 0.6053530000 2.1716300000
H 1.4871730000 2.3563380000 2.3552020000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258523 (Hartree/Particle)
Thermal correction to Energy= 0.276040
Thermal correction to Enthalpy= 0.276984
Thermal correction to Gibbs (Free) Energy= 0.212857
Sum of electronic and zero-point Energies= -828.299480
Sum of electronic and thermal Energies= -828.281963
Sum of electronic and thermal Enthalpies= -828.281018
Sum of electronic and thermal (Free) Energies= -828.345146

1d

cRT

C -0.3165670000 3.6186500000 0.2280920000
C -1.0297140000 2.5951730000 -0.1565810000
C -1.8222960000 1.5996900000 -0.5213120000
C -1.5006270000 0.1989890000 -0.1646700000
C -0.1552970000 -0.2782720000 0.1059070000
C 0.9593510000 0.2702300000 -0.4326100000
H -0.1114040000 -1.1767480000 0.7095190000
C -3.1614270000 1.8426860000 -1.1936860000
O -2.4967240000 -0.5740560000 -0.0904240000
H -3.2867880000 2.9022270000 -1.4266150000
H -3.9770500000 1.5184600000 -0.5399440000
H -3.2402550000 1.2605190000 -2.1181850000
B -2.4386290000 -2.2050120000 0.1727730000
F -3.7495440000 -2.5497860000 0.1441110000
F -1.8350980000 -2.3399810000 1.4045790000
F -1.6804110000 -2.6821040000 -0.8623310000
C -0.4651160000 4.3300820000 1.5530900000
H 0.4557950000 3.9948340000 -0.4460930000
H -1.2613480000 3.8890950000 2.1575930000
H -0.6941230000 5.3906020000 1.3924730000
H 0.4717780000 4.2806730000 2.1210870000
H 0.8476010000 1.1205960000 -1.1003660000
C 2.3319450000 -0.1858960000 -0.2445130000
C 3.3649390000 0.5023840000 -0.9094500000
C 2.6742170000 -1.2807340000 0.5752560000
C 4.6947850000 0.1178180000 -0.7608260000
C 5.0165720000 -0.9671380000 0.0564110000
C 4.0019270000 -1.6641950000 0.7219600000
H 3.1138400000 1.3457310000 -1.5485020000
H 5.4777690000 0.6609580000 -1.2822950000
H 6.0526160000 -1.2724870000 0.1736380000
H 4.2497560000 -2.5114690000 1.3548470000
H 1.8980730000 -1.8354380000 1.0927270000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.253047 (Hartree/Particle)
Thermal correction to Energy= 0.272289
Thermal correction to Enthalpy= 0.273233
Thermal correction to Gibbs (Free) Energy= 0.202903
Sum of electronic and zero-point Energies= -941.406301
Sum of electronic and thermal Energies= -941.387058
Sum of electronic and thermal Enthalpies= -941.386114
Sum of electronic and thermal (Free) Energies= -941.456444

cTS

C 3.4242860000 -0.4801840000 0.1527170000
C 2.1624560000 -0.2125420000 -0.1613580000
C 1.1236540000 0.6703360000 -0.2641230000
C -0.1786350000 0.0630380000 -0.1335740000
C -0.0821200000 -1.3573090000 -0.1143030000
C 1.0993060000 -1.9150370000 -0.6310040000
C 1.2541440000 2.1329290000 -0.5774990000
O -1.2313250000 0.7784120000 -0.0074490000
H 2.2970630000 2.4422470000 -0.6702930000
H 0.7760530000 2.7098040000 0.2237990000
H 0.7145100000 2.3827860000 -1.4983290000
H -0.8458200000 -1.9437160000 0.3832420000
B -2.6581490000 0.0689000000 -0.0406460000
F -3.5519940000 1.0955730000 -0.0081630000
F -2.6920920000 -0.7498320000 1.0802210000
F -2.6697830000 -0.6681670000 -1.2108390000
H 3.9136380000 -1.3278520000 -0.3267660000
C 4.2124740000 0.2392300000 1.2149080000
H 3.6560180000 1.0786090000 1.6389420000
H 5.1544900000 0.6151480000 0.7949890000
H 4.4779300000 -0.4476240000 2.0291800000
H 1.4007940000 -1.6211680000 -1.6364100000
C 1.6050360000 -3.2382360000 -0.2302300000
C 2.3980540000 -3.9797120000 -1.1228130000
C 1.3261120000 -3.7788300000 1.0377980000
C 2.8845850000 -5.2362770000 -0.7674860000

H 2.6177500000 -3.5723230000 -2.1073110000
C 1.8087820000 -5.0355110000 1.3906950000
H 0.7348550000 -3.2060910000 1.7469180000
C 2.5885850000 -5.7671200000 0.4895420000
H 3.4887210000 -5.8020070000 -1.4709980000
H 1.5822220000 -5.4445180000 2.3711540000
H 2.9664420000 -6.7466580000 0.7688840000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.251856 (Hartree/Particle)
Thermal correction to Energy= 0.270099
Thermal correction to Enthalpy= 0.271044
Thermal correction to Gibbs (Free) Energy= 0.203911
Sum of electronic and zero-point Energies= -941.378092
Sum of electronic and thermal Energies= -941.359848
Sum of electronic and thermal Enthalpies= -941.358904
Sum of electronic and thermal (Free) Energies= -941.426037

cPT

C -1.6986210000 2.5207750000 0.1431760000
C -0.6529890000 1.6725080000 0.3249560000
C 0.7173380000 1.7827860000 -0.0774070000
C 1.4371000000 0.6041520000 0.3033140000
C 0.5639910000 -0.2052710000 1.0423040000
C -0.8152500000 0.3302220000 1.0532660000
C 1.4093720000 2.8814920000 -0.8052040000
O 2.6723410000 0.3936050000 -0.0166070000
H 0.9100420000 3.1039800000 -1.7557860000
H 2.4411290000 2.5853900000 -1.0062690000
H 1.4144900000 3.8076260000 -0.2160220000
H 0.8676820000 -1.1308150000 1.5149870000
B 3.1366570000 -1.1012220000 -0.0242500000
F 3.1144930000 -1.5424310000 1.2951840000
F 4.3776450000 -1.1001860000 -0.5879800000
F 2.1745700000 -1.7790110000 -0.7829570000
H -2.6646290000 2.1573320000 0.4946310000
C -1.7422860000 3.8736340000 -0.4846470000
H -0.7692420000 4.2644590000 -0.7776150000
H -2.2093160000 4.5868810000 0.2081610000
H -2.3905040000 3.8497000000 -1.3725450000
C -1.8357030000 -0.6259660000 0.4287690000
H -1.1366110000 0.5256930000 2.0898410000
C -1.4747560000 -1.4585060000 -0.6407740000
C -2.4233070000 -2.3027560000 -1.2184500000
C -3.7350010000 -2.3262770000 -0.7399620000
C -4.0942900000 -1.5103200000 0.3335480000
C -3.1461310000 -0.6697640000 0.9192120000
H -0.4480590000 -1.4735030000 -0.9990310000
H -2.1306460000 -2.9507910000 -2.0398180000
H -4.4693410000 -2.9871150000 -1.1921270000
H -5.1081550000 -1.5342590000 0.7239160000
H -3.4260350000 -0.0529030000 1.7709610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.254618 (Hartree/Particle)
Thermal correction to Energy= 0.272539
Thermal correction to Enthalpy= 0.273484
Thermal correction to Gibbs (Free) Energy= 0.207148
Sum of electronic and zero-point Energies= -941.408160
Sum of electronic and thermal Energies= -941.390239
Sum of electronic and thermal Enthalpies= -941.389295
Sum of electronic and thermal (Free) Energies= -941.455630

ccRT

C 0.0015360000 3.5534160000 -0.9003880000
C -0.8212930000 2.6793290000 -0.3878820000
C 1.1555090000 4.2067100000 -0.1776020000
H -0.1429770000 3.8336570000 -1.9460170000
C -1.7223450000 1.8411590000 0.0999170000
H 2.1061710000 3.9529850000 -0.6628750000
H 1.2037140000 3.8979340000 0.8701740000
H 1.0559750000 5.2982890000 -0.2093780000
C -1.5505960000 0.3762620000 -0.0266840000
C -3.0379260000 2.3260930000 0.6814880000
C -0.2650330000 -0.2777950000 -0.2044570000
O -2.6228130000 -0.2903240000 0.0086520000
H -3.8726290000 1.9930540000 0.0568380000
H -3.0499720000 3.4161770000 0.7457820000
H -3.1969130000 1.9055940000 1.6802860000
C 0.9063110000 0.2210260000 0.2556740000
H -0.3226430000 -1.2576090000 -0.6630030000
B -2.7384270000 -1.9398440000 0.0083200000
H 0.8933080000 1.1691580000 0.7872640000
C 2.2191780000 -0.4069400000 0.1528220000
F -4.0780830000 -2.1359620000 0.0774260000
F -2.0282880000 -2.3226560000 1.1142670000
F -2.1599630000 -2.3315430000 -1.1797410000
C 3.3258540000 0.2529710000 0.7207770000
C 2.4331430000 -1.6424800000 -0.4916210000
C 4.6035860000 -0.2951780000 0.6471380000
H 3.1739300000 1.2049320000 1.2241220000
C 3.7089390000 -2.1889820000 -0.5638330000
H 1.5976170000 -2.1779790000 -0.9309190000
C 4.7982710000 -1.5185020000 0.0035830000
H 5.4448050000 0.2288000000 1.0919120000
H 3.8573590000 -3.1429940000 -1.0614930000
H 5.7930900000 -1.9512780000 -0.0546770000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.252994 (Hartree/Particle)
Thermal correction to Energy= 0.272245
Thermal correction to Enthalpy= 0.273189
Thermal correction to Gibbs (Free) Energy= 0.202861
Sum of electronic and zero-point Energies= -941.406156
Sum of electronic and thermal Energies= -941.386905
Sum of electronic and thermal Enthalpies= -941.385961
Sum of electronic and thermal (Free) Energies= -941.456290

ccTS

C -3.4062070000 0.2154080000 0.6327940000
C -2.1466380000 0.2221140000 0.2022010000
C -4.5524640000 -0.6110110000 0.1319240000
H -3.6216420000 0.8557860000 1.4924830000
C -0.9999200000 0.9548340000 0.0545340000
H -4.8890540000 -1.3219490000 0.8976880000
H -4.3026930000 -1.1713690000 -0.7702000000
H -5.4048440000 0.0431140000 -0.0917300000
C 0.2106440000 0.1720110000 0.0352180000
C -0.9468090000 2.4401480000 -0.1536360000
C -0.0845460000 -1.2187040000 0.0169240000
O 1.3604570000 0.7290980000 0.0912270000
H -0.2533030000 2.8720920000 0.5778530000
H -1.9282030000 2.9057900000 -0.0456780000
H -0.5372560000 2.6811350000 -1.1420280000
C -1.3716590000 -1.5916430000 -0.4119020000
H 0.6240450000 -1.9281960000 0.4283780000
B 2.6646430000 -0.1688580000 -0.0960850000
H -1.7001520000 -1.2415460000 -1.3903940000
C -1.9755460000 -2.8714860000 0.0044200000
F 3.6937480000 0.7224950000 -0.1155540000
F 2.4688340000 -0.8484530000 -1.2847350000
F 2.6801510000 -1.0319740000 0.9908210000
C -2.7556690000 -3.6126670000 -0.8993640000
C -1.7675190000 -3.3821020000 1.2973490000
C -3.2981860000 -4.8408880000 -0.5287630000
H -2.9184150000 -3.2301150000 -1.9046510000
C -2.3133110000 -4.6081690000 1.6691850000
H -1.1821350000 -2.8080210000 2.0105780000
C -3.0780930000 -5.3406140000 0.7570790000
H -3.8886340000 -5.4092480000 -1.2417250000
H -2.1447210000 -4.9924020000 2.6711160000
H -3.5034070000 -6.2968200000 1.0487690000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.251665 (Hartree/Particle)
Thermal correction to Energy= 0.269920
Thermal correction to Enthalpy= 0.270864
Thermal correction to Gibbs (Free) Energy= 0.203750
Sum of electronic and zero-point Energies= -941.375746
Sum of electronic and thermal Energies= -941.357491
Sum of electronic and thermal Enthalpies= -941.356547
Sum of electronic and thermal (Free) Energies= -941.423661

ccPT

C 1.4339470000 2.7429260000 0.0214890000
C 0.5403070000 1.7285490000 0.1488640000

C -0.8113330000 1.7631310000 -0.3194110000
C -1.4891380000 0.5447630000 0.0060160000
C -0.5783370000 -0.2614210000 0.7023430000
C 0.7588250000 0.3826300000 0.8404210000
C -1.5252330000 2.8576590000 -1.0179130000
O -2.7227660000 0.3353810000 -0.3128320000
H -0.8968160000 3.7146630000 -1.2664930000
H -2.3675170000 3.1915150000 -0.3965810000
H -1.9864890000 2.4580730000 -1.9301540000
H -0.8106840000 -1.2472950000 1.0826970000
B -3.3585260000 -1.0379810000 0.1013890000
F -4.6478010000 -0.9882000000 -0.3436780000
F -3.2399500000 -1.1118210000 1.4861210000
F -2.5843250000 -2.0173800000 -0.5109400000
C 2.8348120000 2.7730890000 0.5296450000
H 1.1070890000 3.6382020000 -0.5059930000
H 3.1487490000 1.8281780000 0.9757260000
H 2.9456430000 3.5712070000 1.2777830000
H 3.5274150000 3.0233160000 -0.2853860000
H 0.9747390000 0.5568200000 1.9068200000
C 1.8787070000 -0.4988410000 0.2812710000
C 1.9029880000 -0.8448680000 -1.0764570000
C 2.8676450000 -1.0082250000 1.1299100000
C 3.8747950000 -1.8366510000 0.6300430000
C 3.8986030000 -2.1675210000 -0.7246680000
C 2.9090440000 -1.6697090000 -1.5762840000
H 1.1284630000 -0.4740290000 -1.7427230000
H 2.9149640000 -1.9312220000 -2.6307310000
H 4.6793070000 -2.8141900000 -1.1151040000
H 2.8488660000 -0.7605480000 2.1891620000
H 4.6359120000 -2.2242750000 1.3015510000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.253996 (Hartree/Particle)
Thermal correction to Energy= 0.272216
Thermal correction to Enthalpy= 0.273160
Thermal correction to Gibbs (Free) Energy= 0.205165
Sum of electronic and zero-point Energies= -941.411749
Sum of electronic and thermal Energies= -941.393529
Sum of electronic and thermal Enthalpies= -941.392585
Sum of electronic and thermal (Free) Energies= -941.460579

2a

cRT

C -3.0559440000 -1.5272380000 -0.1191040000
C -2.0478550000 -0.7183380000 0.0635170000
C -1.0381370000 0.1328430000 0.1789170000
C 0.3285910000 -0.4377110000 0.1647860000
C 0.6275090000 -1.7739670000 0.7045760000
C -0.0363100000 -2.3223680000 1.7302580000
H 1.4969690000 -2.2573210000 0.2729500000
C -1.2494320000 1.6706880000 0.2094020000
O 1.2446920000 0.2602150000 -0.3355840000
C -2.7317770000 1.9831560000 0.4875260000
C -0.8592520000 2.2900200000 -1.1534630000
C -0.3970420000 2.2907750000 1.3395730000
B 2.8856460000 -0.1056590000 -0.3747100000
F 3.3859970000 0.9835220000 -1.0038070000
F 2.9530600000 -1.2754620000 -1.0884890000
F 3.2093600000 -0.2338400000 0.9451210000
H -1.4571360000 1.8560760000 -1.9634770000
H 0.1967940000 2.1376080000 -1.3818060000
H -1.0554480000 3.3688410000 -1.1322870000
H -3.0638130000 1.5548520000 1.4403510000
H -3.3849190000 1.5983520000 -0.3024680000
H -2.8705290000 3.0684740000 0.5395100000
H -0.6711250000 1.8727710000 2.3157710000
H -0.5743480000 3.3715680000 1.3788840000
H 0.6727780000 2.1343070000 1.1831060000
H -3.5605970000 -1.9314370000 0.7604380000
C -3.5845170000 -1.9621010000 -1.4663130000
H -3.0197880000 -1.5086560000 -2.2845550000
H -4.6393380000 -1.6804460000 -1.5709810000
H -3.5265010000 -3.0527430000 -1.5655760000
H -0.8627530000 -1.8216760000 2.2239150000
H 0.2632240000 -3.2865390000 2.1309680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256102 (Hartree/Particle)
Thermal correction to Energy= 0.274787
Thermal correction to Enthalpy= 0.275731
Thermal correction to Gibbs (Free) Energy= 0.208710
Sum of electronic and zero-point Energies= -828.274388
Sum of electronic and thermal Energies= -828.255703
Sum of electronic and thermal Enthalpies= -828.254759
Sum of electronic and thermal (Free) Energies= -828.321780

cTS

C -3.0561480000 -1.4172650000 -0.7370090000
C -1.9028420000 -0.8960290000 -0.3343680000
C -0.9861240000 0.1045870000 -0.1882870000
C 0.3882550000 -0.3771500000 -0.2011520000
C 0.4378750000 -1.8072710000 -0.1471880000
C -0.6882750000 -2.4461690000 0.3387730000
C -1.3362900000 1.5806310000 0.0516660000
O 1.3880760000 0.4039790000 -0.3288360000
C -2.8519200000 1.7853780000 0.2261420000
C -0.8537490000 2.3919530000 -1.1783010000
C -0.6203860000 2.0868980000 1.3265490000
H 1.2525880000 -2.3275120000 -0.6387010000
B 2.8808300000 -0.1786710000 -0.1728300000
F 2.8647850000 -0.8793710000 1.0164880000
F 3.6668730000 0.9311650000 -0.1709090000
F 3.0600460000 -1.0092160000 -1.2646460000
H -3.4749300000 -2.2526410000 -0.1771350000
C -3.8089920000 -0.9974810000 -1.9725060000
H -3.9113720000 -1.8434190000 -2.6641460000
H -3.3083780000 -0.1812010000 -2.4981200000
H -4.8243430000 -0.6761150000 -1.7063130000
H -0.9541600000 1.5312140000 2.2108640000
H -0.8643120000 3.1436690000 1.4843360000
H 0.4644780000 1.9958950000 1.2468050000
H -3.2451180000 1.2115560000 1.0724110000
H -3.4130070000 1.5010130000 -0.6698830000
H -3.0512370000 2.8451490000 0.4181350000
H 0.2222040000 2.2854080000 -1.3297090000
H -1.0788450000 3.4531560000 -1.0199430000
H -1.3695180000 2.0702720000 -2.0907490000
H -0.8930250000 -3.4753690000 0.0437990000
H -1.1491670000 -2.1630720000 1.2815310000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255831 (Hartree/Particle)
Thermal correction to Energy= 0.273198
Thermal correction to Enthalpy= 0.274142
Thermal correction to Gibbs (Free) Energy= 0.211028
Sum of electronic and zero-point Energies= -828.248355
Sum of electronic and thermal Energies= -828.230989
Sum of electronic and thermal Enthalpies= -828.230044
Sum of electronic and thermal (Free) Energies= -828.293158

cPT

C 2.9098960000 -1.6145440000 0.0966150000
C 1.6382280000 -1.2388690000 -0.2099580000
C 0.8762000000 -0.0187390000 -0.0954710000
C -0.5274330000 -0.3691350000 -0.0300500000
C -0.6537990000 -1.7250210000 -0.3609520000
C 0.6559320000 -2.3425980000 -0.6064370000
C 1.3123850000 1.4342490000 -0.1606260000
O -1.4688640000 0.4694090000 0.2585460000
C 2.7853180000 1.6551430000 -0.5579000000
C 1.0299810000 2.0951140000 1.2178190000
C 0.4496170000 2.1418900000 -1.2515640000
H -1.6037150000 -2.2392700000 -0.4157310000
B -2.9638260000 -0.0172900000 0.1899810000
F -3.1516330000 -0.4787340000 -1.1082870000
F -3.7064340000 1.0842230000 0.5020270000
F -3.0762200000 -1.0558500000 1.1054990000
H 3.1495150000 -2.6430750000 -0.1767250000
C 3.9930840000 -0.9365360000 0.8724800000
H 4.4731020000 -1.6732100000 1.5275970000
H 3.6293610000 -0.1162810000 1.4914810000
H 4.7803500000 -0.5519560000 0.2091100000
H 0.6613010000 1.7241630000 -2.2424970000
H 0.7221470000 3.2026360000 -1.2683720000
H -0.6176650000 2.0595430000 -1.0523150000

H 3.0736160000 1.0398910000 -1.4175310000
H 3.4823430000 1.4646100000 0.2578580000
H 2.9159130000 2.7033560000 -0.8454860000
H -0.0256390000 2.0136970000 1.4842340000
H 1.2983960000 3.1563680000 1.1626110000
H 1.6318780000 1.6346830000 2.0100650000
H 0.7921530000 -3.2812960000 -0.0495490000
H 0.7991160000 -2.5951660000 -1.6699150000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258416 (Hartree/Particle)
Thermal correction to Energy= 0.275649
Thermal correction to Enthalpy= 0.276593
Thermal correction to Gibbs (Free) Energy= 0.212806
Sum of electronic and zero-point Energies= -828.277390
Sum of electronic and thermal Energies= -828.260157
Sum of electronic and thermal Enthalpies= -828.259213
Sum of electronic and thermal (Free) Energies= -828.323000

ccRT

C 3.0342850000 -1.1985990000 -0.9606770000
C 2.0220290000 -0.5139320000 -0.5023200000
C 0.9970790000 0.2262790000 -0.1027710000
C -0.3256140000 -0.4358620000 -0.0433880000
C -0.4738910000 -1.8693700000 0.2580540000
C 0.3488910000 -2.5447670000 1.0704860000
C 1.1319030000 1.7479320000 0.1728080000
O -1.3401730000 0.2681880000 -0.2710930000
C 2.6209620000 2.1193140000 0.3046460000
C 0.4188060000 2.1029970000 1.4970320000
C 0.5209800000 2.5569710000 -0.9957670000
H -1.3658340000 -2.3314580000 -0.1505710000
B -2.9473460000 -0.2161360000 -0.1660350000
F -3.5920000000 0.9291850000 -0.4899690000
F -3.0684390000 -0.6225700000 1.1314800000
F -3.0543050000 -1.2280510000 -1.0863350000
H 1.0191530000 2.3120290000 -1.9410770000
H 0.6623820000 3.6284500000 -0.8094990000
H -0.5476090000 2.3661690000 -1.1069750000
H 3.1736850000 1.9222080000 -0.6195720000
H 3.1061880000 1.5633890000 1.1154660000
H 2.7103760000 3.1877560000 0.5288500000
H -0.6533240000 1.8976850000 1.4563100000
H 0.5469880000 3.1714210000 1.7048100000
H 0.8484860000 1.5464330000 2.3387570000
C 4.0324100000 -1.9643400000 -0.1260740000
H 3.1717280000 -1.2328000000 -2.0435310000
H 3.8364260000 -1.8535220000 0.9435640000
H 5.0502970000 -1.6103160000 -0.3282420000
H 4.0029200000 -3.0316130000 -0.3782030000
H 1.2036790000 -2.0803130000 1.5510130000
H 0.1582300000 -3.5871510000 1.3090660000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256072 (Hartree/Particle)
Thermal correction to Energy= 0.274757
Thermal correction to Enthalpy= 0.275701
Thermal correction to Gibbs (Free) Energy= 0.208740
Sum of electronic and zero-point Energies= -828.274349
Sum of electronic and thermal Energies= -828.255664
Sum of electronic and thermal Enthalpies= -828.254720
Sum of electronic and thermal (Free) Energies= -828.321681

ccTS

C 3.1568030000 -0.9071400000 -0.6645270000
C 1.9422390000 -0.5731710000 -0.2449860000
C 0.9013550000 0.3068340000 -0.1366700000
C -0.3966980000 -0.3451830000 -0.0896540000
C -0.2587050000 -1.7668820000 0.0300270000
C 0.9366700000 -2.2341430000 0.5424440000
C 1.0608960000 1.8294460000 -0.0112210000
O -1.4945130000 0.2900030000 -0.2238500000
C 2.5404840000 2.2450600000 0.0788430000
C 0.3265400000 2.3299330000 1.2548610000
C 0.4351870000 2.4771530000 -1.2740700000
H -1.0010600000 -2.4103110000 -0.4296400000
B -2.8898260000 -0.4804040000 -0.0022240000
F -3.8188670000 0.5124980000 -0.0123890000
F -2.7475650000 -1.1281910000 1.2093340000
F -2.9837020000 -1.3685690000 -1.0587320000
H 0.9569580000 2.1540100000 -2.1823800000
H 0.5278150000 3.5671150000 -1.2013310000
H -0.6226540000 2.2257480000 -1.3705370000
H 3.1021910000 1.9653490000 -0.8187330000
H 3.0382810000 1.7973530000 0.9459180000
H 2.6014100000 3.3337990000 0.1818390000
H -0.7376390000 2.0875300000 1.2290390000
H 0.4272370000 3.4189030000 1.3275840000
H 0.7633640000 1.8925730000 2.1604980000
C 4.1128540000 -1.8823940000 -0.0384130000
H 3.4874320000 -0.4486780000 -1.5992340000
H 3.7278100000 -2.3034950000 0.8934840000
H 5.0647300000 -1.3827640000 0.1820370000
H 4.3399570000 -2.7056330000 -0.7276340000
H 1.3551460000 -1.8381120000 1.4635200000
H 1.2619610000 -3.2478910000 0.3117970000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255725 (Hartree/Particle)
Thermal correction to Energy= 0.273087
Thermal correction to Enthalpy= 0.274031
Thermal correction to Gibbs (Free) Energy= 0.210939
Sum of electronic and zero-point Energies= -828.247723
Sum of electronic and thermal Energies= -828.230361
Sum of electronic and thermal Enthalpies= -828.229417
Sum of electronic and thermal (Free) Energies= -828.292509

ccPT

C 3.1707370000 -0.8406690000 -0.0000020000
C 1.8105360000 -0.8662370000 0.0000000000
C 0.8694050000 0.2296130000 0.0000010000
C -0.4717290000 -0.3171920000 0.0000020000
C -0.3768170000 -1.7123660000 0.0000040000
C 1.0245220000 -2.1635550000 0.0000030000
C 1.0887120000 1.7305700000 0.0000000000
O -1.5496370000 0.4021990000 0.0000020000
C 2.5516900000 2.2094670000 0.0000000000
C 0.4009260000 2.3115590000 1.2716500000
C 0.4009250000 2.3115590000 -1.2716480000
H -1.2372980000 -2.3672610000 0.0000060000
B -2.9432930000 -0.3203350000 -0.0000010000
F -3.8631140000 0.6886570000 -0.0000020000
F -2.9695760000 -1.1098070000 1.1444300000
F -2.9695720000 -1.1098060000 -1.1444330000
H 0.8882400000 1.9410920000 -2.1807970000
H 0.5019340000 3.4025480000 -1.2538040000
H -0.6588170000 2.0588920000 -1.3070980000
H 3.0981800000 1.8890250000 -0.8936920000
H 3.0981810000 1.8890240000 0.8936910000
H 2.5537500000 3.3044630000 0.0000010000
H -0.6588160000 2.0588920000 1.3071000000
H 0.5019340000 3.4025480000 1.2538050000
H 0.8882420000 1.9410930000 2.1807980000
C 4.0627290000 -2.0386380000 -0.0000030000
H 3.6868280000 0.1098180000 -0.0000040000
H 3.5234060000 -2.9878480000 0.0000000000
H 4.7247160000 -2.0145960000 0.8768620000
H 4.7247110000 -2.0145980000 -0.8768710000
H 1.2544590000 -2.7875290000 0.8778060000
H 1.2544570000 -2.7875300000 -0.8778000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258796 (Hartree/Particle)
Thermal correction to Energy= 0.275910
Thermal correction to Enthalpy= 0.276854
Thermal correction to Gibbs (Free) Energy= 0.213635
Sum of electronic and zero-point Energies= -828.289964
Sum of electronic and thermal Energies= -828.272850
Sum of electronic and thermal Enthalpies= -828.271906
Sum of electronic and thermal (Free) Energies= -828.335124

2b

cRT

C -3.0407550000 -1.2786700000 -0.6350480000
C -2.0568620000 -0.5205550000 -0.2308840000

C -1.0704840000 0.2905470000 0.1180820000
C 0.3154260000 -0.2144530000 -0.0539980000
C 0.6779060000 -1.6103980000 0.1810050000
C 0.0171970000 -2.4225900000 1.0264850000
H 1.5895810000 -1.9381250000 -0.3071940000
C -1.3158800000 1.7508530000 0.5839470000
O 1.1824020000 0.6195750000 -0.4237770000
C -2.7973600000 1.9288630000 0.9655440000
C -0.9735800000 2.7416360000 -0.5537680000
C -0.4480760000 2.0489030000 1.8275970000
B 2.8278520000 0.3821760000 -0.5214440000
F 3.2524230000 1.5892190000 -0.9694580000
F 2.9864110000 -0.6529100000 -1.4113180000
F 3.1763140000 0.0715500000 0.7638380000
H -1.5783460000 2.5344660000 -1.4444100000
H 0.0802910000 2.6924400000 -0.8318770000
H -1.1978900000 3.7639120000 -0.2256150000
H -3.0950860000 1.2387830000 1.7635320000
H -3.4609030000 1.7637390000 0.1104260000
H -2.9603010000 2.9506540000 1.3253450000
H -0.6991500000 1.3739410000 2.6549110000
H -0.6347020000 3.0742460000 2.1666910000
H 0.6204660000 1.9565630000 1.6180150000
H -3.5292130000 -1.9271190000 0.0949810000
C -3.5648980000 -1.3356040000 -2.0511670000
H -3.0172080000 -0.6561240000 -2.7088030000
H -4.6277440000 -1.0655660000 -2.0765500000
H -3.4776760000 -2.3529200000 -2.4517450000
H -0.8520870000 -2.0431580000 1.5597410000
C 0.4194720000 -3.8291420000 1.3289300000
H 1.2991370000 -4.1367760000 0.7572500000
H -0.4055840000 -4.5194370000 1.1060620000
H 0.6389620000 -3.9440700000 2.3987660000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284349 (Hartree/Particle)
Thermal correction to Energy= 0.304629
Thermal correction to Enthalpy= 0.305573
Thermal correction to Gibbs (Free) Energy= 0.234580
Sum of electronic and zero-point Energies= -867.569615
Sum of electronic and thermal Energies= -867.549334
Sum of electronic and thermal Enthalpies= -867.548390
Sum of electronic and thermal (Free) Energies= -867.619384

cTS

C -2.9669140000 -1.3748230000 0.1185320000
C -1.7826070000 -0.8032010000 0.3101480000
C -0.9538880000 0.2880320000 0.3230150000
C 0.4119250000 -0.0558470000 -0.0315650000
C 0.5883980000 -1.4695990000 -0.0749300000
C -0.3518030000 -2.2440770000 0.6047470000
H 1.3305980000 -1.8952720000 -0.7422360000
C -1.3618230000 1.7037180000 0.7487200000
O 1.2916280000 0.8238870000 -0.3308870000
C -2.8031800000 1.7490560000 1.2871220000
C -1.2539040000 2.6238510000 -0.4951340000
C -0.4068740000 2.2106030000 1.8563000000
B 2.8121850000 0.3771690000 -0.5431260000
F 3.4921530000 1.5507820000 -0.6599950000
F 2.8133880000 -0.4008020000 -1.6900350000
F 3.1309970000 -0.3635470000 0.5802860000
H -1.9435450000 2.3036340000 -1.2850480000
H -0.2394420000 2.6297910000 -0.8988220000
H -1.5207580000 3.6480530000 -0.2091120000
H -2.9348960000 1.0893240000 2.1517280000
H -3.5384010000 1.4670050000 0.5270850000
H -3.0346760000 2.7708020000 1.6069440000
H -0.4741240000 1.5799830000 2.7507950000
H -0.6921730000 3.2291040000 2.1434900000
H 0.6313590000 2.2285100000 1.5199440000
H -3.1927980000 -2.2971040000 0.6530550000
C -4.0095990000 -0.9106560000 -0.8643020000
H -3.6937440000 -0.0141640000 -1.4024540000
H -4.9530770000 -0.6965240000 -0.3451980000
H -4.2207850000 -1.6985150000 -1.5988200000
H -0.5594130000 -2.0087290000 1.6478490000
C -0.5902140000 -3.6878930000 0.2464260000
H -0.4881650000 -3.8666910000 -0.8273620000
H -1.5825500000 -4.0217210000 0.5658660000
H 0.1403710000 -4.3173490000 0.7712680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.283932 (Hartree/Particle)
Thermal correction to Energy= 0.302929
Thermal correction to Enthalpy= 0.303873
Thermal correction to Gibbs (Free) Energy= 0.237196
Sum of electronic and zero-point Energies= -867.541136
Sum of electronic and thermal Energies= -867.522140
Sum of electronic and thermal Enthalpies= -867.521195
Sum of electronic and thermal (Free) Energies= -867.587872

cPT

C -2.9257580000 1.1796130000 0.1521290000
C -1.6473280000 0.9070280000 -0.2161170000
C -0.8134700000 -0.2686040000 -0.1080410000
C 0.5640120000 0.1610340000 -0.0388470000
C 0.6068880000 1.5039200000 -0.4292490000
C -0.7357110000 2.0600370000 -0.6907870000
H 1.5267290000 2.0655640000 -0.5287390000
C -1.1724950000 -1.7420780000 -0.1928000000
O 1.5507090000 -0.6120020000 0.2820470000
C -2.6130880000 -2.0281420000 -0.6634230000
C -0.9189830000 -2.3859060000 1.1995840000
C -0.2283190000 -2.4130770000 -1.2375480000
B 3.0116010000 -0.0341330000 0.2183190000
F 3.8184940000 -1.0760550000 0.5734970000
F 3.0444350000 1.0364200000 1.1027960000
F 3.1914540000 0.4001390000 -1.0911940000
H -1.5776880000 -1.9600520000 1.9653680000
H 0.1185250000 -2.2465620000 1.5111090000
H -1.1255740000 -3.4604220000 1.1354570000
H -2.8720150000 -1.4430300000 -1.5528540000
H -3.3648440000 -1.8443740000 0.1031200000
H -2.6881840000 -3.0866670000 -0.9326900000
H -0.4039290000 -2.0012110000 -2.2379400000
H -0.4587750000 -3.4833410000 -1.2697070000
H 0.8233100000 -2.2895310000 -0.9842180000
H -3.2740190000 2.1789420000 -0.1047140000
C -3.8933130000 0.4168310000 0.9999740000
H -3.4372380000 -0.4141570000 1.5381130000
H -4.7328680000 0.0339020000 0.4033160000
H -4.3291190000 1.1019730000 1.7381100000
H -0.8834810000 2.1425810000 -1.7819330000
C -0.9424130000 3.4567330000 -0.0787580000
H -0.8805990000 3.4228010000 1.0134220000
H -1.9084900000 3.8856620000 -0.3619980000
H -0.1649980000 4.1357510000 -0.4437830000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.286868 (Hartree/Particle)
Thermal correction to Energy= 0.305579
Thermal correction to Enthalpy= 0.306523
Thermal correction to Gibbs (Free) Energy= 0.239712
Sum of electronic and zero-point Energies= -867.562861
Sum of electronic and thermal Energies= -867.544150
Sum of electronic and thermal Enthalpies= -867.543205
Sum of electronic and thermal (Free) Energies= -867.610016

ccRT

C -3.0467970000 0.6495930000 -1.2360350000
C -2.0151080000 0.0916230000 -0.6614900000
C -4.0985990000 1.4838890000 -0.5452950000
H -3.1640220000 0.5083650000 -2.3125730000
C -0.9667270000 -0.5270500000 -0.1404550000
H -3.9144600000 1.5599460000 0.5296600000
H -5.0925030000 1.0444730000 -0.6927570000
H -4.1260420000 2.4957900000 -0.9684080000
C 0.3292750000 0.1959920000 -0.1704160000
C -1.0346970000 -1.9898790000 0.3744150000
C 0.4270080000 1.6447480000 -0.0013670000
O 1.3628370000 -0.4963870000 -0.3612020000
C -0.3885600000 -2.9498930000 -0.6523450000
C -2.5061260000 -2.3988030000 0.5746250000
C -0.3058550000 -2.0945890000 1.7331010000
C -0.4544050000 2.3791200000 0.7016460000
H 1.3283340000 2.0944210000 -0.4043930000
B 2.9453070000 0.0175390000 -0.2770830000

H 0.6715550000 -2.7361310000 -0.7967790000
H -0.8934330000 -2.8781010000 -1.6227740000
H -0.4882220000 -3.9828430000 -0.2972380000
H -3.0149790000 -1.7405230000 1.2885660000
H -2.5498330000 -3.4201690000 0.9682500000
H -3.0663510000 -2.3764050000 -0.3656920000
H 0.7532180000 -1.8371920000 1.6549510000
H -0.3733100000 -3.1230480000 2.1057740000
H -0.7684700000 -1.4388170000 2.4808170000
H -1.3101400000 1.8885780000 1.1610620000
C -0.3207330000 3.8473610000 0.9448580000
F 3.6189050000 -1.1237750000 -0.5622680000
F 3.0618590000 0.4684180000 1.0085740000
F 3.0491450000 1.0036070000 -1.2284480000
H 0.5602480000 4.2663050000 0.4512650000
H -1.2124520000 4.3788540000 0.5858440000
H -0.2496110000 4.0529710000 2.0212710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284308 (Hartree/Particle)
Thermal correction to Energy= 0.304598
Thermal correction to Enthalpy= 0.305542
Thermal correction to Gibbs (Free) Energy= 0.234600
Sum of electronic and zero-point Energies= -867.569423
Sum of electronic and thermal Energies= -867.549133
Sum of electronic and thermal Enthalpies= -867.548189
Sum of electronic and thermal (Free) Energies= -867.619131

ccTS

C 2.8624530000 -1.1950170000 0.6710790000
C 1.6972470000 -0.7713550000 0.1832290000
C 3.1050740000 -2.2957690000 1.6624440000
H 3.7576320000 -0.6976210000 0.2918300000
C 0.9428170000 0.2721860000 -0.2855060000
H 2.1788730000 -2.6942010000 2.0825710000
H 3.7096780000 -1.9074740000 2.4920260000
H 3.6776950000 -3.1206400000 1.2178530000
C -0.0879460000 -0.1520740000 -1.2149290000
C 1.0890770000 1.7329630000 0.1626920000
C -0.1671730000 -1.5720890000 -1.2772200000
O -0.7618240000 0.6699050000 -1.9273460000
C 1.5249310000 2.5643990000 -1.0727780000
C 2.1461820000 1.9002640000 1.2691290000
C -0.2680840000 2.2536850000 0.6930800000
C 0.3681890000 -2.2947100000 -0.2108730000
H -0.4845260000 -2.0446570000 -2.2011970000
B -1.9898300000 0.1349330000 -2.8007730000
H 0.7927280000 2.4959240000 -1.8792880000
H 2.4970920000 2.2275510000 -1.4513070000
H 1.6229450000 3.6164180000 -0.7801880000
H 1.9009320000 1.3137530000 2.1612090000
H 2.1923640000 2.9544620000 1.5630200000
H 3.1461680000 1.6077840000 0.9320940000
H -1.0512350000 2.1880460000 -0.0645320000
H -0.1645560000 3.3040630000 0.9888130000
H -0.5868820000 1.6874960000 1.5763620000
H 0.0328290000 -2.0551370000 0.7976330000
C 0.7927170000 -3.7293170000 -0.4084380000
F -2.5858070000 1.2665570000 -3.2672270000
F -2.7630790000 -0.6031730000 -1.9235330000
F -1.4255410000 -0.6610630000 -3.7849650000
H 1.2640860000 -3.8809770000 -1.3833160000
H 1.4817180000 -4.0656660000 0.3694560000
H -0.0933310000 -4.3760800000 -0.3548560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.283898 (Hartree/Particle)
Thermal correction to Energy= 0.302848
Thermal correction to Enthalpy= 0.303793
Thermal correction to Gibbs (Free) Energy= 0.237158
Sum of electronic and zero-point Energies= -867.538867
Sum of electronic and thermal Energies= -867.519917
Sum of electronic and thermal Enthalpies= -867.518973
Sum of electronic and thermal (Free) Energies= -867.585608

ccPT

C -3.1173400000 -0.3455910000 -0.3262760000
C -1.7793810000 -0.5250190000 -0.1582950000
C -0.7499430000 0.4842720000 -0.0358590000
C 0.5395430000 -0.1693960000 -0.0990380000
C 0.3236910000 -1.5454190000 -0.1986870000
C -1.1110500000 -1.8945790000 -0.1678310000
C -0.8406800000 1.9898320000 0.1321080000
O 1.6758500000 0.4545050000 -0.0601540000
C -2.2552550000 2.5915360000 0.2215570000
C -0.1125680000 2.6571410000 -1.0717810000
C -0.0962320000 2.3529100000 1.4534080000
H 1.1254150000 -2.2705100000 -0.2459420000
B 2.9998980000 -0.3845870000 -0.1038450000
F 4.0050930000 0.5379630000 -0.0461350000
F 2.9641260000 -1.1073980000 -1.2917380000
F 2.9528450000 -1.2382560000 0.9935110000
H -0.6148440000 1.9287780000 2.3208540000
H -0.0931280000 3.4433690000 1.5607920000
H 0.9348840000 1.9998900000 1.4457730000
H -2.8444630000 2.1618140000 1.0388890000
H -2.8130490000 2.4956420000 -0.7162690000
H -2.1585470000 3.6635700000 0.4226810000
H 0.9232790000 2.3263180000 -1.1484290000
H -0.1259930000 3.7435620000 -0.9287010000
H -0.6303090000 2.4328890000 -2.0114710000
C -4.1344130000 -1.4138400000 -0.5638590000
H -3.5191680000 0.6584240000 -0.3172430000
H -3.7127570000 -2.4151530000 -0.6588280000
H -4.6972160000 -1.1906310000 -1.4804210000
H -4.8747570000 -1.4199150000 0.2492360000
H -1.3880240000 -2.4574690000 -1.0733100000
C -1.4434110000 -2.7749450000 1.0675620000
H -1.2100550000 -2.2366060000 1.9910810000
H -0.8448090000 -3.6907990000 1.0454210000
H -2.4990870000 -3.0584860000 1.0875410000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.287428 (Hartree/Particle)
Thermal correction to Energy= 0.305995
Thermal correction to Enthalpy= 0.306939
Thermal correction to Gibbs (Free) Energy= 0.240616
Sum of electronic and zero-point Energies= -867.573836
Sum of electronic and thermal Energies= -867.555269
Sum of electronic and thermal Enthalpies= -867.554325
Sum of electronic and thermal (Free) Energies= -867.620648

2c

c/s RT

C -0.6181640000 3.0664880000 -0.9099040000
C 0.0425510000 2.0731750000 -0.3780420000
C 0.7672230000 1.0795950000 0.1119910000
C 0.3329200000 -0.3017570000 -0.2174520000
C -1.0748940000 -0.6783060000 -0.3195090000
C -2.0660950000 -0.0604660000 0.3492800000
H -1.2713080000 -1.5702490000 -0.9052540000
H -1.8324370000 0.7877930000 0.9923820000
C -3.5064400000 -0.4826390000 0.3235140000
C 2.0801760000 1.3167780000 0.9053550000
O 1.2408440000 -1.1513310000 -0.4151580000
C 2.1464750000 2.7845890000 1.3670790000
C 3.3075750000 1.0214370000 0.0112810000
C 2.1008650000 0.4065860000 2.1542180000
C -4.3933150000 0.6789430000 -0.1683510000
C -3.9449710000 -0.9593440000 1.7235290000
H -3.6096890000 -1.3216200000 -0.3762650000
H -4.3178630000 1.5442790000 0.5021840000
H -5.4437490000 0.3684570000 -0.1949300000
H -4.1077640000 1.0022530000 -1.1749650000
H -3.8475910000 -0.1545420000 2.4628060000
H -3.3401790000 -1.8067750000 2.0613930000
H -4.9949490000 -1.2722980000 1.7048660000
B 1.0491680000 -2.7906240000 -0.6187260000
F 2.3317250000 -3.1994080000 -0.7821470000
F 0.2548900000 -2.9219870000 -1.7326240000
F 0.4470180000 -3.1847430000 0.5447360000
H 3.2996710000 1.6573540000 -0.8817290000
H 3.3363910000 -0.0217840000 -0.3069370000
H 4.2258770000 1.2386030000 0.5704220000
H 1.2895190000 3.0492400000 1.9973330000
H 2.1698440000 3.4773790000 0.5195650000

H 3.0579340000 2.9407000000 1.9544140000
H 1.2519050000 0.6228410000 2.8141940000
H 3.0194880000 0.5877530000 2.7238610000
H 2.0744270000 -0.6542050000 1.8930110000
H -1.4232620000 3.5226200000 -0.3305600000
C -0.3588420000 3.6425710000 -2.2825900000
H 0.4604220000 3.1239390000 -2.7865830000
H -0.1055500000 4.7073010000 -2.2088930000
H -1.2568140000 3.5640580000 -2.9074930000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341354 (Hartree/Particle)
Thermal correction to Energy= 0.364391
Thermal correction to Enthalpy= 0.365335
Thermal correction to Gibbs (Free) Energy= 0.287386
Sum of electronic and zero-point Energies= -946.140735
Sum of electronic and thermal Energies= -946.117698
Sum of electronic and thermal Enthalpies= -946.116754
Sum of electronic and thermal (Free) Energies= -946.194703

c/s TS

C 2.7957740000 -0.7229200000 0.6232880000
C 1.5816940000 -0.3235640000 0.2442090000
C 0.6041920000 0.6412820000 0.2948140000
C -0.7221050000 0.0793250000 0.1411080000
C -0.6492710000 -1.2825280000 -0.2532670000
C 0.5629690000 -1.7357260000 -0.7918260000
C 0.8285680000 -3.2378620000 -0.8283790000
C 0.8439500000 2.1532440000 0.3900180000
O -1.7934430000 0.7363120000 0.3955410000
C 2.3367630000 2.5169950000 0.2969270000
C 0.2841030000 2.6375940000 1.7531020000
C 0.0978870000 2.8698090000 -0.7624900000
C 2.2905820000 -3.6262210000 -1.0984150000
C -0.0809860000 -3.8422650000 -1.9251020000
H 0.5267630000 -3.6644570000 0.1365720000
H 2.6914090000 -3.0968700000 -1.9726180000
H 2.3584610000 -4.6991370000 -1.3074480000
H 2.9379730000 -3.4218710000 -0.2417410000
H 0.1869110000 -3.4514130000 -2.9142260000
H -1.1375000000 -3.6180040000 -1.7514040000
H 0.0392820000 -4.9310720000 -1.9493420000
H 0.9772070000 -1.2064900000 -1.6521580000
H -1.4620400000 -1.9538640000 0.0021360000
B -3.2063530000 0.1050800000 0.0165510000
F -3.0901190000 -0.2808270000 -1.3081120000
F -4.0962270000 1.1128990000 0.2347220000
F -3.3671070000 -0.9885540000 0.8543510000
H 3.3518410000 -1.3902420000 -0.0287480000
C 3.4413280000 -0.4077860000 1.9465040000
H 3.6512860000 -1.3340550000 2.4973980000
H 2.8095620000 0.2266370000 2.5719410000
H 4.4053570000 0.0942560000 1.7909770000
H 0.4834640000 2.5489700000 -1.7375330000
H 0.2574950000 3.9509420000 -0.6795960000
H -0.9760860000 2.6790740000 -0.7325930000
H 2.7850460000 2.1574940000 -0.6357280000
H 2.9168570000 2.1157050000 1.1327650000
H 2.4402500000 3.6072820000 0.3191680000
H -0.7802430000 2.4128660000 1.8476800000
H 0.4190630000 3.7227230000 1.8324300000
H 0.8169980000 2.1694640000 2.5892150000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341296 (Hartree/Particle)
Thermal correction to Energy= 0.362842
Thermal correction to Enthalpy= 0.363786
Thermal correction to Gibbs (Free) Energy= 0.290928
Sum of electronic and zero-point Energies= -946.107420
Sum of electronic and thermal Energies= -946.085874
Sum of electronic and thermal Enthalpies= -946.084930
Sum of electronic and thermal (Free) Energies= -946.157787

c/s PT

C 2.8823770000 0.1409220000 0.3827710000
C 1.6269650000 0.0318860000 -0.1204730000
C 0.5029430000 0.9520520000 -0.1312360000
C -0.7079860000 0.1753730000 -0.1416210000
C -0.3620640000 -1.0993930000 -0.5950410000
C 1.0981960000 -1.3284780000 -0.6269930000
C 1.5562340000 -2.6339350000 0.1223560000
C 0.4659030000 2.4666600000 -0.2558440000
O -1.8915750000 0.6264010000 0.1285010000
C 1.7929640000 3.0996550000 -0.7232110000
C 0.0213730000 3.0539540000 1.1134310000
C -0.5995770000 2.8481890000 -1.3276280000
C 2.7742640000 -3.2758820000 -0.5614970000
C 0.4260840000 -3.6697020000 0.2584920000
H 1.8394260000 -2.3313880000 1.1380920000
H 2.5049260000 -3.6410690000 -1.5609020000
H 3.1346400000 -4.1328650000 0.0180530000
H 3.6141280000 -2.5825990000 -0.6841110000
H 0.0798830000 -4.0198540000 -0.7222280000
H -0.4377860000 -3.2696270000 0.7998900000
H 0.7920380000 -4.5446160000 0.8071520000
H 1.4188340000 -1.4201790000 -1.6792500000
H -1.1049470000 -1.8194010000 -0.9082920000
B -3.0545650000 -0.4245360000 0.2389170000
F -3.2338710000 -0.9517380000 -1.0358070000
F -4.1268690000 0.2764970000 0.7061980000
F -2.5976140000 -1.4078900000 1.1171110000
H 3.5087250000 -0.7380020000 0.2475040000
C 3.5209400000 1.1860980000 1.2423830000
H 4.0254120000 0.6877340000 2.0801400000
H 2.8141260000 1.9048760000 1.6562240000
H 4.3026290000 1.7323030000 0.6963400000
H -0.3104330000 2.4665520000 -2.3135570000
H -0.6479150000 3.9404420000 -1.3912840000
H -1.5895210000 2.4681830000 -1.0797270000
H 2.1893630000 2.5896630000 -1.6082440000
H 2.5672790000 3.1118290000 0.0421080000
H 1.6040070000 4.1418330000 -1.0008010000
H -0.9510590000 2.6532160000 1.4096760000
H -0.0610680000 4.1431830000 1.0223160000
H 0.7462330000 2.8350410000 1.9054390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344148 (Hartree/Particle)
Thermal correction to Energy= 0.365402
Thermal correction to Enthalpy= 0.366347
Thermal correction to Gibbs (Free) Energy= 0.294441
Sum of electronic and zero-point Energies= -946.127542
Sum of electronic and thermal Energies= -946.106287
Sum of electronic and thermal Enthalpies= -946.105343
Sum of electronic and thermal (Free) Energies= -946.177249

cc/s RT

C 1.5718800000 2.5218590000 -1.3767870000
C 0.6186900000 1.8977990000 -0.7382150000
C 2.9156050000 2.9041360000 -0.8045000000
H 1.3898430000 2.7911980000 -2.4193810000
C -0.4031900000 1.3025030000 -0.1424910000
H 3.0001450000 2.6276760000 0.2497650000
H 3.0726790000 3.9861210000 -0.8896320000
H 3.7246390000 2.4137240000 -1.3600640000
C -0.5113050000 -0.1698540000 -0.2932920000
C -1.5203420000 2.0996380000 0.5832340000
C 0.6571170000 -1.0458570000 -0.3537140000
O -1.6727610000 -0.6484050000 -0.3798370000
C -1.0366870000 3.5366260000 0.8547000000
C -1.8415530000 1.4256720000 1.9363380000
C -2.7917440000 2.1626160000 -0.2958920000
C 1.8334480000 -0.7765980000 0.2416760000
H 0.4855880000 -2.0042650000 -0.8326620000
B -2.0948200000 -2.2573250000 -0.3876900000
H -0.8263300000 4.0776340000 -0.0735160000
H -0.1277380000 3.5481140000 1.4676210000
H -1.8145510000 4.0863680000 1.3957750000
H -2.2144220000 0.4062080000 1.8118460000
H -2.6136360000 2.0028050000 2.4578970000
H -0.9555910000 1.3952600000 2.5823000000
H -2.5734330000 2.6331260000 -1.2617010000
H -3.5534040000 2.7693210000 0.2089090000
H -3.2076300000 1.1708540000 -0.4797050000
H 1.9592230000 0.1594730000 0.7853930000
C 3.0074260000 -1.7125920000 0.2689220000
F -3.4455610000 -2.1861710000 -0.4829040000

F -1.6101110000 -2.7183640000 0.8056330000
F -1.4648080000 -2.7853810000 -1.4890090000
C 4.2462750000 -1.0400210000 -0.3560620000
C 3.2932980000 -2.1617610000 1.7167350000
H 2.7558380000 -2.6001050000 -0.3254050000
H 5.0982400000 -1.7289020000 -0.3426990000
H 4.0610170000 -0.7474400000 -1.3950960000
H 4.5337520000 -0.1423930000 0.2056110000
H 3.5394480000 -1.3038300000 2.3548370000
H 2.4281730000 -2.6721520000 2.1515980000
H 4.1451600000 -2.8506780000 1.7380560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341301 (Hartree/Particle)
Thermal correction to Energy= 0.364340
Thermal correction to Enthalpy= 0.365284
Thermal correction to Gibbs (Free) Energy= 0.287427
Sum of electronic and zero-point Energies= -946.140524
Sum of electronic and thermal Energies= -946.117486
Sum of electronic and thermal Enthalpies= -946.116541
Sum of electronic and thermal (Free) Energies= -946.194398

cc/s TS

C 3.1575220000 -0.9790530000 -0.2945380000
C 1.8508800000 -0.7754830000 -0.0843110000
C 4.1271070000 -1.7753290000 0.5247200000
H 3.5929190000 -0.4629060000 -1.1521810000
C 0.8889000000 0.2084140000 -0.1151990000
H 3.6580460000 -2.2604950000 1.3817250000
H 4.8951560000 -1.0872750000 0.9050750000
H 4.6533130000 -2.5307310000 -0.0702230000
C -0.4576790000 -0.3198540000 -0.1438890000
C 1.1542980000 1.7187060000 -0.0138610000
C -0.4478080000 -1.7299660000 -0.0120970000
O -1.4966510000 0.4080420000 -0.3323280000
C 2.6466270000 2.0620190000 0.1430130000
C 0.3922980000 2.2957530000 1.2043060000
C 0.6344150000 2.3770880000 -1.3200440000
C 0.7042930000 -2.3483320000 0.4951250000
H -1.2563390000 -2.3014940000 -0.4557960000
B -2.9441620000 -0.2312280000 -0.1490760000
H 3.2351230000 1.7636300000 -0.7306330000
H 3.0853120000 1.5957520000 1.0317570000
H 2.7510810000 3.1472000000 0.2500630000
H -0.6819850000 2.1176640000 1.1329720000
H 0.5575120000 3.3781320000 1.2566120000
H 0.7595070000 1.8556630000 2.1391460000
H 1.1758400000 1.9970750000 -2.1943670000
H 0.7997190000 3.4594930000 -1.2653390000
H -0.4321180000 2.1964380000 -1.4629550000
H 1.0485670000 -2.0709110000 1.4938820000
C 0.8431990000 -3.8404620000 0.1744190000
F -3.7931450000 0.8321060000 -0.2107320000
F -2.9103590000 -0.8672300000 1.0806300000
F -3.0899310000 -1.1377970000 -1.1885970000
C 2.2599380000 -4.4234860000 0.1872500000
C -0.0533370000 -4.6119180000 1.1704830000
H 0.4361010000 -3.9906900000 -0.8335430000
H 2.2114940000 -5.4939840000 -0.0403260000
H 2.9012180000 -3.9538740000 -0.5626440000
H 2.7351780000 -4.3214950000 1.1694430000
H 0.3116980000 -4.4924840000 2.1981970000
H -1.0907080000 -4.2649720000 1.1404280000
H -0.0427290000 -5.6815680000 0.9326690000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341439 (Hartree/Particle)
Thermal correction to Energy= 0.362765
Thermal correction to Enthalpy= 0.363709
Thermal correction to Gibbs (Free) Energy= 0.291288
Sum of electronic and zero-point Energies= -946.100741
Sum of electronic and thermal Energies= -946.079414
Sum of electronic and thermal Enthalpies= -946.078470
Sum of electronic and thermal (Free) Energies= -946.150892

cc/s PT

C -2.8377260000 0.7755860000 -0.7228080000
C -1.6192440000 0.2579070000 -0.4201130000
C -0.4101810000 1.0045660000 -0.1199090000
C 0.7198730000 0.1440450000 -0.3664500000
C 0.2305890000 -1.0969830000 -0.7782280000
C -1.2258480000 -1.2117570000 -0.5696440000
C -0.2162610000 2.4206510000 0.3875010000
O 1.9664160000 0.4880790000 -0.2304550000
C -1.4967570000 3.2380830000 0.6434180000
C 0.6654500000 3.1989080000 -0.6304820000
C 0.5444700000 2.3057070000 1.7448890000
C -1.4933690000 -2.0614210000 0.7460790000
H 0.8722480000 -1.8906170000 -1.1349630000
C -2.9794650000 -2.3629790000 0.9664640000
H -3.5782140000 -1.4526840000 1.0637760000
H -3.1037210000 -2.9396910000 1.8899820000
H -3.3937520000 -2.9657330000 0.1482470000
C -0.6616330000 -3.3546130000 0.7531130000
H -1.1409370000 -1.4302270000 1.5727900000
H -0.8626530000 -3.9652540000 -0.1369010000
H -0.9192420000 -3.9580780000 1.6304620000
H 0.4114060000 -3.1432220000 0.7948050000
H -1.7264680000 -1.7133650000 -1.4081670000
B 3.0258760000 -0.6603940000 -0.2003740000
F 4.1977070000 -0.0635900000 0.1637830000
F 3.0501120000 -1.2273220000 -1.4704050000
F 2.5570550000 -1.5884650000 0.7376390000
H -0.0745860000 1.8035410000 2.4970990000
H 0.7624120000 3.3170420000 2.1062410000
H 1.4842440000 1.7638370000 1.6363010000
H -2.2108020000 2.7106590000 1.2846130000
H -1.9991990000 3.5338880000 -0.2837200000
H -1.2167820000 4.1640680000 1.1566620000
H 1.6228130000 2.7025180000 -0.7927410000
H 0.8519230000 4.2043910000 -0.2365300000
H 0.1499750000 3.3024440000 -1.5922670000
C -4.0431070000 0.0413250000 -1.2153200000
H -2.9618610000 1.8502040000 -0.6805950000
H -3.9025250000 -1.0366190000 -1.2953450000
H -4.3260810000 0.4267060000 -2.2049210000
H -4.9035100000 0.2337720000 -0.5595390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344829 (Hartree/Particle)
Thermal correction to Energy= 0.365749
Thermal correction to Enthalpy= 0.366693
Thermal correction to Gibbs (Free) Energy= 0.296127
Sum of electronic and zero-point Energies= -946.140004
Sum of electronic and thermal Energies= -946.119084
Sum of electronic and thermal Enthalpies= -946.118139
Sum of electronic and thermal (Free) Energies= -946.188706

c/d RT

C -1.4690180000 -2.8855120000 -0.9443540000
C -1.3789230000 -1.6994200000 -0.4049980000
C -1.3374240000 -0.4729050000 0.0921430000
C -0.1210380000 0.3301120000 -0.1904580000
C 1.2119490000 -0.2622280000 -0.2694120000
C 1.5748960000 -1.3682930000 0.4066740000
H 1.9318880000 0.3126650000 -0.8394300000
H 0.8356820000 -1.8689650000 1.0303170000
C 2.9514320000 -1.9733340000 0.4451600000
C -2.5381330000 0.1616800000 0.8437300000
O -0.2841620000 1.5657580000 -0.3721490000
C -3.5277470000 -0.9420760000 1.2616820000
C -3.2738310000 1.1665030000 -0.0740120000
C -2.0326710000 0.8765710000 2.1172130000
C 3.4514640000 -2.0241640000 1.9066440000
C 3.9714490000 -1.2947670000 -0.4755400000
H 2.8277480000 -3.0187690000 0.1145350000
H 3.5989610000 -1.0121780000 2.2996130000
H 4.4080410000 -2.5547670000 1.9616480000
H 2.7396160000 -2.5415230000 2.5601320000
H 4.1498740000 -0.2564440000 -0.1738540000
H 3.6367330000 -1.2917730000 -1.5183710000
H 4.9288760000 -1.8244960000 -0.4314080000
B 0.9071760000 2.7102820000 -0.5470430000
F 0.1801530000 3.8464840000 -0.6867650000
F 1.6041560000 2.3285190000 -1.6688530000
F 1.6245700000 2.6075410000 0.6137920000
H -3.6333350000 0.6708370000 -0.9834070000

H -2.6295320000 1.9977900000 -0.3643430000
H -4.1452050000 1.5719140000 0.4545720000
H -3.0513180000 -1.6889930000 1.9072660000
H -3.9472360000 -1.4626940000 0.3946460000
H -4.3576960000 -0.4946060000 1.8193960000
H -1.5278670000 0.1732260000 2.7906570000
H -2.8841600000 1.3032960000 2.6594830000
H -1.3420980000 1.6913640000 1.8866630000
H -1.1503380000 -3.7479450000 -0.3555850000
C -1.9817050000 -3.1667130000 -2.3377260000
H -2.2752560000 -2.2470960000 -2.8498820000
H -2.8492780000 -3.8367610000 -2.2980150000
H -1.2107990000 -3.6671770000 -2.9362670000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341714 (Hartree/Particle)
Thermal correction to Energy= 0.364192
Thermal correction to Enthalpy= 0.365137
Thermal correction to Gibbs (Free) Energy= 0.289251
Sum of electronic and zero-point Energies= -946.139658
Sum of electronic and thermal Energies= -946.117180
Sum of electronic and thermal Enthalpies= -946.116236
Sum of electronic and thermal (Free) Energies= -946.192122

c/d TS

C 2.7778430000 -1.1428250000 -0.2231060000
C 1.5164900000 -0.8404480000 0.0672530000
C 0.1795940000 -1.1408860000 0.0996490000
C -0.6509060000 0.0389880000 -0.0591410000
C 0.1278310000 1.2290170000 0.0247540000
C 1.3769890000 1.1251020000 0.6390340000
C 2.4957270000 2.1195850000 0.3945220000
C -0.4091400000 -2.5308630000 0.3709550000
O -1.9048610000 -0.0252610000 -0.3112200000
C 0.6807390000 -3.5580830000 0.7265070000
C -1.1454610000 -2.9936720000 -0.9131530000
C -1.4122830000 -2.4520430000 1.5469920000
C 2.3363320000 3.3126100000 1.3636020000
C 2.5983390000 2.5832690000 -1.0644510000
H 3.4345730000 1.6140460000 0.6624830000
H 1.4154200000 3.8674730000 1.1537180000
H 3.1813590000 4.0012610000 1.2544790000
H 2.3002710000 2.9834740000 2.4080910000
H 1.7193820000 3.1638850000 -1.3652630000
H 2.6897160000 1.7318340000 -1.7477020000
H 3.4762970000 3.2241700000 -1.1988620000
H 1.4217930000 0.6703950000 1.6289590000
H -0.2023230000 2.1136830000 -0.5081480000
B -2.7801150000 1.3094880000 -0.2940740000
F -2.4938960000 1.9161700000 0.9157140000
F -4.0634210000 0.8713080000 -0.4179860000
F -2.3297640000 2.0653330000 -1.3661070000
H 3.5724810000 -0.6579540000 0.3433620000
C 3.2232600000 -2.0389120000 -1.3492050000
H 3.8713780000 -1.4889830000 -2.0435970000
H 2.3772260000 -2.4397780000 -1.9119170000
H 3.8143210000 -2.8769770000 -0.9569250000
H -0.9106700000 -2.1365090000 2.4695750000
H -1.8433530000 -3.4441310000 1.7236800000
H -2.2277580000 -1.7571050000 1.3386890000
H 1.2495220000 -3.2565880000 1.6129250000
H 1.3863460000 -3.7149770000 -0.0951930000
H 0.2079840000 -4.5220460000 0.9436980000
H -1.9378680000 -2.2956200000 -1.1906090000
H -1.5949110000 -3.9777930000 -0.7354890000
H -0.4501230000 -3.0874320000 -1.7556950000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341008 (Hartree/Particle)
Thermal correction to Energy= 0.362665
Thermal correction to Enthalpy= 0.363610
Thermal correction to Gibbs (Free) Energy= 0.290770
Sum of electronic and zero-point Energies= -946.111606
Sum of electronic and thermal Energies= -946.089949
Sum of electronic and thermal Enthalpies= -946.089005
Sum of electronic and thermal (Free) Energies= -946.161844

c/d PT

C -2.6600700000 1.3360890000 0.1412720000
C -1.4905810000 0.7859590000 -0.2767400000
C -0.9448190000 -0.5550990000 -0.2039430000
C 0.4922800000 -0.4503000000 -0.2409120000
C 0.7980600000 0.8076780000 -0.7650470000
C -0.3752810000 1.7001310000 -0.8216590000
C -0.1086810000 3.0652520000 -0.1085400000
C -1.6343070000 -1.9098900000 -0.2103230000
O 1.3174210000 -1.3909780000 0.0945660000
C -3.1010000000 -1.8741230000 -0.6883340000
C -1.5323310000 -2.5041110000 1.2230490000
C -0.8802790000 -2.8531200000 -1.1946310000
C 0.8938730000 3.9077380000 -0.9132980000
C 0.3605760000 2.8744540000 1.3426550000
H -1.0578680000 3.6180220000 -0.1024010000
H 1.8882370000 3.4476400000 -0.9322620000
H 1.0034130000 4.8985500000 -0.4593210000
H 0.5653210000 4.0492320000 -1.9500830000
H 1.2976360000 2.3075410000 1.3895980000
H -0.3834850000 2.3350830000 1.9393780000
H 0.5276130000 3.8467190000 1.8191110000
H -0.6344490000 1.9258060000 -1.8704580000
H 1.8017650000 1.0827690000 -1.0613710000
B 2.8285750000 -0.9980830000 0.2576530000
F 3.2895370000 -0.6438820000 -1.0065370000
F 3.4323180000 -2.1047250000 0.7776900000
F 2.8427930000 0.1054500000 1.1126750000
H -2.7664980000 2.3963660000 -0.0853160000
C -3.7662460000 0.8086670000 0.9989540000
H -4.0158650000 1.5662840000 1.7524780000
H -3.5126100000 -0.1142510000 1.5201160000
H -4.6826960000 0.6441560000 0.4151480000
H -0.9448620000 -2.4727400000 -2.2206090000
H -1.3650160000 -3.8348540000 -1.1698680000
H 0.1689540000 -2.9742490000 -0.9304230000
H -3.2032520000 -1.3132090000 -1.6240690000
H -3.7902250000 -1.4541800000 0.0420570000
H -3.4304800000 -2.9000940000 -0.8822370000
H -0.4880620000 -2.5901570000 1.5333550000
H -1.9823710000 -3.5036180000 1.2259420000
H -2.0664300000 -1.8901080000 1.9569610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344025 (Hartree/Particle)
Thermal correction to Energy= 0.365330
Thermal correction to Enthalpy= 0.366274
Thermal correction to Gibbs (Free) Energy= 0.294398
Sum of electronic and zero-point Energies= -946.132796
Sum of electronic and thermal Energies= -946.111492
Sum of electronic and thermal Enthalpies= -946.110548
Sum of electronic and thermal (Free) Energies= -946.182423

cc/s RT

C 1.1071500000 2.7942660000 -1.2969260000
C 0.2583680000 2.0058880000 -0.6937970000
C 2.2718760000 3.5016420000 -0.6472190000
H 0.9710000000 2.9585920000 -2.3679830000
C -0.6606940000 1.2287480000 -0.1415430000
H 2.3122330000 3.3110190000 0.4284680000
H 2.1946590000 4.5846050000 -0.8016130000
H 3.2189530000 3.1762290000 -1.0953740000
C -0.4290330000 -0.2359160000 -0.1950390000
C -1.9900800000 1.7927100000 0.4286310000
C 0.9015200000 -0.8334100000 -0.1000870000
O -1.4446530000 -0.9667370000 -0.3393470000
C -1.8589390000 3.3132160000 0.6372730000
C -2.2894250000 1.1338980000 1.7940170000
C -3.1516930000 1.5262620000 -0.5577180000
C 1.9228770000 -0.2820660000 0.5811590000
H 0.9818990000 -1.8251650000 -0.5283240000
B -1.4914600000 -2.6277490000 -0.2897560000
H -1.6799280000 3.8397700000 -0.3056900000
H -1.0394820000 3.5577520000 1.3233500000
H -2.7872370000 3.7026910000 1.0692670000
H -2.4224410000 0.0527030000 1.7102310000
H -3.2137000000 1.5534920000 2.2074010000
H -1.4842370000 1.3306550000 2.5123920000
H -2.9473710000 1.9856140000 -1.5319210000
H -4.0734730000 1.9709580000 -0.1632370000

H -3.3206480000 0.4587010000 -0.7066340000
H 1.7755510000 0.6853620000 1.0591590000
C 3.2802330000 -0.8970880000 0.7919750000
F -2.8135360000 -2.8711520000 -0.4670400000
F -0.9968900000 -2.9282100000 0.9503560000
F -0.6838610000 -3.0344090000 -1.3249840000
C 3.4494850000 -2.2912950000 0.1785240000
C 4.3736430000 0.0771370000 0.2980570000
H 3.4036400000 -0.9839720000 1.8841980000
H 4.4420290000 -2.6883590000 0.4159850000
H 2.7037170000 -2.9948460000 0.5623250000
H 3.3560680000 -2.2597450000 -0.9134010000
H 4.3144040000 0.2081720000 -0.7885910000
H 4.2783350000 1.0637380000 0.7659100000
H 5.3673970000 -0.3153410000 0.5388130000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341529 (Hartree/Particle)
Thermal correction to Energy= 0.364409
Thermal correction to Enthalpy= 0.365353
Thermal correction to Gibbs (Free) Energy= 0.288172
Sum of electronic and zero-point Energies= -946.139412
Sum of electronic and thermal Energies= -946.116533
Sum of electronic and thermal Enthalpies= -946.115588
Sum of electronic and thermal (Free) Energies= -946.192770

cc/d TS

C -2.4673400000 1.4869200000 0.5282930000
C -1.3131770000 0.9209770000 0.1668380000
C -3.8175260000 1.3475080000 -0.1070220000
H -2.4294730000 2.1369410000 1.4047890000
C 0.0465390000 1.1097430000 0.0918890000
H -3.7805890000 0.7944880000 -1.0468590000
H -4.2163250000 2.3483600000 -0.3173710000
H -4.5372930000 0.8599610000 0.5635290000
C 0.7863260000 -0.1339620000 0.0858760000
C 0.7436110000 2.4685680000 -0.0684880000
C -0.0900470000 -1.2467690000 -0.0074060000
O 2.0608270000 -0.1908440000 0.2115220000
C -0.2510720000 3.6370140000 -0.1910760000
C 1.6333740000 2.4483100000 -1.3350450000
C 1.6241640000 2.6968070000 1.1891380000
C -1.3955030000 -1.0251380000 -0.4651830000
H 0.2244030000 -2.2007970000 0.4024940000
B 2.8129880000 -1.5805970000 -0.0002740000
H -0.8594030000 3.7600310000 0.7108620000
H -0.9248600000 3.5142220000 -1.0458890000
H 0.3090550000 4.5669280000 -0.3373800000
H 2.3846000000 1.6578610000 -1.2905070000
H 2.1519830000 3.4093010000 -1.4301480000
H 1.0266390000 2.3049560000 -2.2371050000
H 1.0111940000 2.7366150000 2.0972350000
H 2.1452260000 3.6564720000 1.0916990000
H 2.3694260000 1.9079180000 1.3041110000
H -1.5254030000 -0.5466080000 -1.4365350000
C -2.4587730000 -2.0663630000 -0.1045100000
F 4.1351130000 -1.2545000000 0.0239650000
F 2.3611200000 -2.0571240000 -1.2182700000
F 2.4072800000 -2.3916030000 1.0494160000
C -2.9379340000 -1.9623510000 1.3554930000
C -3.6258290000 -2.1432960000 -1.0987790000
H -1.9193420000 -3.0226340000 -0.1822460000
H -3.5587610000 -2.8281830000 1.6100160000
H -2.0909220000 -1.9387860000 2.0492180000
H -3.5354840000 -1.0604680000 1.5208920000
H -4.2905440000 -1.2770810000 -1.0279960000
H -3.2665060000 -2.2151120000 -2.1319640000
H -4.2316770000 -3.0334140000 -0.8977680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340995 (Hartree/Particle)
Thermal correction to Energy= 0.362558
Thermal correction to Enthalpy= 0.363502
Thermal correction to Gibbs (Free) Energy= 0.291026
Sum of electronic and zero-point Energies= -946.103933
Sum of electronic and thermal Energies= -946.082370
Sum of electronic and thermal Enthalpies= -946.081425
Sum of electronic and thermal (Free) Energies= -946.153901

cc/d PT

C -2.8245090000 0.7573630000 -0.6932690000
C -1.6049770000 0.2015990000 -0.4662780000
C -0.3761070000 0.9232770000 -0.1877040000
C 0.7332200000 0.0500130000 -0.4831840000
C 0.2173310000 -1.1816130000 -0.8862600000
C -1.2453530000 -1.2625490000 -0.7100710000
C -0.1389440000 2.3258520000 0.3411110000
O 1.9868380000 0.3794410000 -0.3676400000
C -1.3900310000 3.1687880000 0.6540050000
C 0.7260970000 3.1055450000 -0.6904190000
C 0.6602250000 2.1723850000 1.6731670000
C -1.5521650000 -2.2796290000 0.4733790000
H 0.8457820000 -2.0059320000 -1.2003540000
C -0.8830210000 -1.8785870000 1.7954480000
H 0.2059430000 -1.8218060000 1.7081540000
H -1.1225530000 -2.6204900000 2.5653190000
H -1.2515870000 -0.9086980000 2.1534540000
C -3.0487610000 -2.5486480000 0.6666550000
H -1.0929130000 -3.2200110000 0.1397990000
H -3.5768510000 -1.6610180000 1.0323610000
H -3.1844190000 -3.3409060000 1.4114380000
H -3.5319320000 -2.8842100000 -0.2582250000
H -1.7402180000 -1.6611550000 -1.6066700000
B 3.0232580000 -0.7763420000 -0.2156260000
F 4.2095870000 -0.1654770000 0.0722550000
F 3.0340260000 -1.4884930000 -1.4119130000
F 2.5405830000 -1.5778190000 0.8260120000
H 0.0504000000 1.6778820000 2.4376070000
H 0.9160040000 3.1733390000 2.0386390000
H 1.5809530000 1.6069160000 1.5306400000
H -2.0915740000 2.6516340000 1.3171220000
H -1.9196900000 3.4892440000 -0.2496550000
H -1.0680580000 4.0809090000 1.1673500000
H 1.6684850000 2.5947950000 -0.8904250000
H 0.9435100000 4.1001580000 -0.2849040000
H 0.1831390000 3.2361940000 -1.6337080000
C -4.0626700000 0.0824600000 -1.1865420000
H -2.9271150000 1.8279490000 -0.5740800000
H -3.9395060000 -0.9820400000 -1.3820790000
H -4.3959640000 0.5694620000 -2.1134850000
H -4.8825940000 0.2125390000 -0.4664560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344942 (Hartree/Particle)
Thermal correction to Energy= 0.365810
Thermal correction to Enthalpy= 0.366754
Thermal correction to Gibbs (Free) Energy= 0.296372
Sum of electronic and zero-point Energies= -946.140402
Sum of electronic and thermal Energies= -946.119534
Sum of electronic and thermal Enthalpies= -946.118589
Sum of electronic and thermal (Free) Energies= -946.188972

c/u RT

C 0.2730940000 -3.1417120000 0.8167370000
C 0.6577660000 -1.9908830000 0.3334400000
C 1.0977930000 -0.8201620000 -0.1007920000
C 0.2147300000 0.3548210000 0.1099780000
C -1.2412960000 0.2723080000 0.0219500000
C -1.8900420000 -0.6212190000 -0.7479610000
H -1.7730470000 1.0574870000 0.5455880000
H -1.3084820000 -1.3476480000 -1.3137350000
C -3.3793090000 -0.7116440000 -0.9407750000
C 2.5164050000 -0.6348960000 -0.7032040000
O 0.7781760000 1.4482820000 0.3800960000
C 3.0969830000 -2.0082540000 -1.0891830000
C 3.4553830000 0.0279650000 0.3321960000
C 2.4287000000 0.2372390000 -1.9759770000
C -4.1848430000 0.3560370000 -0.1927600000
C -3.8566500000 -2.1380020000 -0.5849380000
H -3.5518020000 -0.5800020000 -2.0217830000
H -4.0643340000 0.2577720000 0.8925170000
H -5.2509060000 0.2507380000 -0.4199460000
H -3.8774050000 1.3673940000 -0.4775940000
H -3.7194150000 -2.3380020000 0.4838870000
H -3.3063520000 -2.9013220000 -1.1473910000
H -4.9209330000 -2.2504630000 -0.8176000000
B 0.0509670000 2.9371820000 0.5083580000

F 1.1097100000 3.7383250000 0.7840950000
F -0.8544280000 2.8019590000 1.5338470000
F -0.5244340000 3.1205580000 -0.7195410000
H 3.5223130000 -0.5807310000 1.2415510000
H 3.1141200000 1.0267850000 0.6084950000
H 4.4636780000 0.1112750000 -0.0914410000
H 2.4606700000 -2.5263270000 -1.8160650000
H 3.2147900000 -2.6602030000 -0.2174910000
H 4.0846750000 -1.8714270000 -1.5428570000
H 1.7842740000 -0.2296010000 -2.7308420000
H 3.4275320000 0.3472470000 -2.4134990000
H 2.0451990000 1.2384110000 -1.7647810000
H -0.2617160000 -3.8279440000 0.1572460000
C 0.5069770000 -3.6070790000 2.2352280000
H 1.0461900000 -2.8571920000 2.8192640000
H 1.0868820000 -4.5381580000 2.2415470000
H -0.4479660000 -3.8149500000 2.7331320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341529 (Hartree/Particle)
Thermal correction to Energy= 0.364434
Thermal correction to Enthalpy= 0.365378
Thermal correction to Gibbs (Free) Energy= 0.287957
Sum of electronic and zero-point Energies= -946.139681
Sum of electronic and thermal Energies= -946.116776
Sum of electronic and thermal Enthalpies= -946.115832
Sum of electronic and thermal (Free) Energies= -946.193253

c/u TS

C -2.6924860000 1.0429020000 -0.2881180000
C -1.4400510000 0.7261810000 0.0338470000
C -0.1068760000 1.0441950000 0.0709930000
C 0.7412510000 -0.1280730000 -0.0391200000
C -0.0187390000 -1.3229590000 0.0857080000
C -1.2896520000 -1.2187900000 0.6606540000
C -2.3340830000 -2.3014220000 0.4102630000
C 0.4635570000 2.4481000000 0.3101320000
O 1.9981010000 -0.0536050000 -0.2770960000
C -0.6379100000 3.4756370000 0.6267710000
C 1.2106000000 2.8825380000 -0.9778560000
C 1.4539620000 2.4116770000 1.4994460000
C -2.7077490000 -2.4537740000 -1.0746660000
C -3.5735460000 -2.1637990000 1.3072840000
H -1.8256840000 -3.2320360000 0.7105170000
H -3.2480280000 -1.5731980000 -1.4386760000
H -3.3524290000 -3.3278150000 -1.2160960000
H -1.8199230000 -2.5873450000 -1.7009690000
H -4.1841720000 -1.2955880000 1.0340630000
H -3.2966240000 -2.0645190000 2.3632200000
H -4.2110950000 -3.0490710000 1.2127590000
H -1.3741620000 -0.7363770000 1.6346520000
H 0.3412100000 -2.2336770000 -0.3811310000
B 2.8961230000 -1.3695430000 -0.1945660000
F 2.6133480000 -1.9258830000 1.0399200000
F 4.1724110000 -0.9141370000 -0.3310990000
F 2.4673070000 -2.1820500000 -1.2337290000
H -3.5063060000 0.5989990000 0.2804550000
C -3.0967130000 1.9060170000 -1.4544310000
H -3.7326430000 1.3398790000 -2.1474560000
H -2.2319440000 2.2778840000 -2.0083330000
H -3.6892090000 2.7623460000 -1.1063580000
H 0.9445650000 2.1165930000 2.4245220000
H 1.8723720000 3.4129260000 1.6533590000
H 2.2789650000 1.7201170000 1.3201590000
H -1.2163390000 3.1913070000 1.5125850000
H -1.3332190000 3.6099440000 -0.2072790000
H -0.1736630000 4.4471930000 0.8278190000
H 2.0127980000 2.1849310000 -1.2266680000
H 1.6485330000 3.8755040000 -0.8220350000
H 0.5245820000 2.9466130000 -1.8307900000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340853 (Hartree/Particle)
Thermal correction to Energy= 0.362536
Thermal correction to Enthalpy= 0.363481
Thermal correction to Gibbs (Free) Energy= 0.290695
Sum of electronic and zero-point Energies= -946.108787
Sum of electronic and thermal Energies= -946.087104
Sum of electronic and thermal Enthalpies= -946.086160
Sum of electronic and thermal (Free) Energies= -946.158946

c/u PT

C 2.8777280000 0.1411040000 0.0964250000
C 1.5850000000 0.0314890000 -0.3101460000
C 0.4438150000 0.9175950000 -0.1922500000
C -0.7524170000 0.1193980000 -0.2859900000
C -0.3871950000 -1.0842740000 -0.8904560000
C 1.0737760000 -1.2873830000 -0.9281810000
C 1.4061240000 -2.6806300000 -0.2845220000
C 0.3635510000 2.4354260000 -0.1262620000
O -1.9377240000 0.5068230000 0.0651940000
C 1.6585440000 3.1672550000 -0.5370650000
C -0.0581480000 2.8295400000 1.3176130000
C -0.7385720000 2.9183770000 -1.1167830000
C 0.9836470000 -2.7642970000 1.1909960000
C 2.8497270000 -3.1646580000 -0.4951110000
H 0.7658050000 -3.3766760000 -0.8459180000
H 1.5746890000 -2.0815450000 1.8132170000
H 1.1456380000 -3.7790530000 1.5712110000
H -0.0756500000 -2.5205790000 1.3247050000
H 3.5537320000 -2.6841740000 0.1933020000
H 3.1982900000 -2.9926860000 -1.5209370000
H 2.9082460000 -4.2418710000 -0.3034240000
H 1.4374750000 -1.3154740000 -1.9692760000
H -1.1148960000 -1.8081350000 -1.2366680000
B -3.0454290000 -0.5974860000 0.1959430000
F -3.2698960000 -1.0973380000 -1.0829380000
F -4.1228870000 0.0386530000 0.7383840000
F -2.4992210000 -1.5821910000 1.0216780000
H 3.5221340000 -0.6783480000 -0.2092120000
C 3.5498130000 1.1001520000 1.0270920000
H 4.1514810000 0.5246560000 1.7423400000
H 2.8549280000 1.7188170000 1.5944410000
H 4.2534820000 1.7534520000 0.4928710000
H -0.4622530000 2.6767790000 -2.1496490000
H -0.8194930000 4.0076120000 -1.0372530000
H -1.7113080000 2.4796290000 -0.9006460000
H 2.0700280000 2.7644840000 -1.4692840000
H 2.4363360000 3.1406060000 0.2240290000
H 1.4226640000 4.2221700000 -0.7107290000
H -1.0120610000 2.3677430000 1.5834090000
H -0.1689160000 3.9188330000 1.3699980000
H 0.6942540000 2.5299230000 2.0559210000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344107 (Hartree/Particle)
Thermal correction to Energy= 0.365383
Thermal correction to Enthalpy= 0.366327
Thermal correction to Gibbs (Free) Energy= 0.294323
Sum of electronic and zero-point Energies= -946.129350
Sum of electronic and thermal Energies= -946.108075
Sum of electronic and thermal Enthalpies= -946.107131
Sum of electronic and thermal (Free) Energies= -946.179135

cc/u RT

C 1.0511020000 -2.8723910000 -1.4445130000
C 1.1557820000 -1.7512400000 -0.7830200000
C 0.5325180000 -4.1783970000 -0.8923350000
H 1.3593230000 -2.8722900000 -2.4921970000
C 1.3186490000 -0.5913190000 -0.1649300000
H 0.2635480000 -4.0934340000 0.1638540000
H 1.2917350000 -4.9635770000 -0.9912390000
H -0.3506450000 -4.5092910000 -1.4529070000
C 0.2142260000 0.3934260000 -0.2767890000
C 2.6441570000 -0.2085100000 0.5462810000
C -1.1915670000 -0.0015160000 -0.3365870000
O 0.5381530000 1.6093550000 -0.3321100000
C 3.4923300000 -1.4738950000 0.7743670000
C 2.3314990000 0.4273980000 1.9195330000
C 3.4531910000 0.7797900000 -0.3266480000
C -1.6801390000 -1.1092200000 0.2514580000
H -1.8465290000 0.7233640000 -0.8050460000
B -0.4919190000 2.9131280000 -0.3136730000
H 3.7744900000 -1.9506090000 -0.1699220000
H 2.9584970000 -2.2141190000 1.3818850000
H 4.4128520000 -1.2046570000 1.3037060000
H 1.7526280000 1.3491890000 1.8251680000

H 3.2694510000 0.6723250000 2.4308910000
H 1.7754850000 -0.2685530000 2.5595330000
H 3.6766410000 0.3403500000 -1.3058200000
H 4.4068360000 1.0044770000 0.1664130000
H 2.9164790000 1.7169800000 -0.4817420000
H -0.9944720000 -1.7682280000 0.7821610000
C -3.1276500000 -1.5146770000 0.3150750000
F 0.3777960000 3.9524680000 -0.3604250000
F -1.1755430000 2.7682350000 0.8630100000
F -1.2734260000 2.7617140000 -1.4343330000
C -3.5643790000 -1.6330740000 1.7928290000
C -4.0767500000 -0.6125630000 -0.4812260000
H -3.1744310000 -2.5302750000 -0.1132860000
H -4.5853580000 -2.0245300000 1.8561890000
H -2.9083790000 -2.3067640000 2.3561340000
H -3.5432870000 -0.6526010000 2.2811750000
H -4.0878640000 0.4064440000 -0.0781780000
H -3.7913380000 -0.5562120000 -1.5371340000
H -5.0985480000 -1.0030840000 -0.4296290000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341468 (Hartree/Particle)
Thermal correction to Energy= 0.364376
Thermal correction to Enthalpy= 0.365320
Thermal correction to Gibbs (Free) Energy= 0.287995
Sum of electronic and zero-point Energies= -946.139675
Sum of electronic and thermal Energies= -946.116767
Sum of electronic and thermal Enthalpies= -946.115822
Sum of electronic and thermal (Free) Energies= -946.193148

cc/u TS

C -2.4568070000 1.7125540000 0.5200180000
C -1.3147560000 1.1312200000 0.1531860000
C -3.8061870000 1.5946550000 -0.1270220000
H -2.4169930000 2.3401760000 1.4128920000
C 0.0512800000 1.2121910000 0.0729650000
H -3.7700380000 1.0600310000 -1.0786660000
H -4.2012660000 2.5999580000 -0.3212090000
H -4.5291310000 1.0962520000 0.5325300000
C 0.6924390000 -0.0888420000 0.0843720000
C 0.8463700000 2.5142440000 -0.0976220000
C -0.2691840000 -1.1343850000 0.0082840000
O 1.9563180000 -0.2399900000 0.2253060000
C -0.0691780000 3.7434930000 -0.2405400000
C 1.7416300000 2.4168750000 -1.3559880000
C 1.7307700000 2.6957270000 1.1642820000
C -1.5349270000 -0.8137520000 -0.4857790000
H -0.0413760000 -2.0876950000 0.4723090000
B 2.6004790000 -1.6904610000 0.0549350000
H -0.6842620000 3.9060850000 0.6506990000
H -0.7360620000 3.6585200000 -1.1053970000
H 0.5500950000 4.6360590000 -0.3809640000
H 2.4371090000 1.5778150000 -1.2943430000
H 2.3251390000 3.3389400000 -1.4599810000
H 1.1336430000 2.3019760000 -2.2612860000
H 1.1150980000 2.7917750000 2.0662940000
H 2.3210770000 3.6136320000 1.0594510000
H 2.4159120000 1.8563940000 1.2962000000
H -1.5935310000 -0.3240920000 -1.4583780000
C -2.7444880000 -1.6743370000 -0.1595630000
F 3.9433550000 -1.4667770000 0.0832860000
F 2.1214550000 -2.1618500000 -1.1540730000
F 2.1246250000 -2.4380050000 1.1219320000
C -2.7484550000 -2.9094810000 -1.0888660000
C -2.8244390000 -2.0788780000 1.3194230000
H -3.6392110000 -1.0891780000 -0.4016000000
H -3.6518180000 -3.5053080000 -0.9174070000
H -2.7284830000 -2.6208050000 -2.1456770000
H -1.8784920000 -3.5474730000 -0.8988490000
H -1.9927610000 -2.7314570000 1.6065400000
H -2.8039300000 -1.2004650000 1.9737780000
H -3.7529730000 -2.6269270000 1.5127360000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341020 (Hartree/Particle)
Thermal correction to Energy= 0.362605
Thermal correction to Enthalpy= 0.363549
Thermal correction to Gibbs (Free) Energy= 0.290882
Sum of electronic and zero-point Energies= -946.109034
Sum of electronic and thermal Energies= -946.087450
Sum of electronic and thermal Enthalpies= -946.086505
Sum of electronic and thermal (Free) Energies= -946.159172

cc/u PT

C -3.0158570000 0.4942230000 -0.4452590000
C -1.7076380000 0.1282990000 -0.3887280000
C -0.5494310000 0.9751980000 -0.1875260000
C 0.6324140000 0.1836880000 -0.4318270000
C 0.2281930000 -1.0963930000 -0.8142670000
C -1.2222530000 -1.2930940000 -0.6528010000
C -0.4304600000 2.4316280000 0.2229070000
O 1.8537010000 0.6129580000 -0.3095960000
C -1.7481510000 3.1961810000 0.4453130000
C 0.3769620000 3.1824930000 -0.8757640000
C 0.3652970000 2.4675450000 1.5634750000
C -1.5395110000 -2.3273370000 0.5019150000
H 0.9291570000 -1.8557320000 -1.1349570000
C -1.1281010000 -3.7434740000 0.0746230000
H -1.5854690000 -4.0302980000 -0.8801460000
H -1.4465660000 -4.4714070000 0.8289730000
H -0.0408370000 -3.8326570000 -0.0273000000
C -0.8899140000 -1.9374710000 1.8367030000
H -2.6288680000 -2.3185220000 0.6325990000
H 0.2035530000 -1.9388080000 1.7702130000
H -1.1873090000 -2.6498880000 2.6142830000
H -1.2051790000 -0.9409200000 2.1669360000
H -1.6731120000 -1.6969520000 -1.5717160000
B 2.9782800000 -0.4600890000 -0.1542010000
F 4.1026800000 0.2390120000 0.1767040000
F 3.0726290000 -1.1391780000 -1.3652460000
F 2.5397490000 -1.3241480000 0.8563410000
H -0.1999430000 1.9781160000 2.3647880000
H 0.5183650000 3.5148040000 1.8479350000
H 1.3381330000 1.9852070000 1.4681260000
H -2.3790350000 2.7324480000 1.2110890000
H -2.3267150000 3.3131840000 -0.4775550000
H -1.5038620000 4.2045370000 0.7957080000
H 1.3560350000 2.7298160000 -1.0347640000
H 0.5180410000 4.2216950000 -0.5580240000
H -0.1718540000 3.1904320000 -1.8246150000
C -4.1815800000 -0.3985450000 -0.7246890000
H -3.2762700000 1.5349660000 -0.3068220000
H -3.9079580000 -1.4330010000 -0.9360740000
H -4.7487900000 -0.0102030000 -1.5816890000
H -4.8778660000 -0.3888320000 0.1261390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344682 (Hartree/Particle)
Thermal correction to Energy= 0.365723
Thermal correction to Enthalpy= 0.366667
Thermal correction to Gibbs (Free) Energy= 0.295646
Sum of electronic and zero-point Energies= -946.144973
Sum of electronic and thermal Energies= -946.123932
Sum of electronic and thermal Enthalpies= -946.122988
Sum of electronic and thermal (Free) Energies= -946.194009

2d

cRT

C -0.5978770000 -3.0970720000 -1.2051460000
C -1.0427370000 -2.0543610000 -0.5549830000
C -1.5412650000 -0.9922440000 0.0540900000
C -0.8974780000 0.3207310000 -0.2206080000
C 0.5412010000 0.4948270000 -0.2886790000
C 1.4288390000 -0.3693570000 0.2619620000
H 0.8598920000 1.4211570000 -0.7511090000
C -2.8083610000 -1.0474740000 0.9491120000
O -1.6776990000 1.2977150000 -0.3954470000
C -3.0828430000 -2.5051140000 1.3628550000
C -4.0360820000 -0.5092090000 0.1772760000
C -2.5717840000 -0.2062250000 2.2243980000
B -1.3000720000 2.9019750000 -0.4056930000
F -2.4974460000 3.4740730000 -0.6902310000
F -0.3448190000 3.0647510000 -1.3853590000
F -0.8325520000 3.1138580000 0.8644700000
H -4.2067490000 -1.0921030000 -0.7354090000
H -3.9135130000 0.5387610000 -0.1004090000

H -4.9299510000 -0.5994990000 0.8066500000
H -2.2346180000 -2.9369040000 1.9066870000
H -3.2882920000 -3.1416960000 0.4960150000
H -3.9580970000 -2.5393450000 2.0209280000
H -1.7339720000 -0.6051290000 2.8094020000
H -3.4656180000 -0.2414230000 2.8576730000
H -2.3641680000 0.8431250000 1.9982530000
H 0.1581190000 -3.7236330000 -0.7275790000
C -1.0464750000 -3.5124710000 -2.5868270000
H -1.8009010000 -2.8293980000 -2.9849710000
H -1.4687280000 -4.5247420000 -2.5647560000
H -0.1944620000 -3.5303550000 -3.2774330000
H 1.0431080000 -1.2466100000 0.7755990000
C 2.8800840000 -0.2390830000 0.2693210000
C 3.6395860000 -1.2332400000 0.9165350000
C 3.5603420000 0.8335830000 -0.3436720000
C 4.9478180000 0.9007870000 -0.3079850000
C 5.0295810000 -1.1649140000 0.9506310000
C 5.6871580000 -0.0968940000 0.3375720000
H 3.1264150000 -2.0634790000 1.3960400000
H 5.5985730000 -1.9407020000 1.4548950000
H 6.7717260000 -0.0383680000 0.3630670000
H 3.0002100000 1.6170260000 -0.8439620000
H 5.4580860000 1.7339550000 -0.7825590000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337933 (Hartree/Particle)
Thermal correction to Energy= 0.361183
Thermal correction to Enthalpy= 0.362127
Thermal correction to Gibbs (Free) Energy= 0.282684
Sum of electronic and zero-point Energies= -1059.258913
Sum of electronic and thermal Energies= -1059.235664
Sum of electronic and thermal Enthalpies= -1059.234719
Sum of electronic and thermal (Free) Energies= -1059.314163

cTS

C 1.1213700000 2.4248060000 0.3727690000
C 0.2217980000 1.5136090000 0.0151310000
C -1.0708820000 1.0552020000 -0.0457800000
C -1.1400690000 -0.3930120000 0.0289150000
C 0.1469850000 -0.9752160000 -0.1170340000
C 1.1509710000 -0.1526520000 -0.6611400000
C -2.3115520000 1.9259150000 -0.2742210000
O -2.2359580000 -1.0215080000 0.2522250000
C -1.9421760000 3.3936490000 -0.5545710000
C -3.1823320000 1.8544640000 1.0076470000
C -3.1152630000 1.3822400000 -1.4803480000
H 0.3436760000 -1.9618770000 0.2854920000
B -2.2745120000 -2.6085530000 0.1298310000
F -1.7580870000 -2.8914370000 -1.1217410000
F -3.5904750000 -2.9267680000 0.2838260000
F -1.4534730000 -3.0850780000 1.1425550000
H 2.0739250000 2.4434350000 -0.1563450000
C 0.9992260000 3.3632550000 1.5429360000
H 0.0510100000 3.2421650000 2.0713920000
H 1.0853490000 4.4047720000 1.2060010000
H 1.8172050000 3.1900220000 2.2542680000
H -2.5226090000 1.4339740000 -2.4014290000
H -4.0116380000 1.9961780000 -1.6249180000
H -3.4292970000 0.3485290000 -1.3257170000
H -1.2982920000 3.4890840000 -1.4357540000
H -1.4328260000 3.8624420000 0.2928780000
H -2.8578510000 3.9637400000 -0.7454180000
H -3.4762920000 0.8269610000 1.2310190000
H -4.0892060000 2.4525210000 0.8594280000
H -2.6467650000 2.2623250000 1.8730850000
C 2.5837230000 -0.3650340000 -0.3882100000
H 0.9612870000 0.3041110000 -1.6323740000
C 3.0236850000 -0.9485850000 0.8132300000
C 3.5400070000 0.0315940000 -1.3384040000
C 4.8997770000 -0.1663320000 -1.1052030000
C 5.3222460000 -0.7593550000 0.0860540000
C 4.3813440000 -1.1494110000 1.0442080000
H 2.2963750000 -1.2382680000 1.5666810000
H 6.3815690000 -0.9150620000 0.2701790000
H 4.7085730000 -1.6061040000 1.9738710000
H 3.2105960000 0.4817090000 -2.2724010000
H 5.6272700000 0.1366310000 -1.8528130000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337288 (Hartree/Particle)
Thermal correction to Energy= 0.359256
Thermal correction to Enthalpy= 0.360200
Thermal correction to Gibbs (Free) Energy= 0.285676
Sum of electronic and zero-point Energies= -1059.230325
Sum of electronic and thermal Energies= -1059.208357
Sum of electronic and thermal Enthalpies= -1059.207413
Sum of electronic and thermal (Free) Energies= -1059.281937

cPT

C 0.9005190000 2.5172240000 0.2372940000
C 0.2424750000 1.4544480000 -0.2904370000
C -1.1164010000 0.9739690000 -0.1860070000
C -1.0938310000 -0.4612730000 -0.3322210000
C 0.1084670000 -0.7923530000 -0.9601570000
C 1.0489810000 0.3462440000 -1.0195340000
C -2.4243200000 1.7354530000 -0.0624530000
O -2.0567320000 -1.2554290000 0.0140060000
C -2.3161080000 3.2317780000 -0.4208890000
C -2.9510130000 1.5470510000 1.3889440000
C -3.4589660000 1.1189170000 -1.0496230000
H 0.3265960000 -1.7857290000 -1.3313000000
B -1.7035000000 -2.7786710000 0.1651600000
F -1.4038120000 -3.2535580000 -1.1065780000
F -2.8095130000 -3.3483150000 0.7235620000
F -0.5750330000 -2.8183050000 0.9879010000
H 1.9574590000 2.5654150000 -0.0228510000
C 0.4904880000 3.5360950000 1.2515050000
H -0.4440870000 3.2989150000 1.7594620000
H 0.4031500000 4.5340750000 0.7991110000
H 1.2800170000 3.6123920000 2.0098520000
H -3.1270040000 1.2436920000 -2.0867830000
H -4.4075260000 1.6541160000 -0.9344960000
H -3.6293020000 0.0600180000 -0.8599100000
H -1.8323570000 3.3743600000 -1.3936860000
H -1.7783850000 3.8224850000 0.3191990000
H -3.3261290000 3.6489330000 -0.4907270000
H -3.0831320000 0.4869800000 1.6184080000
H -3.9206020000 2.0499530000 1.4809830000
H -2.2715640000 1.9835160000 2.1292920000
C 2.4301770000 -0.0018280000 -0.4855020000
H 1.1620030000 0.6905510000 -2.0610260000
C 2.5688790000 -0.8953340000 0.5879680000
C 3.5774080000 0.5588900000 -1.0602290000
C 4.8442910000 0.2516180000 -0.5606900000
C 4.9749210000 -0.6304240000 0.5127510000
C 3.8356930000 -1.2065730000 1.0803530000
H 1.6876860000 -1.3678860000 1.0173920000
H 5.9602600000 -0.8759190000 0.8992710000
H 3.9321460000 -1.9059590000 1.9060530000
H 3.4809460000 1.2323240000 -1.9097770000
H 5.7264650000 0.6927450000 -1.0167330000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.339994 (Hartree/Particle)
Thermal correction to Energy= 0.361739
Thermal correction to Enthalpy= 0.362683
Thermal correction to Gibbs (Free) Energy= 0.288880
Sum of electronic and zero-point Energies= -1059.247463
Sum of electronic and thermal Energies= -1059.225718
Sum of electronic and thermal Enthalpies= -1059.224774
Sum of electronic and thermal (Free) Energies= -1059.298577

ccRT

C -0.4542160000 2.9639760000 -1.6235570000
C -0.9722120000 2.0213720000 -0.8812900000
C 0.6220950000 3.9335090000 -1.1985690000
H -0.8243590000 3.0644860000 -2.6460750000
C -1.5535260000 1.0606900000 -0.1831860000
H 0.9149120000 3.7824500000 -0.1560180000
H 0.2720450000 4.9669510000 -1.3095270000
H 1.5119580000 3.8225730000 -1.8306370000
C -0.9926440000 -0.3111700000 -0.3081090000
C -2.8392840000 1.2874610000 0.6564410000
C 0.4325090000 -0.5846760000 -0.3286230000
O -1.8321580000 -1.2493240000 -0.4014040000
C -3.0273330000 2.7943620000 0.9124620000

C -2.6962480000 0.5676790000 2.0169110000
C -4.0778390000 0.7534020000 -0.1009960000
C 1.3684190000 0.2616730000 0.1662820000
H 0.6941480000 -1.5688500000 -0.6980830000
B -1.5570520000 -2.8684080000 -0.2537520000
H -3.1646480000 3.3507220000 -0.0204310000
H -2.1680840000 3.2242400000 1.4405500000
H -3.9168110000 2.9513830000 1.5324970000
H -2.5540780000 -0.5104130000 1.9042070000
H -3.6031260000 0.7251060000 2.6119100000
H -1.8500860000 0.9692940000 2.5879170000
H -4.1811170000 1.2482710000 -1.0737270000
H -4.9814890000 0.9667910000 0.4830670000
H -4.0193770000 -0.3234800000 -0.2659930000
H 1.0360310000 1.2045790000 0.5936130000
C 2.8065170000 0.0310670000 0.2225280000
F -2.7869960000 -3.3884060000 -0.4955970000
F -1.1098700000 -2.9869390000 1.0355380000
F -0.6092830000 -3.1827900000 -1.2032070000
C 3.6220920000 1.0158690000 0.8131390000
C 3.4202190000 -1.1315270000 -0.2879500000
C 5.0021950000 0.8514130000 0.8918760000
H 3.1607170000 1.9156240000 1.2133300000
C 4.7979700000 -1.2944660000 -0.2083050000
H 2.8158670000 -1.9094410000 -0.7433720000
C 5.5936280000 -0.3051620000 0.3805180000
H 5.6148240000 1.6215300000 1.3517810000
H 5.2563560000 -2.1961570000 -0.6040270000
H 6.6701410000 -0.4386490000 0.4409640000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337853 (Hartree/Particle)
Thermal correction to Energy= 0.361135
Thermal correction to Enthalpy= 0.362079
Thermal correction to Gibbs (Free) Energy= 0.282444
Sum of electronic and zero-point Energies= -1059.258655
Sum of electronic and thermal Energies= -1059.235373
Sum of electronic and thermal Enthalpies= -1059.234429
Sum of electronic and thermal (Free) Energies= -1059.314064

ccTS

C 0.9621800000 2.5402130000 -0.6314130000
C 0.1507790000 1.5791500000 -0.1917100000
C 2.2875760000 2.9679280000 -0.0760040000
H 0.6458150000 3.0561210000 -1.5406900000
C -1.1378610000 1.1123700000 -0.1029470000
H 2.5094640000 2.5072040000 0.8874280000
H 2.2917740000 4.0576570000 0.0531490000
H 3.1036740000 2.7260240000 -0.7694310000
C -1.2060650000 -0.3356260000 -0.0595670000
C -2.3871230000 1.9941240000 0.0213000000
C 0.0858940000 -0.9034440000 0.0924220000
O -2.3033710000 -0.9831520000 -0.2051620000
C -2.0389580000 3.4902000000 0.1229650000
C -3.1891980000 1.5865560000 1.2804410000
C -3.2507670000 1.7666460000 -1.2480270000
C 1.1054140000 -0.0589950000 0.5694210000
H 0.2783890000 -1.9101240000 -0.2598190000
B -2.3301610000 -2.5575750000 0.0399120000
H -1.5295070000 3.8581200000 -0.7736300000
H -1.4028550000 3.7039030000 0.9887760000
H -2.9642370000 4.0654800000 0.2360450000
H -3.4881610000 0.5372770000 1.2480090000
H -4.0951610000 2.1998090000 1.3486550000
H -2.6016040000 1.7555730000 2.1906880000
H -2.7107890000 2.0715220000 -2.1521210000
H -4.1593990000 2.3759660000 -1.1762470000
H -3.5419550000 0.7197450000 -1.3502220000
H 0.9436080000 0.4433200000 1.5229850000
C 2.5229260000 -0.3466920000 0.2734010000
F -3.6496390000 -2.8876580000 -0.0401020000
F -1.7670500000 -2.7420330000 1.2897030000
F -1.5452210000 -3.1076530000 -0.9631790000
C 3.5062180000 -0.1468450000 1.2570150000
C 2.9107230000 -0.8487360000 -0.9806590000
C 4.8397470000 -0.4581720000 1.0020960000
H 3.2166330000 0.2359460000 2.2332600000
C 4.2449730000 -1.1548350000 -1.2375030000
H 2.1608040000 -0.9900240000 -1.7544050000
C 5.2115640000 -0.9620490000 -0.2467160000
H 5.5875550000 -0.3111430000 1.7761450000
H 4.5321260000 -1.5425680000 -2.2107160000
H 6.2518840000 -1.2015970000 -0.4483580000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337075 (Hartree/Particle)
Thermal correction to Energy= 0.359058
Thermal correction to Enthalpy= 0.360002
Thermal correction to Gibbs (Free) Energy= 0.285463
Sum of electronic and zero-point Energies= -1059.227825
Sum of electronic and thermal Energies= -1059.205842
Sum of electronic and thermal Enthalpies= -1059.204898
Sum of electronic and thermal (Free) Energies= -1059.279438

ccPT

C -1.1325760000 2.5722040000 -0.6634460000
C -0.4786960000 1.3840040000 -0.5485960000
C 0.8683150000 1.1397450000 -0.0863600000
C 1.1573490000 -0.2715300000 -0.2317470000
C 0.0297770000 -0.8941380000 -0.7718870000
C -1.0888340000 0.0512270000 -0.9838400000
C 1.9252790000 2.0835910000 0.4597730000
O 2.2895170000 -0.8188190000 0.0831830000
C 1.5329800000 3.5670830000 0.5863090000
C 3.1701350000 2.0019500000 -0.4729640000
C 2.3102890000 1.5796010000 1.8838340000
H -0.0284260000 -1.9539250000 -0.9795830000
B 2.4854130000 -2.3564160000 -0.1654530000
F 3.7631240000 -2.6176060000 0.2403410000
F 2.2724630000 -2.5570730000 -1.5250150000
F 1.5103630000 -2.9988660000 0.5881610000
H 1.4593930000 1.6661330000 2.5695760000
H 3.1191880000 2.2108710000 2.2684140000
H 2.6525030000 0.5449700000 1.8670860000
H 0.6775940000 3.7209880000 1.2530150000
H 1.3248940000 4.0312950000 -0.3836670000
H 2.3798730000 4.1075860000 1.0219440000
H 3.5466940000 0.9823190000 -0.5541620000
H 3.9600460000 2.6365300000 -0.0555930000
H 2.9295740000 2.3758760000 -1.4747670000
C -2.5043570000 2.7781160000 -1.2137000000
H -0.6376450000 3.4773620000 -0.3396210000
H -3.0241820000 1.8519880000 -1.4597500000
H -2.4510850000 3.4032160000 -2.1169050000
H -3.1152570000 3.3404030000 -0.4942650000
H -1.3402530000 0.0989620000 -2.0553030000
C -2.3460520000 -0.4052440000 -0.2336350000
C -3.4605510000 -0.8664810000 -0.9428190000
C -4.5937720000 -1.3232280000 -0.2664470000
C -4.6207110000 -1.3271960000 1.1280010000
C -3.5077420000 -0.8768180000 1.8425050000
C -2.3757440000 -0.4245680000 1.1667860000
H -3.4426210000 -0.8723760000 -2.0306530000
H -5.4516320000 -1.6772480000 -0.8314660000
H -5.5003000000 -1.6840490000 1.6562940000
H -3.5169490000 -0.8861190000 2.9288770000
H -1.5086890000 -0.0901570000 1.7303430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340018 (Hartree/Particle)
Thermal correction to Energy= 0.361844
Thermal correction to Enthalpy= 0.362788
Thermal correction to Gibbs (Free) Energy= 0.287506
Sum of electronic and zero-point Energies= -1059.256834
Sum of electronic and thermal Energies= -1059.235008
Sum of electronic and thermal Enthalpies= -1059.234064
Sum of electronic and thermal (Free) Energies= -1059.309346

3a

cRT

C 2.5750720000 -0.0288430000 -0.8098060000
C 1.3429190000 0.3956090000 -0.7870060000
C 0.1170360000 0.8995820000 -0.7355090000
C -1.0334030000 0.0589390000 -0.3580200000
C -1.0125810000 -1.4113260000 -0.4041800000
C -0.3445470000 -2.1173580000 -1.3246960000

H -1.6610820000 -1.8974730000 0.3165270000
C -0.1559520000 2.3785110000 -0.9406850000
O -2.0573320000 0.6760500000 0.0299000000
H 0.7567780000 2.8986100000 -1.2387620000
H -0.5398010000 2.8258370000 -0.0182220000
H -0.9206910000 2.5264400000 -1.7105360000
B -3.5245510000 -0.0208670000 0.4515940000
F -4.2731540000 1.0670000000 0.7466150000
F -3.2121440000 -0.8229370000 1.5218820000
F -3.8877710000 -0.7070340000 -0.6719880000
C 3.5488090000 -0.0761480000 0.3697260000
H 2.9700610000 -0.4049080000 -1.7569660000
H 0.2458010000 -1.6498480000 -2.1053810000
H -0.4100910000 -3.2014360000 -1.3435170000
C 2.9092860000 0.4756500000 1.6533170000
H 2.6039990000 1.5206900000 1.5305110000
H 2.0255630000 -0.1041170000 1.9411820000
H 3.6260800000 0.4295900000 2.4805680000
C 4.7879780000 0.7650070000 -0.0064360000
H 5.5353580000 0.7165420000 0.7942770000
H 5.2573850000 0.3965460000 -0.9263490000
H 4.5208710000 1.8163350000 -0.1596700000
C 3.9659480000 -1.5482550000 0.5799980000
H 4.4187300000 -1.9688320000 -0.3258710000
H 4.7032080000 -1.6214630000 1.3881860000
H 3.1034730000 -2.1680480000 0.8480560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256045 (Hartree/Particle)
Thermal correction to Energy= 0.274702
Thermal correction to Enthalpy= 0.275646
Thermal correction to Gibbs (Free) Energy= 0.208208
Sum of electronic and zero-point Energies= -828.280021
Sum of electronic and thermal Energies= -828.261364
Sum of electronic and thermal Enthalpies= -828.260419
Sum of electronic and thermal (Free) Energies= -828.327857

cTS

C 3.4261570000 -0.3856780000 -0.0216470000
C 2.1495140000 -0.0949310000 -0.2422500000
H 3.8742730000 -1.1916890000 -0.6043620000
C 4.3486920000 0.2173970000 1.0334470000
C 1.0765780000 0.7425190000 -0.3184670000
C 5.5812610000 0.7916660000 0.2959270000
C 3.6663310000 1.3213190000 1.8552830000
C 4.8012410000 -0.9256240000 1.9720380000
C -0.2055110000 0.1036580000 -0.1078720000
C 1.1362830000 2.2017340000 -0.6753160000
H 2.7726130000 0.9477680000 2.3662810000
H 4.3567270000 1.6973190000 2.6182130000
H 3.3719010000 2.1695540000 1.2286330000
H 5.2977200000 1.6090670000 -0.3760050000
H 6.3035710000 1.1827840000 1.0219800000
H 6.0868610000 0.0223270000 -0.2993630000
H 5.2870950000 -1.7343250000 1.4134140000
H 5.5206200000 -0.5466600000 2.7074000000
H 3.9506670000 -1.3502430000 2.5160920000
C -0.0621440000 -1.3186590000 -0.0268190000
O -1.2644060000 0.7932550000 0.0481500000
H 0.8037450000 2.7976940000 0.1836090000
H 0.4448220000 2.4253030000 -1.4947330000
H 2.1452840000 2.5130410000 -0.9522530000
C 1.0832340000 -1.8460180000 -0.6003430000
H -0.7312440000 -1.8887500000 0.6081910000
B -2.6803630000 0.0363780000 0.1317780000
H 1.4700380000 -2.8031080000 -0.2503050000
H 1.3711330000 -1.6082940000 -1.6213610000
F -2.7130570000 -0.7771690000 -0.9835850000
F -3.5974110000 1.0403000000 0.1333580000
F -2.6268260000 -0.6953040000 1.3061640000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255486 (Hartree/Particle)
Thermal correction to Energy= 0.273031
Thermal correction to Enthalpy= 0.273975
Thermal correction to Gibbs (Free) Energy= 0.209397
Sum of electronic and zero-point Energies= -828.252234
Sum of electronic and thermal Energies= -828.234690
Sum of electronic and thermal Enthalpies= -828.233745
Sum of electronic and thermal (Free) Energies= -828.298323

cPT

C 2.3939620000 0.8605200000 -0.0480350000
C 1.0372220000 0.7024730000 -0.0475050000
C 0.1418580000 -0.4180810000 -0.0335740000
C -1.2192280000 0.0379770000 0.0257190000
C -1.2083170000 1.4409390000 0.0168140000
C 0.1682230000 1.9566950000 -0.0540690000
C 0.3766240000 -1.8838420000 -0.0839830000
O -2.2156820000 -0.7807820000 0.0645890000
H 1.3422430000 -2.1701200000 -0.4948630000
H -0.4341190000 -2.3461450000 -0.6575840000
H 0.2896280000 -2.3018360000 0.9302010000
H -2.1017690000 2.0489960000 0.0635520000
B -3.6648770000 -0.1757030000 0.0122200000
F -3.7751950000 0.6544300000 1.1232200000
F -4.5049100000 -1.2502260000 0.0349690000
F -3.7218850000 0.5660780000 -1.1626100000
H 2.6899790000 1.9100280000 -0.1037420000
C 3.5872600000 -0.0783290000 0.0216930000
H 0.3377490000 2.5507370000 -0.9671800000
H 0.4065450000 2.6298900000 0.7849410000
C 3.4898620000 -1.0606000000 1.2119250000
H 3.4045890000 -0.5154130000 2.1581990000
H 2.6390720000 -1.7386300000 1.1376740000
H 4.3994830000 -1.6703360000 1.2568980000
C 4.8503580000 0.7907630000 0.2276450000
H 5.7444710000 0.1601520000 0.2713160000
H 4.9822660000 1.5035350000 -0.5949740000
H 4.7938410000 1.3579550000 1.1640860000
C 3.7454280000 -0.8384120000 -1.3208370000
H 3.8717900000 -0.1381390000 -2.1536690000
H 4.6363500000 -1.4756570000 -1.2780920000
H 2.8861270000 -1.4734040000 -1.5495400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257957 (Hartree/Particle)
Thermal correction to Energy= 0.275351
Thermal correction to Enthalpy= 0.276296
Thermal correction to Gibbs (Free) Energy= 0.212122
Sum of electronic and zero-point Energies= -828.285861
Sum of electronic and thermal Energies= -828.268466
Sum of electronic and thermal Enthalpies= -828.267522
Sum of electronic and thermal (Free) Energies= -828.331696

ccRT

C 2.4760640000 0.3437460000 -0.8439170000
C 1.2753280000 0.6269880000 -0.4225690000
C 0.0656030000 1.0311680000 -0.0559110000
C -1.0922710000 0.1200510000 -0.0795380000
C -0.9835370000 -1.3444670000 -0.1735050000
C -0.0275520000 -2.0657460000 0.4229520000
H -1.8046270000 -1.8233830000 -0.6962220000
C -0.2227210000 2.4860200000 0.2695680000
O -2.2197350000 0.6754670000 -0.0530790000
H 0.7000650000 3.0697180000 0.2623280000
H -0.6955380000 2.5741040000 1.2534550000
H -0.9210990000 2.9085180000 -0.4598110000
B -3.7042330000 -0.1072580000 -0.0213870000
F -4.5643330000 0.9347720000 0.0515970000
F -3.6277260000 -0.8950640000 1.0915760000
F -3.7323190000 -0.8065710000 -1.2029630000
C 3.6875700000 -0.1004630000 -0.0227850000
H 2.6525880000 0.4280050000 -1.9198810000
H 0.7552800000 -1.6144820000 1.0218630000
H -0.0351470000 -3.1502050000 0.3624920000
C 4.0380920000 -1.5503350000 -0.4228120000
H 3.2205140000 -2.2379460000 -0.1801790000
H 4.2369570000 -1.6300340000 -1.4978620000
H 4.9353930000 -1.8854410000 0.1109380000
C 3.4193490000 -0.0159460000 1.4883270000
H 4.3166960000 -0.3058220000 2.0461050000
H 3.1490150000 1.0023840000 1.7882610000
H 2.6093230000 -0.6851590000 1.7979320000
C 4.8623270000 0.8330890000 -0.3897550000
H 4.6426850000 1.8716900000 -0.1189010000
H 5.7699900000 0.5268440000 0.1432820000

H 5.0768530000 0.8008900000 -1.4644430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255952 (Hartree/Particle)
Thermal correction to Energy= 0.274630
Thermal correction to Enthalpy= 0.275574
Thermal correction to Gibbs (Free) Energy= 0.208312
Sum of electronic and zero-point Energies= -828.278842
Sum of electronic and thermal Energies= -828.260164
Sum of electronic and thermal Enthalpies= -828.259220
Sum of electronic and thermal (Free) Energies= -828.326482

ccTS

C -2.3755890000 0.4956790000 0.5499640000
C -1.1168610000 0.4452400000 0.1248470000
C 0.0762340000 1.1007580000 -0.0012480000
C 1.2500400000 0.2582160000 0.0289400000
C 0.8824760000 -1.1254500000 0.0537110000
C -0.3684240000 -1.4316050000 -0.4553440000
H 1.4952820000 -1.8314570000 0.6035150000
C 0.2180770000 2.5829240000 -0.2011290000
O 2.4183970000 0.7565530000 0.1186830000
H -0.7388040000 3.1006670000 -0.1129490000
H 0.6603570000 2.8047270000 -1.1797080000
H 0.9162950000 2.9749240000 0.5478650000
B 3.6882440000 -0.2260130000 0.0356910000
F 4.7581410000 0.6113230000 -0.0125790000
F 3.4831600000 -0.9718130000 -1.1089390000
F 3.6157780000 -1.0025350000 1.1795950000
C -3.6542330000 -0.1640140000 0.0584920000
H -2.5208270000 1.1089520000 1.4454340000
H -0.6767280000 -1.0772580000 -1.4334110000
H -0.8652160000 -2.3491640000 -0.1426010000
C -4.1017780000 -1.2165050000 1.1002160000
H -3.3683320000 -2.0256130000 1.1860940000
H -4.2267690000 -0.7683880000 2.0925490000
H -5.0620870000 -1.6558640000 0.8055890000
C -3.5227020000 -0.8195930000 -1.3267930000
H -4.5107720000 -1.1340260000 -1.6804230000
H -3.1114970000 -0.1208520000 -2.0642700000
H -2.8920360000 -1.7124440000 -1.3040460000
C -4.7212030000 0.9560450000 -0.0176410000
H -4.4465420000 1.7165590000 -0.7569820000
H -5.6892800000 0.5327140000 -0.3086040000
H -4.8496480000 1.4538590000 0.9505190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255368 (Hartree/Particle)
Thermal correction to Energy= 0.272952
Thermal correction to Enthalpy= 0.273897
Thermal correction to Gibbs (Free) Energy= 0.209198
Sum of electronic and zero-point Energies= -828.248305
Sum of electronic and thermal Energies= -828.230720
Sum of electronic and thermal Enthalpies= -828.229776
Sum of electronic and thermal (Free) Energies= -828.294475

ccPT

C 2.3384840000 0.5624420000 0.0000000000
C 1.0565800000 0.1072360000 0.0000000000
C -0.0880860000 0.9735120000 0.0000000000
C -1.3009240000 0.2127410000 0.0000000000
C -0.9411220000 -1.1404310000 0.0000000000
C 0.5296090000 -1.3186180000 0.0000000000
C -0.1427890000 2.4544980000 0.0000000000
O -2.4659030000 0.7717990000 0.0000000000
H 0.8327560000 2.9433850000 -0.0000010000
H -0.7214130000 2.7902300000 0.8707890000
H -0.7214150000 2.7902300000 -0.8707870000
H -1.6556600000 -1.9526540000 0.0000000000
B -3.7207850000 -0.1666500000 0.0000000000
F -4.7995680000 0.6697830000 0.0000000000
F -3.6134680000 -0.9520010000 1.1440630000
F -3.6134680000 -0.9520000000 -1.1440630000
C 3.6785350000 -0.1304830000 0.0000000000
H 2.4464270000 1.6474840000 0.0000000000
H 0.8665400000 -1.8912270000 0.8760240000
H 0.8665400000 -1.8912270000 -0.8760230000
C 4.4392670000 0.3598620000 -1.2612100000
H 4.5154310000 1.4527930000 -1.2866180000
H 5.4562710000 -0.0484470000 -1.2613420000
H 3.9394470000 0.0315240000 -2.1788450000
C 4.4392700000 0.3598670000 1.2612060000
H 5.4562740000 -0.0484410000 1.2613370000
H 4.5154350000 1.4527990000 1.2866080000
H 3.9394520000 0.0315340000 2.1788430000
C 3.6395890000 -1.6668410000 0.0000030000
H 3.1397180000 -2.0642590000 0.8888640000
H 3.1397170000 -2.0642630000 -0.8888540000
H 4.6637080000 -2.0553500000 0.0000030000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258109 (Hartree/Particle)
Thermal correction to Energy= 0.275569
Thermal correction to Enthalpy= 0.276513
Thermal correction to Gibbs (Free) Energy= 0.211251
Sum of electronic and zero-point Energies= -828.295475
Sum of electronic and thermal Energies= -828.278016
Sum of electronic and thermal Enthalpies= -828.277071
Sum of electronic and thermal (Free) Energies= -828.342334

3b

cRT

C -2.6013030000 0.0408890000 -0.7395430000
C -1.3736670000 -0.3877850000 -0.8390970000
C -0.1546570000 -0.9002270000 -0.9290680000
C 1.0076660000 -0.2067790000 -0.3367470000
C 1.0294060000 1.2237100000 -0.0359620000
C 0.3649370000 2.1504700000 -0.7485970000
H 1.7087210000 1.5150160000 0.7583240000
C 0.0992610000 -2.2739260000 -1.5228000000
O 2.0003820000 -0.9399460000 -0.0838270000
H -0.8181960000 -2.6809490000 -1.9531890000
H 0.4696020000 -2.9577090000 -0.7524430000
H 0.8680200000 -2.2220920000 -2.3011940000
B 3.4731170000 -0.4218240000 0.4925520000
F 4.1764280000 -1.5783470000 0.5526160000
F 3.1823040000 0.1434880000 1.7122340000
F 3.8943720000 0.4779230000 -0.4475900000
C -3.5725300000 -0.2243410000 0.4126980000
H -0.2435230000 1.8394330000 -1.5949600000
C 0.4387870000 3.6209710000 -0.4917640000
H 1.0661890000 3.8548930000 0.3726020000
H -0.5656560000 4.0314020000 -0.3202960000
H 0.8428240000 4.1445090000 -1.3683730000
C -2.9352930000 -1.1061020000 1.4977990000
C -4.8190860000 -0.9243760000 -0.1711980000
H -2.6383400000 -2.0813560000 1.0965610000
H -3.6501200000 -1.2797180000 2.3097570000
H -2.0461840000 -0.6319280000 1.9273980000
H -4.5600940000 -1.8972600000 -0.6030800000
H -5.2870720000 -0.3185580000 -0.9563440000
H -5.5650640000 -1.0883710000 0.6154470000
C -3.9793020000 1.1386300000 1.0143540000
H -3.1125000000 1.6563520000 1.4394750000
H -4.7164750000 0.9962120000 1.8133750000
H -4.4285670000 1.7919890000 0.2567270000
H -2.9954670000 0.6624470000 -1.5477290000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284293 (Hartree/Particle)
Thermal correction to Energy= 0.304536
Thermal correction to Enthalpy= 0.305481
Thermal correction to Gibbs (Free) Energy= 0.234246
Sum of electronic and zero-point Energies= -867.574973
Sum of electronic and thermal Energies= -867.554730
Sum of electronic and thermal Enthalpies= -867.553785
Sum of electronic and thermal (Free) Energies= -867.625020

cTS

C 3.4161360000 -0.4239050000 0.0074130000
C 2.1351720000 -0.1560420000 -0.2234130000
H 3.8664820000 -1.2575530000 -0.5342610000
C 4.3442380000 0.2248100000 1.0296950000
C 1.0813910000 0.7122790000 -0.3074000000
C 3.6602140000 1.3436870000 1.8294580000

C 5.5586120000 0.7928110000 0.2573650000
C 4.8272520000 -0.8817130000 1.9963200000
C -0.2062180000 0.0940650000 -0.0970110000
C 1.1675990000 2.1645950000 -0.6806540000
H 3.3520300000 2.1729930000 1.1849630000
H 4.3548420000 1.7451100000 2.5755080000
H 2.7750030000 0.9753980000 2.3587900000
H 5.2541460000 1.5852430000 -0.4349900000
H 6.0663900000 0.0125710000 -0.3217310000
H 6.2859080000 1.2156330000 0.9604140000
H 3.9909710000 -1.3016760000 2.5657570000
H 5.5512640000 -0.4702940000 2.7093560000
H 5.3173280000 -1.7004680000 1.4561210000
C -0.0794630000 -1.3240030000 -0.0212460000
O -1.2615260000 0.7974860000 0.0540150000
H 2.1779660000 2.4510600000 -0.9789070000
H 0.8641030000 2.7775150000 0.1774550000
H 0.4652150000 2.3953920000 -1.4887700000
C 1.0731640000 -1.8749200000 -0.5858590000
H -0.7741530000 -1.8966490000 0.5843850000
B -2.6752170000 0.0573810000 0.1222610000
H 1.3146900000 -1.6131200000 -1.6157310000
C 1.5906200000 -3.2259400000 -0.1645950000
F -2.7139070000 -0.7503970000 -1.0000570000
F -3.5890450000 1.0660640000 0.1266330000
F -2.6433030000 -0.6894650000 1.2904870000
H 1.0873240000 -4.0085070000 -0.7471770000
H 1.4129440000 -3.4202390000 0.8966410000
H 2.6628280000 -3.3222010000 -0.3632360000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.283573 (Hartree/Particle)
Thermal correction to Energy= 0.302738
Thermal correction to Enthalpy= 0.303682
Thermal correction to Gibbs (Free) Energy= 0.235613
Sum of electronic and zero-point Energies= -867.544877
Sum of electronic and thermal Energies= -867.525711
Sum of electronic and thermal Enthalpies= -867.524767
Sum of electronic and thermal (Free) Energies= -867.592837

cPT

C 2.3759840000 0.6338370000 0.1689740000
C 1.0178990000 0.5098480000 0.1094610000
C 0.1161820000 -0.5843460000 -0.1157550000
C -1.2398390000 -0.1518790000 0.0671600000
C -1.2169180000 1.2139230000 0.3766700000
C 0.1580200000 1.7529290000 0.3742380000
C 0.3407000000 -2.0019410000 -0.4974660000
O -2.2410100000 -0.9571520000 -0.0614880000
H 1.3083870000 -2.1975130000 -0.9536720000
H -0.4673860000 -2.3103860000 -1.1702600000
H 0.2336440000 -2.6410280000 0.3917630000
H -2.1051580000 1.7969340000 0.5833510000
B -3.6843220000 -0.3483100000 0.0356830000
F -3.7818340000 0.2158070000 1.3041250000
F -4.5333780000 -1.3957170000 -0.1731660000
F -3.7456100000 0.6366580000 -0.9448920000
H 2.6938620000 1.6654890000 0.3291700000
C 3.5547290000 -0.3233980000 0.0814070000
C 0.3496390000 2.8947960000 -0.6553800000
H 0.3992660000 2.1650180000 1.3695050000
H 0.1613150000 2.5340810000 -1.6709930000
H 1.3644080000 3.3013140000 -0.6086350000
H -0.3485700000 3.7103600000 -0.4440600000
C 4.8176660000 0.4580890000 0.5154630000
H 5.7028760000 -0.1837340000 0.4559570000
H 4.9897580000 1.3278080000 -0.1296600000
H 4.7294080000 0.8128740000 1.5489950000
C 3.4035310000 -1.5364900000 1.0275110000
H 3.2799670000 -1.2057370000 2.0644940000
H 2.5551500000 -2.1730660000 0.7750890000
H 4.3083720000 -2.1529570000 0.9779190000
C 3.7592550000 -0.7790600000 -1.3868680000
H 3.9236430000 0.0818380000 -2.0440320000
H 4.6426220000 -1.4251360000 -1.4503110000
H 2.9044330000 -1.3359640000 -1.7782300000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.286573 (Hartree/Particle)
Thermal correction to Energy= 0.305440
Thermal correction to Enthalpy= 0.306384
Thermal correction to Gibbs (Free) Energy= 0.239017
Sum of electronic and zero-point Energies= -867.571117
Sum of electronic and thermal Energies= -867.552250
Sum of electronic and thermal Enthalpies= -867.551305
Sum of electronic and thermal (Free) Energies= -867.618673

ccRT

C -2.4710520000 -0.6283120000 -0.8348790000
C -1.2693820000 -0.8690760000 -0.3879350000
C -0.0595090000 -1.2401680000 0.0083030000
C 1.1010600000 -0.3305110000 -0.0779460000
C 1.0017390000 1.1209880000 -0.2266840000
C 0.0269420000 1.8735200000 0.3107030000
H 1.8437480000 1.5830760000 -0.7317660000
C 0.2311320000 -2.6700850000 0.4295760000
O 2.2252990000 -0.8990880000 -0.0546730000
H -0.6916980000 -3.2526570000 0.4679430000
H 0.7105900000 -2.6919010000 1.4140050000
H 0.9247280000 -3.1407480000 -0.2742560000
B 3.7074410000 -0.1408440000 -0.0548370000
F 4.5609750000 -1.1901540000 0.0238530000
F 3.6618540000 0.6674690000 1.0475560000
F 3.7400830000 0.5445270000 -1.2466270000
C -3.6950060000 -0.1485140000 -0.0536660000
H -2.6403940000 -0.7894310000 -1.9032800000
H -0.7607770000 1.3944320000 0.8867360000
C -4.0765970000 1.2590450000 -0.5618160000
H -3.2783840000 1.9826460000 -0.3624690000
H -4.2654980000 1.2554090000 -1.6415930000
H -4.9872500000 1.6106010000 -0.0622960000
C -3.4335330000 -0.1134130000 1.4605360000
H -4.3407780000 0.1948060000 1.9920170000
H -3.1397360000 -1.0994240000 1.8365410000
H -2.6416820000 0.5969180000 1.7221320000
C -4.8485190000 -1.1316790000 -0.3531800000
H -4.6082720000 -2.1418650000 -0.0038300000
H -5.7654730000 -0.8056730000 0.1516370000
H -5.0576820000 -1.1856410000 -1.4280610000
C -0.0295030000 3.3647310000 0.2207780000
H 0.7918070000 3.7693730000 -0.3769050000
H -0.9805750000 3.6889300000 -0.2233090000
H 0.0148950000 3.8123440000 1.2225380000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284218 (Hartree/Particle)
Thermal correction to Energy= 0.304474
Thermal correction to Enthalpy= 0.305418
Thermal correction to Gibbs (Free) Energy= 0.234442
Sum of electronic and zero-point Energies= -867.573581
Sum of electronic and thermal Energies= -867.553325
Sum of electronic and thermal Enthalpies= -867.552381
Sum of electronic and thermal (Free) Energies= -867.623357

ccTS

C 2.3890560000 0.4296090000 -0.5594320000
C 1.1159700000 0.3043280000 -0.1739570000
C -0.0453670000 1.0213700000 -0.0500880000
C -1.2541350000 0.2351230000 -0.0473350000
C -0.9490930000 -1.1531830000 -0.0902890000
C 0.3242330000 -1.5416240000 0.3362500000
H -1.6289170000 -1.8319950000 -0.5952920000
C -0.1136240000 2.5085450000 0.1437910000
O -2.4054280000 0.7861270000 -0.0975520000
H 0.8426750000 2.9937890000 -0.0614400000
H -0.4260200000 2.7554910000 1.1661480000
H -0.8855440000 2.9154600000 -0.5191410000
B -3.7056460000 -0.1328600000 0.0327270000
F -4.7402840000 0.7483940000 0.1051990000
F -3.5050060000 -0.8817530000 1.1782700000
F -3.7100720000 -0.9266100000 -1.1045560000
C 3.6924700000 -0.1304920000 -0.0144660000
H 2.5307390000 1.0774240000 -1.4309990000
H 0.6430030000 -1.2410900000 1.3326830000
C 4.2814480000 -1.1548060000 -1.0130400000
H 3.6343780000 -2.0298770000 -1.1251870000
H 4.4142240000 -0.7076040000 -2.0047710000

H 5.2629300000 -1.4984560000 -0.6656450000
C 3.5530030000 -0.7501050000 1.3872210000
H 4.5418210000 -1.0236190000 1.7717810000
H 3.1061390000 -0.0382300000 2.0903310000
H 2.9451230000 -1.6579110000 1.3871400000
C 4.6621220000 1.0757020000 0.0800900000
H 4.2886110000 1.8330420000 0.7781700000
H 5.6425090000 0.7392970000 0.4363140000
H 4.8048920000 1.5530540000 -0.8962810000
C 0.8917770000 -2.8556870000 -0.1461350000
H 0.7394010000 -2.9904800000 -1.2207280000
H 1.9568340000 -2.9553230000 0.0701830000
H 0.3789480000 -3.6770170000 0.3721200000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.283442 (Hartree/Particle)
Thermal correction to Energy= 0.302668
Thermal correction to Enthalpy= 0.303613
Thermal correction to Gibbs (Free) Energy= 0.235677
Sum of electronic and zero-point Energies= -867.537435
Sum of electronic and thermal Energies= -867.518208
Sum of electronic and thermal Enthalpies= -867.517264
Sum of electronic and thermal (Free) Energies= -867.585200

ccPT

C 2.2661120000 0.7174120000 -0.0871910000
C 0.9985350000 0.2209330000 -0.0746370000
C -0.1539800000 1.0641940000 -0.2445910000
C -1.3589660000 0.3276770000 -0.0164280000
C -0.9865330000 -0.9925920000 0.2530250000
C 0.4852380000 -1.1959830000 0.1715240000
C -0.2213180000 2.5105920000 -0.5618610000
O -2.5278020000 0.8771630000 -0.0790670000
H 0.7354520000 2.9600410000 -0.8326780000
H -0.6442630000 3.0485920000 0.2980050000
H -0.9446830000 2.6600840000 -1.3731360000
H -1.6939480000 -1.7888690000 0.4458270000
B -3.7728200000 -0.0460700000 0.1399280000
F -4.8586680000 0.7736560000 0.0260900000
F -3.6198460000 -0.6086820000 1.4045750000
F -3.7001280000 -1.0286380000 -0.8433800000
C 3.6251570000 0.1063660000 0.1811120000
H 2.3385510000 1.7759150000 -0.3370270000
H 0.8688270000 -1.5979230000 1.1197090000
C 0.8197850000 -2.2048180000 -0.9598280000
H 0.4709370000 -1.8232900000 -1.9242300000
H 0.3183740000 -3.1588300000 -0.7694630000
H 1.8936480000 -2.3940840000 -1.0297240000
C 4.4848500000 1.1944600000 0.8715870000
H 5.5002770000 0.8201110000 1.0408430000
H 4.5585160000 2.0985650000 0.2560170000
H 4.0632490000 1.4774780000 1.8427610000
C 3.6127870000 -1.1420970000 1.0838260000
H 3.1238350000 -0.9339800000 2.0418600000
H 3.1146590000 -1.9958630000 0.6197350000
H 4.6437210000 -1.4458760000 1.2966500000
C 4.2676010000 -0.2329250000 -1.1916520000
H 4.3181750000 0.6499720000 -1.8385270000
H 5.2902220000 -0.5975010000 -1.0388680000
H 3.7031500000 -1.0078500000 -1.7197300000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.286700 (Hartree/Particle)
Thermal correction to Energy= 0.305576
Thermal correction to Enthalpy= 0.306520
Thermal correction to Gibbs (Free) Energy= 0.239033
Sum of electronic and zero-point Energies= -867.577471
Sum of electronic and thermal Energies= -867.558595
Sum of electronic and thermal Enthalpies= -867.557651
Sum of electronic and thermal (Free) Energies= -867.625138

3c

c/s RT

C -2.6126900000 -0.2685490000 -0.7149300000
C -1.3929500000 -0.7047660000 -0.8655170000
C -0.1842130000 -1.2263770000 -1.0182980000
C 0.9804340000 -0.6653430000 -0.3034310000
C 1.0295950000 0.7002230000 0.2149580000
C 0.4192770000 1.7473330000 -0.3678990000
H 1.6935440000 0.8453580000 1.0609510000
H -0.1726690000 1.5927570000 -1.2695190000
C 0.5421500000 3.1708430000 0.0953220000
C 0.0512020000 -2.4927780000 -1.8213010000
O 1.9506510000 -1.4550100000 -0.1510130000
H -0.8662160000 -2.8025570000 -2.3263250000
H 0.3910510000 -3.3003710000 -1.1651900000
H 0.8362330000 -2.3358520000 -2.5687700000
C -0.8515280000 3.7724330000 0.3622580000
C 1.3127960000 4.0019750000 -0.9513680000
H 1.1135500000 3.1812970000 1.0323050000
H -1.4597690000 3.7788310000 -0.5510170000
H -0.7584170000 4.8080150000 0.7079370000
H -1.3936620000 3.2057040000 1.1268930000
H 0.7862110000 4.0103280000 -1.9138680000
H 2.3164030000 3.5975840000 -1.1161330000
H 1.4105530000 5.0398830000 -0.6135600000
B 3.4205310000 -1.0679010000 0.5205810000
F 4.1010790000 -2.2343800000 0.4074790000
F 3.1208060000 -0.6952250000 1.8103670000
F 3.8780260000 -0.0402850000 -0.2589460000
C -3.6092560000 -0.6955300000 0.3648720000
C -3.9984100000 0.5594290000 1.1763930000
C -3.0097970000 -1.7577340000 1.2994040000
C -4.8598260000 -1.2612030000 -0.3430410000
H -5.3011250000 -0.5243610000 -1.0248090000
H -5.6228600000 -1.5340340000 0.3955750000
H -4.6136570000 -2.1562070000 -0.9248470000
H -3.1284840000 0.9797640000 1.6931020000
H -4.7524760000 0.3054730000 1.9307950000
H -4.4198290000 1.3388090000 0.5302480000
H -2.1186340000 -1.3812700000 1.8132260000
H -2.7261340000 -2.6607960000 0.7477910000
H -3.7422730000 -2.0451380000 2.0618350000
H -2.9791190000 0.4856500000 -1.4160480000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341277 (Hartree/Particle)
Thermal correction to Energy= 0.364266
Thermal correction to Enthalpy= 0.365211
Thermal correction to Gibbs (Free) Energy= 0.287137
Sum of electronic and zero-point Energies= -946.146124
Sum of electronic and thermal Energies= -946.123135
Sum of electronic and thermal Enthalpies= -946.122191
Sum of electronic and thermal (Free) Energies= -946.200264

c/s TS

C 3.4630730000 -0.5227630000 0.0455300000
C 2.1612690000 -0.2986410000 -0.1350270000
H 3.9364680000 -1.2855870000 -0.5696880000
C 4.3914560000 0.0963230000 1.0857400000
C 1.1335480000 0.6089170000 -0.1414960000
C 5.0215740000 -1.0583320000 1.9003700000
C 3.6724470000 1.0598890000 2.0418810000
C 5.5094520000 0.8440710000 0.3193800000
C -0.1715680000 0.0180170000 0.0005190000
C 1.2639320000 2.0839710000 -0.3915580000
H 5.5480180000 -1.7674870000 1.2504410000
H 5.7479200000 -0.6606030000 2.6187590000
H 4.2583300000 -1.6094770000 2.4607330000
H 3.2718170000 1.9326660000 1.5181850000
H 2.8456100000 0.5650940000 2.5624060000
H 4.3761790000 1.4240440000 2.7985130000
H 6.2423460000 1.2489970000 1.0272500000
H 6.0407920000 0.1758610000 -0.3683630000
H 5.1034820000 1.6777610000 -0.2637890000
C -0.0858080000 -1.3989340000 -0.0525020000
O -1.2124760000 0.7368960000 0.1928420000
H 0.9645710000 2.6327370000 0.5103600000
H 0.5765450000 2.3985420000 -1.1843430000
H 2.2840490000 2.3680140000 -0.6566030000
C 1.0711380000 -1.9460350000 -0.6269440000
H -0.8246470000 -2.0008700000 0.4657000000
B -2.6411420000 0.0357960000 0.1570540000
H 1.3353820000 -1.6376960000 -1.6407990000
C 1.4154630000 -3.4026750000 -0.3343720000
F -2.6734270000 -0.6643950000 -1.0372630000

F -3.5317020000 1.0630540000 0.2338010000
F -2.6641800000 -0.8205220000 1.2493380000
C 2.8607310000 -3.7976250000 -0.6730900000
C 0.4296860000 -4.2872050000 -1.1339190000
H 1.2470210000 -3.5867110000 0.7343910000
H 3.5818650000 -3.3433840000 0.0111450000
H 2.9775450000 -4.8841330000 -0.5989030000
H 3.1242970000 -3.5099810000 -1.6993690000
H -0.6127130000 -4.0598970000 -0.8915740000
H 0.5623340000 -4.1433270000 -2.2131210000
H 0.6114660000 -5.3443730000 -0.9102050000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340912 (Hartree/Particle)
Thermal correction to Energy= 0.362607
Thermal correction to Enthalpy= 0.363552
Thermal correction to Gibbs (Free) Energy= 0.289580
Sum of electronic and zero-point Energies= -946.111405
Sum of electronic and thermal Energies= -946.089710
Sum of electronic and thermal Enthalpies= -946.088765
Sum of electronic and thermal (Free) Energies= -946.162737

c/s PT

C -2.3772150000 0.2449240000 -0.2949380000
C -1.0259370000 0.1123430000 -0.1712670000
H -2.6745390000 1.2340670000 -0.6397730000
C -3.5675300000 -0.6918940000 -0.1273990000
C -0.1566490000 -0.9691200000 0.2234870000
C -4.8390130000 0.1052690000 -0.5024250000
C -3.7212690000 -1.1576170000 1.3407500000
C -3.4662740000 -1.8988210000 -1.0917450000
C 1.1957090000 -0.6541230000 -0.1215410000
C -0.4285630000 -2.2482390000 0.9341740000
H -4.7918770000 0.4654820000 -1.5368550000
H -5.7288630000 -0.5259790000 -0.4074880000
H -4.9719450000 0.9733110000 0.1542020000
H -2.8764280000 -1.7541190000 1.6874190000
H -3.8240310000 -0.2980600000 2.0123250000
H -4.6261000000 -1.7690110000 1.4381810000
H -4.3465110000 -2.5414490000 -0.9742200000
H -3.4336170000 -1.5602370000 -2.1330420000
H -2.5782740000 -2.5101730000 -0.9173380000
C 1.1848950000 0.5801900000 -0.7853120000
O 2.2007130000 -1.4266250000 0.1350900000
H -0.5651260000 -2.0443430000 2.0065610000
H 0.4424880000 -2.9011580000 0.8389280000
H -1.3227820000 -2.7658420000 0.5864640000
C -0.1109090000 1.2613800000 -0.6321070000
H 2.0481440000 0.9820170000 -1.2977020000
B 3.6233470000 -0.8002780000 -0.0438540000
H -0.4546490000 1.7071730000 -1.5773780000
C 0.0182550000 2.4351720000 0.4306710000
F 3.7896130000 -0.5625270000 -1.4043890000
F 4.4963350000 -1.7098690000 0.4739160000
F 3.5925680000 0.4113250000 0.6588490000
C -1.2182580000 3.3429980000 0.4506290000
C 1.2961930000 3.2593790000 0.1991710000
H 0.1088750000 1.9398350000 1.4063820000
H -2.1244950000 2.8088300000 0.7503420000
H -1.0666570000 4.1582190000 1.1670210000
H -1.3948880000 3.7991060000 -0.5319310000
H 2.1978170000 2.6591400000 0.3566620000
H 1.3272520000 3.6739880000 -0.8169180000
H 1.3264990000 4.1022000000 0.8984350000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.343920 (Hartree/Particle)
Thermal correction to Energy= 0.365308
Thermal correction to Enthalpy= 0.366252
Thermal correction to Gibbs (Free) Energy= 0.293702
Sum of electronic and zero-point Energies= -946.137677
Sum of electronic and thermal Energies= -946.116289
Sum of electronic and thermal Enthalpies= -946.115345
Sum of electronic and thermal (Free) Energies= -946.187895

cc/s RT

C -2.4228190000 -1.2033190000 -0.7748410000
C -1.2071660000 -1.3386010000 -0.3204400000
C -3.6693040000 -0.7160090000 -0.0360420000
H -2.5928880000 -1.5004160000 -1.8137530000
C 0.0137630000 -1.6424870000 0.0993070000
C -3.3638410000 -0.3323780000 1.4201470000
C -4.6937200000 -1.8736080000 -0.0597150000
C -4.2499850000 0.4951600000 -0.7963380000
C 1.1642230000 -0.7399710000 -0.1030930000
C 0.3260040000 -3.0141400000 0.6738450000
H -2.9163900000 -1.1684830000 1.9686300000
H -2.6765600000 0.5185020000 1.4787270000
H -4.2873630000 -0.0463550000 1.9357940000
H -5.6312710000 -1.5587920000 0.4137450000
H -4.9231090000 -2.1828670000 -1.0861680000
H -4.3150290000 -2.7479840000 0.4807310000
H -4.4841900000 0.2369370000 -1.8358460000
H -5.1763790000 0.8357910000 -0.3187840000
H -3.5447320000 1.3328660000 -0.8082280000
C 1.0606160000 0.6863400000 -0.4059660000
O 2.2932890000 -1.2963480000 -0.0295680000
H -0.5898910000 -3.5971970000 0.7905600000
H 0.8187340000 -2.9210310000 1.6475060000
H 1.0152060000 -3.5543650000 0.0172660000
C 0.1124980000 1.5054020000 0.0796820000
H 1.8967520000 1.0871720000 -0.9700660000
B 3.7681200000 -0.5354070000 -0.1228910000
H -0.6737550000 1.1037830000 0.7173500000
C 0.1036610000 2.9947060000 -0.1235240000
F 4.6296620000 -1.5630650000 0.0727020000
F 3.7231980000 0.3946310000 0.8803190000
F 3.7945750000 0.0099720000 -1.3851820000
C -1.2379810000 3.4639230000 -0.7173740000
C 0.3967220000 3.7066150000 1.2138920000
H 0.9050930000 3.2482760000 -0.8292230000
H -1.4437320000 2.9786170000 -1.6775650000
H -1.2231680000 4.5473730000 -0.8805880000
H -2.0697570000 3.2424320000 -0.0367310000
H -0.3707010000 3.4722810000 1.9622490000
H 0.4048040000 4.7931300000 1.0709400000
H 1.3684720000 3.4045130000 1.6166610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341292 (Hartree/Particle)
Thermal correction to Energy= 0.364243
Thermal correction to Enthalpy= 0.365188
Thermal correction to Gibbs (Free) Energy= 0.287559
Sum of electronic and zero-point Energies= -946.144241
Sum of electronic and thermal Energies= -946.121290
Sum of electronic and thermal Enthalpies= -946.120346
Sum of electronic and thermal (Free) Energies= -946.197975

cc/s TS

C -2.1152540000 -1.0757610000 -0.5592950000
C -0.8467610000 -0.7483770000 -0.2694580000
C -3.4480060000 -0.8077660000 0.1138450000
H -2.2086470000 -1.7639520000 -1.4070910000
C 0.3550150000 -1.4157080000 -0.2092590000
C -3.3705690000 0.1547440000 1.3064500000
C -3.9051010000 -2.2005490000 0.6347490000
C -4.4863750000 -0.3182670000 -0.9208500000
C 1.5238320000 -0.5836090000 -0.1419970000
C 0.4867070000 -2.9069450000 -0.0934730000
H -2.6315010000 -0.1798010000 2.0435150000
H -3.1135680000 1.1696580000 0.9970050000
H -4.3426910000 0.2009230000 1.8094980000
H -4.8965900000 -2.1123310000 1.0943190000
H -3.9754800000 -2.9323400000 -0.1779230000
H -3.2117600000 -2.5903530000 1.3874070000
H -4.5719940000 -1.0223140000 -1.7567430000
H -5.4731500000 -0.2337050000 -0.4516190000
H -4.2231570000 0.6599290000 -1.3332710000
C 1.1588890000 0.7863190000 -0.1088670000
O 2.7040280000 -1.0773540000 -0.1840440000
H 1.3917330000 -3.2243390000 -0.6209120000
H -0.3840330000 -3.4294910000 -0.4974950000
H 0.6144800000 -3.2080790000 0.9544020000
C -0.1555570000 1.1177930000 0.2587810000
H 1.8483630000 1.5218480000 -0.5088020000
B 3.9496120000 -0.1192670000 0.0711340000
H -0.5073570000 0.8020200000 1.2415640000

C -0.6757810000 2.4827980000 -0.2111630000
F 5.0227520000 -0.9563480000 0.1193190000
F 3.6723790000 0.5288900000 1.2624160000
F 3.9664480000 0.7652300000 -0.9987160000
C -1.7274050000 2.4193160000 -1.3331790000
C -1.1413670000 3.3532300000 0.9682130000
H 0.1963180000 2.9808510000 -0.6553870000
H -1.3899790000 1.7871990000 -2.1605220000
H -1.9060840000 3.4269480000 -1.7248800000
H -2.6835430000 2.0310460000 -0.9738940000
H -2.0221480000 2.9325540000 1.4667370000
H -1.4073290000 4.3568960000 0.6183350000
H -0.3499800000 3.4587410000 1.7182890000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340686 (Hartree/Particle)
Thermal correction to Energy= 0.362461
Thermal correction to Enthalpy= 0.363405
Thermal correction to Gibbs (Free) Energy= 0.290100
Sum of electronic and zero-point Energies= -946.098909
Sum of electronic and thermal Energies= -946.077134
Sum of electronic and thermal Enthalpies= -946.076190
Sum of electronic and thermal (Free) Energies= -946.149496

cc/s PT

C 2.2151220000 -0.9609890000 0.2491180000
C 0.9596390000 -0.4409070000 0.1797860000
C 3.5683820000 -0.5796280000 -0.3142730000
H 2.2684130000 -1.9248850000 0.7568020000
C -0.1821280000 -1.2324590000 0.5809010000
C 3.5697040000 0.5613500000 -1.3448330000
C 4.1164580000 -1.8559530000 -1.0085700000
C 4.5072080000 -0.2335150000 0.8709920000
C -1.3780940000 -0.7006190000 0.0135400000
C -0.2194980000 -2.4769400000 1.3871790000
H 2.9274130000 0.3251640000 -2.2003270000
H 3.2464970000 1.5122290000 -0.9191560000
H 4.5869110000 0.7029200000 -1.7269690000
H 5.1217950000 -1.6634330000 -1.3995920000
H 4.1829660000 -2.6983280000 -0.3104100000
H 3.4784840000 -2.1575530000 -1.8466690000
H 4.5354310000 -1.0436800000 1.6086350000
H 5.5278430000 -0.0799770000 0.5016140000
H 4.1909650000 0.6801550000 1.3837680000
C -1.0086130000 0.4261760000 -0.7262760000
O -2.5479490000 -1.2324740000 0.1852510000
H 0.7004320000 -2.6762870000 1.9399280000
H -0.4379920000 -3.3334850000 0.7334120000
H -1.0671530000 -2.4200080000 2.0803160000
C 0.3918520000 0.8364320000 -0.4448450000
H -1.6977860000 0.9743260000 -1.3535870000
B -3.7697220000 -0.3572870000 -0.2310010000
H 0.9204070000 1.1712270000 -1.3428200000
C 0.3285850000 2.0432640000 0.5929380000
F -4.8753020000 -1.0317510000 0.1976830000
F -3.7033500000 -0.1996540000 -1.6131010000
F -3.5883150000 0.8788840000 0.4041680000
C 1.6880790000 2.6979680000 0.8502750000
C -0.7096840000 3.0980990000 0.1718510000
H -0.0187380000 1.5896220000 1.5307720000
H 2.4348690000 1.9785950000 1.1980290000
H 1.5832030000 3.4654280000 1.6256680000
H 2.0731390000 3.1952130000 -0.0483030000
H -0.5076190000 3.4779740000 -0.8381660000
H -0.6684250000 3.9513840000 0.8577510000
H -1.7282220000 2.6986470000 0.1968560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344282 (Hartree/Particle)
Thermal correction to Energy= 0.365477
Thermal correction to Enthalpy= 0.366421
Thermal correction to Gibbs (Free) Energy= 0.294825
Sum of electronic and zero-point Energies= -946.140309
Sum of electronic and thermal Energies= -946.119114
Sum of electronic and thermal Enthalpies= -946.118170
Sum of electronic and thermal (Free) Energies= -946.189766

c/d RT

C -2.7521040000 -0.0062690000 -0.7113920000
C -1.5904710000 -0.5820780000 -0.8517010000
C -0.4470800000 -1.2379760000 -0.9897880000
C 0.7864510000 -0.7587400000 -0.3334140000
C 0.9859780000 0.6191990000 0.1098610000
C 0.4668430000 1.6878780000 -0.5209610000
H 1.6792900000 0.7329540000 0.9347170000
H -0.1540970000 1.5304470000 -1.4013010000
C 0.7165130000 3.1304570000 -0.1727510000
C -0.3645230000 -2.5699510000 -1.7128080000
O 1.6771010000 -1.6333210000 -0.1575210000
H -1.3216490000 -2.8129680000 -2.1792210000
H -0.0932270000 -3.3660130000 -1.0121800000
H 0.4131720000 -2.5433460000 -2.4835650000
C 1.3398330000 3.8536570000 -1.3876930000
C 1.5498370000 3.3428110000 1.0957480000
H -0.2794320000 3.5772470000 -0.0118700000
H 2.3382140000 3.4568180000 -1.6022080000
H 1.4344250000 4.9257160000 -1.1839410000
H 0.7265510000 3.7334610000 -2.2882280000
H 2.5610730000 2.9369510000 0.9788240000
H 1.0909180000 2.8633050000 1.9670860000
H 1.6420930000 4.4126180000 1.3108880000
B 3.1898230000 -1.3613050000 0.4693480000
F 3.7540030000 -2.5915680000 0.3981840000
F 2.9545820000 -0.9052820000 1.7460810000
F 3.7293890000 -0.4167920000 -0.3618770000
C -3.7630240000 -0.2471470000 0.4115640000
C -3.9898250000 1.0948320000 1.1415400000
C -3.2616810000 -1.3056660000 1.4061720000
C -5.0857190000 -0.7145480000 -0.2340350000
H -5.4595110000 0.0203870000 -0.9569790000
H -5.8556680000 -0.8505010000 0.5346770000
H -4.9548180000 -1.6680810000 -0.7572670000
H -3.0655610000 1.4491890000 1.6108870000
H -4.7470830000 0.9775220000 1.9257560000
H -4.3402900000 1.8712850000 0.4508860000
H -2.3219410000 -0.9981890000 1.8776100000
H -3.0932880000 -2.2692320000 0.9127340000
H -4.0023670000 -1.4582790000 2.1989570000
H -3.0506520000 0.7358330000 -1.4563690000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341473 (Hartree/Particle)
Thermal correction to Energy= 0.364331
Thermal correction to Enthalpy= 0.365276
Thermal correction to Gibbs (Free) Energy= 0.287570
Sum of electronic and zero-point Energies= -946.145242
Sum of electronic and thermal Energies= -946.122383
Sum of electronic and thermal Enthalpies= -946.121439
Sum of electronic and thermal (Free) Energies= -946.199144

c/d TS

C -2.3955860000 -0.0485510000 -0.5466410000
C -1.0972480000 -0.3238600000 -0.6183410000
H -2.7572430000 0.8331350000 -1.0787130000
C -3.4667120000 -0.7612140000 0.2736020000
C -0.0556390000 -1.2114380000 -0.6239740000
C -4.1144050000 0.2794290000 1.2161800000
C -2.9057150000 -1.9266630000 1.1022610000
C -4.5346590000 -1.2828310000 -0.7177060000
C 1.2016690000 -0.6419110000 -0.2044610000
C -0.1138590000 -2.6306170000 -1.1128360000
H -4.5191440000 1.1308080000 0.6561890000
H -4.9400920000 -0.1780440000 1.7736950000
H -3.3879730000 0.6631100000 1.9410290000
H -2.4907560000 -2.7147570000 0.4662210000
H -2.1188680000 -1.5904870000 1.7858770000
H -3.7050850000 -2.3737290000 1.7034600000
H -5.3599630000 -1.7505310000 -0.1679170000
H -4.9525920000 -0.4692050000 -1.3220650000
H -4.1132710000 -2.0296750000 -1.3993290000
C 1.0910520000 0.7702140000 -0.0471410000
O 2.2185330000 -1.3800420000 0.0300730000
H 0.0614330000 -3.3114210000 -0.2702360000
H 0.6872510000 -2.8208350000 -1.8351240000
H -1.0792300000 -2.8689540000 -1.5636720000
C 0.0309830000 1.3891270000 -0.7154580000
H 1.7205700000 1.2763690000 0.6760940000

B 3.6220220000 -0.6825010000 0.3228330000
H -0.0726620000 1.1967560000 -1.7841030000
C -0.5228600000 2.7402020000 -0.3045590000
F 3.8191550000 0.1925000000 -0.7309380000
F 4.5118090000 -1.7113650000 0.3785260000
F 3.4567420000 -0.0066800000 1.5237380000
C 0.2789380000 3.8579450000 -1.0077380000
C -0.5716540000 2.9477780000 1.2147420000
H -1.5507970000 2.7913580000 -0.6913320000
H 0.2818870000 3.7301370000 -2.0960240000
H -0.1608250000 4.8359060000 -0.7829830000
H 1.3202440000 3.8667700000 -0.6675360000
H -1.1243760000 2.1415090000 1.7094200000
H 0.4335550000 2.9832080000 1.6490130000
H -1.0656180000 3.8956510000 1.4537630000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340684 (Hartree/Particle)
Thermal correction to Energy= 0.362479
Thermal correction to Enthalpy= 0.363424
Thermal correction to Gibbs (Free) Energy= 0.289401
Sum of electronic and zero-point Energies= -946.115272
Sum of electronic and thermal Energies= -946.093477
Sum of electronic and thermal Enthalpies= -946.092533
Sum of electronic and thermal (Free) Energies= -946.166556

c/d PT

C -2.4101340000 0.3523300000 -0.3062370000
C -1.0634120000 0.1350280000 -0.3136180000
H -2.6668740000 1.3834490000 -0.5550040000
C -3.6403280000 -0.5072420000 -0.0531980000
C -0.2210640000 -0.9961750000 -0.0307690000
C -4.8835540000 0.3972940000 -0.2222090000
C -3.6531940000 -1.0600400000 1.3931700000
C -3.7422780000 -1.6493580000 -1.0942180000
C 1.1460340000 -0.6587450000 -0.2910810000
C -0.5116530000 -2.3528590000 0.5036850000
H -4.9323590000 0.8216680000 -1.2319690000
H -5.8006760000 -0.1774660000 -0.0556150000
H -4.8721770000 1.2262870000 0.4952270000
H -2.8129570000 -1.7236430000 1.6024870000
H -3.6233750000 -0.2417310000 2.1209480000
H -4.5778670000 -1.6245370000 1.5609900000
H -4.6494900000 -2.2364320000 -0.9101750000
H -3.8050580000 -1.2428100000 -2.1095240000
H -2.8888950000 -2.3301220000 -1.0648670000
C 1.1755130000 0.6330710000 -0.8306300000
O 2.1283510000 -1.4659630000 -0.0521440000
H -0.3858830000 -2.3375580000 1.5971850000
H 0.2437950000 -3.0509210000 0.1297650000
H -1.5104380000 -2.7223640000 0.2827540000
C -0.1425440000 1.2839860000 -0.7498210000
H 2.0774720000 1.0874350000 -1.2194100000
B 3.5563500000 -0.8290220000 -0.0020240000
H -0.4566780000 1.6577940000 -1.7382800000
C -0.1374790000 2.5314070000 0.2142950000
F 3.8480170000 -0.3837710000 -1.2883530000
F 4.3855890000 -1.8147830000 0.4444750000
F 3.4486410000 0.2563670000 0.8750440000
C 0.6789170000 3.6779280000 -0.3988140000
C 0.3646020000 2.1772670000 1.6207400000
H -1.1808270000 2.8674230000 0.2871480000
H 0.3277340000 3.9347490000 -1.4054810000
H 0.5939650000 4.5754530000 0.2236850000
H 1.7430270000 3.4239970000 -0.4631210000
H -0.2419760000 1.3896040000 2.0819210000
H 1.4041580000 1.8306340000 1.6005550000
H 0.3100350000 3.0582360000 2.2698100000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.343580 (Hartree/Particle)
Thermal correction to Energy= 0.365093
Thermal correction to Enthalpy= 0.366038
Thermal correction to Gibbs (Free) Energy= 0.292864
Sum of electronic and zero-point Energies= -946.142044
Sum of electronic and thermal Energies= -946.120531
Sum of electronic and thermal Enthalpies= -946.119586
Sum of electronic and thermal (Free) Energies= -946.192760

cc/d RT

C -2.4968130000 -1.0013840000 -0.8366540000
C -1.2989890000 -1.2366560000 -0.3753920000
C -3.7468690000 -0.5632760000 -0.0739590000
H -2.6481090000 -1.1645710000 -1.9076870000
C -0.1001510000 -1.6398410000 0.0239110000
C -3.4631340000 -0.3403950000 1.4195180000
C -4.7962580000 -1.6869480000 -0.2371290000
C -4.2844710000 0.7337330000 -0.7148010000
C 1.0885330000 -0.7679590000 -0.0520810000
C 0.1470260000 -3.0843170000 0.4259450000
H -3.0430730000 -1.2385670000 1.8853970000
H -2.7604490000 0.4847310000 1.5781400000
H -4.3907730000 -0.0898320000 1.9460790000
H -5.7372300000 -1.3989560000 0.2465760000
H -5.0087470000 -1.8844320000 -1.2943410000
H -4.4496480000 -2.6208110000 0.2186820000
H -4.5071060000 0.5885100000 -1.7785110000
H -5.2102360000 1.0483350000 -0.2185880000
H -3.5586260000 1.5494460000 -0.6313110000
C 1.0511570000 0.6898540000 -0.1496720000
O 2.1927030000 -1.3772930000 -0.0564990000
H -0.7934430000 -3.6383030000 0.4585870000
H 0.6270370000 -3.1341860000 1.4091330000
H 0.8244200000 -3.5669120000 -0.2854820000
C 0.1395080000 1.4664310000 0.4604600000
H 1.9087060000 1.1224410000 -0.6506590000
B 3.6970960000 -0.6731080000 -0.0688010000
H -0.6650720000 0.9953810000 1.0221750000
C 0.1550490000 2.9723950000 0.5002040000
F 4.5156170000 -1.7510220000 -0.0006330000
F 3.6968940000 0.1366120000 1.0354090000
F 3.7422910000 0.0150310000 -1.2589620000
C 1.3394980000 3.6129690000 -0.2319800000
C -1.1932720000 3.5297730000 -0.0061220000
H 0.2277240000 3.2404230000 1.5673070000
H 2.2970430000 3.2565720000 0.1611030000
H 1.3096260000 4.7013070000 -0.1142040000
H 1.3098500000 3.3935670000 -1.3058740000
H -1.3376880000 3.2958060000 -1.0672680000
H -1.2206920000 4.6188800000 0.1073870000
H -2.0387120000 3.1131900000 0.5535480000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341535 (Hartree/Particle)
Thermal correction to Energy= 0.364336
Thermal correction to Enthalpy= 0.365280
Thermal correction to Gibbs (Free) Energy= 0.288274
Sum of electronic and zero-point Energies= -946.143024
Sum of electronic and thermal Energies= -946.120223
Sum of electronic and thermal Enthalpies= -946.119279
Sum of electronic and thermal (Free) Energies= -946.196286

cc/d TS

C -2.1030590000 -1.0338270000 -0.5974960000
C -0.8383820000 -0.7517320000 -0.2500520000
C -3.4408240000 -0.8006560000 0.0824010000
H -2.1908490000 -1.6046740000 -1.5284620000
C 0.3693620000 -1.4046380000 -0.2314320000
C -3.3001290000 -0.3617600000 1.5497740000
C -4.1558090000 -2.1781750000 0.0536900000
C -4.2978810000 0.2030280000 -0.7225950000
C 1.5282800000 -0.5617010000 -0.0995770000
C 0.5239260000 -2.8980040000 -0.2405170000
H -2.7083770000 -1.0873100000 2.1192800000
H -2.8277720000 0.6165120000 1.6501870000
H -4.2895260000 -0.2967910000 2.0162670000
H -5.1425730000 -2.0924880000 0.5228530000
H -4.3007780000 -2.5346400000 -0.9726840000
H -3.5845490000 -2.9358590000 0.6012400000
H -4.4083500000 -0.1181730000 -1.7647870000
H -5.3007640000 0.2752160000 -0.2856960000
H -3.8574480000 1.2037570000 -0.7247540000
C 1.1452320000 0.7965290000 0.0229610000
O 2.7130820000 -1.0378190000 -0.1810630000
H -0.3601740000 -3.4004970000 -0.6398310000
H 0.7124390000 -3.2769140000 0.7722130000
H 1.4042760000 -3.1589550000 -0.8369080000

C -0.1721160000 1.0841660000 0.4186550000
H 1.8170070000 1.5656680000 -0.3437660000
B 3.9514810000 -0.0802390000 0.1145170000
H -0.5094460000 0.7072610000 1.3839080000
C -0.7160250000 2.4561140000 0.0033370000
F 5.0349020000 -0.9049260000 0.0948300000
F 3.6851980000 0.4903040000 1.3466300000
F 3.9397930000 0.8671020000 -0.9002800000
C -1.0524610000 2.5291160000 -1.4979700000
C -1.8504570000 3.0051110000 0.8779700000
H 0.1428370000 3.1267740000 0.1589830000
H -0.2052290000 2.2025070000 -2.1100570000
H -1.2958750000 3.5588430000 -1.7816800000
H -1.9101550000 1.8964970000 -1.7468050000
H -2.8035620000 2.5024640000 0.6895020000
H -2.0009950000 4.0692700000 0.6659050000
H -1.6191690000 2.9115370000 1.9455030000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340541 (Hartree/Particle)
Thermal correction to Energy= 0.362292
Thermal correction to Enthalpy= 0.363236
Thermal correction to Gibbs (Free) Energy= 0.290143
Sum of electronic and zero-point Energies= -946.099957
Sum of electronic and thermal Energies= -946.078205
Sum of electronic and thermal Enthalpies= -946.077261
Sum of electronic and thermal (Free) Energies= -946.150354

cc/d PT

C 2.1694980000 -0.8988050000 0.2897370000
C 0.9245290000 -0.3764050000 0.1068340000
C 3.5521270000 -0.6124880000 -0.2569310000
H 2.1841880000 -1.7892610000 0.9192240000
C -0.2330520000 -1.1275240000 0.5340600000
C 3.6071140000 0.3330200000 -1.4674660000
C 4.1310260000 -1.9858730000 -0.6927940000
C 4.4292420000 -0.0629420000 0.8984380000
C -1.4080800000 -0.6441540000 -0.1150180000
C -0.3088490000 -2.2899160000 1.4527230000
H 2.9946180000 -0.0439560000 -2.2940280000
H 3.2785290000 1.3432790000 -1.2234390000
H 4.6396740000 0.4028260000 -1.8275270000
H 5.1548200000 -1.8570210000 -1.0610550000
H 4.1609760000 -2.6949410000 0.1425520000
H 3.5353570000 -2.4316210000 -1.4971850000
H 4.4161550000 -0.7340260000 1.7648420000
H 5.4680980000 0.0294120000 0.5607540000
H 4.0896700000 0.9235030000 1.2280040000
C -1.0190280000 0.4349650000 -0.9115130000
O -2.5828530000 -1.1597670000 0.0797800000
H 0.5675010000 -2.4084820000 2.0930330000
H -0.4524870000 -3.2123730000 0.8717750000
H -1.2118530000 -2.1898350000 2.0657770000
C 0.3960520000 0.8251150000 -0.6800580000
H -1.7090640000 0.9926580000 -1.5329640000
B -3.8020780000 -0.2539040000 -0.2613630000
H 0.9378550000 0.9898590000 -1.6180900000
C 0.3567210000 2.2187980000 0.0951270000
F -4.9062230000 -0.9420050000 0.1505190000
F -3.7689900000 -0.0149020000 -1.6343450000
F -3.5908600000 0.9386150000 0.4429640000
C -0.3805760000 2.1388890000 1.4405460000
C 1.7319930000 2.8733010000 0.2580510000
H -0.2319020000 2.8698260000 -0.5652560000
H -1.4233700000 1.8295400000 1.3266780000
H -0.3742220000 3.1262630000 1.9152680000
H 0.1145960000 1.4442360000 2.1309700000
H 2.3932240000 2.2743470000 0.8936160000
H 1.6159740000 3.8519480000 0.7372640000
H 2.2272330000 3.0402170000 -0.7043000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344231 (Hartree/Particle)
Thermal correction to Energy= 0.365462
Thermal correction to Enthalpy= 0.366406
Thermal correction to Gibbs (Free) Energy= 0.294673
Sum of electronic and zero-point Energies= -946.140530
Sum of electronic and thermal Energies= -946.119299
Sum of electronic and thermal Enthalpies= -946.118355
Sum of electronic and thermal (Free) Energies= -946.190089

c/u RT

C -2.6377010000 -0.3745640000 -0.7134780000
C -1.4198320000 -0.8269720000 -0.8270200000
C -0.2129920000 -1.3650560000 -0.9290530000
C 0.9700070000 -0.6904940000 -0.3566890000
C 1.0317520000 0.7425790000 -0.0771170000
C 0.3999100000 1.6736620000 -0.8141360000
H 1.7237830000 1.0200630000 0.7088420000
H -0.2227520000 1.3536230000 -1.6480080000
C 0.4952610000 3.1645280000 -0.6298730000
C 0.0049090000 -2.7484750000 -1.5145640000
O 1.9490900000 -1.4432600000 -0.1045470000
H -0.9262220000 -3.1400100000 -1.9297300000
H 0.3711820000 -3.4335180000 -0.7433800000
H 0.7642980000 -2.7188490000 -2.3032810000
C 1.4277560000 3.6064630000 0.5030450000
C -0.9225280000 3.7560340000 -0.4640440000
H 0.8949230000 3.5600130000 -1.5782390000
H 1.0662530000 3.2541690000 1.4764160000
H 1.4793070000 4.6996070000 0.5433380000
H 2.4441690000 3.2254450000 0.3607060000
H -1.3818990000 3.4095400000 0.4689530000
H -1.5803770000 3.4691150000 -1.2926730000
H -0.8764600000 4.8499270000 -0.4337240000
B 3.4307620000 -0.9488430000 0.4594920000
F 4.1207670000 -2.1142290000 0.5083120000
F 3.1586230000 -0.3847140000 1.6844620000
F 3.8604690000 -0.0483500000 -0.4778290000
C -3.5972370000 -0.6150730000 0.4538910000
C -3.9747380000 0.7583740000 1.0505230000
C -2.9595930000 -1.4987100000 1.5372580000
C -4.8625720000 -1.2996710000 -0.1076370000
H -5.3313510000 -0.6925820000 -0.8913300000
H -5.6004930000 -1.4456650000 0.6901030000
H -4.6248090000 -2.2798730000 -0.5351780000
H -3.0939200000 1.2658360000 1.4591090000
H -4.7025240000 0.6335780000 1.8610600000
H -4.4242130000 1.4130240000 0.2942380000
H -2.0571710000 -1.0357370000 1.9510320000
H -2.6837190000 -2.4816470000 1.1397700000
H -3.6660410000 -1.6545890000 2.3600980000
H -3.0316520000 0.2487110000 -1.5203380000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341472 (Hartree/Particle)
Thermal correction to Energy= 0.364328
Thermal correction to Enthalpy= 0.365272
Thermal correction to Gibbs (Free) Energy= 0.287664
Sum of electronic and zero-point Energies= -946.145063
Sum of electronic and thermal Energies= -946.122206
Sum of electronic and thermal Enthalpies= -946.121262
Sum of electronic and thermal (Free) Energies= -946.198871

c/u TS

C -2.2938070000 -0.1919260000 -0.4928110000
C -0.9708720000 -0.3214360000 -0.5719980000
H -2.7575910000 0.6373340000 -1.0251830000
C -3.2739420000 -1.0359620000 0.3176920000
C 0.1321620000 -1.1322300000 -0.5970720000
C -4.0964730000 -0.0851920000 1.2180030000
C -2.5795380000 -2.0922060000 1.1906940000
C -4.2252630000 -1.7243140000 -0.6916520000
C 1.3548620000 -0.4804700000 -0.1998110000
C 0.1682470000 -2.5477840000 -1.0986580000
H -4.5957820000 0.6938820000 0.6296960000
H -4.8702620000 -0.6479780000 1.7530400000
H -3.4599970000 0.4043980000 1.9631920000
H -2.0430040000 -2.8314690000 0.5886440000
H -1.8655100000 -1.6331460000 1.8826810000
H -3.3260230000 -2.6303480000 1.7852590000
H -4.9910490000 -2.2958850000 -0.1539640000
H -4.7371300000 -0.9907480000 -1.3254180000
H -3.6807540000 -2.4151010000 -1.3444870000
C 1.1561260000 0.9193650000 -0.0481240000
O 2.4248940000 -1.1494470000 0.0089250000
H 0.4269730000 -3.2184500000 -0.2695670000

H 0.9575410000 -2.6680260000 -1.8486980000
H -0.7892240000 -2.8590680000 -1.5206590000
C 0.0338530000 1.4713610000 -0.6782280000
H 1.7844230000 1.4802040000 0.6356180000
B 3.7869630000 -0.3622580000 0.2599890000
H -0.0932830000 1.2823690000 -1.7447190000
C -0.5179240000 2.8166540000 -0.2194270000
F 3.9043190000 0.5103150000 -0.8077130000
F 4.7411900000 -1.3325650000 0.3054480000
F 3.6092100000 0.3172770000 1.4573580000
C -0.9369340000 2.8270900000 1.2602830000
C -1.6256400000 3.3616510000 -1.1337640000
H 0.3407230000 3.5007840000 -0.3183630000
H -0.1269100000 2.4838330000 1.9116890000
H -1.2098550000 3.8410950000 1.5717140000
H -1.8031780000 2.1777230000 1.4264800000
H -1.3267210000 3.3379380000 -2.1882150000
H -2.5565130000 2.7930630000 -1.0301840000
H -1.8524590000 4.4016160000 -0.8764970000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340511 (Hartree/Particle)
Thermal correction to Energy= 0.362351
Thermal correction to Enthalpy= 0.363295
Thermal correction to Gibbs (Free) Energy= 0.289079
Sum of electronic and zero-point Energies= -946.112314
Sum of electronic and thermal Energies= -946.090474
Sum of electronic and thermal Enthalpies= -946.089530
Sum of electronic and thermal (Free) Energies= -946.163746

c/u PT

C -2.3350160000 0.1722470000 -0.3837890000
C -0.9734150000 0.0891310000 -0.3274990000
H -2.6803140000 1.1250260000 -0.7813850000
C -3.4875830000 -0.7680400000 -0.0567550000
C -0.0520120000 -0.9452550000 0.0697180000
C -4.8024640000 -0.0090970000 -0.3543750000
C -3.4991340000 -1.1541770000 1.4423160000
C -3.4542900000 -2.0225740000 -0.9649350000
C 1.2844310000 -0.5640780000 -0.2734170000
C -0.2446220000 -2.2406400000 0.7743630000
H -4.8584530000 0.2920080000 -1.4071090000
H -5.6681880000 -0.6449990000 -0.1412540000
H -4.8889640000 0.8931070000 0.2625880000
H -2.6082240000 -1.7036330000 1.7488240000
H -3.5735400000 -0.2601330000 2.0711670000
H -4.3714810000 -1.7843520000 1.6514450000
H -4.3102350000 -2.6674170000 -0.7343940000
H -3.5231870000 -1.7372940000 -2.0203700000
H -2.5447040000 -2.6144110000 -0.8436470000
C 1.2183720000 0.6589520000 -0.9515310000
O 2.3192600000 -1.2842700000 0.0186660000
H -0.1663190000 -2.0680380000 1.8588370000
H 0.5793780000 -2.9120920000 0.5162410000
H -1.2006140000 -2.7225760000 0.5814920000
C -0.1298060000 1.2468550000 -0.8821260000
H 2.0805200000 1.1338400000 -1.4035490000
B 3.7065970000 -0.5664910000 -0.0262610000
H -0.4924060000 1.5395490000 -1.8801570000
C -0.0730710000 2.5765860000 -0.0213470000
F 3.9404180000 -0.2121880000 -1.3524200000
F 4.6041020000 -1.4632220000 0.4730970000
F 3.5570460000 0.5791570000 0.7642100000
C 0.4551100000 2.3417040000 1.4009470000
C -1.4014210000 3.3452430000 -0.0091090000
H 0.6578100000 3.2033220000 -0.5505110000
H 1.4604630000 1.9090310000 1.4010770000
H 0.4956950000 3.2941170000 1.9411450000
H -0.2066440000 1.6737860000 1.9665240000
H -1.8133710000 3.4759310000 -1.0174400000
H -2.1537390000 2.8432740000 0.6093330000
H -1.2451210000 4.3437010000 0.4143760000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.343887 (Hartree/Particle)
Thermal correction to Energy= 0.365294
Thermal correction to Enthalpy= 0.366238
Thermal correction to Gibbs (Free) Energy= 0.293172
Sum of electronic and zero-point Energies= -946.139247
Sum of electronic and thermal Energies= -946.117839
Sum of electronic and thermal Enthalpies= -946.116895
Sum of electronic and thermal (Free) Energies= -946.189962

cc/u RT

C -2.5742760000 -1.0269610000 -0.8334690000
C -1.3893780000 -1.2872190000 -0.3539060000
C -3.7775260000 -0.4191130000 -0.1116770000
H -2.7442220000 -1.2729210000 -1.8854980000
C -0.2015680000 -1.6810830000 0.0848640000
C -3.5255190000 -0.2641510000 1.3965650000
C -4.9781410000 -1.3648600000 -0.3373560000
C -4.0820990000 0.9559110000 -0.7454620000
C 1.0014610000 -0.8388740000 -0.0714500000
C 0.0163660000 -3.0804580000 0.6330980000
H -3.2859920000 -1.2269180000 1.8609720000
H -2.6995630000 0.4249450000 1.6034790000
H -4.4193880000 0.1356120000 1.8883170000
H -5.8806220000 -0.9494530000 0.1262310000
H -5.1821730000 -1.5025770000 -1.4057390000
H -4.7929410000 -2.3512900000 0.1018790000
H -4.2637650000 0.8667320000 -1.8228300000
H -4.9766910000 1.3962130000 -0.2890340000
H -3.2484980000 1.6522590000 -0.6015630000
C 0.9738930000 0.5962810000 -0.3473040000
O 2.0977670000 -1.4561080000 0.0117770000
H -0.9339340000 -3.6125260000 0.7128260000
H 0.4879730000 -3.0383660000 1.6206800000
H 0.6906410000 -3.6441750000 -0.0192680000
C 0.0458640000 1.4382480000 0.1389170000
H 1.8342360000 0.9627830000 -0.8949380000
B 3.6078710000 -0.7683180000 -0.0500070000
H -0.7526720000 1.0386090000 0.7607010000
C 0.0349200000 2.9345950000 -0.0253480000
F 4.4162090000 -1.8385180000 0.1451210000
F 3.5957960000 0.1528570000 0.9626400000
F 3.6791010000 -0.2101160000 -1.3054430000
C 0.0853800000 3.6054170000 1.3657230000
C 1.1284250000 3.4788800000 -0.9508450000
H -0.9457830000 3.1843870000 -0.4652010000
H -0.7181090000 3.2448200000 2.0184370000
H -0.0207430000 4.6912440000 1.2679690000
H 1.0413240000 3.3978800000 1.8589980000
H 2.1267360000 3.2804670000 -0.5446320000
H 1.0224270000 4.5632090000 -1.0616970000
H 1.0734950000 3.0318260000 -1.9492510000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341401 (Hartree/Particle)
Thermal correction to Energy= 0.364262
Thermal correction to Enthalpy= 0.365206
Thermal correction to Gibbs (Free) Energy= 0.287814
Sum of electronic and zero-point Energies= -946.143871
Sum of electronic and thermal Energies= -946.121010
Sum of electronic and thermal Enthalpies= -946.120066
Sum of electronic and thermal (Free) Energies= -946.197458

cc/u TS

C -2.2329100000 -1.0627790000 -0.5516840000
C -0.9608040000 -0.8817780000 -0.1821840000
C -3.5560970000 -0.6217150000 0.0525850000
H -2.3546540000 -1.6690180000 -1.4556590000
C 0.2357020000 -1.5478280000 -0.1170910000
C -3.4230640000 -0.0846200000 1.4886710000
C -4.4440870000 -1.8925040000 0.0886730000
C -4.2346590000 0.4222550000 -0.8653170000
C 1.4041060000 -0.7056070000 -0.0710190000
C 0.3773850000 -3.0391750000 -0.0165430000
H -2.9143780000 -0.8089210000 2.1347250000
H -2.8750230000 0.8595030000 1.5347460000
H -4.4179520000 0.0982090000 1.9097560000
H -5.4343850000 -1.6441810000 0.4872730000
H -4.5812690000 -2.3148010000 -0.9135340000
H -4.0052930000 -2.6669240000 0.7275410000
H -4.3593330000 0.0321330000 -1.8819150000
H -5.2290300000 0.6744230000 -0.4783340000
H -3.6512690000 1.3456210000 -0.9301700000
C 1.0329940000 0.6655230000 -0.0274260000

O 2.5817830000 -1.1952000000 -0.1579400000
H 1.1710370000 -3.3647860000 -0.6982970000
H -0.5528960000 -3.5574390000 -0.2579190000
H 0.6974780000 -3.3345280000 0.9905330000
C -0.2567910000 0.9677830000 0.4221790000
H 1.6859800000 1.3997130000 -0.4863810000
B 3.8336760000 -0.2255970000 0.0317120000
H -0.5481800000 0.5940480000 1.4034680000
C -0.9098630000 2.2884380000 0.0444670000
F 4.9123480000 -1.0559630000 0.0392210000
F 3.6054230000 0.4328510000 1.2269770000
F 3.7936590000 0.6462760000 -1.0475870000
C -0.3584950000 3.4056990000 0.9586210000
C -0.7519820000 2.6431550000 -1.4411110000
H -1.9807810000 2.2002650000 0.2582550000
H -0.5046680000 3.1697860000 2.0186470000
H -0.8709200000 4.3510860000 0.7480850000
H 0.7139810000 3.5561130000 0.7936680000
H 0.2963380000 2.8167290000 -1.7072930000
H -1.3046210000 3.5602500000 -1.6727680000
H -1.1342760000 1.8427310000 -2.0838970000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340577 (Hartree/Particle)
Thermal correction to Energy= 0.362406
Thermal correction to Enthalpy= 0.363350
Thermal correction to Gibbs (Free) Energy= 0.289731
Sum of electronic and zero-point Energies= -946.107548
Sum of electronic and thermal Energies= -946.085719
Sum of electronic and thermal Enthalpies= -946.084774
Sum of electronic and thermal (Free) Energies= -946.158394

cc/u PT

C 2.2580130000 -1.0225890000 0.0937440000
C 0.9861040000 -0.5650300000 -0.0631490000
C 3.6239400000 -0.4273200000 -0.1773910000
H 2.3317390000 -2.0333870000 0.4955020000
C -0.1619070000 -1.3954110000 0.1957080000
C 3.6537610000 0.7068170000 -1.2190920000
C 4.5273350000 -1.5777870000 -0.6879380000
C 4.1890310000 0.0807260000 1.1769440000
C -1.3573760000 -0.7367750000 -0.2227360000
C -0.2239520000 -2.7568540000 0.7805230000
H 3.2230720000 0.3820990000 -2.1726590000
H 3.1233520000 1.6014370000 -0.8854270000
H 4.6930860000 0.9982160000 -1.4073270000
H 5.5479290000 -1.2126840000 -0.8464120000
H 4.5738630000 -2.4021790000 0.0331730000
H 4.1605810000 -1.9788770000 -1.6396260000
H 4.2072440000 -0.7172280000 1.9276730000
H 5.2170460000 0.4355590000 1.0375490000
H 3.5924210000 0.9076200000 1.5753670000
C -0.9798080000 0.4915650000 -0.7722400000
O -2.5378220000 -1.2508440000 -0.0726600000
H 0.7155580000 -3.1033720000 1.2144580000
H -0.5471690000 -3.4704440000 0.0096070000
H -1.0152590000 -2.7770480000 1.5398460000
C 0.4642740000 0.7725490000 -0.5827980000
H -1.6870120000 1.1765960000 -1.2213030000
B -3.7378470000 -0.2579750000 -0.1549770000
H 0.9412510000 1.0458380000 -1.5330040000
C 0.6658600000 1.9906880000 0.4055010000
F -4.8418120000 -0.9772930000 0.1987640000
F -3.7771500000 0.2298870000 -1.4595120000
F -3.4327840000 0.7762750000 0.7388850000
C 0.2485980000 3.3033810000 -0.2726840000
C -0.0671480000 1.7941280000 1.7403730000
H 1.7415350000 2.0472260000 0.6115960000
H 0.7729170000 3.4549210000 -1.2240750000
H 0.4828660000 4.1538570000 0.3770110000
H -0.8288640000 3.3307310000 -0.4696330000
H -1.1525740000 1.7340490000 1.6034310000
H 0.1478780000 2.6360320000 2.4078390000
H 0.2557120000 0.8793230000 2.2507680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.343892 (Hartree/Particle)
Thermal correction to Energy= 0.365286
Thermal correction to Enthalpy= 0.366231
Thermal correction to Gibbs (Free) Energy= 0.293823
Sum of electronic and zero-point Energies= -946.148369
Sum of electronic and thermal Energies= -946.126974
Sum of electronic and thermal Enthalpies= -946.126030
Sum of electronic and thermal (Free) Energies= -946.198438

3d

cRT

C -2.6261000000 1.1486860000 -0.6435230000
C -2.0269470000 0.0034180000 -0.8191350000
C -1.4886950000 -1.1955440000 -0.9866870000
C -0.1869760000 -1.5401680000 -0.3745170000
C 0.8207440000 -0.5594840000 -0.0059830000
C 0.9744620000 0.6319450000 -0.6300660000
H 1.5116660000 -0.8931890000 0.7587800000
H 0.3032800000 0.8785770000 -1.4486500000
C 1.9920870000 1.6380600000 -0.3463020000
C -2.2308930000 -2.3187610000 -1.6881200000
O -0.0046240000 -2.7732120000 -0.1670490000
H -3.1621160000 -1.9494330000 -2.1230770000
H -2.4577010000 -3.1227730000 -0.9809230000
H -1.6130360000 -2.7542270000 -2.4808320000
C 2.9606310000 1.4892900000 0.6673680000
C 2.0051970000 2.8157900000 -1.1180410000
B 1.3841490000 -3.4631490000 0.3989270000
F 1.0663360000 -4.7813070000 0.4198950000
F 1.5753400000 -2.8985120000 1.6422050000
F 2.3354660000 -3.1009620000 -0.5167870000
C -3.5430310000 1.5326450000 0.5195290000
C -2.9194060000 2.7521250000 1.2330880000
C -3.7101010000 0.3734640000 1.5141480000
C -4.9160040000 1.9243640000 -0.0691060000
H -4.8222550000 2.7439800000 -0.7916230000
H -5.5902550000 2.2565720000 0.7292170000
H -5.3842450000 1.0752800000 -0.5790220000
H -1.9422850000 2.5021830000 1.6604170000
H -3.5716490000 3.0903310000 2.0470200000
H -2.7827180000 3.5926510000 0.5420400000
H -2.7485170000 0.0756300000 1.9459910000
H -4.1515240000 -0.5059460000 1.0323890000
H -4.3698970000 0.6741990000 2.3355640000
H -2.4635860000 1.9340200000 -1.3864040000
C 2.9469020000 3.8148730000 -0.8864370000
C 3.8974110000 3.6526860000 0.1228750000
C 3.9007360000 2.4867950000 0.8968240000
H 1.2665340000 2.9407740000 -1.9063390000
H 2.9411720000 4.7163040000 -1.4925850000
H 4.6358260000 4.4283820000 0.3056840000
H 2.9806960000 0.5877190000 1.2712330000
H 4.6424750000 2.3563260000 1.6795580000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337828 (Hartree/Particle)
Thermal correction to Energy= 0.361053
Thermal correction to Enthalpy= 0.361998
Thermal correction to Gibbs (Free) Energy= 0.282283
Sum of electronic and zero-point Energies= -1059.263962
Sum of electronic and thermal Energies= -1059.240737
Sum of electronic and thermal Enthalpies= -1059.239793
Sum of electronic and thermal (Free) Energies= -1059.319507

cTS

C 1.7397660000 1.3868420000 -0.5154680000
C 0.4407830000 1.1183450000 -0.6047160000
H 2.4269350000 0.7249520000 -1.0455930000
C 2.4318180000 2.4310420000 0.3525340000
C -0.8726050000 1.5080370000 -0.5817440000
C 1.4460150000 3.2883950000 1.1600090000
C 3.2703180000 3.3314680000 -0.5857740000
C 3.3783360000 1.6798170000 1.3184740000
C -1.7874270000 0.4571950000 -0.2051700000
C -1.4018870000 2.8481480000 -1.0036460000
H 0.7946220000 3.8797800000 0.5088580000
H 1.9975880000 3.9873070000 1.7984580000
H 0.8134000000 2.6710350000 1.8066890000
H 3.9837140000 2.7425840000 -1.1740560000
H 3.8408220000 4.0587820000 0.0038040000

H 2.6307740000 3.8847880000 -1.2821840000
H 2.8159660000 1.0264660000 1.9941840000
H 3.9421910000 2.3968090000 1.9268050000
H 4.0991950000 1.0606590000 0.7720570000
C -1.1197230000 -0.7947640000 -0.1345330000
O -3.0147720000 0.7122530000 0.0546040000
H -0.6265800000 3.4725940000 -1.4517310000
H -1.8123210000 3.3666820000 -0.1277650000
H -2.2329160000 2.7267760000 -1.7067070000
C 0.1188810000 -0.8731990000 -0.8011900000
H -1.5076790000 -1.5866010000 0.4953300000
B -4.0210520000 -0.4986770000 0.2820980000
C 1.1708410000 -1.8288570000 -0.4092460000
H 0.1343520000 -0.6268650000 -1.8632850000
F -3.8877780000 -1.2995770000 -0.8381780000
F -5.2426580000 0.0892130000 0.4153290000
F -3.5750630000 -1.1453600000 1.4277370000
C 2.0730960000 -2.3082790000 -1.3736760000
C 1.3047490000 -2.2664810000 0.9203190000
C 3.0724200000 -3.2152480000 -1.0250340000
H 1.9761740000 -1.9796520000 -2.4062090000
C 2.3005500000 -3.1748520000 1.2676520000
H 0.6270150000 -1.8870250000 1.6802390000
C 3.1864260000 -3.6513730000 0.2963300000
H 3.7569060000 -3.5848130000 -1.7832790000
H 2.3902960000 -3.5095480000 2.2971680000
H 3.9642280000 -4.3585940000 0.5705240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.336928 (Hartree/Particle)
Thermal correction to Energy= 0.359064
Thermal correction to Enthalpy= 0.360008
Thermal correction to Gibbs (Free) Energy= 0.284113
Sum of electronic and zero-point Energies= -1059.233948
Sum of electronic and thermal Energies= -1059.211813
Sum of electronic and thermal Enthalpies= -1059.210868
Sum of electronic and thermal (Free) Energies= -1059.286763

cPT

C -2.2055260000 -0.6618760000 -0.3855150000
C -0.8443650000 -0.6518410000 -0.4802990000
C 0.1993710000 -1.5569550000 -0.0943470000
C 1.4819020000 -0.9731550000 -0.3604180000
C 1.2756740000 0.2228300000 -1.0537350000
C -0.1574690000 0.5733370000 -1.1251010000
C -0.4671180000 1.9230250000 -0.4734030000
C 0.1764830000 -2.9101180000 0.5185110000
O 2.5893350000 -1.5361270000 -0.0008370000
H -0.7585780000 -3.4498800000 0.3928520000
H 0.3869570000 -2.8133190000 1.5944210000
H 1.0108900000 -3.4946990000 0.1162090000
C -1.4526000000 2.7578300000 -1.0135030000
C 0.2317660000 2.3396370000 0.6696150000
H -0.4820060000 0.6313920000 -2.1775310000
H 2.0790530000 0.8298000000 -1.4514330000
B 3.8423190000 -0.6016250000 0.0983110000
F 4.1332440000 -0.1708050000 -1.1923750000
F 4.8239590000 -1.3609830000 0.6629760000
F 3.4333360000 0.4731120000 0.8947710000
H -2.6524430000 0.2568600000 -0.7674970000
C -3.2447350000 -1.6350510000 0.1500510000
C -3.3056090000 -2.9086570000 -0.7308730000
H -3.5516770000 -2.6530290000 -1.7673590000
H -2.3643020000 -3.4628270000 -0.7424580000
H -4.0877530000 -3.5783660000 -0.3548820000
C -4.6216320000 -0.9350970000 0.0648570000
H -5.4112710000 -1.5983220000 0.4334240000
H -4.6396210000 -0.0213090000 0.6699260000
H -4.8666250000 -0.6636290000 -0.9688210000
C -2.9881110000 -1.9894750000 1.6344600000
H -2.9783900000 -1.0847450000 2.2516580000
H -3.7938910000 -2.6370130000 1.9991740000
H -2.0437850000 -2.5119520000 1.7919380000
C -0.0741140000 3.5610880000 1.2694870000
C -1.0749710000 4.3786410000 0.7397900000
C -1.7613560000 3.9765930000 -0.4065030000
H -1.9746740000 2.4609370000 -1.9209990000
H -1.3079910000 5.3302900000 1.2093770000
H -2.5290870000 4.6141100000 -0.8366730000
H 1.0381270000 1.7286280000 1.0686170000
H 0.4804040000 3.8777700000 2.1484090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.339568 (Hartree/Particle)
Thermal correction to Energy= 0.361534
Thermal correction to Enthalpy= 0.362478
Thermal correction to Gibbs (Free) Energy= 0.287266
Sum of electronic and zero-point Energies= -1059.254076
Sum of electronic and thermal Energies= -1059.232110
Sum of electronic and thermal Enthalpies= -1059.231166
Sum of electronic and thermal (Free) Energies= -1059.306378

ccRT

C -2.0026700000 -2.1227710000 -0.8729370000
C -0.8030050000 -2.0948740000 -0.3602790000
C -3.3396640000 -1.8506180000 -0.1833720000
H -2.0767710000 -2.3766040000 -1.9342480000
C 0.4367300000 -2.1974080000 0.0983030000
C -3.1793210000 -1.6833440000 1.3360210000
C -4.2617540000 -3.0565460000 -0.4707690000
C -3.9565350000 -0.5758650000 -0.8001370000
C 1.4070630000 -1.0884800000 -0.0248590000
C 0.9803530000 -3.5171410000 0.6177480000
H -2.7253610000 -2.5715890000 1.7887480000
H -2.5528820000 -0.8206970000 1.5879740000
H -4.1581560000 -1.5280190000 1.8034640000
H -5.2523490000 -2.8900050000 -0.0314290000
H -4.3936860000 -3.2093410000 -1.5483920000
H -3.8513910000 -3.9792210000 -0.0457490000
H -4.0798970000 -0.6789780000 -1.8845090000
H -4.9457640000 -0.3842010000 -0.3670380000
H -3.3270440000 0.3015720000 -0.6167950000
C 1.0440640000 0.3071730000 -0.2132390000
O 2.6197990000 -1.4427510000 0.0032530000
H 1.4253760000 -3.3871180000 1.6100830000
H 1.7712850000 -3.8882460000 -0.0414380000
H 0.1838170000 -4.2618070000 0.6776750000
C -0.0875520000 0.8670170000 0.2719080000
H 1.8083940000 0.9029020000 -0.6977890000
B 3.9273410000 -0.4337190000 -0.0220300000
H -0.7747300000 0.2401260000 0.8331230000
C -0.4794340000 2.2689590000 0.1632240000
F 4.9654020000 -1.3030750000 0.0518130000
F 3.7519320000 0.3688230000 1.0730880000
F 3.8269350000 0.2407120000 -1.2202000000
C 0.2653540000 3.2211450000 -0.5618640000
C -1.6576490000 2.6910370000 0.8089030000
C -0.1595960000 4.5423420000 -0.6358430000
H 1.1799880000 2.9258090000 -1.0659270000
C -2.0823440000 4.0152410000 0.7340100000
H -2.2380330000 1.9692110000 1.3786630000
C -1.3338850000 4.9447190000 0.0102360000
H 0.4263010000 5.2643610000 -1.1973560000
H -2.9931390000 4.3216290000 1.2405620000
H -1.6604100000 5.9791630000 -0.0501200000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337834 (Hartree/Particle)
Thermal correction to Energy= 0.361015
Thermal correction to Enthalpy= 0.361959
Thermal correction to Gibbs (Free) Energy= 0.283109
Sum of electronic and zero-point Energies= -1059.262499
Sum of electronic and thermal Energies= -1059.239318
Sum of electronic and thermal Enthalpies= -1059.238374
Sum of electronic and thermal (Free) Energies= -1059.317224

ccTS

C 2.4363080000 0.3945090000 -0.2777850000
C 1.1225430000 0.2451160000 -0.0803050000
C 3.6602210000 -0.2879850000 0.3058240000
H 2.6851720000 1.1674940000 -0.1129360000
C -0.0268240000 0.9961750000 -0.0429380000
C 3.3596120000 -1.0564770000 1.6036090000
C 4.6712220000 0.8427770000 0.6216490000
C 4.2835440000 -1.2312430000 -0.7511310000
C -1.2418050000 0.2720120000 -0.3160200000
C -0.0816460000 2.4510530000 0.3195870000

H 2.8646710000 -0.4128990000 2.3399330000
H 2.7311040000 -1.9299290000 1.4215900000
H 4.2950430000 -1.4155950000 2.0474960000
H 5.5975590000 0.4137970000 1.0201880000
H 4.9263820000 1.4163440000 -0.2771930000
H 4.2716680000 1.5389420000 1.3677840000
H 4.5204170000 -0.6889200000 -1.6738760000
H 5.2165000000 -1.6591620000 -0.3650200000
H 3.6073030000 -2.0527250000 -1.0028900000
C -0.9747750000 -1.1131000000 -0.4642550000
O -2.3574900000 0.8789230000 -0.4710450000
H -0.4885420000 2.5856170000 1.3300050000
H -0.7757820000 2.9573730000 -0.3601760000
H 0.9012180000 2.9245080000 0.2705650000
C 0.2236830000 -1.5980750000 0.0977580000
H -1.6141180000 -1.7256540000 -1.0893490000
B -3.6881750000 0.0175300000 -0.6320260000
H 0.3767900000 -1.4478650000 1.1658040000
C 0.8248230000 -2.8366130000 -0.4440210000
F -4.6929540000 0.9368930000 -0.6350190000
F -3.6981860000 -0.8418300000 0.4521310000
F -3.5431960000 -0.6700670000 -1.8289000000
C 0.9116420000 -3.0378070000 -1.8322430000
C 1.2706560000 -3.8535920000 0.4166060000
C 1.4320490000 -4.2240350000 -2.3446770000
H 0.5776820000 -2.2530350000 -2.5058320000
C 1.7845230000 -5.0432910000 -0.0961700000
H 1.1879980000 -3.7203400000 1.4925920000
C 1.8698470000 -5.2290830000 -1.4777580000
H 1.4963590000 -4.3654620000 -3.4197790000
H 2.1135980000 -5.8260790000 0.5812660000
H 2.2748640000 -6.1542220000 -1.8781670000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.336703 (Hartree/Particle)
Thermal correction to Energy= 0.358884
Thermal correction to Enthalpy= 0.359828
Thermal correction to Gibbs (Free) Energy= 0.284423
Sum of electronic and zero-point Energies= -1059.225992
Sum of electronic and thermal Energies= -1059.203811
Sum of electronic and thermal Enthalpies= -1059.202867
Sum of electronic and thermal (Free) Energies= -1059.278272

ccPT

C -1.6848710000 -1.8466940000 -0.2246140000
C -0.5354830000 -1.1456720000 -0.0194220000
C 0.7358880000 -1.5978470000 -0.5124360000
C 1.7910300000 -0.7377440000 -0.0726440000
C 1.2034930000 0.2756560000 0.6912370000
C -0.2807920000 0.1456960000 0.7632620000
C 1.0546720000 -2.7971410000 -1.3239550000
O 3.0293500000 -0.9535130000 -0.3741740000
H 0.1834340000 -3.3203430000 -1.7213010000
H 1.6469230000 -3.4946880000 -0.7152060000
H 1.7195270000 -2.5021590000 -2.1449830000
C -0.9308080000 1.4262140000 0.2215120000
H 1.7532680000 1.0905350000 1.1431590000
C -0.9361610000 1.7060000000 -1.1513320000
C -1.4491620000 2.3771300000 1.1083830000
H -0.5964480000 0.0216470000 1.8086280000
B 4.0983150000 0.0435950000 0.1901770000
F 5.3013240000 -0.4258620000 -0.2533990000
F 3.9557820000 0.0141280000 1.5747570000
F 3.7601610000 1.2963930000 -0.3105730000
C -3.1136420000 -1.6561740000 0.2303730000
H -1.5747880000 -2.7219290000 -0.8649590000
C -3.2819440000 -0.8266180000 1.5160550000
H -2.7031250000 -1.2528090000 2.3434960000
H -2.9860710000 0.2147740000 1.3765150000
H -4.3364180000 -0.8302770000 1.8141420000
C -3.7124720000 -3.0643740000 0.4668020000
H -4.7701720000 -2.9806710000 0.7392320000
H -3.6460950000 -3.6868280000 -0.4333510000
H -3.1949760000 -3.5859510000 1.2801170000
C -3.8792600000 -0.9755800000 -0.9383140000
H -3.8049880000 -1.5620100000 -1.8612040000
H -4.9410550000 -0.8908550000 -0.6782590000
H -3.4905670000 0.0280350000 -1.1352700000
C -1.4771160000 2.8996830000 -1.6276860000
C -2.0039810000 3.8380880000 -0.7370780000
C -1.9851060000 3.5754790000 0.6327170000
H -0.5118710000 0.9908190000 -1.8509150000
H -1.4764030000 3.1012450000 -2.6952530000
H -2.4198980000 4.7700510000 -1.1091680000
H -1.4324630000 2.1812490000 2.1781970000
H -2.3852950000 4.3017590000 1.3346640000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.339376 (Hartree/Particle)
Thermal correction to Energy= 0.361478
Thermal correction to Enthalpy= 0.362423
Thermal correction to Gibbs (Free) Energy= 0.286238
Sum of electronic and zero-point Energies= -1059.260762
Sum of electronic and thermal Energies= -1059.238659
Sum of electronic and thermal Enthalpies= -1059.237715
Sum of electronic and thermal (Free) Energies= -1059.313899

4a

cRT

C 2.5719870000 -0.2972720000 -0.7293590000
C 1.3627540000 0.1757650000 -0.6054010000
C 0.1468260000 0.6745430000 -0.4226910000
C -0.9726020000 -0.2909960000 -0.3555310000
C -0.9652740000 -1.5588150000 -1.1042810000
C -0.3694260000 -1.7111700000 -2.2937380000
H -1.5662020000 -2.3499190000 -0.6695920000
C -0.1038050000 2.1867790000 -0.1753530000
O -1.9501250000 0.0012950000 0.3775620000
B -3.3776200000 -0.8644640000 0.5464960000
F -4.0554650000 -0.0931050000 1.4291980000
F -2.9772070000 -2.0864020000 1.0268380000
F -3.8790520000 -0.8983300000 -0.7229940000
C 3.4886770000 -0.7874080000 0.3932310000
H 2.9908770000 -0.3714370000 -1.7359940000
H 0.1749020000 -0.9080420000 -2.7796130000
H -0.4469660000 -2.6495030000 -2.8354590000
C -1.2814660000 2.6676320000 -1.0535520000
H -2.2164100000 2.1609220000 -0.8034910000
H -1.4334470000 3.7425640000 -0.9032780000
H -1.0718540000 2.5065880000 -2.1179560000
C -0.4154180000 2.4436990000 1.3178570000
H -0.5462650000 3.5201070000 1.4825160000
H -1.3263540000 1.9344190000 1.6362810000
H 0.4120430000 2.1056400000 1.9527000000
C 1.1518990000 2.9897560000 -0.5635940000
H 2.0162300000 2.7190550000 0.0516120000
H 1.4228850000 2.8343490000 -1.6142610000
H 0.9586270000 4.0583490000 -0.4197780000
C 2.8230210000 -0.6539510000 1.7714690000
H 2.5787310000 0.3896370000 1.9989530000
H 1.8980600000 -1.2380060000 1.8280360000
H 3.4992200000 -1.0184660000 2.5526730000
C 4.7843380000 0.0517660000 0.3494490000
H 5.4928880000 -0.3047850000 1.1064630000
H 5.2742230000 -0.0200220000 -0.6289460000
H 4.5781520000 1.1093550000 0.5478740000
C 3.8235180000 -2.2694070000 0.1144990000
H 4.2940650000 -2.3947260000 -0.8680750000
H 4.5202510000 -2.6497950000 0.8708120000
H 2.9207930000 -2.8893270000 0.1401380000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340871 (Hartree/Particle)
Thermal correction to Energy= 0.363531
Thermal correction to Enthalpy= 0.364476
Thermal correction to Gibbs (Free) Energy= 0.288280
Sum of electronic and zero-point Energies= -946.131937
Sum of electronic and thermal Energies= -946.109276
Sum of electronic and thermal Enthalpies= -946.108332
Sum of electronic and thermal (Free) Energies= -946.184527

cTS

C -2.7001410000 -0.4737260000 -0.0394690000
C -1.3919180000 -0.2430950000 0.0620690000
C -3.6599390000 -0.1191430000 -1.1719850000
H -3.1529570000 -1.0998400000 0.7311870000

C -0.2303060000 0.4646040000 -0.0756960000
C -4.7919620000 0.7593800000 -0.5891110000
C -4.2681250000 -1.4511040000 -1.6763420000
C -2.9753810000 0.5946690000 -2.3469130000
C 0.9308040000 -0.3992560000 -0.2740910000
C -0.0823450000 1.9839860000 0.0979990000
H -5.2946400000 0.2595370000 0.2472210000
H -4.4099110000 1.7197860000 -0.2287230000
H -5.5444670000 0.9596450000 -1.3608990000
H -5.0130460000 -1.2522730000 -2.4555060000
H -3.4972370000 -2.1024540000 -2.1024300000
H -4.7672730000 -1.9964180000 -0.8665880000
H -2.1522210000 -0.0033810000 -2.7522200000
H -3.6997900000 0.7599790000 -3.1520140000
H -2.5749680000 1.5706790000 -2.0593410000
C 0.5982880000 -1.7653070000 -0.0372330000
O 2.0528730000 0.0481270000 -0.6877530000
C 0.9945820000 2.2671040000 1.1754930000
C 0.3644090000 2.6009510000 -1.2516260000
C -1.3966560000 2.6414450000 0.5550280000
C -0.5630540000 -1.9795580000 0.6948590000
H 1.1266720000 -2.5488280000 -0.5682660000
B 3.3297990000 -0.9245720000 -0.7301430000
H 1.9673570000 1.8584140000 0.8967570000
H 1.1021380000 3.3503750000 1.3019880000
H 0.7017590000 1.8450940000 2.1442560000
H 1.3085820000 2.1702070000 -1.5905960000
H -0.3897260000 2.4453440000 -2.0307340000
H 0.5012030000 3.6812820000 -1.1247690000
H -1.7494790000 2.2232430000 1.5041740000
H -1.2297070000 3.7139220000 0.7022630000
H -2.1963370000 2.5303490000 -0.1826050000
H -0.7081010000 -1.5368180000 1.6775110000
H -1.1158700000 -2.9097490000 0.5581770000
F 4.3632610000 -0.0971570000 -1.0457600000
F 3.0367050000 -1.8700780000 -1.6981200000
F 3.3986560000 -1.4791780000 0.5324350000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340920 (Hartree/Particle)
Thermal correction to Energy= 0.362198
Thermal correction to Enthalpy= 0.363142
Thermal correction to Gibbs (Free) Energy= 0.291704
Sum of electronic and zero-point Energies= -946.102080
Sum of electronic and thermal Energies= -946.080803
Sum of electronic and thermal Enthalpies= -946.079858
Sum of electronic and thermal (Free) Energies= -946.151297

cPT

C 2.3630060000 -0.9760290000 -0.5835260000
C 1.0241850000 -0.7220620000 -0.6677090000
C 3.5055310000 -0.5650450000 0.3301980000
H 2.6636760000 -1.8181240000 -1.2111800000
C 0.0772790000 0.2767210000 -0.2481860000
C 4.5419030000 0.2722930000 -0.4623990000
C 4.1947650000 -1.8973140000 0.7405700000
C 3.0731130000 0.1399770000 1.6276470000
C -1.2142800000 -0.3615680000 -0.0820250000
C 0.1891460000 1.7931530000 -0.2174090000
H 4.8751510000 -0.2618190000 -1.3596770000
H 4.1400840000 1.2383440000 -0.7756510000
H 5.4224720000 0.4542540000 0.1646300000
H 5.0500180000 -1.6863090000 1.3918200000
H 3.5062820000 -2.5504800000 1.2883240000
H 4.5644880000 -2.4454760000 -0.1336880000
H 2.3366190000 -0.4625490000 2.1706510000
H 3.9440490000 0.2705930000 2.2794090000
H 2.6429940000 1.1268850000 1.4622640000
C -1.1495200000 -1.6327990000 -0.6638540000
O -2.2308080000 0.2123690000 0.4748650000
C -0.9218210000 2.3489380000 -1.1647190000
C -0.0811010000 2.3180500000 1.2193750000
C 1.5239930000 2.3398890000 -0.7530750000
C 0.1795680000 -1.8925860000 -1.2248730000
H -1.9775770000 -2.3289190000 -0.6718010000
B -3.6450200000 -0.4650230000 0.3474590000
H -1.9194870000 2.0341180000 -0.8610390000
H -0.8774240000 3.4432370000 -1.1388110000
H -0.7471390000 2.0292690000 -2.1983160000
H -1.0616550000 1.9948650000 1.5733560000
H 0.6789680000 1.9717460000 1.9266840000
H -0.0562240000 3.4136800000 1.2042460000
H 1.7620290000 1.9241950000 -1.7383680000
H 1.4412870000 3.4263520000 -0.8625230000
H 2.3654000000 2.1499080000 -0.0883790000
H 0.1878410000 -1.8201520000 -2.3242780000
H 0.5641840000 -2.8912550000 -0.9753680000
F -4.5004670000 0.3830400000 0.9897260000
F -3.5409010000 -1.7173450000 0.9431150000
F -3.8774180000 -0.5807960000 -1.0171320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.343360 (Hartree/Particle)
Thermal correction to Energy= 0.364632
Thermal correction to Enthalpy= 0.365576
Thermal correction to Gibbs (Free) Energy= 0.293282
Sum of electronic and zero-point Energies= -946.120172
Sum of electronic and thermal Energies= -946.098900
Sum of electronic and thermal Enthalpies= -946.097956
Sum of electronic and thermal (Free) Energies= -946.170249

ccRT

C 2.4160520000 -0.2204380000 -0.9158750000
C 1.2726310000 0.1640310000 -0.4179950000
C 3.6919830000 -0.6535940000 -0.1940900000
H 2.4791430000 -0.2499250000 -2.0076050000
C 0.0844390000 0.6246470000 -0.0432670000
C 3.6254660000 -0.3894180000 1.3181250000
C 4.8656040000 0.1446440000 -0.8033910000
C 3.9011990000 -2.1610650000 -0.4598000000
C -1.0265730000 -0.3500270000 0.0068590000
C -0.1896780000 2.1404040000 0.1585170000
H 3.4504520000 0.6707380000 1.5306770000
H 2.8295610000 -0.9692170000 1.7961150000
H 4.5711920000 -0.6767810000 1.7911210000
H 5.8133990000 -0.1692490000 -0.3506520000
H 4.9399840000 -0.0185750000 -1.8850250000
H 4.7456500000 1.2198990000 -0.6304970000
H 3.9606620000 -2.3718160000 -1.5339110000
H 4.8350680000 -2.5030810000 0.0022950000
H 3.0773080000 -2.7527210000 -0.0459850000
C -0.8236630000 -1.7690290000 0.3454790000
O -2.1770560000 0.0666730000 -0.2786680000
C -0.9337700000 2.7159280000 -1.0699440000
C -1.0292410000 2.3537810000 1.4382810000
C 1.1440740000 2.8934750000 0.3211220000
C 0.0631740000 -2.1868150000 1.2565810000
H -1.5273980000 -2.4542050000 -0.1146410000
B -3.6044390000 -0.8155300000 -0.2399320000
H -1.9109710000 2.2504750000 -1.2076880000
H -1.0816620000 3.7941240000 -0.9340750000
H -0.3460870000 2.5705670000 -1.9839390000
H -2.0118280000 1.8817110000 1.3704980000
H -0.5120980000 1.9575930000 2.3206430000
H -1.1840490000 3.4270130000 1.5977470000
H 0.9424310000 3.9577150000 0.4845290000
H 1.7138900000 2.5237940000 1.1817120000
H 1.7748900000 2.8035520000 -0.5689250000
H 0.7142780000 -1.4996750000 1.7856730000
H 0.1252020000 -3.2356900000 1.5320330000
F -4.5077780000 0.1221560000 -0.6119770000
F -3.6837160000 -1.2376800000 1.0560420000
F -3.4007910000 -1.8234900000 -1.1490350000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340825 (Hartree/Particle)
Thermal correction to Energy= 0.363507
Thermal correction to Enthalpy= 0.364451
Thermal correction to Gibbs (Free) Energy= 0.288110
Sum of electronic and zero-point Energies= -946.130230
Sum of electronic and thermal Energies= -946.107549
Sum of electronic and thermal Enthalpies= -946.106605
Sum of electronic and thermal (Free) Energies= -946.182946

ccTS

C -2.4579150000 0.1463710000 0.2491960000
C -1.1763600000 -0.0577720000 -0.0429940000

C -3.7520840000 -0.4007960000 -0.3358710000
H -2.6218490000 0.8207950000 1.0949060000
C 0.1062710000 0.4257450000 -0.0647130000
C -3.5808320000 -1.0851140000 -1.7035690000
C -4.6996250000 0.8126900000 -0.5052800000
C -4.3795610000 -1.3886030000 0.6760250000
C 1.1130130000 -0.5931370000 0.1843360000
C 0.4815370000 1.8857200000 -0.3612780000
H -3.0399020000 -0.4428360000 -2.4078430000
H -3.0541690000 -2.0400530000 -1.6295640000
H -4.5658590000 -1.2964400000 -2.1341420000
H -5.6776700000 0.4775770000 -0.8687470000
H -4.8558170000 1.3348620000 0.4458590000
H -4.2974910000 1.5332850000 -1.2259350000
H -4.5358630000 -0.9147410000 1.6518090000
H -5.3529650000 -1.7370400000 0.3110280000
H -3.7387670000 -2.2641460000 0.8265830000
C 0.5293410000 -1.8985770000 0.2056010000
O 2.3311950000 -0.3123600000 0.4423690000
C 1.1021840000 2.4875020000 0.9269120000
C 1.5124510000 1.9360010000 -1.5141100000
C -0.7420730000 2.7295050000 -0.7625800000
C -0.6784460000 -2.0395500000 -0.4552880000
H 0.9478100000 -2.6583130000 0.8565420000
B 3.4082240000 -1.4981560000 0.5667030000
H 1.9905980000 1.9352570000 1.2386780000
H 1.3897690000 3.5278000000 0.7346140000
H 0.3795640000 2.4844400000 1.7513360000
H 2.4205250000 1.3810190000 -1.2715990000
H 1.0875510000 1.5256820000 -2.4379690000
H 1.7901560000 2.9783570000 -1.7083790000
H -0.4144510000 3.7507020000 -0.9853820000
H -1.2350380000 2.3326790000 -1.6569660000
H -1.4856910000 2.7875120000 0.0387010000
H -0.8011210000 -1.7027260000 -1.4792310000
H -1.3502970000 -2.8499670000 -0.1754770000
F 4.6031590000 -0.8519380000 0.6379960000
F 3.2304480000 -2.2612220000 -0.5710290000
F 3.0581370000 -2.1880010000 1.7142870000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340788 (Hartree/Particle)
Thermal correction to Energy= 0.362094
Thermal correction to Enthalpy= 0.363038
Thermal correction to Gibbs (Free) Energy= 0.291069
Sum of electronic and zero-point Energies= -946.100164
Sum of electronic and thermal Energies= -946.078858
Sum of electronic and thermal Enthalpies= -946.077913
Sum of electronic and thermal (Free) Energies= -946.149883

ccPT

C 2.4211890000 0.1069880000 0.0000000000
C 1.1181460000 -0.2928510000 0.0000000000
C 3.7363080000 -0.6406840000 0.0000000000
H 2.5946390000 1.1742250000 0.0000000000
C -0.0528230000 0.5621800000 0.0000000000
C 3.6818740000 -2.1767530000 -0.0000020000
C 4.5101210000 -0.1675440000 1.2608870000
C 4.5101230000 -0.1675410000 -1.2608850000
C -1.2361830000 -0.2737240000 0.0000000000
C -0.2012630000 2.0763200000 0.0000000000
H 3.1821510000 -2.5733660000 0.8888650000
H 3.1821510000 -2.5733630000 -0.8888710000
H 4.7043480000 -2.5699460000 -0.0000020000
H 5.5166740000 -0.6011130000 1.2614610000
H 4.6139000000 0.9231160000 1.2858120000
H 4.0025880000 -0.4826980000 2.1790020000
H 4.6139020000 0.9231190000 -1.2858070000
H 5.5166760000 -0.6011100000 -1.2614590000
H 4.0025910000 -0.4826930000 -2.1790020000
C -0.8291520000 -1.6085660000 0.0000000000
O -2.4513300000 0.1809100000 0.0000000000
C -1.0093930000 2.4707050000 -1.2729840000
C -1.0093920000 2.4707060000 1.2729840000
C 1.0889860000 2.9179240000 0.0000000000
C 0.6357470000 -1.7330890000 0.0000000000
H -1.5182170000 -2.4419120000 0.0000000000
B -3.6427640000 -0.8377400000 0.0000000000
H -1.9738940000 1.9650330000 -1.3121890000
H -1.1810140000 3.5528530000 -1.2544460000
H -0.4425470000 2.2335220000 -2.1806810000
H -1.9738940000 1.9650330000 1.3121890000
H -0.4425470000 2.2335220000 2.1806810000
H -1.1810140000 3.5528530000 1.2544460000
H 0.8020230000 3.9747610000 0.0000000000
H 1.7007330000 2.7553760000 0.8940020000
H 1.7007330000 2.7553760000 -0.8940020000
H 0.9927880000 -2.2933850000 0.8758260000
H 0.9927880000 -2.2933850000 -0.8758260000
F -4.7683300000 -0.0636890000 0.0000000000
F -3.4917700000 -1.6136460000 1.1445210000
F -3.4917700000 -1.6136460000 -1.1445220000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344196 (Hartree/Particle)
Thermal correction to Energy= 0.365244
Thermal correction to Enthalpy= 0.366188
Thermal correction to Gibbs (Free) Energy= 0.293205
Sum of electronic and zero-point Energies= -946.138981
Sum of electronic and thermal Energies= -946.117933
Sum of electronic and thermal Enthalpies= -946.116988
Sum of electronic and thermal (Free) Energies= -946.189972

4b

cRT

C 2.5918590000 0.3717150000 0.4992920000
C 1.3918640000 -0.1411890000 0.5265420000
C 0.1863690000 -0.6907080000 0.5040850000
C -0.9495450000 0.1862530000 0.1261880000
C -1.0189420000 1.5946160000 0.5116760000
C -0.4287300000 2.0984610000 1.6109230000
H -1.6686500000 2.2091810000 -0.1023980000
C -0.0485870000 -2.2050920000 0.7520160000
O -1.8680870000 -0.3353880000 -0.5591000000
B -3.3238710000 0.3523420000 -0.9740830000
F -3.8996920000 -0.6389440000 -1.6984040000
F -2.9949970000 1.4765090000 -1.6937530000
F -3.9057190000 0.6155500000 0.2353750000
C 3.5125930000 0.4954520000 -0.7159950000
H 0.1573220000 1.4407860000 2.2496730000
C -0.5524580000 3.5190620000 2.0565090000
H -1.1554500000 4.1149940000 1.3661440000
H 0.4407420000 3.9799740000 2.1460730000
H -1.0088020000 3.5703550000 3.0540210000
C -0.3195170000 -2.9363310000 -0.5838700000
H -0.4368100000 -4.0102270000 -0.3938690000
H -1.2254830000 -2.5712220000 -1.0699340000
H 0.5212940000 -2.8078320000 -1.2756170000
C -1.2476220000 -2.3898670000 1.7099320000
H -2.1750650000 -1.9896520000 1.2929960000
H -1.4012160000 -3.4578510000 1.9023200000
H -1.0612580000 -1.9014330000 2.6741820000
C 1.2007100000 -2.8212080000 1.4090930000
H 2.0793400000 -2.7518620000 0.7594270000
H 1.4426720000 -2.3292220000 2.3582810000
H 1.0182060000 -3.8814780000 1.6155750000
C 2.8623350000 -0.0786820000 -1.9840700000
C 4.8193420000 -0.2657080000 -0.4027130000
C 3.8256470000 1.9941220000 -0.9211210000
H 2.6339410000 -1.1441020000 -1.8694780000
H 3.5411190000 0.0295840000 -2.8373490000
H 1.9299740000 0.4421780000 -2.2274010000
H 2.9153940000 2.5594860000 -1.1488310000
H 4.5259480000 2.1257940000 -1.7544670000
H 4.2836140000 2.4326670000 -0.0262620000
H 4.6291600000 -1.3348100000 -0.2570010000
H 5.2985490000 0.1196860000 0.5052400000
H 5.5307010000 -0.1560420000 -1.2299370000
H 3.0005650000 0.7690270000 1.4319320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.369102 (Hartree/Particle)
Thermal correction to Energy= 0.393367
Thermal correction to Enthalpy= 0.394311
Thermal correction to Gibbs (Free) Energy= 0.314100
Sum of electronic and zero-point Energies= -985.427118
Sum of electronic and thermal Energies= -985.402853

Sum of electronic and thermal Enthalpies= -985.401909
Sum of electronic and thermal (Free) Energies= -985.482120

cTS

C -2.3853130000 0.6079030000 -0.5181250000
C -1.0942470000 0.2751910000 -0.5563060000
H -2.7425680000 1.2793020000 -1.3006100000
C -3.4339160000 0.3462600000 0.5599620000
C -0.0369290000 -0.5691780000 -0.3167220000
C -2.8848680000 -0.4117870000 1.7773190000
C -4.6076980000 -0.4315060000 -0.0809920000
C -3.9492830000 1.7312420000 1.0242440000
C 1.1950560000 0.1662800000 -0.0680410000
C -0.0456610000 -2.0973310000 -0.4545550000
H -2.0318270000 0.1120390000 2.2216920000
H -3.6642290000 -0.4959740000 2.5428040000
H -2.5640860000 -1.4251390000 1.5228380000
H -5.4167060000 -0.5552400000 0.6485840000
H -5.0158920000 0.1045190000 -0.9459470000
H -4.2964460000 -1.4258020000 -0.4161090000
H -4.3543960000 2.3109830000 0.1863330000
H -4.7497010000 1.6058220000 1.7626040000
H -3.1486050000 2.3169970000 1.4891900000
C 1.0348480000 1.5375570000 -0.3928910000
O 2.2358460000 -0.3823610000 0.4401820000
C 0.2530900000 -2.7296150000 0.9290640000
C 1.0612620000 -2.5149390000 -1.4566920000
C -1.3893260000 -2.6257990000 -0.9867290000
C -0.0636690000 1.8478110000 -1.2088880000
H 1.6400320000 2.2902580000 0.1005610000
B 3.5987690000 0.4417400000 0.5160670000
H 1.2157170000 -2.3917260000 1.3176690000
H -0.5244920000 -2.4811780000 1.6592200000
H 0.2830230000 -3.8206420000 0.8252960000
H 1.0633620000 -3.6062730000 -1.5571350000
H 0.8738130000 -2.0885800000 -2.4494250000
H 2.0516600000 -2.2005380000 -1.1233030000
H -1.6378440000 -2.1901610000 -1.9607600000
H -1.3235480000 -3.7120080000 -1.1119470000
H -2.2181070000 -2.4226270000 -0.3035920000
C -0.6582690000 3.2352460000 -1.1975100000
H -0.1338140000 1.3532300000 -2.1776710000
F 3.8162370000 0.9042730000 -0.7693170000
F 4.5163140000 -0.4654180000 0.9533820000
F 3.3602840000 1.4817400000 1.4022730000
H -0.7702860000 3.6243560000 -0.1815800000
H -1.6302360000 3.2679610000 -1.6979490000
H 0.0085950000 3.9112570000 -1.7484330000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.369034 (Hartree/Particle)
Thermal correction to Energy= 0.391946
Thermal correction to Enthalpy= 0.392891
Thermal correction to Gibbs (Free) Energy= 0.317995
Sum of electronic and zero-point Energies= -985.393988
Sum of electronic and thermal Energies= -985.371076
Sum of electronic and thermal Enthalpies= -985.370132
Sum of electronic and thermal (Free) Energies= -985.445027

cPT

C 2.4105540000 -0.7509840000 -0.4173380000
C 1.0594760000 -0.6340270000 -0.5291910000
H 2.8080780000 -1.6213320000 -0.9397510000
C 3.4852370000 -0.1238070000 0.4561570000
C 0.0509720000 0.3406540000 -0.1943330000
C 2.9526230000 0.7058850000 1.6365900000
C 4.4691070000 0.6911520000 -0.4211160000
C 4.2728370000 -1.3230560000 1.0547960000
C -1.1806810000 -0.3602820000 0.1084900000
C 0.0249880000 1.8444770000 -0.4189160000
H 2.2622620000 0.1142860000 2.2480630000
H 3.7882090000 1.0105340000 2.2764750000
H 2.4345630000 1.6127820000 1.3277890000
H 5.3121380000 1.0316170000 0.1912690000
H 4.8735650000 0.0760780000 -1.2333790000
H 3.9949710000 1.5681000000 -0.8671480000
H 4.7169770000 -1.9459150000 0.2697180000
H 5.0850660000 -0.9527540000 1.6900490000
H 3.6258340000 -1.9582440000 1.6701460000
C -1.0565340000 -1.6568020000 -0.3909330000
O -2.1958860000 0.2058990000 0.6768980000
C -0.3253020000 2.5949580000 0.8948670000
C -1.1169630000 2.0988670000 -1.4612610000
C 1.3088090000 2.4247300000 -1.0383880000
C 0.2690590000 -1.9048220000 -0.9899430000
H -1.8587520000 -2.3830120000 -0.3509010000
B -3.6643060000 -0.2751970000 0.4250090000
H -1.2855310000 2.2631790000 1.2910680000
H 0.4417040000 2.4454580000 1.6616310000
H -0.3817900000 3.6678320000 0.6783350000
H -1.2243730000 3.1820200000 -1.5869100000
H -0.8472990000 1.6737160000 -2.4349650000
H -2.0789860000 1.6878310000 -1.1547170000
H 1.6314860000 1.8516070000 -1.9142320000
H 1.1056450000 3.4488150000 -1.3688700000
H 2.1402350000 2.4772070000 -0.3356070000
C 0.8313920000 -3.2974280000 -0.6679220000
H 0.1948360000 -1.8074210000 -2.0864260000
F -3.9492320000 0.1120710000 -0.8777970000
F -4.4131810000 0.3694130000 1.3693900000
F -3.6895080000 -1.6631900000 0.5609130000
H 1.0181790000 -3.4125850000 0.4046190000
H 1.7603010000 -3.5033460000 -1.2079360000
H 0.1051450000 -4.0594220000 -0.9704600000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.371908 (Hartree/Particle)
Thermal correction to Energy= 0.394516
Thermal correction to Enthalpy= 0.395460
Thermal correction to Gibbs (Free) Energy= 0.321218
Sum of electronic and zero-point Energies= -985.405657
Sum of electronic and thermal Energies= -985.383050
Sum of electronic and thermal Enthalpies= -985.382106
Sum of electronic and thermal (Free) Energies= -985.456347

ccRT

C 2.3974440000 0.1477120000 -1.0275780000
C 1.2562080000 0.4292370000 -0.4579090000
C 0.0673030000 0.8064840000 -0.0069030000
C -1.0371000000 -0.1789910000 -0.1046550000
C -0.8463650000 -1.6121670000 0.1129640000
C 0.0634630000 -2.1178820000 0.9640650000
H -1.5720970000 -2.2539500000 -0.3755540000
C -0.2282860000 2.2651930000 0.4386520000
O -2.1714590000 0.2718990000 -0.4138400000
B -3.6031730000 -0.5734630000 -0.4707630000
F -4.4771210000 0.3929490000 -0.8463080000
F -3.7503210000 -1.0395730000 0.8065090000
F -3.3946740000 -1.5592190000 -1.4056720000
C 3.6955790000 -0.3629120000 -0.4041670000
H 0.7205400000 -1.4367680000 1.4998160000
C 0.2092450000 -3.5718420000 1.2776140000
H -0.4788100000 -4.1879520000 0.6925090000
H 0.0208450000 -3.7547510000 2.3439440000
H 1.2367630000 -3.9076920000 1.0822300000
C -0.9620370000 3.0312810000 -0.6876850000
H -1.1221740000 4.0709320000 -0.3768990000
H -0.3607720000 3.0436610000 -1.6043180000
H -1.9319030000 2.5866180000 -0.9155500000
C 1.0939510000 2.9926300000 0.7466980000
H 1.7381550000 3.0584780000 -0.1358430000
H 0.8783220000 4.0127760000 1.0828160000
H 1.6556040000 2.4886820000 1.5421210000
C -1.0893150000 2.2516920000 1.7217440000
H -2.0595980000 1.7751560000 1.5631540000
H -0.5744650000 1.7290150000 2.5371930000
H -1.2722730000 3.2811830000 2.0502330000
C 3.6355760000 -0.3931970000 1.1306980000
C 4.8311800000 0.5830440000 -0.8544060000
C 3.9642860000 -1.7828090000 -0.9504950000
H 3.4117730000 0.5972830000 1.5413100000
H 4.5996760000 -0.7175430000 1.5383560000
H 2.8741260000 -1.0920780000 1.4914980000
H 3.1711790000 -2.4773060000 -0.6518780000
H 4.9176990000 -2.1654940000 -0.5667510000
H 4.0175790000 -1.7851650000 -2.0454080000
H 4.6716320000 1.5996570000 -0.4784020000

H 4.8985980000 0.6329920000 -1.9475670000
H 5.7959070000 0.2266490000 -0.4744770000
H 2.4434870000 0.2954800000 -2.1105770000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.369079 (Hartree/Particle)
Thermal correction to Energy= 0.393362
Thermal correction to Enthalpy= 0.394306
Thermal correction to Gibbs (Free) Energy= 0.314011
Sum of electronic and zero-point Energies= -985.425100
Sum of electronic and thermal Energies= -985.400818
Sum of electronic and thermal Enthalpies= -985.399874
Sum of electronic and thermal (Free) Energies= -985.480168

ccTS

C 2.3403720000 0.1479570000 -0.6085600000
C 1.0731910000 0.0411680000 -0.1927310000
H 2.4628310000 0.7309230000 -1.5257650000
C 3.6651240000 -0.3488870000 -0.0489550000
C -0.1180030000 0.7227030000 -0.1030230000
C 3.5753080000 -0.8358930000 1.4082640000
C 4.2501030000 -1.4481310000 -0.9672420000
C 4.6209850000 0.8723470000 -0.0893760000
C -0.2588470000 2.2456030000 0.0421060000
C -1.2772970000 -0.1505020000 -0.0901220000
H 2.9839960000 -1.7477100000 1.5148230000
H 4.5794840000 -1.0565360000 1.7870720000
H 3.1366290000 -0.0664760000 2.0535670000
H 3.6219000000 -2.3428210000 -0.9841640000
H 5.2478650000 -1.7386440000 -0.6176220000
H 4.3483310000 -1.0881260000 -1.9977890000
H 5.6148950000 0.5784380000 0.2670200000
H 4.2576700000 1.6854730000 0.5481700000
H 4.7311570000 1.2616810000 -1.1081290000
C -0.9796300000 2.7761430000 -1.2259940000
C 1.0978590000 2.9612040000 0.1711620000
C -1.1006830000 2.5723230000 1.2997160000
C -0.8855190000 -1.5122920000 -0.0281140000
O -2.4763990000 0.2827930000 -0.2141020000
H -0.3882100000 2.5773330000 -2.1275350000
H -1.1064170000 3.8616180000 -1.1387660000
H -1.9643660000 2.3212750000 -1.3459600000
H 1.7201880000 2.8374010000 -0.7205580000
H 0.9225430000 4.0344530000 0.3032890000
H 1.6659520000 2.6062000000 1.0380500000
H -1.2166270000 3.6588470000 1.3866690000
H -2.0950530000 2.1256470000 1.2507470000
H -0.6006920000 2.2158570000 2.2082860000
C 0.4069510000 -1.7890230000 0.4286630000
H -1.5187250000 -2.2682640000 -0.4809480000
B -3.7011910000 -0.7244740000 -0.0315160000
C 1.0436860000 -3.0999920000 0.0244880000
H 0.6932190000 -1.4172140000 1.4107850000
F -3.6287000000 -1.5988000000 -1.1051870000
F -4.8000150000 0.0802290000 -0.0379370000
F -3.4674980000 -1.3680950000 1.1703020000
H 1.0509110000 -3.2253590000 -1.0622420000
H 2.0627860000 -3.2108520000 0.3967800000
H 0.4511980000 -3.9214860000 0.4483200000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.368982 (Hartree/Particle)
Thermal correction to Energy= 0.391881
Thermal correction to Enthalpy= 0.392825
Thermal correction to Gibbs (Free) Energy= 0.317816
Sum of electronic and zero-point Energies= -985.387987
Sum of electronic and thermal Energies= -985.365089
Sum of electronic and thermal Enthalpies= -985.364144
Sum of electronic and thermal (Free) Energies= -985.439153

ccPT

C -2.3435400000 0.2823900000 -0.1251870000
C -1.0685970000 -0.1631710000 0.0575060000
H -2.4653660000 1.3563240000 -0.1505630000
C -3.6786720000 -0.4137550000 -0.3179840000
C 0.1165590000 0.6775630000 0.0781990000
C -3.6355750000 -1.8636230000 -0.8359180000
C -4.4228830000 -0.3610920000 1.0446330000
C -4.4755080000 0.4333280000 -1.3434930000
C 0.2878980000 2.1837320000 0.2035270000
C 1.2822540000 -0.1716010000 -0.0423450000
H -3.1959630000 -2.5608600000 -0.1198330000
H -4.6585870000 -2.2051200000 -1.0295060000
H -3.0814830000 -1.9347090000 -1.7782170000
H -3.9084010000 -0.9543920000 1.8072610000
H -5.4369710000 -0.7608350000 0.9263220000
H -4.5076930000 0.6666690000 1.4150220000
H -5.4797610000 0.0162330000 -1.4760580000
H -3.9813580000 0.4407810000 -2.3216740000
H -4.5849420000 1.4716760000 -1.0096160000
C 1.2013660000 2.4342320000 1.4439470000
C -0.9839270000 3.0297300000 0.4094970000
C 1.0024980000 2.7005430000 -1.0794530000
C 0.8550340000 -1.4972550000 0.0025790000
O 2.5002250000 0.2668330000 -0.1430890000
H 0.6958800000 2.1249840000 2.3660770000
H 1.4027550000 3.5090030000 1.5129600000
H 2.1512480000 1.9068800000 1.3620220000
H -1.5826820000 2.6930440000 1.2626810000
H -0.6747330000 4.0593730000 0.6179440000
H -1.6168770000 3.0695040000 -0.4834120000
H 1.1819880000 3.7761850000 -0.9701200000
H 1.9577750000 2.1995500000 -1.2366120000
H 0.3702290000 2.5508490000 -1.9622580000
C -0.6104570000 -1.6146130000 0.1504470000
H 1.5327830000 -2.3407460000 -0.0037560000
B 3.6670180000 -0.7700640000 -0.2683120000
C -0.9597520000 -2.2922670000 1.5044850000
H -1.0275230000 -2.2254940000 -0.6603850000
F 3.6186830000 -1.5532690000 0.8815740000
F 4.8011060000 -0.0158040000 -0.3754280000
F 3.3898230000 -1.5353880000 -1.3960380000
H -0.5704260000 -1.6972770000 2.3362820000
H -2.0387900000 -2.4041810000 1.6344280000
H -0.5046990000 -3.2864840000 1.5536630000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.372832 (Hartree/Particle)
Thermal correction to Energy= 0.395280
Thermal correction to Enthalpy= 0.396224
Thermal correction to Gibbs (Free) Energy= 0.321453
Sum of electronic and zero-point Energies= -985.420577
Sum of electronic and thermal Energies= -985.398129
Sum of electronic and thermal Enthalpies= -985.397185
Sum of electronic and thermal (Free) Energies= -985.471956

4c

c/s RT

C 2.5987740000 0.2119670000 0.2694630000
C 1.4184450000 -0.3133510000 0.4554510000
C 3.5632970000 -0.0762900000 -0.8822630000
H 2.9532820000 0.9458280000 0.9977030000
C 0.2358920000 -0.8910680000 0.6085490000
C 4.8849160000 -0.5981480000 -0.2772330000
C 3.8255810000 1.2534810000 -1.6232430000
C 2.9891310000 -1.1125500000 -1.8605130000
C -0.9146810000 -0.2705240000 -0.0936640000
C 0.0470590000 -2.2171190000 1.3931980000
H 5.3109320000 0.1209310000 0.4326940000
H 4.7308050000 -1.5450110000 0.2519980000
H 5.6249210000 -0.7669110000 -1.0686280000
H 4.5545910000 1.1033710000 -2.4284230000
H 2.9039160000 1.6451240000 -2.0676300000
H 4.2275120000 2.0160470000 -0.9452060000
H 2.0479700000 -0.7680320000 -2.3024600000
H 3.6979130000 -1.2935920000 -2.6762520000
H 2.7979230000 -2.0697050000 -1.3628210000
C -1.0467120000 1.1753720000 -0.2603470000
O -1.7883600000 -1.0512000000 -0.5560770000
C -1.1800200000 -2.0934930000 2.3250870000
C -0.1462390000 -3.4008290000 0.4163610000
C 1.2919230000 -2.4877240000 2.2586910000
C -0.5307210000 2.0773850000 0.5946750000
H -1.6863210000 1.4880030000 -1.0791560000
B -3.2475720000 -0.6306250000 -1.2271900000
H -2.1047900000 -1.9199390000 1.7693740000

H -1.3017780000 -3.0216230000 2.8951580000
H -1.0484220000 -1.2758680000 3.0442760000
H -1.0456860000 -3.2838100000 -0.1899680000
H 0.7150140000 -3.4961590000 -0.2553380000
H -0.2317950000 -4.3336960000 0.9869660000
H 1.4789890000 -1.6703520000 2.9647060000
H 1.1406860000 -3.4055070000 2.8374310000
H 2.1917280000 -2.6194440000 1.6488850000
H 0.0448010000 1.7340950000 1.4541290000
C -0.7272080000 3.5621580000 0.4914960000
F -3.7698570000 -1.8438590000 -1.5354120000
F -2.9300470000 0.1527600000 -2.3115250000
F -3.8792730000 0.0448420000 -0.2187130000
H -1.2865800000 3.7749540000 -0.4283740000
C 0.6370170000 4.2763990000 0.4134950000
C -1.5515180000 4.0730360000 1.6911930000
H 0.4936670000 5.3591980000 0.3265580000
H 1.2319210000 4.0898200000 1.3164940000
H 1.2174580000 3.9386470000 -0.4516590000
H -2.5350140000 3.5941390000 1.7289720000
H -1.0367680000 3.8701460000 2.6386020000
H -1.6991600000 5.1561780000 1.6150160000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426086 (Hartree/Particle)
Thermal correction to Energy= 0.453110
Thermal correction to Enthalpy= 0.454054
Thermal correction to Gibbs (Free) Energy= 0.366972
Sum of electronic and zero-point Energies= -1063.998273
Sum of electronic and thermal Energies= -1063.971249
Sum of electronic and thermal Enthalpies= -1063.970305
Sum of electronic and thermal (Free) Energies= -1064.057388

c/s TS

C -2.3572990000 0.1722670000 -0.2276440000
C -1.0477010000 -0.0474610000 -0.3683220000
C -3.3499930000 -0.3943200000 0.7847800000
H -2.7833180000 0.9822860000 -0.8206310000
C 0.0487830000 -0.8839910000 -0.3199520000
C -4.4985630000 -1.0841410000 0.0110530000
C -3.9310520000 0.8165750000 1.5573830000
C -2.7185030000 -1.3637300000 1.7943900000
C 1.2498570000 -0.1585190000 0.0502290000
C 0.1066020000 -2.3459130000 -0.7807410000
H -4.9669970000 -0.3964650000 -0.7029400000
H -4.1428930000 -1.9569390000 -0.5450580000
H -5.2731780000 -1.4184300000 0.7113170000
H -4.6976750000 0.4780260000 2.2640040000
H -3.1519870000 1.3345620000 2.1279780000
H -4.3976280000 1.5406930000 0.8789770000
H -1.8802230000 -0.8978020000 2.3233450000
H -3.4651960000 -1.6581770000 2.5402520000
H -2.3526850000 -2.2771130000 1.3194030000
C 1.0208510000 1.2407520000 0.0097260000
O 2.3357130000 -0.7429040000 0.4071790000
C 1.2004150000 -2.4784060000 -1.8727360000
C 0.4829500000 -3.2428890000 0.4266250000
C -1.2240610000 -2.8224060000 -1.3888750000
C -0.1221120000 1.6501980000 -0.7031280000
H 1.6360690000 1.9053420000 0.6024590000
B 3.6593880000 0.1175010000 0.5952940000
H 2.1841770000 -2.1872970000 -1.5010320000
H 1.2532830000 -3.5216490000 -2.2043250000
H 0.9592930000 -1.8619320000 -2.7469590000
H 1.4399030000 -2.9420160000 0.8574300000
H -0.2805900000 -3.2021710000 1.2105390000
H 0.5647480000 -4.2825300000 0.0882970000
H -1.5250360000 -2.2009830000 -2.2394330000
H -1.1056700000 -3.8499110000 -1.7495790000
H -2.0407760000 -2.8209160000 -0.6629250000
H -0.1731440000 1.3473380000 -1.7504560000
C -0.8163480000 2.9898150000 -0.4404750000
F 4.6366470000 -0.8062580000 0.8158630000
F 3.4179930000 0.9563610000 1.6747910000
F 3.8015180000 0.8320940000 -0.5820530000
H -1.5836710000 2.8156790000 0.3260490000
C -1.5142070000 3.4999730000 -1.7122600000
C 0.1422880000 4.0607880000 0.1160740000
H -2.0778440000 4.4162020000 -1.5076370000
H -0.7781640000 3.7278750000 -2.4932590000
H -2.2142550000 2.7624310000 -2.1232000000
H 0.5593760000 3.7774330000 1.0869450000
H 0.9750460000 4.2486850000 -0.5708360000
H -0.4004910000 5.0021730000 0.2532000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426246 (Hartree/Particle)
Thermal correction to Energy= 0.451765
Thermal correction to Enthalpy= 0.452709
Thermal correction to Gibbs (Free) Energy= 0.371734
Sum of electronic and zero-point Energies= -1063.960709
Sum of electronic and thermal Energies= -1063.935191
Sum of electronic and thermal Enthalpies= -1063.934246
Sum of electronic and thermal (Free) Energies= -1064.015222

c/s PT

C -2.3686560000 0.2131940000 -0.1538340000
C -1.0245810000 0.2340730000 -0.3492310000
C -3.3278400000 -0.6419810000 0.6608040000
H -2.8723120000 1.1134150000 -0.4998430000
C 0.0573360000 -0.7111220000 -0.1896520000
C -4.3202250000 -1.3647570000 -0.2842170000
C -4.1431870000 0.3692420000 1.5152060000
C -2.6570410000 -1.6234540000 1.6357990000
C 1.2376510000 0.0109600000 0.2241380000
C 0.1851170000 -2.1404360000 -0.6947040000
H -4.8259280000 -0.6504880000 -0.9444160000
H -3.8237910000 -2.1087190000 -0.9115160000
H -5.0893490000 -1.8745480000 0.3076290000
H -4.8819700000 -0.1678960000 2.1204210000
H -3.4938170000 0.9307950000 2.1964030000
H -4.6819580000 1.0871570000 0.8860380000
H -1.9479790000 -1.1025860000 2.2888250000
H -3.4197070000 -2.0852800000 2.2727070000
H -2.1237570000 -2.4305020000 1.1353950000
C 1.0213840000 1.3574860000 -0.0683730000
O 2.3061160000 -0.5643050000 0.6775150000
C 1.3012570000 -2.0921050000 -1.7947730000
C 0.6485760000 -3.0982160000 0.4357870000
C -1.0745640000 -2.6958140000 -1.3829640000
C -0.3212600000 1.6136630000 -0.6350400000
H 1.7943730000 2.1032280000 0.0546290000
B 3.7176410000 0.0806050000 0.4904050000
H 2.2392410000 -1.6682640000 -1.4349550000
H 1.4877200000 -3.1177750000 -2.1321170000
H 0.9617690000 -1.5111670000 -2.6601320000
H 1.5956700000 -2.7689910000 0.8641920000
H -0.0938060000 -3.1664630000 1.2372130000
H 0.7794570000 -4.1000520000 0.0110670000
H -1.4741310000 -1.9959830000 -2.1245910000
H -0.8079130000 -3.6193800000 -1.9075970000
H -1.8717960000 -2.9469190000 -0.6831150000
H -0.2163820000 1.6369620000 -1.7339790000
C -1.0169530000 2.9446130000 -0.2097460000
F 4.5623060000 -0.6895730000 1.2394740000
F 3.6462360000 1.4027120000 0.9314000000
F 3.9629830000 0.0180950000 -0.8764660000
H -1.6368430000 2.7282030000 0.6696310000
C -1.9211090000 3.4807180000 -1.3344420000
C -0.0150610000 4.0387160000 0.1993230000
H -2.4841590000 4.3570220000 -0.9954520000
H -1.3143100000 3.7890660000 -2.1955850000
H -2.6436760000 2.7414020000 -1.6971960000
H 0.5668970000 3.7588270000 1.0829000000
H 0.6868000000 4.2687780000 -0.6116190000
H -0.5542710000 4.9618010000 0.4387620000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.428822 (Hartree/Particle)
Thermal correction to Energy= 0.454150
Thermal correction to Enthalpy= 0.455094
Thermal correction to Gibbs (Free) Energy= 0.374822
Sum of electronic and zero-point Energies= -1063.969838
Sum of electronic and thermal Energies= -1063.944511
Sum of electronic and thermal Enthalpies= -1063.943567
Sum of electronic and thermal (Free) Energies= -1064.023839

cc/s RT

C -2.3168660000 -0.9457560000 -1.0778010000
C -1.1666450000 -0.9829290000 -0.4585970000
C -3.6636680000 -0.4091750000 -0.5977410000
H -2.3343750000 -1.3737580000 -2.0845450000
C 0.0356660000 -1.1603390000 0.0697040000
C -4.0942070000 0.7331760000 -1.5437350000
C -3.6048230000 0.0996520000 0.8502240000
C -4.6840200000 -1.5658610000 -0.6961070000
C 1.0907890000 -0.1781050000 -0.2826000000
C 0.4109920000 -2.4354250000 0.8761980000
H -3.3880310000 1.5693380000 -1.5007640000
H -5.0856510000 1.1082430000 -1.2627390000
H -4.1475210000 0.3897640000 -2.5835110000
H -2.9190750000 0.9470330000 0.9490130000
H -3.2766930000 -0.6878950000 1.5373650000
H -4.5967520000 0.4362550000 1.1723040000
H -4.7431730000 -1.9597550000 -1.7175730000
H -5.6837000000 -1.2153020000 -0.4131720000
H -4.4111120000 -2.3918310000 -0.0301370000
C 0.8615800000 1.2624730000 -0.3546720000
O 2.2311000000 -0.6511320000 -0.5329980000
C 1.2798070000 -2.0405690000 2.0916980000
C 1.1755960000 -3.4355530000 -0.0230590000
C -0.8691420000 -3.1182030000 1.3930870000
C -0.0416500000 1.9165830000 0.3979400000
H 1.5726190000 1.8086480000 -0.9658890000
B 3.6418450000 0.1923300000 -0.7696900000
H 1.5278410000 -2.9371410000 2.6712280000
H 2.2182800000 -1.5665350000 1.7937490000
H 0.7403260000 -1.3541760000 2.7558890000
H 2.1207930000 -3.0217980000 -0.3775550000
H 1.3885900000 -4.3486860000 0.5462170000
H 0.5706490000 -3.7156910000 -0.8933590000
H -1.4509700000 -2.4487110000 2.0376290000
H -1.5147390000 -3.4474910000 0.5727840000
H -0.5983320000 -4.0006440000 1.9831980000
H -0.6944930000 1.3517950000 1.0626300000
C -0.1663750000 3.4128570000 0.4567050000
F 4.5288260000 -0.8102350000 -0.9881050000
F 3.8005750000 0.8747000000 0.4061000000
F 3.4039670000 0.9985370000 -1.8572060000
C 0.2451690000 3.9150140000 1.8568770000
C -1.5974820000 3.8651240000 0.1077880000
H 0.5239870000 3.8438590000 -0.2794730000
H -0.4101370000 3.5006080000 2.6330960000
H 0.1710540000 5.0073300000 1.9033180000
H 1.2752430000 3.6299440000 2.0926490000
H -2.3271890000 3.4570950000 0.8181170000
H -1.8849920000 3.5443240000 -0.8992540000
H -1.6691030000 4.9577890000 0.1486590000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426226 (Hartree/Particle)
Thermal correction to Energy= 0.453183
Thermal correction to Enthalpy= 0.454128
Thermal correction to Gibbs (Free) Energy= 0.367482
Sum of electronic and zero-point Energies= -1063.995606
Sum of electronic and thermal Energies= -1063.968649
Sum of electronic and thermal Enthalpies= -1063.967704
Sum of electronic and thermal (Free) Energies= -1064.054350

cc/s TS

C -2.1570290000 -0.7381500000 -0.5361420000
C -0.8957040000 -0.3782350000 -0.2349970000
C -3.5164670000 -0.4951240000 0.0998350000
H -2.2285520000 -1.4281290000 -1.3807770000
C 0.3543570000 -0.9700470000 -0.1721250000
C -4.5401450000 -0.0731230000 -0.9803050000
C -3.5153590000 0.4910860000 1.2749130000
C -3.9632310000 -1.8837240000 0.6431320000
C 1.4401430000 -0.0155810000 -0.1410620000
C 0.6471970000 -2.4751580000 -0.0295100000
H -4.2914770000 0.8893540000 -1.4339040000
H -5.5392760000 0.0081240000 -0.5375220000
H -4.5904620000 -0.8176100000 -1.7835390000
H -3.3001520000 1.5117750000 0.9575510000
H -2.7820830000 0.2035860000 2.0371960000
H -4.5017760000 0.4973640000 1.7516860000
H -3.9508990000 -2.6507130000 -0.1387450000
H -4.9880580000 -1.8085590000 1.0252440000
H -3.3184580000 -2.2182440000 1.4615250000
C 0.9500570000 1.3078100000 -0.0926000000
O 2.6778930000 -0.3508170000 -0.2132160000
C 1.4722280000 -2.7220810000 1.2584890000
C 1.4676850000 -2.9111690000 -1.2747060000
C -0.6114160000 -3.3559100000 0.0415730000
C -0.3934770000 1.5149330000 0.2660230000
H 1.5725040000 2.1076540000 -0.4777960000
B 3.8073580000 0.7357160000 0.0533910000
H 1.7060230000 -3.7900440000 1.3390440000
H 2.4109200000 -2.1667180000 1.2551640000
H 0.8985010000 -2.4374570000 2.1487050000
H 2.4030930000 -2.3564240000 -1.3557420000
H 1.7026600000 -3.9786370000 -1.1897430000
H 0.8901940000 -2.7660570000 -2.1954120000
H -1.2531650000 -3.0896300000 0.8866460000
H -1.2067410000 -3.3122310000 -0.8756640000
H -0.3027190000 -4.3983840000 0.1760900000
H -0.7110690000 1.2004100000 1.2612360000
C -0.9935310000 2.8498980000 -0.2162500000
F 4.9641010000 0.0158600000 0.0945940000
F 3.4647210000 1.3367050000 1.2526690000
F 3.7335250000 1.6297790000 -1.0055470000
C -1.4770190000 3.7164580000 0.9594930000
C -2.0452450000 2.7476810000 -1.3337430000
H -0.1472340000 3.3809580000 -0.6706370000
H -2.3354030000 3.2739380000 1.4768590000
H -1.7822290000 4.7054290000 0.5995830000
H -0.6795110000 3.8606280000 1.6965440000
H -1.7051930000 2.0962860000 -2.1449700000
H -2.2281340000 3.7437590000 -1.7522230000
H -3.0006050000 2.3690460000 -0.9651870000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426563 (Hartree/Particle)
Thermal correction to Energy= 0.451940
Thermal correction to Enthalpy= 0.452885
Thermal correction to Gibbs (Free) Energy= 0.372481
Sum of electronic and zero-point Energies= -1063.945987
Sum of electronic and thermal Energies= -1063.920610
Sum of electronic and thermal Enthalpies= -1063.919666
Sum of electronic and thermal (Free) Energies= -1064.000069

cc/s PT

C -2.2659750000 0.6132050000 -0.2393880000
C -1.0229840000 0.0943820000 -0.0490160000
C -3.6037570000 0.0668150000 -0.7047070000
H -2.3327590000 1.6867220000 -0.1107970000
C 0.1652270000 0.9247430000 0.1221560000
C -4.6003150000 0.2013490000 0.4770600000
C -3.6266210000 -1.3729490000 -1.2426240000
C -4.0741050000 1.0102110000 -1.8450020000
C 1.3021980000 0.1814320000 -0.3605530000
C 0.3369770000 2.3169510000 0.7032650000
H -4.3387310000 -0.4692930000 1.3017930000
H -5.6119430000 -0.0534030000 0.1399510000
H -4.6244120000 1.2253880000 0.8668860000
H -3.3547580000 -2.1096700000 -0.4852330000
H -2.9596780000 -1.4909570000 -2.1034650000
H -4.6410330000 -1.6128630000 -1.5810110000
H -4.1366390000 2.0514350000 -1.5082330000
H -5.0694080000 0.7091270000 -2.1907530000
H -3.3911320000 0.9698030000 -2.7008030000
C 0.8629760000 -1.0986100000 -0.6943770000
O 2.5170920000 0.6432390000 -0.4427590000
C 0.9438710000 3.2441910000 -0.3874840000
C 1.3520150000 2.1756410000 1.8816640000
C -0.9257720000 2.9926560000 1.2760630000
C -0.5239950000 -1.3392060000 -0.2436930000
H 1.5074490000 -1.8430510000 -1.1407890000
B 3.6680050000 -0.3962000000 -0.6077380000
H 1.1229890000 4.2326060000 0.0508570000
H 1.8884270000 2.8509230000 -0.7653390000
H 0.2476890000 3.3665120000 -1.2253300000
H 2.2895320000 1.7237300000 1.5583090000
H 1.5628940000 3.1759110000 2.2761960000
H 0.9242640000 1.5755380000 2.6929850000

H -1.5991960000 3.3663430000 0.4977650000
H -1.4880860000 2.3338490000 1.9460310000
H -0.6120470000 3.8650970000 1.8588860000
H -1.1007490000 -1.9299580000 -0.9598890000
C -0.4557220000 -2.1350690000 1.1346540000
F 4.8246820000 0.3162980000 -0.4721200000
F 3.5136160000 -0.9880960000 -1.8579130000
F 3.4765660000 -1.3445250000 0.4054100000
C 0.5042840000 -3.3332680000 1.0476590000
C -1.8289660000 -2.5751800000 1.6489870000
H -0.0329700000 -1.4179050000 1.8511250000
H 0.2217480000 -4.0132230000 0.2332940000
H 0.4679640000 -3.9063280000 1.9808330000
H 1.5388340000 -3.0130300000 0.8905220000
H -2.2799510000 -3.3332280000 0.9973920000
H -2.5246730000 -1.7357480000 1.7410900000
H -1.7201740000 -3.0260880000 2.6421030000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.430158 (Hartree/Particle)
Thermal correction to Energy= 0.455002
Thermal correction to Enthalpy= 0.455946
Thermal correction to Gibbs (Free) Energy= 0.377096
Sum of electronic and zero-point Energies= -1063.984809
Sum of electronic and thermal Energies= -1063.959964
Sum of electronic and thermal Enthalpies= -1063.959020
Sum of electronic and thermal (Free) Energies= -1064.037870

c/d RT

C 2.5989920000 0.7439470000 0.3356220000
C 1.5565110000 -0.0284740000 0.4773780000
C 3.5766620000 0.7644500000 -0.8406730000
H 2.8105010000 1.4685730000 1.1261220000
C 0.5215410000 -0.8493770000 0.5831530000
C 4.9903000000 0.4749290000 -0.2903810000
C 3.5436860000 2.1802210000 -1.4575780000
C 3.2057050000 -0.2767550000 -1.9078270000
C -0.7468350000 -0.4216480000 -0.0567470000
C 0.6290670000 -2.2483070000 1.2472940000
H 5.2752270000 1.2004180000 0.4810120000
H 5.0457390000 -0.5265800000 0.1504060000
H 5.7314480000 0.5337330000 -1.0963820000
H 4.2692680000 2.2555110000 -2.2761890000
H 2.5513480000 2.4118150000 -1.8596540000
H 3.7966020000 2.9458490000 -0.7141750000
H 2.2041410000 -0.0959960000 -2.3127880000
H 3.9179890000 -0.2340060000 -2.7393360000
H 3.2264440000 -1.2932760000 -1.4995770000
C -1.1698190000 0.9760660000 -0.1127010000
O -1.4593360000 -1.3254290000 -0.5698660000
C -0.5737280000 -2.4636630000 2.1940030000
C 0.6605370000 -3.3573030000 0.1694080000
C 1.9236250000 -2.3287170000 2.0778690000
C -0.8306930000 1.8919420000 0.8135380000
H -1.8698390000 1.2079930000 -0.9064090000
B -2.9799320000 -1.1490210000 -1.2082650000
H -1.5272890000 -2.4431180000 1.6608720000
H -0.4846710000 -3.4408260000 2.6823520000
H -0.5987070000 -1.6994890000 2.9804330000
H -0.2575900000 -3.3765430000 -0.4196870000
H 1.5073490000 -3.2140340000 -0.5120750000
H 0.7815310000 -4.3336120000 0.6545040000
H 1.9551300000 -1.5548200000 2.8535310000
H 1.9788740000 -3.3046390000 2.5724850000
H 2.8163410000 -2.2173490000 1.4537640000
H -0.1859330000 1.5909020000 1.6379670000
C -1.3096840000 3.3166800000 0.8705530000
F -3.2703850000 -2.4185750000 -1.5875650000
F -2.8295720000 -0.2574370000 -2.2445220000
F -3.7162990000 -0.6633690000 -0.1616760000
H -0.3982090000 3.9384400000 0.8817730000
C -2.0344990000 3.5635680000 2.2129740000
C -2.1713630000 3.7470220000 -0.3214530000
H -2.2985240000 4.6219150000 2.3122270000
H -2.9567410000 2.9746850000 2.2676400000
H -1.4060780000 3.2900420000 3.0683640000
H -1.6453330000 3.6094060000 -1.2722230000
H -3.1044870000 3.1739780000 -0.3644330000
H -2.4338930000 4.8065060000 -0.2329990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426286 (Hartree/Particle)
Thermal correction to Energy= 0.453169
Thermal correction to Enthalpy= 0.454113
Thermal correction to Gibbs (Free) Energy= 0.367526
Sum of electronic and zero-point Energies= -1063.997338
Sum of electronic and thermal Energies= -1063.970455
Sum of electronic and thermal Enthalpies= -1063.969511
Sum of electronic and thermal (Free) Energies= -1064.056097

c/d TS

C 2.3674650000 0.2489160000 0.3793540000
C 1.0654420000 -0.0378880000 0.4461670000
C 3.4349410000 -0.2182600000 -0.6075600000
H 2.7292280000 1.0296250000 1.0506270000
C -0.0002140000 -0.9006740000 0.3165050000
C 4.5466150000 -0.9444090000 0.1880850000
C 4.0439850000 1.0519850000 -1.2512090000
C 2.8869740000 -1.1217660000 -1.7220010000
C -1.2212240000 -0.1947680000 -0.0363890000
C -0.0191100000 -2.3924180000 0.6768520000
H 4.9552300000 -0.3020920000 0.9770980000
H 4.1758520000 -1.8605510000 0.6572350000
H 5.3700340000 -1.2140930000 -0.4837780000
H 4.8694930000 0.7753720000 -1.9172170000
H 3.2995770000 1.5943220000 -1.8440810000
H 4.4409930000 1.7367990000 -0.4924730000
H 2.0781400000 -0.6285150000 -2.2717220000
H 3.6854340000 -1.3552660000 -2.4350500000
H 2.5036630000 -2.0696740000 -1.3367000000
C -1.0510070000 1.2041160000 0.1113560000
O -2.2695550000 -0.7950710000 -0.4693380000
C -1.1378630000 -2.6383290000 1.7224400000
C -0.3253040000 -3.2155320000 -0.6008690000
C 1.3099950000 -2.8644190000 1.2913960000
C 0.0563350000 1.6082650000 0.8774050000
H -1.6673300000 1.8873780000 -0.4609830000
B -3.6244130000 0.0214770000 -0.6354580000
H -2.1207590000 -2.3562160000 1.3417750000
H -1.1621570000 -3.7033350000 1.9798500000
H -0.9442840000 -2.0764040000 2.6439770000
H -1.2807210000 -2.9214700000 -1.0395630000
H 0.4583420000 -3.0903950000 -1.3557110000
H -0.3749100000 -4.2788870000 -0.3384060000
H 1.5683810000 -2.2894440000 2.1874230000
H 1.2164230000 -3.9160600000 1.5832670000
H 2.1440180000 -2.7917280000 0.5892230000
H 0.1140360000 1.2429060000 1.9041380000
C 0.6572550000 2.9973050000 0.7305890000
F -4.5527390000 -0.9235480000 -0.9552600000
F -3.3890340000 0.9483420000 -1.6415790000
F -3.8318150000 0.6380970000 0.5863830000
H 1.6845860000 2.9488730000 1.1174240000
C -0.1160630000 3.9794090000 1.6383110000
C 0.7104360000 3.4952970000 -0.7196260000
H 0.3475250000 4.9713410000 1.6005230000
H -1.1575070000 4.0790340000 1.3133300000
H -0.1198030000 3.6476100000 2.6827140000
H 1.2230600000 2.7790180000 -1.3706790000
H -0.2937340000 3.6589980000 -1.1257280000
H 1.2460400000 4.4490410000 -0.7752490000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426221 (Hartree/Particle)
Thermal correction to Energy= 0.451740
Thermal correction to Enthalpy= 0.452684
Thermal correction to Gibbs (Free) Energy= 0.372055
Sum of electronic and zero-point Energies= -1063.963812
Sum of electronic and thermal Energies= -1063.938293
Sum of electronic and thermal Enthalpies= -1063.937349
Sum of electronic and thermal (Free) Energies= -1064.017978

c/d PT

C -2.3039640000 0.5551400000 -0.3689120000
C -0.9821760000 0.2838630000 -0.5657370000
C -3.4336710000 0.0486190000 0.5162510000
H -2.6007950000 1.4973700000 -0.8307150000

C -0.0806830000 -0.8257830000 -0.3496780000
C -4.5513350000 -0.5743110000 -0.3587480000
C -4.0229980000 1.3252950000 1.1823250000
C -3.0091370000 -0.8950620000 1.6547580000
C 1.2551980000 -0.3004420000 -0.1874260000
C -0.2843630000 -2.3247800000 -0.5204070000
H -4.8842080000 0.1296490000 -1.1302630000
H -4.2255920000 -1.4897060000 -0.8580090000
H -5.4171490000 -0.8163130000 0.2685470000
H -4.8710390000 1.0518890000 1.8197950000
H -3.2786970000 1.8293470000 1.8087230000
H -4.3818070000 2.0415800000 0.4342550000
H -2.1881020000 -0.4610370000 2.2360770000
H -3.8547530000 -1.0479420000 2.3345230000
H -2.6946950000 -1.8787880000 1.3094670000
C 1.2607100000 0.9843490000 -0.7272310000
O 2.2565410000 -0.9685490000 0.2912930000
C 0.7850390000 -2.8245690000 -1.5421800000
C -0.0308600000 -3.0459280000 0.8327810000
C -1.6523290000 -2.7115990000 -1.1088060000
C -0.0907590000 1.4668120000 -1.0600330000
H 2.1693550000 1.5561440000 -0.8595910000
B 3.5792530000 -0.1767480000 0.5933270000
H 1.8013150000 -2.6319970000 -1.1994390000
H 0.6591210000 -3.9050510000 -1.6706930000
H 0.6424600000 -2.3502200000 -2.5198370000
H 0.9709780000 -2.8242020000 1.2058170000
H -0.7592970000 -2.7540390000 1.5943800000
H -0.1166460000 -4.1275030000 0.6766330000
H -1.8543570000 -2.1687880000 -2.0388900000
H -1.6468760000 -3.7814200000 -1.3429600000
H -2.4815430000 -2.5374370000 -0.4262220000
H -0.2302790000 1.4920200000 -2.1545180000
C -0.3450790000 2.9073050000 -0.5192860000
F 4.3976560000 -1.0740140000 1.2150450000
F 3.2041880000 0.8974170000 1.3984550000
F 4.0620730000 0.2725620000 -0.6322180000
H -1.4010950000 3.1498430000 -0.6951590000
C 0.4828740000 3.9321160000 -1.3125550000
C -0.0616520000 3.0101820000 0.9878750000
H 0.2384570000 4.9485860000 -0.9855670000
H 1.5590630000 3.7921760000 -1.1608800000
H 0.2818910000 3.8693400000 -2.3888680000
H -0.6912810000 2.3228480000 1.5641440000
H 0.9834070000 2.7690200000 1.2157250000
H -0.2605570000 4.0258380000 1.3470730000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.428706 (Hartree/Particle)
Thermal correction to Energy= 0.454164
Thermal correction to Enthalpy= 0.455108
Thermal correction to Gibbs (Free) Energy= 0.374491
Sum of electronic and zero-point Energies= -1063.974293
Sum of electronic and thermal Energies= -1063.948836
Sum of electronic and thermal Enthalpies= -1063.947891
Sum of electronic and thermal (Free) Energies= -1064.028509

cc/d RT

C -2.3758350000 -0.6871840000 -1.0864990000
C -1.2394840000 -0.8739590000 -0.4691130000
C -3.6973280000 -0.1433070000 -0.5477600000
H -2.4008510000 -0.9711820000 -2.1427840000
C -0.0584330000 -1.1926600000 0.0414870000
C -4.0367580000 1.1519980000 -1.3173660000
C -3.6373920000 0.1386750000 0.9608810000
C -4.7845320000 -1.2047850000 -0.8300340000
C 1.0557360000 -0.2362450000 -0.1677350000
C 0.2260910000 -2.5882150000 0.6651770000
H -3.2818270000 1.9257530000 -1.1417990000
H -5.0092060000 1.5434530000 -0.9952840000
H -4.0889960000 0.9705020000 -2.3972950000
H -2.8950040000 0.9080490000 1.1954580000
H -3.3827090000 -0.7645660000 1.5258800000
H -4.6102640000 0.4960100000 1.3169410000
H -4.8476880000 -1.4362490000 -1.8998410000
H -5.7661450000 -0.8376900000 -0.5076320000
H -4.5763010000 -2.1370770000 -0.2936550000
C 0.9096580000 1.2147640000 -0.0782190000
O 2.1779790000 -0.7377690000 -0.4456190000
C 1.0959380000 -2.4230540000 1.9315680000
C 0.9443660000 -3.4979430000 -0.3594800000
C -1.1011760000 -3.2565330000 1.0702130000
C 0.0459030000 1.8276390000 0.7514590000
H 1.6589450000 1.7762930000 -0.6226360000
B 3.6204780000 0.0687330000 -0.6048010000
H 1.2707090000 -3.4050140000 2.3859340000
H 2.0701220000 -1.9811950000 1.7090380000
H 0.5922860000 -1.7963330000 2.6777710000
H 1.9178010000 -3.0966850000 -0.6453870000
H 1.0944580000 -4.4926730000 0.0778120000
H 0.3376960000 -3.6170870000 -1.2648120000
H -1.6523890000 -2.6496160000 1.7981970000
H -1.7516210000 -3.4271220000 0.2065770000
H -0.8934380000 -4.2280360000 1.5320220000
H -0.6452500000 1.2193370000 1.3328870000
C -0.0182710000 3.3096620000 1.0135740000
F 4.4787260000 -0.9495860000 -0.8612360000
F 3.7837770000 0.6862090000 0.6063200000
F 3.4259070000 0.9391350000 -1.6507660000
C -1.4454920000 3.8393190000 0.7527350000
C 1.0323570000 4.1324840000 0.2592890000
H 0.1683770000 3.4247720000 2.0942850000
H -1.6989650000 3.7657550000 -0.3111910000
H -1.5170330000 4.8926070000 1.0446460000
H -2.1974940000 3.2813910000 1.3220350000
H 0.8832680000 4.0710460000 -0.8252300000
H 2.0484020000 3.7912280000 0.4818480000
H 0.9591300000 5.1870380000 0.5452390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426358 (Hartree/Particle)
Thermal correction to Energy= 0.453200
Thermal correction to Enthalpy= 0.454144
Thermal correction to Gibbs (Free) Energy= 0.368041
Sum of electronic and zero-point Energies= -1063.994492
Sum of electronic and thermal Energies= -1063.967651
Sum of electronic and thermal Enthalpies= -1063.966707
Sum of electronic and thermal (Free) Energies= -1064.052809

cc/d TS

C 2.1445010000 0.6826300000 -0.5602110000
C 0.8881530000 0.3693170000 -0.1953550000
C 3.5037850000 0.4811290000 0.0924180000
H 2.2095830000 1.2611610000 -1.4855910000
C -0.3606230000 0.9537200000 -0.1488240000
C 4.3858490000 -0.4737120000 -0.7450790000
C 3.4136920000 0.0256280000 1.5587780000
C 4.1804380000 1.8797600000 0.0669310000
C -1.4423820000 -0.0074480000 -0.0680230000
C -0.6484390000 2.4633850000 -0.0861590000
H 3.9931170000 -1.4926910000 -0.7578650000
H 5.3994780000 -0.5071830000 -0.3289220000
H 4.4618570000 -0.1300640000 -1.7832930000
H 2.9834120000 -0.9703860000 1.6662080000
H 2.8079570000 0.7244460000 2.1467830000
H 4.4156200000 -0.0023170000 2.0017440000
H 4.2787220000 2.2605720000 -0.9561900000
H 5.1860900000 1.8070070000 0.4965360000
H 3.6140470000 2.6121090000 0.6506300000
C -0.9413040000 -1.3215870000 0.0428090000
O -2.6794110000 0.3200810000 -0.1688860000
C -1.4953190000 2.7777260000 1.1723790000
C -1.4430930000 2.8431770000 -1.3651110000
C 0.6207550000 3.3310230000 -0.0299040000
C 0.4032120000 -1.4947280000 0.4209280000
H -1.5463520000 -2.1452830000 -0.3204640000
B -3.8093110000 -0.7638600000 0.1142600000
H -1.7176650000 3.8507890000 1.1996120000
H -2.4401310000 2.2327790000 1.1751490000
H -0.9430010000 2.5275520000 2.0861540000
H -2.3783840000 2.2860020000 -1.4362250000
H -1.6778190000 3.9136690000 -1.3356430000
H -0.8500000000 2.6532010000 -2.2675440000
H 1.2391560000 3.0942620000 0.8424000000
H 1.2369180000 3.2320070000 -0.9286630000
H 0.3259140000 4.3832440000 0.0480150000
H 0.7066110000 -1.1360190000 1.4045930000
C 1.0316600000 -2.8222630000 -0.0340020000

F -4.9704880000 -0.0503910000 0.1002800000
F -3.4910900000 -1.3158230000 1.3426610000
F -3.7043280000 -1.6962490000 -0.9083900000
C 2.1948300000 -3.3445450000 0.8195810000
C 1.3481330000 -2.8473160000 -1.5409800000
H 0.2108080000 -3.5403160000 0.1134310000
H 3.1293560000 -2.8073520000 0.6388180000
H 2.3797720000 -4.3981360000 0.5827760000
H 1.9672380000 -3.2843140000 1.8903770000
H 0.4722760000 -2.5601410000 -2.1322570000
H 1.6445620000 -3.8562850000 -1.8479940000
H 2.1627610000 -2.1628640000 -1.7947880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426302 (Hartree/Particle)
Thermal correction to Energy= 0.451657
Thermal correction to Enthalpy= 0.452601
Thermal correction to Gibbs (Free) Energy= 0.372612
Sum of electronic and zero-point Energies= -1063.948413
Sum of electronic and thermal Energies= -1063.923059
Sum of electronic and thermal Enthalpies= -1063.922115
Sum of electronic and thermal (Free) Energies= -1064.002104

cc/d PT

C -2.2455660000 0.6135160000 -0.2063320000
C -1.0223090000 0.0209370000 -0.1197700000
C -3.6308310000 0.1772570000 -0.6471720000
H -2.2474830000 1.6738020000 0.0144250000
C 0.2019220000 0.8053420000 -0.0006330000
C -4.5466710000 0.1752940000 0.6053950000
C -3.7357580000 -1.1707300000 -1.3777980000
C -4.1347410000 1.2830770000 -1.6140030000
C 1.2769450000 0.0469390000 -0.5958230000
C 0.4755530000 2.1519150000 0.6434920000
H -4.2608530000 -0.6113860000 1.3102710000
H -5.5858320000 0.0004730000 0.3027300000
H -4.5076530000 1.1354440000 1.1323960000
H -3.4677320000 -2.0146930000 -0.7416850000
H -3.1049020000 -1.1912530000 -2.2732020000
H -4.7710180000 -1.3242090000 -1.7028380000
H -4.1400460000 2.2683350000 -1.1336810000
H -5.1588540000 1.0599180000 -1.9331310000
H -3.5067360000 1.3443340000 -2.5098520000
C 0.7924290000 -1.2246440000 -0.8808420000
O 2.4890440000 0.4972200000 -0.7659300000
C 1.0795480000 3.1136830000 -0.4185550000
C 1.5319430000 1.8805730000 1.7660970000
C -0.7140160000 2.8627310000 1.3204650000
C -0.6015840000 -1.4168400000 -0.4236680000
H 1.4230690000 -2.0128680000 -1.2745140000
B 3.6708040000 -0.4963310000 -0.5923340000
H 1.3129570000 4.0679730000 0.0672080000
H 1.9919560000 2.7064430000 -0.8540680000
H 0.3573640000 3.3104300000 -1.2197730000
H 2.3839110000 1.3004190000 1.4127330000
H 1.8938390000 2.8473830000 2.1336230000
H 1.0681480000 1.3504580000 2.6051040000
H -1.4044520000 3.3171360000 0.6016510000
H -1.2772930000 2.2014210000 1.9872040000
H -0.3175540000 3.6817630000 1.9298880000
H -1.2184380000 -1.8946860000 -1.1910320000
C -0.5624310000 -2.4075920000 0.8259540000
F 4.8060220000 0.2464330000 -0.7546230000
F 3.5354930000 -1.5083350000 -1.5427320000
F 3.5234270000 -1.0100870000 0.7030340000
C -1.9525050000 -2.8334380000 1.3100020000
C 0.2855220000 -1.8828060000 1.9932010000
H -0.0659860000 -3.3053560000 0.4333880000
H -2.5282130000 -1.9800520000 1.6854080000
H -1.8507090000 -3.5483030000 2.1343440000
H -2.5321410000 -3.3272890000 0.5232940000
H -0.1358560000 -0.9597750000 2.4115670000
H 1.3235570000 -1.6883390000 1.7090880000
H 0.2913850000 -2.6269960000 2.7973970000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.430102 (Hartree/Particle)
Thermal correction to Energy= 0.454982
Thermal correction to Enthalpy= 0.455926
Thermal correction to Gibbs (Free) Energy= 0.376771
Sum of electronic and zero-point Energies= -1063.984089
Sum of electronic and thermal Energies= -1063.959209
Sum of electronic and thermal Enthalpies= -1063.958265
Sum of electronic and thermal (Free) Energies= -1064.037421

c/u RT

C 2.6064180000 0.1879430000 0.3030070000
C 1.4405770000 -0.3787580000 0.4557040000
C 3.5170120000 0.1040160000 -0.9232270000
H 2.9891120000 0.8009470000 1.1229600000
C 0.2712160000 -0.9917570000 0.5678580000
C 4.8704350000 -0.4873220000 -0.4721140000
C 3.7323000000 1.5397890000 -1.4509290000
C 2.9050440000 -0.7701970000 -2.0285350000
C -0.9151590000 -0.2847270000 0.0253190000
C 0.1313890000 -2.4293190000 1.1366970000
H 5.3241360000 0.1147690000 0.3242470000
H 4.7498190000 -1.5093820000 -0.0963110000
H 5.5728580000 -0.5146460000 -1.3136900000
H 4.4226850000 1.5329060000 -2.3027640000
H 2.7870400000 1.9832830000 -1.7827240000
H 4.1603290000 2.1894720000 -0.6779500000
H 1.9406880000 -0.3743010000 -2.3647820000
H 3.5750680000 -0.8058920000 -2.8947780000
H 2.7463430000 -1.7980150000 -1.6838830000
C -1.0675710000 1.1673330000 0.0924560000
O -1.8045140000 -0.9956280000 -0.5142000000
C -1.0547090000 -2.4792140000 2.1265570000
C -0.0914770000 -3.4442920000 -0.0090340000
C 1.4160120000 -2.8125800000 1.8950320000
C -0.5259540000 1.9262600000 1.0631320000
H -1.7440010000 1.5877020000 -0.6418390000
B -3.2853740000 -0.4863260000 -1.0633020000
H -2.0053210000 -2.2397400000 1.6438660000
H -1.1381690000 -3.4878360000 2.5472060000
H -0.9029380000 -1.7824450000 2.9599430000
H -1.0166170000 -3.2458180000 -0.5523160000
H 0.7418050000 -3.4169960000 -0.7210110000
H -0.1445090000 -4.4578220000 0.4070180000
H 1.6242860000 -2.1158820000 2.7152860000
H 1.3007810000 -3.8140160000 2.3239770000
H 2.2898320000 -2.8280970000 1.2354630000
H 0.0899490000 1.4466970000 1.8225830000
C -0.7065760000 3.4098140000 1.2361500000
F -3.8273460000 -1.6452390000 -1.5136770000
F -3.0022000000 0.4373690000 -2.0418980000
F -3.8769890000 0.0483940000 0.0490270000
H -1.1608650000 3.5442230000 2.2317620000
C -1.6237690000 4.0654140000 0.1982150000
C 0.6789730000 4.0929330000 1.2840740000
H -1.7399640000 5.1317230000 0.4188980000
H -1.2075470000 3.9779180000 -0.8123200000
H -2.6197740000 3.6110390000 0.1948420000
H 1.3216930000 3.6506980000 2.0542440000
H 1.1915870000 4.0003750000 0.3197180000
H 0.5685230000 5.1590690000 1.5092250000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426273 (Hartree/Particle)
Thermal correction to Energy= 0.453165
Thermal correction to Enthalpy= 0.454109
Thermal correction to Gibbs (Free) Energy= 0.367488
Sum of electronic and zero-point Energies= -1063.997209
Sum of electronic and thermal Energies= -1063.970317
Sum of electronic and thermal Enthalpies= -1063.969373
Sum of electronic and thermal (Free) Energies= -1064.055994

c/u TS

C -2.3089980000 0.0321200000 -0.2930560000
C -0.9816930000 -0.0848220000 -0.4055340000
C -3.2711180000 -0.5827600000 0.7223190000
H -2.7945580000 0.7506420000 -0.9509910000
C 0.1699240000 -0.8353590000 -0.2983170000
C -4.3094910000 -1.4313940000 -0.0519690000
C -4.0196540000 0.5840980000 1.4137870000
C -2.5767310000 -1.4244860000 1.8028240000
C 1.3198560000 -0.0091660000 0.0273390000

C 0.3435280000 -2.3125640000 -0.6801740000
H -4.8281200000 -0.8310390000 -0.8087740000
H -3.8434180000 -2.2817890000 -0.5578830000
H -5.0643660000 -1.8192020000 0.6421570000
H -4.7951010000 0.1871740000 2.0791740000
H -3.3379050000 1.1914420000 2.0182210000
H -4.5094580000 1.2395480000 0.6838850000
H -1.8114530000 -0.8431140000 2.3281440000
H -3.3138100000 -1.7567390000 2.5423400000
H -2.0996500000 -2.3172810000 1.3925250000
C 1.0157690000 1.3597060000 -0.1512680000
O 2.4308880000 -0.4987520000 0.4459960000
C 1.4516530000 -2.4136990000 -1.7616760000
C 0.7812980000 -3.1145020000 0.5724920000
C -0.9388660000 -2.9263070000 -1.2675910000
C -0.1518070000 1.6467260000 -0.8865620000
H 1.5952870000 2.1197100000 0.3605650000
B 3.7081950000 0.4401770000 0.5554880000
H 2.4062040000 -2.0224480000 -1.4062830000
H 1.5922250000 -3.4657060000 -2.0347710000
H 1.1652830000 -1.8686460000 -2.6690830000
H 1.7112990000 -2.7212320000 0.9869810000
H 0.0140300000 -3.0904100000 1.3534750000
H 0.9409260000 -4.1613300000 0.2883520000
H -1.2910190000 -2.3687740000 -2.1424160000
H -0.7303760000 -3.9533250000 -1.5864250000
H -1.7533010000 -2.9681350000 -0.5409200000
H -0.2083440000 1.2637930000 -1.9066410000
C -0.7891390000 3.0290450000 -0.7407670000
F 4.7225540000 -0.4047770000 0.8947990000
F 3.4083230000 1.3835480000 1.5292140000
F 3.8411930000 1.0223910000 -0.6933770000
H 0.0352970000 3.7052320000 -1.0213780000
C -1.1861590000 3.3822330000 0.7010950000
C -1.9278770000 3.3016220000 -1.7361370000
H -1.4875940000 4.4333220000 0.7651460000
H -2.0287550000 2.7708310000 1.0388190000
H -0.3558980000 3.2304400000 1.3980940000
H -1.6516810000 3.0112140000 -2.7566160000
H -2.8481070000 2.7713600000 -1.4679470000
H -2.1673160000 4.3701840000 -1.7497090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426136 (Hartree/Particle)
Thermal correction to Energy= 0.451707
Thermal correction to Enthalpy= 0.452651
Thermal correction to Gibbs (Free) Energy= 0.371811
Sum of electronic and zero-point Energies= -1063.959804
Sum of electronic and thermal Energies= -1063.934232
Sum of electronic and thermal Enthalpies= -1063.933288
Sum of electronic and thermal (Free) Energies= -1064.014129

c/u PT

C -2.2681100000 0.2986760000 -0.3597710000
C -0.9258460000 0.1818880000 -0.5788870000
C -3.3000990000 -0.3033030000 0.5836600000
H -2.6940030000 1.1622000000 -0.8657200000
C 0.0940730000 -0.8183680000 -0.3504290000
C -4.3612300000 -1.0907340000 -0.2273060000
C -4.0244540000 0.9182280000 1.2208540000
C -2.7311710000 -1.1380810000 1.7437010000
C 1.3718220000 -0.1526340000 -0.2534580000
C 0.0519130000 -2.3369380000 -0.4688320000
H -4.8008500000 -0.4629670000 -1.0110970000
H -3.9443040000 -1.9799950000 -0.7048670000
H -5.1713780000 -1.4085820000 0.4392610000
H -4.8148870000 0.5676650000 1.8937260000
H -3.3327300000 1.5339670000 1.8060690000
H -4.4898990000 1.5542380000 0.4592000000
H -1.9522210000 -0.5832480000 2.2782660000
H -3.5316370000 -1.3613230000 2.4578220000
H -2.3097780000 -2.0911130000 1.4281960000
C 1.2272560000 1.0867190000 -0.8708240000
O 2.4499400000 -0.6857290000 0.2278060000
C 1.1372940000 -2.7470030000 -1.5139630000
C 0.4303060000 -2.9818490000 0.8936810000
C -1.2808020000 -2.8959470000 -0.9961500000
C -0.1784260000 1.4305130000 -1.1488390000
H 2.0656450000 1.7410690000 -1.0755190000
B 3.6581900000 0.2743560000 0.5213890000
H 2.1357000000 -2.4290920000 -1.2144820000
H 1.1323940000 -3.8385370000 -1.6048950000
H 0.9089700000 -2.3256820000 -2.4996070000
H 1.4142310000 -2.6412220000 1.2217670000
H -0.2980350000 -2.7461110000 1.6744610000
H 0.4573980000 -4.0708500000 0.7715740000
H -1.5823980000 -2.4007010000 -1.9257790000
H -1.1551560000 -3.9619560000 -1.2133680000
H -2.0979550000 -2.8098540000 -0.2830990000
H -0.3777880000 1.4176630000 -2.2337150000
C -0.4442730000 2.8875040000 -0.6372370000
F 4.5770560000 -0.4975740000 1.1702880000
F 3.1381130000 1.3068520000 1.3018300000
F 4.0954380000 0.7572910000 -0.7080800000
H 0.3589940000 3.4647550000 -1.1190640000
C -0.2434200000 3.0232650000 0.8808370000
C -1.7601040000 3.5297800000 -1.1049450000
H -0.3203850000 4.0743910000 1.1802210000
H -1.0077600000 2.4662610000 1.4355910000
H 0.7404520000 2.6560620000 1.1929080000
H -1.9620760000 3.3295860000 -2.1645720000
H -2.6218480000 3.1909380000 -0.5203730000
H -1.7030060000 4.6170740000 -0.9812060000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.428916 (Hartree/Particle)
Thermal correction to Energy= 0.454265
Thermal correction to Enthalpy= 0.455209
Thermal correction to Gibbs (Free) Energy= 0.375109
Sum of electronic and zero-point Energies= -1063.970204
Sum of electronic and thermal Energies= -1063.944854
Sum of electronic and thermal Enthalpies= -1063.943910
Sum of electronic and thermal (Free) Energies= -1064.024011

cc/u RT

C -2.4732420000 -0.5756120000 -1.0865470000
C -1.3480370000 -0.8358310000 -0.4765620000
C -3.7260790000 0.1210440000 -0.5577280000
H -2.5405800000 -0.8973920000 -2.1299760000
C -0.1828070000 -1.2117350000 0.0338630000
C -3.8976820000 1.4490550000 -1.3282800000
C -3.6488570000 0.3957180000 0.9518720000
C -4.9304800000 -0.8011900000 -0.8506490000
C 0.9816380000 -0.3305860000 -0.2244670000
C 0.0179740000 -2.5931490000 0.7154500000
H -3.0542720000 2.1237650000 -1.1441510000
H -4.8178290000 1.9564900000 -1.0143010000
H -3.9607020000 1.2774840000 -2.4091760000
H -2.8330800000 1.0837930000 1.1955900000
H -3.4959170000 -0.5291240000 1.5185040000
H -4.5818620000 0.8539090000 1.2989780000
H -5.0119640000 -1.0225290000 -1.9213790000
H -5.8636530000 -0.3196060000 -0.5354500000
H -4.8401370000 -1.7523210000 -0.3144060000
C 0.8834990000 1.1271580000 -0.2678660000
O 2.0863550000 -0.8987900000 -0.4360000000
C 0.8879320000 -2.4273560000 1.9816980000
C 0.6901960000 -3.5814780000 -0.2669600000
C -1.3474390000 -3.1695940000 1.1348130000
C 0.0293190000 1.8305530000 0.4968250000
H 1.6377390000 1.6166820000 -0.8724960000
B 3.5573100000 -0.1583060000 -0.6426850000
H 1.0000340000 -3.3981830000 2.4779140000
H 1.8880520000 -2.0544520000 1.7490180000
H 0.4180720000 -1.7407340000 2.6965300000
H 1.6850680000 -3.2451470000 -0.5627440000
H 0.7849340000 -4.5638990000 0.2115830000
H 0.0815690000 -3.7053060000 -1.1703630000
H -1.8678020000 -2.5050770000 1.8346560000
H -2.0017150000 -3.3361540000 0.2731990000
H -1.1977600000 -4.1327710000 1.6348730000
H -0.6498960000 1.2882860000 1.1521890000
C -0.0393830000 3.3299300000 0.6041790000
F 4.3833420000 -1.2229200000 -0.7974670000
F 3.7286030000 0.5574390000 0.5114260000
F 3.4042310000 0.6226360000 -1.7639720000
C 0.8775550000 4.0782860000 -0.3693500000
C 0.2219480000 3.7528220000 2.0674920000

H -1.0838180000 3.6028390000 0.3755330000
H 1.9326100000 3.8635300000 -0.1651610000
H 0.7313020000 5.1589490000 -0.2690410000
H 0.6715370000 3.8061500000 -1.4101240000
H 1.2493900000 3.5108350000 2.3608620000
H -0.4575390000 3.2464580000 2.7627080000
H 0.0789170000 4.8327730000 2.1814650000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426257 (Hartree/Particle)
Thermal correction to Energy= 0.453147
Thermal correction to Enthalpy= 0.454091
Thermal correction to Gibbs (Free) Energy= 0.367539
Sum of electronic and zero-point Energies= -1063.995391
Sum of electronic and thermal Energies= -1063.968501
Sum of electronic and thermal Enthalpies= -1063.967556
Sum of electronic and thermal (Free) Energies= -1064.054109

cc/u TS

C -2.2515450000 -0.6431790000 -0.5721710000
C -0.9857410000 -0.4490180000 -0.1791320000
C -3.5985490000 -0.2569810000 0.0219780000
H -2.3511460000 -1.2299040000 -1.4896660000
C 0.2419960000 -1.0668060000 -0.1091380000
C -4.3065760000 0.7791470000 -0.8828160000
C -3.5146840000 0.2415240000 1.4759640000
C -4.4440530000 -1.5585110000 0.0108690000
C 1.3512520000 -0.1324000000 -0.0828660000
C 0.4700990000 -2.5815060000 0.0136880000
H -3.7645130000 1.7279660000 -0.9225460000
H -5.3159830000 0.9801690000 -0.5050110000
H -4.4016000000 0.4048050000 -1.9085630000
H -3.0117820000 1.2068380000 1.5659570000
H -2.9862830000 -0.4803800000 2.1087960000
H -4.5245890000 0.3652380000 1.8826770000
H -4.5451340000 -1.9628440000 -1.0029230000
H -5.4506450000 -1.3498720000 0.3910620000
H -3.9953570000 -2.3323820000 0.6426500000
C 0.8862550000 1.2038390000 -0.0060830000
O 2.5740980000 -0.4973670000 -0.2069520000
C 1.3280820000 -2.8778330000 1.2680710000
C 1.2220470000 -3.0499810000 -1.2608440000
C -0.8410650000 -3.3792410000 0.1294600000
C -0.4242910000 1.4059720000 0.4424290000
H 1.4881580000 1.9930800000 -0.4423100000
B 3.7382120000 0.5704340000 -0.0001100000
H 1.5067890000 -3.9570260000 1.3389450000
H 2.2947360000 -2.3733720000 1.2280180000
H 0.8068560000 -2.5647280000 2.1806940000
H 2.1787700000 -2.5369150000 -1.3719290000
H 1.4115840000 -4.1274890000 -1.1898550000
H 0.6210080000 -2.8721010000 -2.1604190000
H -1.4301340000 -3.0727140000 1.0007550000
H -1.4689140000 -3.2805660000 -0.7614860000
H -0.6012470000 -4.4418220000 0.2457870000
H -0.6864230000 1.0166680000 1.4261960000
C -1.1485140000 2.6940940000 0.0751640000
F 4.8811310000 -0.1708430000 -0.0136110000
F 3.4649230000 1.1813610000 1.2109720000
F 3.6250850000 1.4599270000 -1.0590520000
C -1.0175920000 3.0649870000 -1.4092240000
C -0.6448720000 3.8318040000 0.9918660000
H -2.2113860000 2.5555230000 0.2962070000
H 0.0183870000 3.2957510000 -1.6797880000
H -1.6196640000 3.9526150000 -1.6325730000
H -1.3600160000 2.2492270000 -2.0551630000
H 0.4180260000 4.0350050000 0.8220880000
H -0.7735480000 3.5841640000 2.0515240000
H -1.2035390000 4.7523580000 0.7889740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426136 (Hartree/Particle)
Thermal correction to Energy= 0.451631
Thermal correction to Enthalpy= 0.452575
Thermal correction to Gibbs (Free) Energy= 0.371954
Sum of electronic and zero-point Energies= -1063.957813
Sum of electronic and thermal Energies= -1063.932318
Sum of electronic and thermal Enthalpies= -1063.931374
Sum of electronic and thermal (Free) Energies= -1064.011995

cc/u PT

C -2.3263420000 0.6286870000 -0.1891100000
C -1.0466780000 0.1613820000 -0.1972840000
C -3.6859880000 -0.0205750000 -0.3804900000
H -2.4345270000 1.6904720000 -0.0164490000
C 0.1484000000 0.9835990000 -0.0802360000
C -4.3074070000 -0.2012040000 1.0316240000
C -3.7181960000 -1.3605890000 -1.1388540000
C -4.5533860000 0.9928820000 -1.1707380000
C 1.2890260000 0.1742210000 -0.4378440000
C 0.3501060000 2.4303850000 0.3449980000
H -3.7410660000 -0.9225010000 1.6295670000
H -5.3368590000 -0.5669930000 0.9380360000
H -4.3360360000 0.7465090000 1.5810110000
H -3.2259460000 -2.1701550000 -0.5960110000
H -3.2570530000 -1.2712630000 -2.1285220000
H -4.7611980000 -1.6615170000 -1.2886170000
H -4.6144170000 1.9584530000 -0.6553600000
H -5.5729460000 0.6082960000 -1.2836070000
H -4.1458170000 1.1677580000 -2.1730030000
C 0.8342370000 -1.1046940000 -0.7507970000
O 2.5240980000 0.5865380000 -0.4436340000
C 1.0605360000 3.1840920000 -0.8169580000
C 1.2832660000 2.4083310000 1.5956800000
C -0.9016670000 3.2411490000 0.7324080000
C -0.5995320000 -1.2736630000 -0.4600640000
H 1.4938180000 -1.8873700000 -1.1016710000
B 3.6433010000 -0.4966930000 -0.3659570000
H 1.2655230000 4.2112730000 -0.4947100000
H 2.0032470000 2.7083130000 -1.0878850000
H 0.4150290000 3.2298870000 -1.7018280000
H 2.2214930000 1.8925200000 1.3934980000
H 1.5059850000 3.4433890000 1.8786450000
H 0.7840200000 1.9257900000 2.4436900000
H -1.5586080000 3.4410040000 -0.1209830000
H -1.4813480000 2.7681940000 1.5322230000
H -0.5701760000 4.2152820000 1.1073650000
H -1.1259570000 -1.7109690000 -1.3165700000
C -0.8110890000 -2.2590890000 0.7624370000
F 4.8049410000 0.1947150000 -0.1738800000
F 3.6092350000 -1.2182720000 -1.5561760000
F 3.3004900000 -1.3211200000 0.7130000000
C -0.0236760000 -1.8357410000 2.0098660000
C -0.4684950000 -3.6974850000 0.3493520000
H -1.8798320000 -2.2232410000 1.0051650000
H 1.0574950000 -1.8614480000 1.8357810000
H -0.2544880000 -2.5141410000 2.8389150000
H -0.2871580000 -0.8218780000 2.3330080000
H 0.5997770000 -3.8096850000 0.1333630000
H -1.0307390000 -4.0118410000 -0.5384530000
H -0.7121880000 -4.3910040000 1.1618300000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.430083 (Hartree/Particle)
Thermal correction to Energy= 0.455015
Thermal correction to Enthalpy= 0.455959
Thermal correction to Gibbs (Free) Energy= 0.376539
Sum of electronic and zero-point Energies= -1063.991638
Sum of electronic and thermal Energies= -1063.966706
Sum of electronic and thermal Enthalpies= -1063.965762
Sum of electronic and thermal (Free) Energies= -1064.045182

4d

cRT

C 1.2183920000 2.4771640000 0.1250470000
C 1.3010780000 1.2031360000 0.4001640000
C 1.4226970000 -0.0922430000 0.6404500000
C 0.4915440000 -1.0094240000 -0.0685680000
C -0.9214460000 -0.7245420000 -0.2382060000
C -1.6100700000 0.1450640000 0.5407960000
H -1.4134800000 -1.3261000000 -0.9928870000
H -1.0730250000 0.6672960000 1.3288330000
C -3.0332320000 0.4478140000 0.4592080000
C 2.5371620000 -0.6870600000 1.5426590000
O 0.9967510000 -2.0719310000 -0.5277610000
C -3.8922270000 -0.1385820000 -0.4933000000

C -3.5759130000 1.3723040000 1.3728500000
B 0.2054950000 -3.4047820000 -1.0826460000
F 1.2306080000 -4.1963480000 -1.4890940000
F -0.6132440000 -2.9673160000 -2.1015350000
F -0.4740770000 -3.8428500000 0.0234700000
C 1.8909720000 3.2135160000 -1.0343490000
C 3.6614280000 -1.3061220000 0.6794130000
H 4.4596370000 -1.6783940000 1.3333320000
H 3.2966270000 -2.1360260000 0.0723790000
H 4.0974460000 -0.5542210000 0.0111790000
C 1.9245120000 -1.7649050000 2.4665620000
H 1.4729190000 -2.5866310000 1.9042680000
H 2.7075930000 -2.1879400000 3.1061690000
H 1.1577690000 -1.3327350000 3.1212410000
C 3.1401210000 0.4266610000 2.4185650000
H 3.6170850000 1.2057710000 1.8148730000
H 2.3782240000 0.9041100000 3.0455860000
H 3.9021280000 -0.0006490000 3.0797040000
C 0.7803430000 3.8583030000 -1.8928240000
C 2.7327670000 2.2637970000 -1.9002620000
C 2.7896710000 4.3197740000 -0.4395560000
H 2.2131420000 5.0064620000 0.1919180000
H 3.2501410000 4.9085610000 -1.2419130000
H 3.5918890000 3.8914370000 0.1715570000
H 2.1192030000 1.4659040000 -2.3322870000
H 3.5335870000 1.7951460000 -1.3176180000
H 3.1961750000 2.8167750000 -2.7249940000
H 0.1275420000 3.0953360000 -2.3306580000
H 1.2210680000 4.4406280000 -2.7107920000
H 0.1573560000 4.5359360000 -1.2966010000
H 0.6014820000 3.1040600000 0.7741580000
C -4.9271340000 1.7055450000 1.3384420000
C -5.7631780000 1.1169270000 0.3879590000
C -5.2409610000 0.1943210000 -0.5256980000
H -3.5027170000 -0.8596090000 -1.2048130000
H -2.9244990000 1.8284390000 2.1145810000
H -5.3277610000 2.4204480000 2.0514080000
H -5.8910080000 -0.2671310000 -1.2634580000
H -6.8187470000 1.3724240000 0.3584710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.422683 (Hartree/Particle)
Thermal correction to Energy= 0.449929
Thermal correction to Enthalpy= 0.450874
Thermal correction to Gibbs (Free) Energy= 0.362166
Sum of electronic and zero-point Energies= -1177.116375
Sum of electronic and thermal Energies= -1177.089129
Sum of electronic and thermal Enthalpies= -1177.088184
Sum of electronic and thermal (Free) Energies= -1177.176892

cTS

C 1.5492810000 1.4903160000 -0.2678780000
C 0.3588570000 0.9002130000 -0.4013860000
C 2.0417470000 2.5050040000 0.7586540000
H 2.3582470000 1.0861050000 -0.8788220000
C -1.0179090000 0.9079280000 -0.3247910000
C 0.9894610000 2.8790590000 1.8126500000
C 3.2524730000 1.8524310000 1.4723480000
C 2.5308840000 3.7650650000 0.0052300000
C -1.5422930000 -0.4089150000 0.0033990000
C -1.9481930000 2.0614090000 -0.7192920000
H 1.4364600000 3.5418140000 2.5619930000
H 0.1354300000 3.4046340000 1.3785670000
H 0.6127300000 1.9908480000 2.3311490000
H 4.0406030000 1.5830320000 0.7597960000
H 3.6796910000 2.5524760000 2.1997620000
H 2.9561510000 0.9432830000 2.0064470000
H 2.9820340000 4.4707830000 0.7127720000
H 3.2896210000 3.5110120000 -0.7442050000
H 1.7081820000 4.2744980000 -0.5059990000
C -0.5364180000 -1.3926550000 -0.1272840000
O -2.7526870000 -0.5930140000 0.3931580000
C -2.7512070000 2.5100690000 0.5292490000
C -2.9344790000 1.5558750000 -1.8045870000
C -1.1801890000 3.2602370000 -1.3027660000
C 0.6247130000 -0.9836500000 -0.8288050000
H -0.6230930000 -2.3472140000 0.3771010000
B -3.3152740000 -2.0715390000 0.5320500000
H -3.4437820000 3.3092310000 0.2399480000
H -3.3294010000 1.6820670000 0.9437140000
H -2.0915790000 2.9013660000 1.3109550000
H -3.5383270000 0.7196890000 -1.4486550000
H -1.8969170000 4.0272240000 -1.6156680000
H -0.5044520000 3.7182830000 -0.5763990000
H -0.5909210000 2.9737200000 -2.1807980000
H -3.6091850000 2.3726660000 -2.0851960000
H -2.3972400000 1.2413280000 -2.7072750000
C 1.9358990000 -1.6200770000 -0.5751000000
H 0.4974270000 -0.6855590000 -1.8705910000
F -3.0882510000 -2.6676060000 -0.6959990000
F -4.6323310000 -1.9056890000 0.8436820000
F -2.5685150000 -2.6721890000 1.5373880000
C 2.8766110000 -1.7234140000 -1.6124790000
C 2.2688850000 -2.1239580000 0.6941810000
C 4.1138020000 -2.3282100000 -1.3942120000
H 2.6274190000 -1.3420490000 -2.6004530000
C 3.5030240000 -2.7305030000 0.9116930000
H 1.5558830000 -2.0354990000 1.5096490000
C 4.4282610000 -2.8338160000 -0.1316140000
H 4.8278870000 -2.4096570000 -2.2087730000
H 3.7462720000 -3.1212680000 1.8956310000
H 5.3913220000 -3.3061080000 0.0409410000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.422398 (Hartree/Particle)
Thermal correction to Energy= 0.448303
Thermal correction to Enthalpy= 0.449247
Thermal correction to Gibbs (Free) Energy= 0.366575
Sum of electronic and zero-point Energies= -1177.082656
Sum of electronic and thermal Energies= -1177.056752
Sum of electronic and thermal Enthalpies= -1177.055807
Sum of electronic and thermal (Free) Energies= -1177.138479

cPT

C -1.7159270000 1.3067660000 0.3226420000
C -0.5446310000 0.6298780000 0.4562580000
C -2.2041940000 2.4613150000 -0.5359720000
H -2.5571040000 0.7904920000 0.7868720000
C 0.8516820000 0.8489370000 0.1957110000
C -1.2414910000 2.8806610000 -1.6595860000
C -3.5051330000 1.9407440000 -1.2094080000
C -2.5881210000 3.6621560000 0.3651450000
C 1.4692140000 -0.4236210000 -0.1256340000
C 1.7276590000 2.0526950000 0.5078390000
H -1.7259550000 3.6289420000 -2.2966880000
H -0.3148330000 3.3201220000 -1.2920320000
H -0.9818680000 2.0231440000 -2.2902960000
H -4.2621550000 1.6703180000 -0.4645940000
H -3.9269420000 2.7209670000 -1.8528190000
H -3.3086420000 1.0579770000 -1.8275360000
H -3.0658830000 4.4394690000 -0.2425250000
H -3.3009390000 3.3595240000 1.1409130000
H -1.7186520000 4.1016470000 0.8594510000
C 0.6067310000 -1.4306290000 0.3087830000
O 2.6469250000 -0.5220740000 -0.6508590000
C 2.4972770000 2.5153710000 -0.7594750000
C 2.7648270000 1.5664260000 1.5755120000
C 0.9802390000 3.2400040000 1.1402410000
C -0.6440040000 -0.8901760000 0.8799990000
H 0.8449540000 -2.4845650000 0.2481880000
B 3.5678670000 -1.7665820000 -0.4113680000
H 3.1499500000 3.3515980000 -0.4839120000
H 3.1088310000 1.7076590000 -1.1628800000
H 1.8144880000 2.8636520000 -1.5412070000
H 3.3317200000 0.6911840000 1.2574230000
H 1.7172300000 3.9550520000 1.5208410000
H 0.3508410000 3.7782680000 0.4316170000
H 0.3577010000 2.9239690000 1.9841700000
H 3.4663510000 2.3866870000 1.7642440000
H 2.2601960000 1.3335740000 2.5204030000
C -1.8889410000 -1.6717020000 0.5151160000
H -0.5649550000 -0.8620000000 1.9788250000
F 3.9806710000 -1.6564940000 0.9096500000
F 4.5808320000 -1.6333490000 -1.3196110000
F 2.7992610000 -2.9119340000 -0.6130750000
C -2.8278310000 -2.0146010000 1.4949390000
C -2.1137900000 -2.0762200000 -0.8094030000
C -3.9711170000 -2.7444210000 1.1620010000

H -2.6591890000 -1.7176960000 2.5280570000
C -3.2529050000 -2.8056760000 -1.1436350000
H -1.3876490000 -1.8208930000 -1.5781220000
C -4.1857530000 -3.1408370000 -0.1579430000
H -4.6877580000 -3.0074900000 1.9351280000
H -3.4114400000 -3.1170120000 -2.1724190000
H -5.0726590000 -3.7115140000 -0.4188380000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.424541 (Hartree/Particle)
Thermal correction to Energy= 0.450417
Thermal correction to Enthalpy= 0.451361
Thermal correction to Gibbs (Free) Energy= 0.368498
Sum of electronic and zero-point Energies= -1177.090220
Sum of electronic and thermal Energies= -1177.064344
Sum of electronic and thermal Enthalpies= -1177.063400
Sum of electronic and thermal (Free) Energies= -1177.146263

ccRT

C -0.1086060000 2.6650610000 -1.1542390000
C -0.7343490000 1.7421760000 -0.4719790000
C -1.4922600000 0.8270810000 0.1127490000
C -1.2355060000 -0.5950240000 -0.2368730000
C 0.0950090000 -1.1700260000 -0.3134930000
C 1.1564830000 -0.6761920000 0.3678030000
H 0.1565030000 -2.0926330000 -0.8780950000
H 1.0021170000 0.2043210000 0.9859270000
C 2.5053370000 -1.2294000000 0.3989930000
C -2.7231520000 1.1858450000 0.9897860000
O -2.2561230000 -1.2948350000 -0.4884170000
C 2.8991190000 -2.3372000000 -0.3796220000
C 3.4601660000 -0.6295180000 1.2431180000
B -2.3313480000 -2.9324570000 -0.6576560000
F -3.6419200000 -3.1277600000 -0.9518350000
F -1.9280030000 -3.3915220000 0.5681760000
F -1.4647080000 -3.2463240000 -1.6821100000
C 1.1190160000 3.4917050000 -0.7770350000
C -2.7852280000 0.2324470000 2.2045460000
H -3.6502210000 0.4876110000 2.8273820000
H -2.8863730000 -0.8143890000 1.9062880000
H -1.8873690000 0.3285870000 2.8274800000
C -4.0242060000 1.0756810000 0.1600120000
H -4.1949630000 0.0572320000 -0.1921570000
H -4.8783850000 1.3772190000 0.7787350000
H -3.9869640000 1.7417590000 -0.7099170000
C -2.5872260000 2.6306170000 1.5052830000
H -1.6771370000 2.7608790000 2.1027030000
H -2.5619120000 3.3541880000 0.6841980000
H -3.4449570000 2.8736550000 2.1422070000
C 2.2733310000 3.0985640000 -1.7259780000
C 1.5444410000 3.2731690000 0.6827640000
C 0.7624310000 4.9797200000 -0.9903720000
H 0.4476410000 5.1697810000 -2.0232830000
H 1.6328770000 5.6133270000 -0.7829130000
H -0.0515760000 5.2909290000 -0.3262100000
H 1.8599640000 2.2395680000 0.8566270000
H 0.7286790000 3.5047290000 1.3761820000
H 2.3923770000 3.9223610000 0.9290940000
H 2.5508180000 2.0470180000 -1.5950790000
H 3.1586020000 3.7142640000 -1.5254380000
H 1.9931660000 3.2455340000 -2.7756070000
H -0.5152590000 2.8887620000 -2.1449700000
C 4.7634000000 -1.1150340000 1.3102790000
C 5.1367380000 -2.2119300000 0.5318760000
C 4.2003940000 -2.8200910000 -0.3119500000
H 2.1833750000 -2.8204300000 -1.0369400000
H 3.1680820000 0.2213500000 1.8538460000
H 5.4853070000 -0.6405600000 1.9687850000
H 4.4886820000 -3.6749590000 -0.9168420000
H 6.1523460000 -2.5945920000 0.5815270000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.422655 (Hartree/Particle)
Thermal correction to Energy= 0.449937
Thermal correction to Enthalpy= 0.450881
Thermal correction to Gibbs (Free) Energy= 0.361099
Sum of electronic and zero-point Energies= -1177.114292
Sum of electronic and thermal Energies= -1177.087010
Sum of electronic and thermal Enthalpies= -1177.086066
Sum of electronic and thermal (Free) Energies= -1177.175848

ccTS

C 1.2646780000 1.8485020000 -0.5739420000
C 0.2418750000 1.1010380000 -0.1387300000
C 2.6617310000 2.1270860000 -0.0441800000
H 1.0527130000 2.3874530000 -1.5015040000
C -1.1366630000 1.0853850000 -0.0978520000
C 3.7156430000 1.4072240000 -0.9194430000
C 2.8370930000 1.7518650000 1.4369900000
C 2.8691070000 3.6569930000 -0.1885730000
C -1.6906290000 -0.2537940000 -0.0511100000
C -2.0388590000 2.3264240000 -0.0302880000
H 3.6288870000 0.3206040000 -0.8441260000
H 4.7240560000 1.6949510000 -0.5986590000
H 3.6082360000 1.6859840000 -1.9742440000
H 2.8099410000 0.6724360000 1.5913110000
H 2.0619560000 2.2163260000 2.0573740000
H 3.8099700000 2.1065490000 1.7959490000
H 2.7650600000 3.9799680000 -1.2311020000
H 3.8764040000 3.9280180000 0.1474830000
H 2.1473290000 4.2180600000 0.4151900000
C -0.6668530000 -1.2162370000 0.1102880000
O -2.9396310000 -0.4977240000 -0.2159550000
C -2.9772290000 2.2186610000 1.1969770000
C -2.8810710000 2.3669140000 -1.3339610000
C -1.2471020000 3.6415830000 0.0849670000
C 0.5784760000 -0.7547290000 0.5869040000
H -0.8147540000 -2.2306990000 -0.2406390000
B -3.4934810000 -1.9708840000 0.0255050000
H -3.6371670000 3.0934160000 1.2259350000
H -3.5984900000 1.3226860000 1.1567920000
H -2.4004200000 2.2042140000 2.1294870000
H -3.4896110000 1.4678200000 -1.4444850000
H -3.5475140000 3.2368650000 -1.3023360000
H -2.2376800000 2.4674930000 -2.2160590000
H -0.6033690000 3.6545990000 0.9712670000
H -0.6239410000 3.8323300000 -0.7939930000
H -1.9537250000 4.4740750000 0.1727870000
H 0.5987050000 -0.2757580000 1.5653480000
C 1.7879630000 -1.5479630000 0.2641940000
F -4.8469630000 -1.8403130000 -0.0670550000
F -3.0371440000 -2.3327430000 1.2804430000
F -2.9293970000 -2.7541430000 -0.9710540000
C 1.9940000000 -2.0295400000 -1.0397130000
C 2.7115930000 -1.8896610000 1.2655820000
C 3.0978900000 -2.8265300000 -1.3344850000
H 1.2877880000 -1.7653210000 -1.8224300000
C 3.8121690000 -2.6931960000 0.9724910000
H 2.5504820000 -1.5459720000 2.2845260000
C 4.0099040000 -3.1592260000 -0.3290790000
H 3.2471120000 -3.1890100000 -2.3475630000
H 4.5115890000 -2.9593710000 1.7598520000
H 4.8701450000 -3.7815190000 -0.5592670000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.422244 (Hartree/Particle)
Thermal correction to Energy= 0.448111
Thermal correction to Enthalpy= 0.449055
Thermal correction to Gibbs (Free) Energy= 0.366573
Sum of electronic and zero-point Energies= -1177.076236
Sum of electronic and thermal Energies= -1177.050370
Sum of electronic and thermal Enthalpies= -1177.049426
Sum of electronic and thermal (Free) Energies= -1177.131908

ccPT

C -1.6091550000 1.7180190000 -0.2454280000
C -0.5692700000 0.8358270000 -0.2627610000
C -3.0458080000 1.6484780000 -0.7236100000
H -1.4038200000 2.6736740000 0.2152100000
C 0.7888590000 1.1275060000 0.1603160000
C -3.9209070000 1.3378660000 0.5228180000
C -3.3490400000 0.6289530000 -1.8361230000
C -3.4118440000 3.0605460000 -1.2466210000
C 1.6370490000 0.0124590000 -0.2037190000
C 1.3999950000 2.3381140000 0.8527620000
H -3.6999740000 0.3447180000 0.9249380000
H -4.9804080000 1.3699890000 0.2420580000

H -3.7618680000 2.0755070000 1.3177440000
H -3.2469370000 -0.4022390000 -1.4944040000
H -2.7019920000 0.7829220000 -2.7072450000
H -4.3847960000 0.7597700000 -2.1694250000
H -3.2574290000 3.8281240000 -0.4791590000
H -4.4665140000 3.0891870000 -1.5413870000
H -2.8098630000 3.3290460000 -2.1224410000
C 0.8343810000 -0.9780100000 -0.7664340000
O 2.9211400000 -0.0232800000 -0.0173910000
C 2.4778840000 2.9399920000 -0.0970950000
C 2.0835220000 1.8244090000 2.1575980000
C 0.4551730000 3.4832380000 1.2661410000
C -0.5939810000 -0.5905840000 -0.8132320000
H 1.2055860000 -1.9451800000 -1.0772330000
B 3.7317920000 -1.2502130000 -0.5607770000
H 2.9663240000 3.7764000000 0.4156880000
H 3.2352750000 2.2037880000 -0.3656590000
H 2.0146400000 3.3279230000 -1.0116080000
H 2.8128450000 1.0412440000 1.9534130000
H 2.5983930000 2.6665310000 2.6332610000
H 1.3350520000 1.4450920000 2.8632830000
H 0.0225730000 4.0081680000 0.4079080000
H -0.3490780000 3.1505920000 1.9313360000
H 1.0444570000 4.2213100000 1.8204940000
H -0.9501900000 -0.5944280000 -1.8519280000
C -1.4195560000 -1.6204670000 -0.0250460000
F 5.0355090000 -0.9699370000 -0.2630670000
F 3.4654920000 -1.3141800000 -1.9242290000
F 3.2337180000 -2.3724450000 0.0925320000
C -1.4427520000 -1.6125690000 1.3752990000
C -2.0852580000 -2.6461560000 -0.7068400000
C -2.1442580000 -2.5926740000 2.0769820000
H -0.9086170000 -0.8394120000 1.9208480000
C -2.7823680000 -3.6314720000 -0.0050890000
H -2.0571040000 -2.6769620000 -1.7937720000
C -2.8171580000 -3.6050500000 1.3891000000
H -2.1558750000 -2.5705670000 3.1631920000
H -3.2955310000 -4.4186160000 -0.5504910000
H -3.3587430000 -4.3707690000 1.9371480000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.425512 (Hartree/Particle)
Thermal correction to Energy= 0.451173
Thermal correction to Enthalpy= 0.452118
Thermal correction to Gibbs (Free) Energy= 0.368926
Sum of electronic and zero-point Energies= -1177.103416
Sum of electronic and thermal Energies= -1177.077755
Sum of electronic and thermal Enthalpies= -1177.076811
Sum of electronic and thermal (Free) Energies= -1177.160002

5a

cRT

C 1.9749300000 1.2793880000 0.4708240000
C 0.7401320000 0.9653200000 0.7815300000
C -0.4731910000 0.6033940000 1.1657470000
C -1.5522380000 0.3868420000 0.1773950000
C -1.5184380000 0.9338220000 -1.1863470000
C -0.9616240000 2.1099370000 -1.5017970000
H -2.0612780000 0.3521150000 -1.9233000000
C -0.8001820000 0.2784650000 2.6129440000
H 2.2332710000 2.3401690000 0.4579550000
C 3.0659530000 0.3493080000 0.1230860000
O -2.5139940000 -0.3191400000 0.5674870000
H 0.0608090000 0.4770790000 3.2541860000
H -1.0869900000 -0.7733060000 2.7092590000
H -1.6507410000 0.8763290000 2.9575170000
C 4.3386180000 0.8706920000 -0.1570140000
C 2.8747990000 -1.0417880000 0.0631700000
C 3.9317990000 -1.8841860000 -0.2660090000
H 1.8934550000 -1.4581810000 0.2733850000
C 5.1968490000 -1.3553010000 -0.5417230000
H 3.7693500000 -2.9575540000 -0.3095500000
C 5.3965950000 0.0243740000 -0.4862210000
H 4.4970530000 1.9456930000 -0.1144310000
H 6.0196930000 -2.0162110000 -0.7990820000
H 6.3757100000 0.4440710000 -0.6997240000
B -3.9079850000 -0.6669000000 -0.3170050000
F -4.6109170000 -1.4130750000 0.5646570000
F -3.4363470000 -1.3432290000 -1.4136280000
F -4.4182150000 0.5674620000 -0.5965860000
H -1.0102180000 2.4884440000 -2.5186800000
H -0.4829320000 2.7469450000 -0.7658980000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.224463 (Hartree/Particle)
Thermal correction to Energy= 0.242113
Thermal correction to Enthalpy= 0.243057
Thermal correction to Gibbs (Free) Energy= 0.176366
Sum of electronic and zero-point Energies= -902.109637
Sum of electronic and thermal Energies= -902.091987
Sum of electronic and thermal Enthalpies= -902.091043
Sum of electronic and thermal (Free) Energies= -902.157734

cTS

C -1.9319680000 0.5675150000 -0.6727310000
C -0.6741930000 0.1266130000 -0.7541460000
C -3.0758880000 -0.1708780000 -0.1318870000
H -2.1376790000 1.5868680000 -0.9982650000
C 0.2666550000 -0.8188980000 -0.9884340000
C -4.3544850000 0.4118460000 -0.2121120000
C -2.9488170000 -1.4441060000 0.4562400000
C 1.5416550000 -0.5970680000 -0.3255580000
C 0.0897060000 -1.9932230000 -1.9129550000
C -5.4750400000 -0.2644580000 0.2630890000
H -4.4639280000 1.3977490000 -0.6574360000
C -4.0700940000 -2.1152250000 0.9318820000
H -1.9658290000 -1.8956420000 0.5518510000
C 1.5751190000 0.6785420000 0.3284720000
O 2.4294590000 -1.5055270000 -0.3034490000
H -0.9432730000 -2.0935230000 -2.2514280000
H 0.3918240000 -2.9071360000 -1.3892280000
H 0.7486830000 -1.9011650000 -2.7841630000
C -5.3370850000 -1.5305750000 0.8355010000
H -6.4552800000 0.1979710000 0.1896520000
H -3.9565170000 -3.0954340000 1.3861720000
C 0.6964900000 1.6364360000 -0.1395690000
H 2.1381290000 0.7852310000 1.2492090000
B 3.8792270000 -1.1820690000 0.3344990000
H -6.2098210000 -2.0573530000 1.2106830000
H 0.6042590000 1.8597280000 -1.1993170000
H 0.3856390000 2.4523480000 0.5122030000
F 4.6121990000 -2.2939260000 0.0645620000
F 3.6328960000 -0.9658450000 1.6781810000
F 4.2969970000 -0.0378120000 -0.3111900000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.223916 (Hartree/Particle)
Thermal correction to Energy= 0.240480
Thermal correction to Enthalpy= 0.241424
Thermal correction to Gibbs (Free) Energy= 0.177763
Sum of electronic and zero-point Energies= -902.085844
Sum of electronic and thermal Energies= -902.069280
Sum of electronic and thermal Enthalpies= -902.068336
Sum of electronic and thermal (Free) Energies= -902.131998

cPT

C -1.8019990000 1.3346480000 0.0194780000
C -0.4611070000 1.0444310000 0.0552720000
C 0.2734840000 -0.1548590000 -0.1641850000
C 1.6787730000 0.0878690000 0.0293760000
C 1.8436040000 1.4451530000 0.3419010000
C 0.5504130000 2.1554300000 0.3058340000
C -0.1702580000 -1.4924130000 -0.6374250000
C -2.9764670000 0.4791840000 0.0404520000
O 2.5589260000 -0.8462580000 -0.1035980000
H -1.1724640000 -1.4899480000 -1.0672660000
H -0.1451490000 -2.2153080000 0.1903090000
H 0.5616230000 -1.8612670000 -1.3648180000
C -4.1689280000 0.9624620000 -0.5423930000
C -3.0065830000 -0.7761070000 0.6840700000
C -4.1725600000 -1.5342590000 0.7030750000
H -2.1247460000 -1.1295720000 1.2064390000
C -5.3314050000 -1.0591700000 0.0818970000
H -4.1826690000 -2.4926540000 1.2139270000
C -5.3269910000 0.1937200000 -0.5387790000
H -4.1689460000 1.9411380000 -1.0156080000

H -6.2396150000 -1.6547940000 0.0978430000
H -6.2295710000 0.5728150000 -1.0090160000
B 4.0751610000 -0.4409080000 -0.0454420000
F 4.2503920000 0.5091860000 -1.0446040000
F 4.7653620000 -1.6003550000 -0.2511060000
F 4.2788450000 0.1219100000 1.2111140000
H 0.5149420000 2.8937190000 -0.5124100000
H 0.3465860000 2.7212300000 1.2280660000
H -2.0353500000 2.4003630000 -0.0044980000
H 2.7968820000 1.8956920000 0.5829280000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.226610 (Hartree/Particle)
Thermal correction to Energy= 0.242789
Thermal correction to Enthalpy= 0.243734
Thermal correction to Gibbs (Free) Energy= 0.181083
Sum of electronic and zero-point Energies= -902.126145
Sum of electronic and thermal Energies= -902.109966
Sum of electronic and thermal Enthalpies= -902.109022
Sum of electronic and thermal (Free) Energies= -902.171673

ccRT

C 1.8734090000 0.8771420000 -1.0749970000
C 0.6802240000 1.0028120000 -0.5459900000
C 3.0788590000 0.3386310000 -0.4178940000
H 1.9886730000 1.1790080000 -2.1179510000
C -0.5192730000 1.2050230000 -0.0271560000
C 4.2299830000 0.1077220000 -1.1874930000
C 3.1144470000 0.0463170000 0.9571110000
C -1.5828600000 0.1824440000 -0.1396890000
C -0.9118640000 2.5264530000 0.6098700000
C 5.3837940000 -0.4114810000 -0.6021530000
H 4.2156230000 0.3342850000 -2.2508040000
C 4.2669960000 -0.4737670000 1.5389450000
H 2.2388870000 0.2439390000 1.5702950000
C -1.3263970000 -1.2224710000 -0.4868700000
O -2.7515390000 0.5932680000 0.0633650000
H -0.0516270000 3.1966980000 0.6634790000
H -1.3066450000 2.3647600000 1.6183930000
H -1.7056130000 3.0052840000 0.0277520000
C 5.4057420000 -0.7061590000 0.7617970000
H 6.2655460000 -0.5853520000 -1.2125810000
H 4.2800340000 -0.6927230000 2.6030750000
C -0.2150400000 -1.8914230000 -0.1540820000
H -2.1551220000 -1.7225360000 -0.9761050000
B -4.1470950000 -0.3547360000 0.0919550000
H 6.3047570000 -1.1097230000 1.2188520000
H 0.6034930000 -1.4455420000 0.4008990000
H -0.1127250000 -2.9430040000 -0.4063600000
F -4.2140500000 -0.8752170000 -1.1755020000
F -5.0933760000 0.5636740000 0.3910040000
F -3.8798630000 -1.2756810000 1.0629390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.224556 (Hartree/Particle)
Thermal correction to Energy= 0.242147
Thermal correction to Enthalpy= 0.243092
Thermal correction to Gibbs (Free) Energy= 0.176919
Sum of electronic and zero-point Energies= -902.110128
Sum of electronic and thermal Energies= -902.092537
Sum of electronic and thermal Enthalpies= -902.091592
Sum of electronic and thermal (Free) Energies= -902.157765

ccTS

C -1.6270780000 -1.3878120000 -0.8345580000
C -0.3836310000 -1.2273060000 -0.3641870000
C -2.8807980000 -0.8911860000 -0.2675840000
H -1.7085600000 -1.8943270000 -1.7993590000
C 0.8688640000 -1.7020080000 -0.1495940000
C -3.9922840000 -0.7136360000 -1.1133040000
C -3.0287720000 -0.6095340000 1.1049430000
C 1.9013330000 -0.6844820000 -0.0531520000
C 1.2227380000 -3.1520870000 0.0325900000
C -5.2005380000 -0.2388210000 -0.6110920000
H -3.8959490000 -0.9394410000 -2.1724010000
C -4.2379460000 -0.1332560000 1.6039880000
H -2.2049950000 -0.8044570000 1.7855120000
C 1.3376990000 0.6325660000 -0.1134060000
O 3.1303960000 -1.0043350000 -0.0283320000
H 0.3554450000 -3.8018690000 -0.0978990000
H 1.6595370000 -3.3237580000 1.0230270000
H 1.9936560000 -3.4249200000 -0.6977310000
C -5.3258850000 0.0587900000 0.7481870000
H -6.0456490000 -0.1013290000 -1.2796140000
H -4.3371710000 0.0738650000 2.6657870000
C 0.0059610000 0.7464600000 0.2375350000
H 1.8972070000 1.4230860000 -0.6017010000
B 4.2417180000 0.1490150000 0.1881170000
H -6.2698430000 0.4253030000 1.1412480000
H -0.3756440000 0.3428180000 1.1716650000
H -0.5919620000 1.5687450000 -0.1529820000
F 4.1646160000 0.9308810000 -0.9499580000
F 5.4060800000 -0.5373580000 0.3270460000
F 3.8267830000 0.8258410000 1.3159450000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.223607 (Hartree/Particle)
Thermal correction to Energy= 0.240191
Thermal correction to Enthalpy= 0.241135
Thermal correction to Gibbs (Free) Energy= 0.177607
Sum of electronic and zero-point Energies= -902.083891
Sum of electronic and thermal Energies= -902.067307
Sum of electronic and thermal Enthalpies= -902.066363
Sum of electronic and thermal (Free) Energies= -902.129891

ccPT

C -1.7663860000 0.8555910000 0.0000010000
C -0.5092840000 0.3071460000 0.0000010000
C 0.6869250000 1.0821560000 0.0000010000
C 1.8425490000 0.2292110000 0.0000000000
C 1.3854920000 -1.0920890000 0.0000000000
C -0.0993820000 -1.1529260000 0.0000000000
C 0.8531240000 2.5558810000 0.0000010000
O 3.0444830000 0.7034960000 0.0000000000
H -0.0835040000 3.1161630000 0.0000010000
H 1.4537530000 2.8481840000 -0.8712860000
H 1.4537520000 2.8481840000 0.8712890000
H 2.0347450000 -1.9569590000 -0.0000010000
C -3.0861070000 0.2552250000 0.0000000000
H -1.7948830000 1.9434840000 0.0000010000
C -4.1913850000 1.1377780000 -0.0000010000
C -5.4974060000 0.6621080000 -0.0000020000
C -5.7352390000 -0.7139480000 -0.0000010000
C -4.6572860000 -1.6063820000 0.0000010000
C -3.3510570000 -1.1340150000 0.0000010000
H -4.0092020000 2.2094380000 -0.0000020000
H -6.3283030000 1.3613190000 -0.0000030000
H -6.7536610000 -1.0915980000 -0.0000010000
H -4.8396960000 -2.6770380000 0.0000020000
H -2.5375540000 -1.8476730000 0.0000030000
B 4.2322590000 -0.3190910000 0.0000000000
F 5.3653800000 0.4430550000 0.0000000000
F 4.0730240000 -1.0947090000 -1.1441930000
F 4.0730240000 -1.0947110000 1.1441910000
H -0.4814060000 -1.6915690000 -0.8801690000
H -0.4814050000 -1.6915690000 0.8801690000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.226668 (Hartree/Particle)
Thermal correction to Energy= 0.243123
Thermal correction to Enthalpy= 0.244068
Thermal correction to Gibbs (Free) Energy= 0.179902
Sum of electronic and zero-point Energies= -902.132316
Sum of electronic and thermal Energies= -902.115861
Sum of electronic and thermal Enthalpies= -902.114917
Sum of electronic and thermal (Free) Energies= -902.179083

5b

cRT

C 2.0267080000 0.5326490000 1.1916000000
C 0.8017120000 0.0659890000 1.2473070000
C -0.3984040000 -0.4830020000 1.3276280000
C -1.4925020000 -0.0661310000 0.4182030000
C -1.5208700000 1.2199570000 -0.2729310000
C -0.9785150000 2.3489420000 0.2177260000

H -2.0999100000 1.2347200000 -1.1902970000
H -0.4747680000 2.3257050000 1.1815270000
C -1.0568080000 3.6805300000 -0.4553060000
C -0.6931740000 -1.6460500000 2.2590060000
H 2.2729280000 1.3757610000 1.8403590000
C 3.1226820000 0.0436350000 0.3334750000
O -2.4074480000 -0.9148840000 0.2574630000
H 0.1741310000 -1.8654590000 2.8849160000
H -0.9553770000 -2.5367210000 1.6798120000
H -1.5505910000 -1.4160820000 2.9006820000
C 4.3862270000 0.6461850000 0.4359490000
C 2.9451440000 -1.0060080000 -0.5841960000
C 4.0061220000 -1.4390340000 -1.3729990000
H 1.9708620000 -1.4779310000 -0.6771500000
C 5.2619790000 -0.8335640000 -1.2620540000
H 3.8538230000 -2.2509200000 -2.0787690000
C 5.4483050000 0.2102100000 -0.3552380000
H 4.5345180000 1.4596490000 1.1423380000
H 6.0879320000 -1.1740000000 -1.8801620000
H 6.4202140000 0.6869810000 -0.2626170000
B -3.8098210000 -0.6886760000 -0.6238870000
F -4.4456860000 -1.8706760000 -0.4449960000
F -3.3697360000 -0.4526630000 -1.9040550000
F -4.3926370000 0.3947090000 -0.0282470000
H -1.5783370000 3.6249850000 -1.4145830000
H -0.0486310000 4.0824900000 -0.6246440000
H -1.5772060000 4.4050880000 0.1849800000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.252725 (Hartree/Particle)
Thermal correction to Energy= 0.271953
Thermal correction to Enthalpy= 0.272898
Thermal correction to Gibbs (Free) Energy= 0.202483
Sum of electronic and zero-point Energies= -941.404836
Sum of electronic and thermal Energies= -941.385607
Sum of electronic and thermal Enthalpies= -941.384663
Sum of electronic and thermal (Free) Energies= -941.455077

cTS

C -1.8928450000 0.5517440000 -0.7317600000
C -0.6338710000 0.1055870000 -0.7763580000
C -3.0386780000 -0.1319130000 -0.1278930000
H -2.0975900000 1.5428640000 -1.1372650000
C 0.2695470000 -0.8978360000 -0.9231440000
C -4.3170930000 0.4412160000 -0.2649430000
C -2.9149230000 -1.3449230000 0.5770810000
C 1.5599230000 -0.6326290000 -0.3169450000
C 0.0394900000 -2.1603910000 -1.7066230000
C -5.4397450000 -0.1878500000 0.2666800000
H -4.4247770000 1.3814340000 -0.8005280000
C -4.0382270000 -1.9686650000 1.1092230000
H -1.9323950000 -1.7848340000 0.7192320000
C 1.6344790000 0.7076750000 0.1703790000
O 2.4321230000 -1.5544610000 -0.2016550000
H -1.0054820000 -2.2741240000 -2.0014270000
H 0.3415230000 -3.0182510000 -1.0951070000
H 0.6722440000 -2.1800970000 -2.6018630000
C -5.3046790000 -1.3955650000 0.9544890000
H -6.4194970000 0.2659860000 0.1470930000
H -3.9265090000 -2.9021430000 1.6535420000
C 0.7541510000 1.6325250000 -0.3846880000
H 2.2420790000 0.9236300000 1.0430620000
B 3.8922550000 -1.1876900000 0.3559760000
H -6.1789990000 -1.8850340000 1.3739300000
C 0.3710770000 2.9015080000 0.3281920000
H 0.6855030000 1.6944780000 -1.4704260000
F 4.3256140000 -0.1449050000 -0.4388720000
F 4.6015900000 -2.3404650000 0.2210460000
F 3.6894040000 -0.7903380000 1.6675920000
H 0.4133260000 2.7894860000 1.4147870000
H -0.6392980000 3.2199330000 0.0504700000
H 1.0520780000 3.7112230000 0.0351620000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.251957 (Hartree/Particle)
Thermal correction to Energy= 0.270168
Thermal correction to Enthalpy= 0.271113
Thermal correction to Gibbs (Free) Energy= 0.203860
Sum of electronic and zero-point Energies= -941.379056
Sum of electronic and thermal Energies= -941.360845
Sum of electronic and thermal Enthalpies= -941.359901
Sum of electronic and thermal (Free) Energies= -941.427153

cPT

C -1.8107470000 1.1338560000 -0.3053700000
C -0.4711460000 0.8594630000 -0.1987400000
C 0.2471880000 -0.3707420000 -0.1804680000
C 1.6554480000 -0.1158020000 -0.0451290000
C 1.8369850000 1.2722790000 -0.0126270000
C 0.5567400000 1.9971710000 -0.1821450000
C 0.3256940000 3.1083030000 0.8633920000
C -0.2151750000 -1.7676300000 -0.3938450000
C -2.9854230000 0.2989710000 -0.1130710000
O 2.5233150000 -1.0703830000 0.0055960000
H -1.2190990000 -1.8338070000 -0.8141850000
H -0.1958470000 -2.3216700000 0.5553680000
H 0.5097110000 -2.2763720000 -1.0392740000
C -4.1727070000 0.6413280000 -0.7970900000
C -3.0207600000 -0.7872730000 0.7865780000
C -4.1864500000 -1.5262810000 0.9593650000
H -2.1427450000 -1.0174430000 1.3797370000
C -5.3399440000 -1.2001590000 0.2400040000
H -4.2004020000 -2.3514220000 1.6654790000
C -5.3303040000 -0.1115870000 -0.6373610000
H -4.1691840000 1.4943450000 -1.4710040000
H -6.2479200000 -1.7804850000 0.3766350000
H -6.2286510000 0.1543150000 -1.1867370000
H 0.5441880000 2.4682280000 -1.1817070000
B 4.0426510000 -0.6801170000 -0.0292260000
F 4.2185010000 0.0531500000 -1.1973310000
F 4.7200840000 -1.8650970000 -0.0081770000
F 4.2657850000 0.1169270000 1.0902540000
H 1.1512140000 3.8264700000 0.8327960000
H 0.2738020000 2.6889600000 1.8729510000
H -0.6005170000 3.6569870000 0.6674600000
H -2.0478120000 2.1698950000 -0.5503730000
H 2.7977600000 1.7494470000 0.1305450000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255019 (Hartree/Particle)
Thermal correction to Energy= 0.272719
Thermal correction to Enthalpy= 0.273663
Thermal correction to Gibbs (Free) Energy= 0.207758
Sum of electronic and zero-point Energies= -941.411833
Sum of electronic and thermal Energies= -941.394134
Sum of electronic and thermal Enthalpies= -941.393189
Sum of electronic and thermal (Free) Energies= -941.459095

ccRT

C -1.8601650000 -1.0185390000 -1.1135800000
C -0.6701690000 -1.1686650000 -0.5822110000
C -3.0737960000 -0.5263540000 -0.4350730000
H -1.9668080000 -1.2592220000 -2.1732170000
C 0.5276870000 -1.3915190000 -0.0706440000
C -4.2172520000 -0.2448660000 -1.1994950000
C -3.1254790000 -0.3273280000 0.9560740000
C 1.5892510000 -0.3571810000 -0.1253790000
C 0.9269590000 -2.7463120000 0.4872150000
C -5.3781370000 0.2332030000 -0.5933590000
H -4.1912750000 -0.4000090000 -2.2753780000
C -4.2850450000 0.1518550000 1.5589870000
H -2.2568670000 -0.5670220000 1.5640960000
C 1.3279530000 1.0635120000 -0.3385400000
O 2.7629390000 -0.7921700000 0.0042440000
H 1.7200330000 -3.1870010000 -0.1249600000
H 0.0692590000 -3.4218350000 0.5051390000
H 1.3253630000 -2.6422240000 1.5019630000
C -5.4156110000 0.4356340000 0.7870200000
H -6.2535750000 0.4466560000 -1.2003900000
H -4.3102980000 0.2975320000 2.6354430000
C 0.2029180000 1.6956690000 0.0419990000
H 2.1582020000 1.6191970000 -0.7616600000
B 4.1505560000 0.1353670000 0.0988990000
H -6.3203320000 0.8064130000 1.2603500000
C -0.0346020000 3.1603730000 -0.1325680000
H -0.5899740000 1.1412200000 0.5390240000
F 5.1058940000 -0.8089090000 0.2700280000

F 3.9205760000 0.9477410000 1.1738540000
F 4.1974810000 0.7991800000 -1.1031320000
H -0.1862880000 3.6433510000 0.8419080000
H -0.9540470000 3.3303140000 -0.7088420000
H 0.7976930000 3.6541720000 -0.6413520000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.252810 (Hartree/Particle)
Thermal correction to Energy= 0.271986
Thermal correction to Enthalpy= 0.272930
Thermal correction to Gibbs (Free) Energy= 0.203038
Sum of electronic and zero-point Energies= -941.405344
Sum of electronic and thermal Energies= -941.386168
Sum of electronic and thermal Enthalpies= -941.385224
Sum of electronic and thermal (Free) Energies= -941.455116

ccTS

C -1.5573320000 -1.4851090000 -0.8653720000
C -0.2995590000 -1.2458210000 -0.4612150000
C -2.7929590000 -0.8604460000 -0.3988390000
H -1.6674350000 -2.1892620000 -1.6937210000
C 0.9281760000 -1.7583060000 -0.1822400000
C -3.9237710000 -0.8595930000 -1.2393870000
C -2.9110870000 -0.2883690000 0.8845220000
C 2.0136840000 -0.8032280000 -0.2844420000
C 1.1996930000 -3.1678480000 0.2613130000
C -5.1198340000 -0.2808180000 -0.8250570000
H -3.8514930000 -1.3088580000 -2.2267580000
C -4.1083280000 0.2910830000 1.2952970000
H -2.0717680000 -0.3366410000 1.5721480000
C 1.5205430000 0.5037940000 -0.5713130000
O 3.2282400000 -1.1819760000 -0.2120100000
H 1.9575670000 -3.6075810000 -0.3978420000
H 0.2984620000 -3.7834330000 0.2396960000
H 1.6245240000 -3.1826660000 1.2718140000
C -5.2150000000 0.3011010000 0.4417710000
H -5.9793740000 -0.2844620000 -1.4892930000
H -4.1839190000 0.7217550000 2.2897760000
C 0.1855370000 0.7602920000 -0.2614750000
H 2.1255460000 1.1796430000 -1.1668420000
B 4.3940900000 -0.0788080000 -0.2078800000
H -6.1498780000 0.7480780000 0.7674900000
C -0.5932320000 1.8356340000 -0.9707010000
H -0.1574140000 0.5604760000 0.7536570000
F 5.5294880000 -0.7918270000 0.0224640000
F 4.0491090000 0.8006840000 0.7995530000
F 4.3352430000 0.5157910000 -1.4578520000
H -0.4915710000 2.7845970000 -0.4277340000
H -1.6598810000 1.5938990000 -0.9946780000
H -0.2406320000 1.9840010000 -1.9949640000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.251732 (Hartree/Particle)
Thermal correction to Energy= 0.269930
Thermal correction to Enthalpy= 0.270874
Thermal correction to Gibbs (Free) Energy= 0.203871
Sum of electronic and zero-point Energies= -941.377074
Sum of electronic and thermal Energies= -941.358876
Sum of electronic and thermal Enthalpies= -941.357932
Sum of electronic and thermal (Free) Energies= -941.424935

ccPT

C -1.7181760000 0.9919450000 -0.0039420000
C -0.4693440000 0.4240430000 -0.0170310000
C 0.7309420000 1.1937400000 -0.0008480000
C 1.8802640000 0.3363890000 -0.0427110000
C 1.4124790000 -0.9812000000 -0.0549550000
C -0.0731440000 -1.0496950000 -0.0159890000
C 0.9045290000 2.6671660000 0.0219670000
O 3.0859450000 0.8008710000 -0.0547590000
H -0.0222940000 3.2287420000 0.1526050000
H 1.3881740000 2.9865250000 -0.9113330000
H 1.6130820000 2.9311560000 0.8166960000
C -0.5701540000 -1.8440150000 1.2160350000
H 2.0571220000 -1.8503500000 -0.0559380000
C -3.0434930000 0.4089760000 -0.0940120000
H -0.4384150000 -1.5514900000 -0.9257690000
H -1.7350820000 2.0742240000 0.1119120000
C -4.1340960000 1.2098360000 0.3180380000
C -5.4369410000 0.7287590000 0.2783780000
C -5.6893610000 -0.5604650000 -0.1989650000
C -4.6298370000 -1.3586830000 -0.6402210000
C -3.3235940000 -0.8840930000 -0.5916240000
H -3.9408110000 2.2142390000 0.6861370000
H -6.2567200000 1.3582080000 0.6117990000
H -6.7075770000 -0.9363740000 -0.2407540000
H -4.8250760000 -2.3515130000 -1.0348850000
H -2.5226560000 -1.5024390000 -0.9775630000
B 4.2642130000 -0.2313190000 -0.0977240000
F 5.4038710000 0.5207710000 -0.1143610000
F 4.0705810000 -0.9892050000 -1.2487020000
F 4.1259510000 -1.0221610000 1.0389350000
H -0.2169520000 -1.3742350000 2.1389230000
H -0.1826710000 -2.8671170000 1.1834710000
H -1.6628020000 -1.8908110000 1.2438310000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255141 (Hartree/Particle)
Thermal correction to Energy= 0.273007
Thermal correction to Enthalpy= 0.273952
Thermal correction to Gibbs (Free) Energy= 0.207295
Sum of electronic and zero-point Energies= -941.417333
Sum of electronic and thermal Energies= -941.399467
Sum of electronic and thermal Enthalpies= -941.398523
Sum of electronic and thermal (Free) Energies= -941.465180

5c

c/s RT

C 2.0886990000 0.1767080000 1.2190950000
C 0.8953730000 -0.3669910000 1.2609570000
C -0.2685850000 -0.9907170000 1.3249830000
C -1.3771900000 -0.6333250000 0.4079990000
C -1.4770670000 0.6553080000 -0.2706750000
C -1.0239820000 1.8134940000 0.2424200000
H -2.0405810000 0.6420130000 -1.1979120000
H -0.5372090000 1.8177890000 1.2171120000
C -1.1876380000 3.1562470000 -0.4090010000
C -0.4992350000 -2.1782760000 2.2433070000
H 2.2758070000 1.0287300000 1.8757810000
C 3.2196890000 -0.2349260000 0.3657430000
O -2.2370270000 -1.5353080000 0.2304410000
H 0.3744960000 -2.3500410000 2.8751670000
H -0.7013650000 -3.0778770000 1.6539090000
H -1.3746020000 -2.0073820000 2.8791920000
C 0.1883250000 3.8218940000 -0.6112750000
C -2.1161620000 4.0485730000 0.4402250000
H -1.6531280000 3.0093700000 -1.3919160000
H 0.6907850000 3.9884510000 0.3499150000
H 0.0694850000 4.7961420000 -1.0983860000
H 0.8441870000 3.2055600000 -1.2349940000
H -1.6977030000 4.2137820000 1.4409190000
H -3.1053340000 3.5944300000 0.5557150000
H -2.2403800000 5.0272140000 -0.0368560000
C 4.4410640000 0.4471170000 0.4806660000
C 3.1163680000 -1.2877340000 -0.5596560000
C 4.2082000000 -1.6462010000 -1.3437630000
H 2.1752280000 -1.8209620000 -0.6621450000
C 5.4216250000 -0.9617550000 -1.2203970000
H 4.1132310000 -2.4616150000 -2.0554990000
C 5.5342070000 0.0858320000 -0.3058570000
H 4.5318990000 1.2637870000 1.1930420000
H 6.2718780000 -1.2441610000 -1.8347930000
H 6.4726860000 0.6237000000 -0.2035230000
B -3.6401780000 -1.3834240000 -0.6604630000
F -4.2112030000 -2.6002620000 -0.4942890000
F -3.2046840000 -1.1150180000 -1.9360160000
F -4.2901600000 -0.3381470000 -0.0646470000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309727 (Hartree/Particle)
Thermal correction to Energy= 0.331709
Thermal correction to Enthalpy= 0.332653
Thermal correction to Gibbs (Free) Energy= 0.255283
Sum of electronic and zero-point Energies= -1019.976000
Sum of electronic and thermal Energies= -1019.954018
Sum of electronic and thermal Enthalpies= -1019.953073

Sum of electronic and thermal (Free) Energies= -1020.030444

c/s TS

C -1.7329650000 1.0285050000 0.2086960000
C -0.5604450000 0.4153920000 -0.0056410000
C 0.1753440000 -0.7221820000 0.1162740000
C 1.6044480000 -0.5258580000 0.0063050000
C 1.9093790000 0.8164010000 -0.3565100000
C 0.9000190000 1.5720920000 -0.9578130000
C 1.0087730000 3.0888480000 -0.9809860000
C -0.3948550000 -2.1062890000 0.2558830000
H -2.1054850000 1.7042850000 -0.5582470000
C -2.5556110000 0.9268030000 1.4147090000
O 2.4229280000 -1.4660220000 0.2812700000
H -1.4670560000 -2.0899120000 0.4601340000
H 0.1245390000 -2.6240550000 1.0701490000
H -0.2086940000 -2.6927460000 -0.6518080000
C -0.3347210000 3.8097590000 -1.1672950000
C 1.9859370000 3.4767680000 -2.1151020000
H 1.4457330000 3.4145200000 -0.0285780000
H -0.8641350000 3.4440280000 -2.0571000000
H -0.1665190000 4.8831370000 -1.3059120000
H -0.9870130000 3.6855320000 -0.2987100000
H 1.5918070000 3.1740250000 -3.0929120000
H 2.9643730000 3.0038520000 -1.9862090000
H 2.1282510000 4.5631700000 -2.1307180000
C -3.8281220000 1.5305890000 1.4164850000
C -2.1319870000 0.2428340000 2.5713430000
C -2.9656970000 0.1500510000 3.6805600000
H -1.1400260000 -0.1976120000 2.6003130000
C -4.2333590000 0.7408060000 3.6631700000
H -2.6237710000 -0.3776760000 4.5663970000
C -4.6608170000 1.4326710000 2.5277450000
H -4.1629830000 2.0693630000 0.5333120000
H -4.8798800000 0.6684470000 4.5330790000
H -5.6417240000 1.8992140000 2.5096210000
H 0.3862460000 1.1574120000 -1.8274080000
H 2.8452830000 1.2543450000 -0.0252370000
B 3.9830480000 -1.2487800000 0.0014330000
F 4.0598140000 -0.8474200000 -1.3191040000
F 4.5451250000 -2.4609130000 0.2602600000
F 4.3750580000 -0.2410700000 0.8694530000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309266 (Hartree/Particle)
Thermal correction to Energy= 0.330016
Thermal correction to Enthalpy= 0.330960
Thermal correction to Gibbs (Free) Energy= 0.257769
Sum of electronic and zero-point Energies= -1019.946855
Sum of electronic and thermal Energies= -1019.926105
Sum of electronic and thermal Enthalpies= -1019.925161
Sum of electronic and thermal (Free) Energies= -1019.998352

c/s PT

C -1.8394490000 0.7232570000 -0.5112920000
C -0.5105080000 0.4583760000 -0.2874410000
C 0.1487430000 -0.7877350000 -0.0559070000
C 1.5722470000 -0.6026780000 -0.0875280000
C 1.8195320000 0.7406320000 -0.3857060000
C 0.5677500000 1.5317970000 -0.4799510000
C 0.5545130000 2.7324450000 0.5369710000
C -0.3902260000 -2.1687150000 0.0600200000
H -2.0441390000 1.6834770000 -0.9817740000
C -3.0400900000 -0.0473130000 -0.2229480000
O 2.3987540000 -1.5803170000 0.0888480000
H -1.3897150000 -2.2802330000 -0.3620680000
H -0.4298240000 -2.4714420000 1.1162610000
H 0.3141040000 -2.8570590000 -0.4182870000
C -0.7077940000 3.6028480000 0.4318320000
C 1.8056070000 3.6115580000 0.3613900000
H 0.5841680000 2.2904640000 1.5419950000
H -0.8457630000 3.9868570000 -0.5877460000
H -0.6174480000 4.4695740000 1.0959020000
H -1.6129720000 3.0632910000 0.7238160000
H 1.8761350000 4.0000230000 -0.6628940000
H 2.7308960000 3.0742610000 0.5859370000
H 1.7547990000 4.4721020000 1.0370890000
C -4.1674650000 0.1221880000 -1.0563300000
C -3.1631830000 -0.8818570000 0.9076820000
C -4.3542070000 -1.5521950000 1.1678390000
H -2.3330310000 -0.9655830000 1.6005980000
C -5.4456150000 -1.4072360000 0.3067020000
H -4.4361650000 -2.1808620000 2.0497410000
C -5.3492550000 -0.5657060000 -0.8058150000
H -4.0977010000 0.7862010000 -1.9142520000
H -6.3733920000 -1.9336600000 0.5116240000
H -6.1997650000 -0.4391770000 -1.4692980000
H 0.4656570000 1.9631680000 -1.4911240000
H 2.8146200000 1.1427580000 -0.5075980000
B 3.9303730000 -1.2750200000 -0.0302050000
F 4.1245100000 -0.7635800000 -1.3102120000
F 4.5561840000 -2.4683630000 0.1902700000
F 4.2075330000 -0.3063380000 0.9305230000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311941 (Hartree/Particle)
Thermal correction to Energy= 0.332418
Thermal correction to Enthalpy= 0.333362
Thermal correction to Gibbs (Free) Energy= 0.260329
Sum of electronic and zero-point Energies= -1019.977977
Sum of electronic and thermal Energies= -1019.957500
Sum of electronic and thermal Enthalpies= -1019.956556
Sum of electronic and thermal (Free) Energies= -1020.029589

cc/s RT

C -1.7292370000 -1.5076190000 -1.0649180000
C -0.5294330000 -1.5929970000 -0.5411630000
C 0.6799060000 -1.7517950000 -0.0330540000
C 1.7017030000 -0.6809260000 -0.1324800000
C 1.3872840000 0.7199370000 -0.3957720000
C 0.2407170000 1.3251520000 -0.0353860000
C 1.1332330000 -3.0696070000 0.5703950000
O 2.8913380000 -1.0678790000 0.0078110000
H 1.9388140000 -3.5022150000 -0.0311090000
H 0.3017400000 -3.7757310000 0.6189010000
H 1.5333850000 -2.9138600000 1.5778160000
H 2.1970010000 1.2902440000 -0.8390310000
B 4.2418680000 -0.0881010000 0.0655950000
F 4.2645430000 0.5341840000 -1.1593310000
F 5.2325780000 -0.9890780000 0.2686730000
F 3.9843140000 0.7541020000 1.1115880000
C -2.9536210000 -1.0356630000 -0.3913080000
C -4.1132530000 -0.8204850000 -1.1530970000
C -3.0001020000 -0.7911840000 0.9929360000
C -5.2850860000 -0.3634620000 -0.5516190000
H -4.0914300000 -1.0110160000 -2.2233540000
C -4.1708100000 -0.3333250000 1.5911300000
H -2.1180080000 -0.9789500000 1.5997000000
C -5.3176970000 -0.1161180000 0.8215600000
H -6.1728680000 -0.2017100000 -1.1566960000
H -4.1917520000 -0.1526180000 2.6623690000
H -6.2309290000 0.2379810000 1.2913030000
H -1.8371360000 -1.7905870000 -2.1139120000
H -0.5342540000 0.7623340000 0.4833220000
C -0.0596420000 2.7797790000 -0.2545220000
H 0.7927780000 3.2366630000 -0.7731870000
C -0.2478490000 3.4937400000 1.0993690000
H -1.0880650000 3.0628380000 1.6579280000
H 0.6509610000 3.4137030000 1.7191740000
H -0.4611850000 4.5566770000 0.9401150000
C -1.3138390000 2.9326410000 -1.1398480000
H -1.5390390000 3.9938560000 -1.2946930000
H -1.1682050000 2.4679680000 -2.1206990000
H -2.1883980000 2.4666830000 -0.6701270000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309834 (Hartree/Particle)
Thermal correction to Energy= 0.331769
Thermal correction to Enthalpy= 0.332713
Thermal correction to Gibbs (Free) Energy= 0.255780
Sum of electronic and zero-point Energies= -1019.976525
Sum of electronic and thermal Energies= -1019.954589
Sum of electronic and thermal Enthalpies= -1019.953645
Sum of electronic and thermal (Free) Energies= -1020.030578

cc/s TS

C -1.5669860000 0.5439580000 -0.2400930000
C -0.2827460000 0.1274590000 -0.2448260000
C 0.4702580000 -0.9820900000 -0.4842350000
C 1.8889040000 -0.7353710000 -0.6078100000
C 2.1821810000 0.6392280000 -0.4052700000
C 1.2306800000 1.4294820000 0.2522230000
C -0.0542660000 -2.3892660000 -0.5321320000
O 2.6949560000 -1.6664400000 -0.9438470000
H 0.3250730000 -2.8789200000 -1.4364590000
H -1.1454370000 -2.4209810000 -0.5292200000
H 0.3237810000 -2.9740860000 0.3149780000
H 3.0309330000 1.0732750000 -0.9239430000
B 4.2684080000 -1.3793430000 -0.9221940000
F 4.4831890000 -0.4346130000 -1.9140290000
F 4.8372500000 -2.5907470000 -1.1699010000
F 4.5245960000 -0.8690650000 0.3369480000
C -2.2748730000 1.2999150000 0.7843790000
C -3.4539860000 1.9926380000 0.4449660000
C -1.8520620000 1.3125050000 2.1299010000
C -4.1637820000 2.7047220000 1.4067500000
H -3.8008320000 1.9772820000 -0.5853600000
C -2.5647170000 2.0244440000 3.0899860000
H -0.9841230000 0.7294480000 2.4235380000
C -3.7183240000 2.7283110000 2.7312950000
H -5.0663190000 3.2399650000 1.1258450000
H -2.2301710000 2.0185660000 4.1235350000
H -4.2757130000 3.2789790000 3.4836250000
H -2.1510390000 0.2988680000 -1.1310430000
H 0.9277000000 1.1552000000 1.2651210000
C 1.2983770000 2.9371790000 0.0126670000
H 1.6338500000 3.0856100000 -1.0217300000
C 2.3811790000 3.5160480000 0.9518360000
H 2.0947420000 3.3904920000 2.0033760000
H 3.3502550000 3.0284680000 0.8060770000
H 2.5053400000 4.5884540000 0.7636930000
C -0.0197540000 3.7010320000 0.1897040000
H 0.1546510000 4.7678930000 0.0108940000
H -0.7847220000 3.3629120000 -0.5138860000
H -0.4194050000 3.5947620000 1.2034350000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.308880 (Hartree/Particle)
Thermal correction to Energy= 0.329646
Thermal correction to Enthalpy= 0.330590
Thermal correction to Gibbs (Free) Energy= 0.257571
Sum of electronic and zero-point Energies= -1019.940727
Sum of electronic and thermal Energies= -1019.919961
Sum of electronic and thermal Enthalpies= -1019.919017
Sum of electronic and thermal (Free) Energies= -1019.992036

cc/s PT

C -1.6927040000 -1.1999510000 -0.2335930000
C -0.4456650000 -0.6459470000 -0.1136060000
C 0.7413030000 -1.4238510000 -0.3174300000
C 1.8916120000 -0.7009830000 0.1292330000
C 1.4377130000 0.5257670000 0.6206030000
C 0.0071340000 0.7573080000 0.2967110000
C 0.8795780000 -2.8053910000 -0.8433060000
O 3.0964570000 -1.1709340000 0.0641880000
H -0.0133680000 -3.1833020000 -1.3451310000
H 1.1389610000 -3.4872910000 -0.0211560000
H 1.7336960000 -2.8382130000 -1.5296170000
C -0.0908810000 1.8056120000 -0.8918970000
H 2.0809250000 1.2422820000 1.1113260000
C -3.0224670000 -0.7047760000 0.0884640000
C -1.5246770000 2.2767030000 -1.1550510000
H -2.1985860000 1.4524950000 -1.4018450000
H -1.5301320000 2.9757370000 -1.9992260000
H -1.9389370000 2.8065170000 -0.2883800000
C 0.8453430000 3.0039280000 -0.6602670000
H 0.2682660000 1.2689710000 -1.7802220000
H 0.6302820000 3.5029390000 0.2938150000
H 0.7039630000 3.7430160000 -1.4565120000
H 1.8980950000 2.7041520000 -0.6653110000
H -0.5370860000 1.1678830000 1.1555340000
H -1.7057020000 -2.2185680000 -0.6185120000
C -4.1209840000 -1.3318850000 -0.5417200000
C -5.4255650000 -0.9246940000 -0.2874470000
C -5.6693090000 0.1002900000 0.6306070000
C -4.5989070000 0.7089520000 1.2922470000
C -3.2919390000 0.3143450000 1.0272710000
H -3.9350480000 -2.1358100000 -1.2495880000
H -6.2528580000 -1.4114320000 -0.7956490000
H -6.6881430000 0.4122260000 0.8417190000
H -4.7855190000 1.4874420000 2.0263660000
H -2.4788270000 0.7720630000 1.5769320000
B 4.2535400000 -0.1490540000 0.3063440000
F 5.4061020000 -0.8194430000 0.0171160000
F 4.1558350000 0.2630270000 1.6323270000
F 3.9995250000 0.9252020000 -0.5544070000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.312260 (Hartree/Particle)
Thermal correction to Energy= 0.332688
Thermal correction to Enthalpy= 0.333632
Thermal correction to Gibbs (Free) Energy= 0.261567
Sum of electronic and zero-point Energies= -1019.980764
Sum of electronic and thermal Energies= -1019.960335
Sum of electronic and thermal Enthalpies= -1019.959391
Sum of electronic and thermal (Free) Energies= -1020.031456

c/d RT

C -2.2056300000 0.2674360000 -1.2428970000
C -1.0468940000 -0.3471020000 -1.2756300000
C 0.0775170000 -1.0408020000 -1.3257500000
C 1.2246900000 -0.6977300000 -0.4518800000
C 1.4145100000 0.6173830000 0.1518220000
C 1.0190370000 1.7671430000 -0.4249180000
H 1.9940890000 0.6159500000 1.0672550000
H 0.5164760000 1.7277180000 -1.3898910000
C 1.2640060000 3.1539300000 0.1040440000
C 0.2191340000 -2.2892190000 -2.1790640000
H -2.3574830000 1.0907880000 -1.9438380000
C -3.3400740000 -0.0290010000 -0.3473970000
O 2.0358500000 -1.6372190000 -0.2402590000
H -0.6770120000 -2.4447630000 -2.7831330000
H 0.3827650000 -3.1647640000 -1.5433130000
H 1.0882750000 -2.2055010000 -2.8404310000
C 2.0651530000 3.9688900000 -0.9361860000
C 1.9253260000 3.1997590000 1.4857100000
H 0.2689140000 3.6241780000 0.1805240000
H 3.0715160000 3.5538820000 -1.0598480000
H 2.1624680000 5.0096000000 -0.6089560000
H 1.5747250000 3.9672140000 -1.9165020000
H 2.9307020000 2.7643030000 1.4595550000
H 1.3387820000 2.6553630000 2.2334570000
H 2.0196390000 4.2372630000 1.8231750000
C -4.5225690000 0.7155690000 -0.4794010000
C -3.2777920000 -1.0326630000 0.6345330000
C -4.3716490000 -1.2824180000 1.4570360000
H -2.3667800000 -1.6133310000 0.7505600000
C -5.5462490000 -0.5363660000 1.3163440000
H -4.3085810000 -2.0608910000 2.2123480000
C -5.6178640000 0.4632020000 0.3456590000
H -4.5814610000 1.4950210000 -1.2354990000
H -6.3981830000 -0.7338960000 1.9608270000
H -6.5259710000 1.0483130000 0.2294350000
B 3.4587830000 -1.5181150000 0.6199160000
F 3.9620490000 -2.7705830000 0.5070690000
F 3.0605530000 -1.1638170000 1.8871020000
F 4.1554520000 -0.5396210000 -0.0347680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309905 (Hartree/Particle)
Thermal correction to Energy= 0.331749
Thermal correction to Enthalpy= 0.332693
Thermal correction to Gibbs (Free) Energy= 0.255803
Sum of electronic and zero-point Energies= -1019.975119
Sum of electronic and thermal Energies= -1019.953274
Sum of electronic and thermal Enthalpies= -1019.952330
Sum of electronic and thermal (Free) Energies= -1020.029221

c/d TS

C -1.9200320000 0.5348730000 -0.8967470000
C -0.6665700000 0.0716170000 -0.8885700000
C 0.2269690000 -0.9496690000 -0.9387280000
C 1.5110190000 -0.6491710000 -0.3363170000

C 1.5971470000 0.7249530000 0.0405300000
C 0.7385520000 1.6131190000 -0.6027110000
C 0.3542040000 2.9630290000 -0.0323670000
C -0.0055640000 -2.2688210000 -1.6222150000
H -2.1067280000 1.4925940000 -1.3830240000
C -3.0822980000 -0.0848940000 -0.2553890000
O 2.3706620000 -1.5686440000 -0.1327480000
H -1.0463460000 -2.3934570000 -1.9273190000
H 0.2732130000 -3.0779670000 -0.9376080000
H 0.6434290000 -2.3686380000 -2.5002870000
C 1.3874650000 4.0214580000 -0.4798020000
C 0.1685230000 2.9570520000 1.4905710000
H -0.6059540000 3.2360240000 -0.4936530000
H 2.3735360000 3.8107320000 -0.0516450000
H 1.0758280000 5.0167770000 -0.1444230000
H 1.4929370000 4.0488910000 -1.5701330000
H 1.1118460000 2.7571420000 2.0107930000
H -0.5567110000 2.1968500000 1.8000690000
H -0.1938400000 3.9325250000 1.8323250000
C -4.3510990000 0.4916180000 -0.4534130000
C -2.9834600000 -1.2400900000 0.5442310000
C -4.1213600000 -1.8057160000 1.1094310000
H -2.0088120000 -1.6802470000 0.7324850000
C -5.3780100000 -1.2306840000 0.8940040000
H -4.0287330000 -2.6949090000 1.7266340000
C -5.4884270000 -0.0793430000 0.1116570000
H -4.4396090000 1.3880140000 -1.0625760000
H -6.2637980000 -1.6745840000 1.3393050000
H -6.4604380000 0.3760100000 -0.0558750000
H 0.6909710000 1.5772880000 -1.6916420000
H 2.2013210000 0.9962990000 0.8990860000
B 3.8268730000 -1.1744910000 0.4092830000
F 4.2871350000 -0.2114730000 -0.4673840000
F 4.5218190000 -2.3439320000 0.3870150000
F 3.6161420000 -0.6594540000 1.6790430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309031 (Hartree/Particle)
Thermal correction to Energy= 0.329909
Thermal correction to Enthalpy= 0.330853
Thermal correction to Gibbs (Free) Energy= 0.257297
Sum of electronic and zero-point Energies= -1019.949584
Sum of electronic and thermal Energies= -1019.928707
Sum of electronic and thermal Enthalpies= -1019.927762
Sum of electronic and thermal (Free) Energies= -1020.001318

c/d PT

C 1.8753820000 0.7905280000 0.5677370000
C 0.5505010000 0.4638230000 0.4282570000
C -0.0980510000 -0.7889100000 0.2208230000
C -1.5218160000 -0.6021220000 0.1820530000
C -1.7830500000 0.7527300000 0.4218570000
C -0.5369830000 1.5252440000 0.6295450000
C -0.4186470000 2.8181120000 -0.2400110000
C 0.4487060000 -2.1709320000 0.1714420000
H 2.0599140000 1.7861270000 0.9732930000
C 3.0918310000 0.0634500000 0.2402110000
O -2.3387360000 -1.5833640000 -0.0139510000
H 1.4624630000 -2.2511260000 0.5651590000
H 0.4465810000 -2.5415470000 -0.8635450000
H -0.2325750000 -2.8328580000 0.7173390000
C -1.4426080000 3.8719540000 0.2067260000
C -0.5438130000 2.5193350000 -1.7404760000
H 0.5817030000 3.2326260000 -0.0533280000
H -2.4708090000 3.5395660000 0.0233410000
H -1.2963280000 4.8036440000 -0.3507620000
H -1.3477030000 4.1020480000 1.2746460000
H -1.5392990000 2.1306690000 -1.9850220000
H 0.1954970000 1.7815410000 -2.0713970000
H -0.3882280000 3.4324790000 -2.3253600000
C 4.2641980000 0.3490940000 0.9740230000
C 3.1792480000 -0.8505230000 -0.8308830000
C 4.3821850000 -1.4840060000 -1.1256460000
H 2.3102360000 -1.0251090000 -1.4554830000
C 5.5219260000 -1.2220630000 -0.3598470000
H 4.4352200000 -2.1750480000 -1.9619090000
C 5.4598150000 -0.3008430000 0.6900850000
H 4.2197210000 1.0738680000 1.7830650000
H 6.4590620000 -1.7198180000 -0.5920080000
H 6.3466760000 -0.0831700000 1.2780360000
H -0.4869070000 1.8490710000 1.6852230000
H -2.7804500000 1.1696620000 0.4468530000
B -3.8738050000 -1.2706220000 0.0060550000
F -4.1405550000 -0.7250910000 1.2580710000
F -4.4912190000 -2.4667760000 -0.2210470000
F -4.0869810000 -0.3261140000 -0.9950440000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311706 (Hartree/Particle)
Thermal correction to Energy= 0.331954
Thermal correction to Enthalpy= 0.332898
Thermal correction to Gibbs (Free) Energy= 0.261018
Sum of electronic and zero-point Energies= -1019.982133
Sum of electronic and thermal Energies= -1019.961885
Sum of electronic and thermal Enthalpies= -1019.960941
Sum of electronic and thermal (Free) Energies= -1020.032821

cc/d RT

C -1.8432720000 -1.2728530000 -1.1853500000
C -0.6516220000 -1.4824090000 -0.6782250000
C 0.5474250000 -1.7650930000 -0.2004220000
C 1.6092150000 -0.7317070000 -0.1310900000
C 1.3528310000 0.7046310000 -0.1662240000
C 0.2339450000 1.2852290000 0.3054930000
C 0.9470860000 -3.1779000000 0.1876450000
O 2.7830290000 -1.1813920000 -0.0571620000
H 1.7391130000 -3.5409350000 -0.4747820000
H 0.0891780000 -3.8504860000 0.1246030000
H 1.3470620000 -3.1981890000 1.2069100000
H 2.1871030000 1.2991070000 -0.5186430000
B 4.1675650000 -0.2721050000 0.1384470000
F 4.2189150000 0.5149020000 -0.9871030000
F 5.1235910000 -1.2286680000 0.2131580000
F 3.9387250000 0.4264880000 1.2921370000
C -3.0572470000 -0.8708160000 -0.4505150000
C -4.2039150000 -0.5049450000 -1.1735170000
C -3.1067790000 -0.8400420000 0.9547420000
C -5.3657650000 -0.1089090000 -0.5124230000
H -4.1797210000 -0.5296920000 -2.2602680000
C -4.2673570000 -0.4423230000 1.6127440000
H -2.2355490000 -1.1462520000 1.5280800000
C -5.4011690000 -0.0738030000 0.8823400000
H -6.2435030000 0.1715580000 -1.0880520000
H -4.2907620000 -0.4268600000 2.6989490000
H -6.3065610000 0.2329700000 1.3982760000
H -1.9514240000 -1.3833910000 -2.2661930000
H -0.5545220000 0.6635250000 0.7258110000
C -0.0463740000 2.7630220000 0.3443970000
H -0.2277870000 3.0066580000 1.4042380000
C -1.3641060000 3.0538180000 -0.4103450000
H -1.2499590000 2.8478220000 -1.4807540000
H -2.1909080000 2.4416480000 -0.0337890000
H -1.6399980000 4.1075330000 -0.2947160000
C 1.1012080000 3.6435030000 -0.1612320000
H 0.8384600000 4.7011940000 -0.0540000000
H 2.0246810000 3.4661720000 0.3996090000
H 1.3073390000 3.4583560000 -1.2220430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310019 (Hartree/Particle)
Thermal correction to Energy= 0.331815
Thermal correction to Enthalpy= 0.332759
Thermal correction to Gibbs (Free) Energy= 0.256362
Sum of electronic and zero-point Energies= -1019.975532
Sum of electronic and thermal Energies= -1019.953736
Sum of electronic and thermal Enthalpies= -1019.952791
Sum of electronic and thermal (Free) Energies= -1020.029188

cc/d TS

C 1.5679350000 -1.1921720000 0.8838050000
C 0.3185850000 -0.9471010000 0.4446370000
C -0.9137370000 -1.5079840000 0.2976030000
C -1.9875600000 -0.5593580000 0.1082560000
C -1.4883520000 0.7716300000 0.0567920000
C -0.1286400000 0.9505420000 -0.2245120000
C -1.1915560000 -2.9832390000 0.2412580000
O -3.2055350000 -0.9393580000 0.0831480000

H -1.9904030000 -3.2213030000 0.9533540000
H -0.3054620000 -3.5763650000 0.4751610000
H -1.5669540000 -3.2705190000 -0.7480890000
H -2.1227220000 1.5843280000 0.3945720000
B -4.3497530000 0.1221940000 -0.2729190000
F -4.3380230000 1.0373460000 0.7684880000
F -5.4869030000 -0.6212380000 -0.3523860000
F -3.9499800000 0.6946220000 -1.4654110000
C 2.8387150000 -0.8343970000 0.2627910000
C 3.9944050000 -0.7229620000 1.0611570000
C 2.9644840000 -0.6578040000 -1.1302240000
C 5.2254790000 -0.4100250000 0.4922260000
H 3.9151770000 -0.8752140000 2.1347670000
C 4.1979360000 -0.3494270000 -1.6968590000
H 2.0965800000 -0.7997210000 -1.7675990000
C 5.3305710000 -0.2181610000 -0.8880400000
H 6.1047460000 -0.3196220000 1.1236270000
H 4.2799610000 -0.2242280000 -2.7728220000
H 6.2927870000 0.0178490000 -1.3333990000
H 1.6418960000 -1.6920060000 1.8531150000
H 0.2687430000 0.5301990000 -1.1500160000
C 0.5488760000 2.2377610000 0.2486030000
H -0.2467500000 2.9963790000 0.2024260000
C 1.6814390000 2.7065370000 -0.6749530000
H 2.5339140000 2.0211720000 -0.6511130000
H 1.3398870000 2.7899650000 -1.7134150000
H 2.0378580000 3.6943920000 -0.3630780000
C 0.9989730000 2.1745690000 1.7217300000
H 1.2963290000 3.1722300000 2.0629310000
H 0.1895920000 1.8225790000 2.3702340000
H 1.8567140000 1.5067530000 1.8469120000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.308707 (Hartree/Particle)
Thermal correction to Energy= 0.329577
Thermal correction to Enthalpy= 0.330521
Thermal correction to Gibbs (Free) Energy= 0.257151
Sum of electronic and zero-point Energies= -1019.942098
Sum of electronic and thermal Energies= -1019.921228
Sum of electronic and thermal Enthalpies= -1019.920284
Sum of electronic and thermal (Free) Energies= -1019.993654

cc/d PT

C -1.6562380000 -1.1290080000 -0.2570110000
C -0.4196140000 -0.5789950000 -0.0407170000
C 0.7790220000 -1.3346520000 -0.2472990000
C 1.9104020000 -0.6219330000 0.2608220000
C 1.4367170000 0.5858830000 0.7797280000
C -0.0053400000 0.7920710000 0.4949810000
C 0.9468570000 -2.6842230000 -0.8429940000
O 3.1205120000 -1.0793890000 0.1865260000
H 0.0885180000 -3.0230000000 -1.4270570000
H 1.1404000000 -3.4172720000 -0.0469610000
H 1.8475030000 -2.6837700000 -1.4671640000
C -0.1416080000 2.0134730000 -0.5095140000
H 2.0767310000 1.3257180000 1.2440040000
C -2.9982060000 -0.6725090000 0.0704520000
C 0.6564460000 1.8074680000 -1.8058550000
H 1.7227860000 1.6489620000 -1.6172170000
H 0.5536830000 2.6931150000 -2.4425720000
H 0.2782770000 0.9501050000 -2.3767210000
C -1.5936230000 2.4027450000 -0.8067690000
H 0.3177190000 2.8512560000 0.0332320000
H -2.1089030000 1.6340300000 -1.3920690000
H -1.6084880000 3.3291450000 -1.3922570000
H -2.1735320000 2.5781020000 0.1054360000
H -0.5528720000 1.0687230000 1.4051230000
H -1.6477750000 -2.1031450000 -0.7442720000
C -4.0715880000 -1.1906650000 -0.6881250000
C -5.3836270000 -0.8119140000 -0.4280770000
C -5.6602530000 0.0669600000 0.6228040000
C -4.6159100000 0.5585710000 1.4112360000
C -3.3005650000 0.1962900000 1.1406330000
H -3.8597700000 -1.8828720000 -1.4992360000
H -6.1917900000 -1.2089810000 -1.0353430000
H -6.6857110000 0.3535010000 0.8377930000
H -4.8298950000 1.2181060000 2.2473090000
H -2.5071520000 0.5537230000 1.7859740000
B 4.2711210000 -0.0358370000 0.3285750000
F 5.4256680000 -0.7200220000 0.0811840000
F 4.1936570000 0.4886370000 1.6170980000
F 3.9943800000 0.9571040000 -0.6181540000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.312287 (Hartree/Particle)
Thermal correction to Energy= 0.332638
Thermal correction to Enthalpy= 0.333583
Thermal correction to Gibbs (Free) Energy= 0.262169
Sum of electronic and zero-point Energies= -1019.981893
Sum of electronic and thermal Energies= -1019.961541
Sum of electronic and thermal Enthalpies= -1019.960597
Sum of electronic and thermal (Free) Energies= -1020.032010

c/u RT

C -2.1173790000 -0.0390000000 -1.2858360000
C -0.9134320000 -0.5603500000 -1.2763030000
C 0.2621710000 -1.1651760000 -1.2742390000
C 1.3891670000 -0.6389960000 -0.4676420000
C 1.4850750000 0.7470530000 -0.0199600000
C 0.9961960000 1.7911790000 -0.7138750000
H 2.0775630000 0.8928950000 0.8751820000
H 0.4771800000 1.6046240000 -1.6525670000
C 1.1224010000 3.2426420000 -0.3381100000
C 0.4921040000 -2.4862640000 -1.9874920000
H -2.3444430000 0.6864550000 -2.0696400000
C -3.2118590000 -0.3212560000 -0.3375600000
O 2.2728310000 -1.4843180000 -0.1680510000
H -0.3960180000 -2.7770920000 -2.5521400000
H 0.7321510000 -3.2701380000 -1.2626220000
H 1.3439170000 -2.4097140000 -2.6718740000
C 1.9100560000 3.4998710000 0.9509200000
C -0.2838180000 3.8818290000 -0.2834360000
H 1.6585390000 3.7248050000 -1.1721690000
H 1.4083290000 3.0560200000 1.8188500000
H 1.9951880000 4.5766900000 1.1308470000
H 2.9221740000 3.0861190000 0.8954110000
H -0.8764340000 3.4489230000 0.5303450000
H -0.8332020000 3.7317320000 -1.2201180000
H -0.2028120000 4.9601490000 -0.1096610000
C -4.4514780000 0.3104930000 -0.5229930000
C -3.0561430000 -1.2020950000 0.7465690000
C -4.1148680000 -1.4428920000 1.6163610000
H -2.1004260000 -1.6943240000 0.9043700000
C -5.3468260000 -0.8099730000 1.4219700000
H -3.9794810000 -2.1257190000 2.4505730000
C -5.5113810000 0.0673050000 0.3496830000
H -4.5828610000 0.9943840000 -1.3582850000
H -6.1711100000 -1.0001140000 2.1035640000
H -6.4646100000 0.5639980000 0.1910290000
B 3.6903040000 -1.1620870000 0.6494070000
F 4.2895140000 -2.3766710000 0.6634130000
F 3.2756550000 -0.7038910000 1.8772640000
F 4.3017510000 -0.2095420000 -0.1186830000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309938 (Hartree/Particle)
Thermal correction to Energy= 0.331775
Thermal correction to Enthalpy= 0.332719
Thermal correction to Gibbs (Free) Energy= 0.255904
Sum of electronic and zero-point Energies= -1019.974941
Sum of electronic and thermal Energies= -1019.953103
Sum of electronic and thermal Enthalpies= -1019.952159
Sum of electronic and thermal (Free) Energies= -1020.028974

c/u TS

C -1.8563250000 0.4738720000 -0.8475400000
C -0.5634070000 0.1268140000 -0.8404690000
C 0.3869840000 -0.8388040000 -0.9337770000
C 1.6592450000 -0.4927230000 -0.3326090000
C 1.6788900000 0.8667950000 0.0924920000
C 0.7550200000 1.7367060000 -0.4871130000
C 0.3660050000 3.0383750000 0.1986020000
C 0.2214840000 -2.1406730000 -1.6681760000
H -2.1320920000 1.4173470000 -1.3150280000
C -2.9560540000 -0.2719450000 -0.2316590000
O 2.5708370000 -1.3719410000 -0.1782650000
H -0.8160420000 -2.3188590000 -1.9571750000

H 0.5673120000 -2.9576170000 -1.0248470000
H 0.8549510000 -2.1618540000 -2.5629230000
C -0.2518780000 2.8188280000 1.5910580000
C -0.5140460000 3.9361960000 -0.6838280000
H 1.3221010000 3.5669230000 0.3452760000
H -1.2166880000 2.3055670000 1.5157250000
H -0.4161370000 3.7801720000 2.0896100000
H 0.4013920000 2.2170250000 2.2308680000
H -1.5148310000 3.5110230000 -0.8214390000
H -0.0689930000 4.0893580000 -1.6738850000
H -0.6408840000 4.9201250000 -0.2203720000
C -4.2751490000 0.1733320000 -0.4425280000
C -2.7497880000 -1.4219770000 0.5552250000
C -3.8312860000 -2.1111930000 1.0932480000
H -1.7375760000 -1.7599750000 0.7554790000
C -5.1374240000 -1.6666460000 0.8638910000
H -3.6562660000 -2.9946250000 1.7007340000
C -5.3552540000 -0.5211280000 0.0953770000
H -4.4471580000 1.0647620000 -1.0410150000
H -5.9789630000 -2.2065660000 1.2884560000
H -6.3667250000 -0.1667470000 -0.0821500000
H 0.6820520000 1.7578420000 -1.5748070000
H 2.2993860000 1.1469260000 0.9372510000
B 4.0129050000 -0.9236320000 0.3557860000
F 4.4121470000 0.0887910000 -0.4947240000
F 4.7644870000 -2.0558850000 0.2855720000
F 3.7980130000 -0.4609180000 1.6451800000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.308903 (Hartree/Particle)
Thermal correction to Energy= 0.329797
Thermal correction to Enthalpy= 0.330741
Thermal correction to Gibbs (Free) Energy= 0.257265
Sum of electronic and zero-point Energies= -1019.947403
Sum of electronic and thermal Energies= -1019.926509
Sum of electronic and thermal Enthalpies= -1019.925565
Sum of electronic and thermal (Free) Energies= -1019.999041

c/u PT

C -1.8341780000 0.7353110000 -0.6138350000
C -0.4907470000 0.4705330000 -0.5186810000
C 0.2063790000 -0.7634140000 -0.3279970000
C 1.6213450000 -0.5426750000 -0.4118150000
C 1.8204830000 0.7913690000 -0.7794280000
C 0.5542690000 1.5555400000 -0.7938650000
C 0.6495020000 2.7610190000 0.2141300000
C -0.2959640000 -2.1548690000 -0.1738640000
H -2.0801370000 1.7103540000 -1.0318600000
C -3.0042840000 -0.0468330000 -0.2400170000
O 2.4883900000 -1.4788070000 -0.1983940000
H -1.3198790000 -2.2878200000 -0.5249160000
H -0.2515090000 -2.4547180000 0.8829680000
H 0.3846460000 -2.8332110000 -0.6988390000
C 0.9539610000 2.2994050000 1.6476550000
C -0.5688000000 3.6932010000 0.1676970000
H 1.5139340000 3.3403630000 -0.1397990000
H 0.1349750000 1.6913770000 2.0517530000
H 1.0711890000 3.1686430000 2.3041760000
H 1.8743860000 1.7081560000 1.7003920000
H -1.4519290000 3.2277020000 0.6199140000
H -0.8213600000 3.9891790000 -0.8582690000
H -0.3593880000 4.6087850000 0.7320470000
C -4.1997700000 0.1394660000 -0.9679570000
C -3.0275800000 -0.9110320000 0.8742960000
C -4.1902470000 -1.5937620000 1.2180900000
H -2.1417590000 -1.0079400000 1.4923400000
C -5.3521770000 -1.4315530000 0.4584860000
H -4.1942560000 -2.2452470000 2.0871500000
C -5.3540510000 -0.5602580000 -0.6350730000
H -4.2060290000 0.8265120000 -1.8104310000
H -6.2575940000 -1.9674460000 0.7285610000
H -6.2590080000 -0.4196990000 -1.2189720000
H 0.3657380000 1.9852380000 -1.7917870000
H 2.7977720000 1.2169230000 -0.9689260000
B 3.9637390000 -1.0233310000 0.0504830000
F 4.4105240000 -0.4300300000 -1.1276060000
F 4.6460970000 -2.1544730000 0.3917020000
F 3.8928840000 -0.0775770000 1.0772700000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.312262 (Hartree/Particle)
Thermal correction to Energy= 0.332483
Thermal correction to Enthalpy= 0.333427
Thermal correction to Gibbs (Free) Energy= 0.262265
Sum of electronic and zero-point Energies= -1019.979789
Sum of electronic and thermal Energies= -1019.959568
Sum of electronic and thermal Enthalpies= -1019.958623
Sum of electronic and thermal (Free) Energies= -1020.029785

cc/u RT

C -1.9112660000 -1.4430330000 -1.1084340000
C -0.7277890000 -1.5952100000 -0.5632510000
C 0.4616680000 -1.8180980000 -0.0326570000
C 1.5402840000 -0.8033610000 -0.1158590000
C 1.3072850000 0.6104280000 -0.3925680000
C 0.1896210000 1.2744780000 -0.0440220000
C 0.8321920000 -3.1559130000 0.5829230000
O 2.7051230000 -1.2516230000 0.0509550000
H 1.6251340000 -3.6330210000 -0.0015060000
H -0.0365180000 -3.8166250000 0.6169420000
H 1.2204440000 -3.0180780000 1.5975840000
H 2.1536540000 1.1267360000 -0.8296140000
B 4.1007100000 -0.3424430000 0.1233130000
F 4.1823070000 0.2554700000 -1.1116350000
F 5.0401390000 -1.2879120000 0.3649610000
F 3.8662760000 0.5332450000 1.1478400000
C -3.1178710000 -0.8992330000 -0.4572080000
C -4.2508290000 -0.6231100000 -1.2389700000
C -3.1726660000 -0.6446860000 0.9248110000
C -5.4041100000 -0.0963060000 -0.6592130000
H -4.2225750000 -0.8208570000 -2.3077880000
C -4.3245990000 -0.1168960000 1.5013290000
H -2.3129420000 -0.8796700000 1.5470550000
C -5.4445050000 0.1610940000 0.7118740000
H -6.2713770000 0.1121570000 -1.2795770000
H -4.3525750000 0.0708980000 2.5712010000
H -6.3433590000 0.5698210000 1.1647070000
H -2.0170080000 -1.7227780000 -2.1584900000
H -0.6094940000 0.7434520000 0.4699760000
C -0.0641640000 2.7440500000 -0.2413290000
H -0.9918170000 2.8070810000 -0.8350380000
C 1.0436520000 3.4869480000 -0.9956700000
H 1.9856730000 3.4704380000 -0.4357640000
H 1.2277900000 3.0472720000 -1.9817700000
H 0.7609720000 4.5346350000 -1.1429570000
C -0.3642570000 3.4031680000 1.1236460000
H -0.6497180000 4.4513000000 0.9836840000
H -1.1848260000 2.8958690000 1.6437690000
H 0.5196420000 3.3734270000 1.7704720000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310009 (Hartree/Particle)
Thermal correction to Energy= 0.331799
Thermal correction to Enthalpy= 0.332743
Thermal correction to Gibbs (Free) Energy= 0.256389
Sum of electronic and zero-point Energies= -1019.975593
Sum of electronic and thermal Energies= -1019.953803
Sum of electronic and thermal Enthalpies= -1019.952859
Sum of electronic and thermal (Free) Energies= -1020.029212

cc/u TS

C -1.6588070000 -1.3365870000 -0.8175220000
C -0.4128240000 -1.1376590000 -0.3573070000
C 0.8264560000 -1.6619420000 -0.1646400000
C 1.8845660000 -0.6775770000 -0.0612410000
C 1.3594640000 0.6468940000 -0.0989350000
C 0.0138370000 0.8075060000 0.2315960000
C 1.1333600000 -3.1233410000 0.0023350000
O 3.1092500000 -1.0320460000 -0.0404570000
H 1.9106250000 -3.4073990000 -0.7169600000
H 0.2503370000 -3.7462360000 -0.1524290000
H 1.5473370000 -3.3226380000 0.9976760000
H 1.9605460000 1.4347620000 -0.5393470000
B 4.2409250000 0.0765510000 0.2010830000
F 4.1822690000 0.9057790000 -0.9083100000
F 5.3944630000 -0.6372320000 0.3069610000
F 3.8596650000 0.7327930000 1.3554040000

C -2.9203420000 -0.8609670000 -0.2549390000
C -4.0481740000 -0.7476570000 -1.0915930000
C -3.0659360000 -0.5488780000 1.1124660000
C -5.2690400000 -0.3089840000 -0.5874140000
H -3.9544980000 -0.9978190000 -2.1454610000
C -4.2878850000 -0.1084650000 1.6132760000
H -2.2263990000 -0.6913330000 1.7866330000
C -5.3921040000 0.0171200000 0.7657330000
H -6.1262120000 -0.2225520000 -1.2491210000
H -4.3842490000 0.1217990000 2.6705920000
H -6.3461700000 0.3542940000 1.1606750000
H -1.7378590000 -1.8728440000 -1.7664550000
H -0.3279960000 0.4041790000 1.1859810000
C -0.8072230000 1.9890120000 -0.2448300000
H -1.8578920000 1.6748080000 -0.2026020000
C -0.4900620000 2.4169750000 -1.6840200000
H 0.5270220000 2.8139890000 -1.7762100000
H -0.5888280000 1.5764550000 -2.3797110000
H -1.1796880000 3.2054130000 -2.0042960000
C -0.6425040000 3.1604790000 0.7489980000
H -1.2892510000 3.9952160000 0.4570100000
H -0.9119760000 2.8653300000 1.7693350000
H 0.3922570000 3.5205600000 0.7646700000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.308768 (Hartree/Particle)
Thermal correction to Energy= 0.329662
Thermal correction to Enthalpy= 0.330606
Thermal correction to Gibbs (Free) Energy= 0.257258
Sum of electronic and zero-point Energies= -1019.947341
Sum of electronic and thermal Energies= -1019.926448
Sum of electronic and thermal Enthalpies= -1019.925504
Sum of electronic and thermal (Free) Energies= -1019.998852

cc/u PT

C -1.7299370000 -1.2520860000 -0.0077540000
C -0.4790790000 -0.7192280000 0.1712070000
C 0.7133860000 -1.4949380000 0.0386360000
C 1.8629220000 -0.6912610000 0.3262260000
C 1.4025230000 0.5768080000 0.6895490000
C -0.0647620000 0.7088050000 0.5133460000
C 0.8729540000 -2.9247390000 -0.3267180000
O 3.0751450000 -1.1364540000 0.2275670000
H -0.0444760000 -3.4064310000 -0.6700550000
H 1.2627620000 -3.4799750000 0.5376030000
H 1.6479900000 -3.0087510000 -1.0981170000
C -0.4182800000 1.7788920000 -0.5881540000
H 2.0598070000 1.3753800000 1.0066210000
C -3.0591090000 -0.6806330000 0.1134930000
C -0.1279420000 3.1957040000 -0.0721930000
H -0.6484980000 3.4003430000 0.8716690000
H -0.4613810000 3.9392030000 -0.8045000000
H 0.9437780000 3.3556940000 0.0905700000
C 0.3030030000 1.5102800000 -1.9180440000
H -1.4993340000 1.6986950000 -0.7591650000
H 1.3918950000 1.5688380000 -1.8109210000
H -0.0077240000 2.2502730000 -2.6638780000
H 0.0597170000 0.5192610000 -2.3173860000
H -0.5306380000 1.0395970000 1.4534860000
H -1.7468250000 -2.2976330000 -0.3103640000
C -4.1284060000 -1.4109940000 -0.4552870000
C -5.4346290000 -0.9399620000 -0.4008620000
C -5.7130200000 0.2672460000 0.2454670000
C -4.6756670000 0.9927390000 0.8390600000
C -3.3664080000 0.5286560000 0.7776020000
H -3.9156850000 -2.3523030000 -0.9557130000
H -6.2364430000 -1.5144830000 -0.8552720000
H -6.7337470000 0.6349400000 0.2980810000
H -4.8910750000 1.9204590000 1.3611710000
H -2.5856700000 1.0895450000 1.2754230000
B 4.2051420000 -0.0615390000 0.1414360000
F 5.3537120000 -0.7518350000 -0.1164810000
F 4.2171090000 0.6164880000 1.3582830000
F 3.8251100000 0.8014510000 -0.8918490000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.312259 (Hartree/Particle)
Thermal correction to Energy= 0.332725
Thermal correction to Enthalpy= 0.333669
Thermal correction to Gibbs (Free) Energy= 0.261785
Sum of electronic and zero-point Energies= -1019.987489
Sum of electronic and thermal Energies= -1019.967023
Sum of electronic and thermal Enthalpies= -1019.966079
Sum of electronic and thermal (Free) Energies= -1020.037963

5d

cRT

C -2.3502340000 0.1661150000 -1.2343550000
C -1.3581810000 -0.6922450000 -1.2696390000
C -0.4180190000 -1.6200560000 -1.3109480000
C 0.8082560000 -1.5061590000 -0.4822310000
C 1.3507540000 -0.2446370000 -0.0121150000
C 1.1724970000 0.9360150000 -0.6517810000
H 1.9931270000 -0.3284660000 0.8560590000
H 0.5861040000 0.9460860000 -1.5669180000
C 1.7250120000 2.2279770000 -0.2631680000
C -0.5919980000 -2.9101400000 -2.0938790000
H -2.3471720000 0.9710850000 -1.9721680000
C -3.4838430000 0.1692770000 -0.2899720000
O 1.3533010000 -2.6060850000 -0.1876440000
H -1.5198330000 -2.8874380000 -2.6690930000
H -0.6101840000 -3.7655050000 -1.4117320000
H 0.2507600000 -3.0613020000 -2.7772290000
C 1.4513200000 3.3461470000 -1.0743490000
C 2.5168450000 2.4117120000 0.8889530000
C -4.4775830000 1.1513880000 -0.4240040000
C -3.6037820000 -0.7787950000 0.7406170000
C -4.6906460000 -0.7427510000 1.6082810000
H -2.8390220000 -1.5414990000 0.8587960000
C -5.6767320000 0.2386750000 1.4651330000
H -4.7692580000 -1.4816600000 2.4009740000
C -5.5663580000 1.1854130000 0.4463320000
H -4.3942920000 1.8906530000 -1.2172720000
H -6.5236960000 0.2640550000 2.1450040000
H -6.3270120000 1.9521900000 0.3278380000
B 2.7874080000 -2.7932080000 0.6198790000
F 3.6951630000 -2.1327570000 -0.1627030000
F 2.9208390000 -4.1414310000 0.6604830000
F 2.5786660000 -2.1975070000 1.8444330000
C 1.9452030000 4.6063600000 -0.7487370000
C 2.7260130000 4.7712040000 0.3966130000
C 3.0099230000 3.6700400000 1.2122650000
H 0.8449300000 3.2168600000 -1.9677530000
H 1.7235660000 5.4571150000 -1.3867160000
H 3.1153280000 5.7523550000 0.6537810000
H 3.6203430000 3.7958040000 2.1018430000
H 2.7501610000 1.5664050000 1.5283420000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.306262 (Hartree/Particle)
Thermal correction to Energy= 0.328472
Thermal correction to Enthalpy= 0.329416
Thermal correction to Gibbs (Free) Energy= 0.250496
Sum of electronic and zero-point Energies= -1133.093800
Sum of electronic and thermal Energies= -1133.071590
Sum of electronic and thermal Enthalpies= -1133.070646
Sum of electronic and thermal (Free) Energies= -1133.149565

cTS

C -1.7841690000 -0.3116250000 -0.9199610000
C -0.4742060000 -0.5764940000 -0.8999140000
H -2.1114370000 0.5911790000 -1.4360040000
C -2.8374530000 -1.0685600000 -0.2416370000
C 0.5633300000 -1.4544970000 -0.8792600000
C -4.1788540000 -0.6980000000 -0.4550170000
C -2.5658100000 -2.1582330000 0.6087270000
C 1.7873660000 -0.9171800000 -0.3186380000
C 0.5358820000 -2.8422850000 -1.4564090000
C -5.2170100000 -1.4067570000 0.1435900000
H -4.4006710000 0.1473130000 -1.1018700000
C -3.6052560000 -2.8617150000 1.2074600000
H -1.5360470000 -2.4372640000 0.8104310000
C 1.6774550000 0.4806190000 -0.0781290000
O 2.7738590000 -1.6832010000 -0.0497910000
H 0.9252420000 -3.5443960000 -0.7102240000
H 1.2037920000 -2.9121150000 -2.3232410000

H -0.4711240000 -3.1443500000 -1.7505380000
C -4.9341900000 -2.4919850000 0.9756740000
H -6.2465520000 -1.1101580000 -0.0361210000
H -3.3798770000 -3.6975950000 1.8637360000
C 0.6633060000 1.1623670000 -0.7697830000
H 2.2824840000 0.9435270000 0.6925690000
B 4.1599010000 -1.0434260000 0.4220680000
H -5.7429450000 -3.0429530000 1.4472420000
H 0.6217340000 1.0466720000 -1.8530080000
C 0.0617990000 2.4155910000 -0.2890560000
F 4.4910650000 -0.1318670000 -0.5615670000
F 5.0060970000 -2.1055250000 0.5212100000
F 3.8862020000 -0.4205350000 1.6315670000
C -0.4789070000 3.3269420000 -1.2127100000
C 0.0006490000 2.7235550000 1.0819160000
C -1.0486740000 4.5232230000 -0.7818980000
H -0.4337770000 3.1001410000 -2.2757650000
C -0.5657650000 3.9198350000 1.5114140000
H 0.3915740000 2.0164770000 1.8081670000
C -1.0911030000 4.8223240000 0.5813970000
H -1.4542330000 5.2225020000 -1.5075300000
H -0.6039890000 4.1480690000 2.5726840000
H -1.5351540000 5.7542650000 0.9199850000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.305322 (Hartree/Particle)
Thermal correction to Energy= 0.326491
Thermal correction to Enthalpy= 0.327435
Thermal correction to Gibbs (Free) Energy= 0.252372
Sum of electronic and zero-point Energies= -1133.068227
Sum of electronic and thermal Energies= -1133.047058
Sum of electronic and thermal Enthalpies= -1133.046113
Sum of electronic and thermal (Free) Energies= -1133.121176

cPT

C -1.8215190000 0.0472320000 -0.7157140000
C -0.4768460000 -0.1765780000 -0.5687490000
C 0.2673260000 -1.3352740000 -0.2164510000
C 1.6696180000 -1.0215050000 -0.1445110000
C 1.8286110000 0.3201320000 -0.5132480000
C 0.5370700000 0.9370150000 -0.9032490000
C 0.2696570000 2.3061660000 -0.2934710000
C -0.1638200000 -2.7490980000 -0.0542250000
C -2.9768310000 -0.7095210000 -0.2648080000
O 2.5506220000 -1.9066810000 0.1807260000
H -1.1732630000 -2.9409710000 -0.4185550000
H -0.1090100000 -3.0401220000 1.0042330000
H 0.5613600000 -3.3923650000 -0.5658410000
C 0.4219190000 2.5124910000 1.0850840000
C -0.1279510000 3.3785490000 -1.0991360000
C -4.1904290000 -0.5655420000 -0.9731200000
C -2.9685350000 -1.5197470000 0.8904220000
C -4.1176030000 -2.1926380000 1.2919830000
H -2.0695790000 -1.5797450000 1.4936750000
C -5.2980500000 -2.0738690000 0.5522970000
H -4.0977400000 -2.8016430000 2.1910960000
C -5.3317040000 -1.2552700000 -0.5806350000
H -4.2202520000 0.0802310000 -1.8470360000
H -6.1930580000 -2.6019170000 0.8685590000
H -6.2510060000 -1.1476840000 -1.1488610000
H 0.5190830000 1.0516450000 -2.0014020000
B 4.0654790000 -1.5058760000 0.0815980000
F 4.2679140000 -1.1143350000 -1.2367860000
F 4.7579180000 -2.6257610000 0.4424610000
F 4.2385890000 -0.4313520000 0.9482990000
H -2.0752680000 0.9795050000 -1.2214840000
H 2.7765040000 0.8412480000 -0.5152730000
C -0.3791770000 4.6336910000 -0.5401650000
C 0.1735200000 3.7645530000 1.6437520000
C -0.2297380000 4.8287970000 0.8326370000
H -0.6839780000 5.4575820000 -1.1796670000
H -0.4198520000 5.8053740000 1.2690800000
H -0.2324130000 3.2357030000 -2.1727600000
H 0.7430930000 1.6900390000 1.7197350000
H 0.3001230000 3.9114650000 2.7127940000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.307676 (Hartree/Particle)
Thermal correction to Energy= 0.328624
Thermal correction to Enthalpy= 0.329568
Thermal correction to Gibbs (Free) Energy= 0.254663
Sum of electronic and zero-point Energies= -1133.094900
Sum of electronic and thermal Energies= -1133.073952
Sum of electronic and thermal Enthalpies= -1133.073008
Sum of electronic and thermal (Free) Energies= -1133.147913

ccRT

C -1.5309770000 -2.0792380000 -1.1645850000
H -1.6008430000 -2.3003390000 -2.2314310000
C -0.3383890000 -2.1177060000 -0.6184090000
C -2.7960940000 -1.7312800000 -0.4906350000
C 0.8689180000 -2.2214820000 -0.0933900000
C -3.9535080000 -1.5435540000 -1.2627660000
C -2.8837610000 -1.5765090000 0.9047570000
C 1.4036920000 -3.5410960000 0.4354030000
C 1.8194810000 -1.0796730000 -0.1070670000
H -3.8999400000 -1.6652420000 -2.3418660000
C -5.1629330000 -1.1988940000 -0.6609390000
H -2.0036270000 -1.7490680000 1.5189370000
C -4.0922140000 -1.2295860000 1.5037970000
H 2.2440970000 -3.8794630000 -0.1785140000
H 0.6216270000 -4.3031710000 0.4266290000
H 1.7798300000 -3.4219840000 1.4570560000
O 3.0355210000 -1.4078830000 -0.0183280000
C 1.4228340000 0.3101150000 -0.2343470000
H -6.0480960000 -1.0567830000 -1.2747540000
C -5.2364860000 -1.0375060000 0.7234330000
H -4.1444060000 -1.1188870000 2.5835250000
B 4.3173300000 -0.3692790000 0.1290440000
C 0.2093980000 0.7933640000 0.1258520000
H 2.2123920000 0.9666690000 -0.5790640000
H -6.1790450000 -0.7712790000 1.1933280000
F 4.2806290000 0.3982920000 -1.0141190000
F 5.3692310000 -1.2206060000 0.2070170000
F 4.0411310000 0.3341800000 1.2701030000
H -0.5284940000 0.1077140000 0.5330410000
C -0.2280060000 2.1822280000 0.0543070000
C 0.6085350000 3.2327140000 -0.3760730000
C -1.5511280000 2.4861760000 0.4305000000
H 1.6365540000 3.0286080000 -0.6579300000
C 0.1308260000 4.5364900000 -0.4302870000
C -2.0279870000 3.7929510000 0.3722800000
H -2.2053870000 1.6836960000 0.7624270000
H 0.7874950000 5.3364610000 -0.7599680000
C -1.1879210000 4.8214290000 -0.0582490000
H -3.0520230000 4.0091290000 0.6631900000
H -1.5555540000 5.8429400000 -0.1016900000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.306443 (Hartree/Particle)
Thermal correction to Energy= 0.328568
Thermal correction to Enthalpy= 0.329512
Thermal correction to Gibbs (Free) Energy= 0.251613
Sum of electronic and zero-point Energies= -1133.094754
Sum of electronic and thermal Energies= -1133.072628
Sum of electronic and thermal Enthalpies= -1133.071684
Sum of electronic and thermal (Free) Energies= -1133.149583

ccTS

C -1.1826300000 -1.6622010000 -1.0482200000
H -1.2160970000 -1.9802120000 -2.0931860000
C 0.0355200000 -1.3812500000 -0.5522500000
C -2.4756120000 -1.5202930000 -0.3875720000
C 1.3372290000 -1.7691620000 -0.4841090000
C -3.6375500000 -1.3503670000 -1.1653510000
C -2.6114370000 -1.6088250000 1.0127670000
C 1.8325150000 -3.1756220000 -0.6643570000
C 2.2651710000 -0.7101630000 -0.1408880000
H -3.5486470000 -1.2945800000 -2.2473520000
C -4.8869200000 -1.2381040000 -0.5634030000
H -1.7350370000 -1.8087370000 1.6226600000
C -3.8633870000 -1.5010540000 1.6121020000
H 2.6306050000 -3.1762890000 -1.4161560000
H 1.0358440000 -3.8534040000 -0.9767980000
H 2.2841850000 -3.5494710000 0.2621160000
O 3.5261410000 -0.9074580000 -0.1894850000
C 1.5800620000 0.5015590000 0.1356390000

H -5.7717070000 -1.0988600000 -1.1780670000
C -5.0038210000 -1.3092960000 0.8275000000
H -3.9529010000 -1.5839310000 2.6917480000
B 4.5205810000 0.2336870000 0.3245860000
C 0.2081540000 0.4057430000 0.4383790000
H 2.0772540000 1.4497960000 -0.0312400000
H -5.9805540000 -1.2316150000 1.2966200000
F 4.3269740000 1.3056590000 -0.5344380000
F 5.7561840000 -0.3323820000 0.2402030000
F 4.1057670000 0.5228000000 1.6100260000
H -0.0857720000 -0.2021520000 1.2951940000
C -0.7094120000 1.5224220000 0.1473550000
C -0.5213610000 2.3251360000 -0.9923560000
C -1.7759960000 1.8159410000 1.0130870000
H 0.2877990000 2.0945080000 -1.6800710000
C -1.3668940000 3.4005660000 -1.2476590000
C -2.6204240000 2.8944550000 0.7588590000
H -1.9343240000 1.2016750000 1.8946750000
H -1.2100410000 4.0132420000 -2.1308710000
C -2.4173360000 3.6888860000 -0.3712830000
H -3.4348020000 3.1161330000 1.4426910000
H -3.0771150000 4.5286190000 -0.5715930000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.304943 (Hartree/Particle)
Thermal correction to Energy= 0.326115
Thermal correction to Enthalpy= 0.327059
Thermal correction to Gibbs (Free) Energy= 0.252335
Sum of electronic and zero-point Energies= -1133.064061
Sum of electronic and thermal Energies= -1133.042889
Sum of electronic and thermal Enthalpies= -1133.041945
Sum of electronic and thermal (Free) Energies= -1133.116668

ccPT

C -1.3714020000 -1.7279330000 -0.2847430000
C -0.1737400000 -1.1074220000 -0.0260210000
C 1.0776510000 -1.6627680000 -0.4213920000
C 2.1633290000 -0.8189910000 -0.0103360000
C 1.6070740000 0.2773480000 0.6533450000
C 0.1154620000 0.2106120000 0.6937090000
C 1.3623920000 -2.9390700000 -1.1232350000
O 3.3964040000 -1.1204440000 -0.2520070000
H 0.4768600000 -3.4634870000 -1.4864660000
H 1.9198030000 -3.6026310000 -0.4480110000
H 2.0455660000 -2.7417530000 -1.9583480000
C -0.4873020000 1.4792830000 0.0845310000
H 2.1800540000 1.0973870000 1.0644440000
C -2.7387530000 -1.3994430000 0.0585660000
C -0.9916890000 2.4855950000 0.9168710000
C -0.4672040000 1.6916700000 -1.2999050000
H -0.2164190000 0.1408960000 1.7412460000
H -1.2936520000 -2.6367330000 -0.8784510000
C -3.7575210000 -2.1546890000 -0.5703190000
C -5.1003710000 -1.9099360000 -0.3140550000
C -5.4635610000 -0.9096020000 0.5920320000
C -4.4736530000 -0.1631640000 1.2385540000
C -3.1290890000 -0.4026480000 0.9811580000
H -3.4767640000 -2.9334630000 -1.2749630000
H -5.8637350000 -2.4981410000 -0.8147530000
H -6.5123150000 -0.7181550000 0.8005590000
H -4.7531240000 0.6064010000 1.9520990000
H -2.3827270000 0.1767290000 1.5061360000
B 4.5053170000 -0.1512320000 0.2855150000
F 5.6906980000 -0.7167760000 -0.0898290000
F 4.3220270000 -0.0862920000 1.6632480000
F 4.2580900000 1.0844670000 -0.3024300000
C -0.9654300000 2.8758140000 -1.8403220000
C -1.4762080000 3.8709830000 -1.0036480000
C -1.4849740000 3.6746620000 0.3773750000
H -0.9922120000 2.3426080000 1.9956940000
H -1.8727390000 4.4457700000 1.0373520000
H -0.9463070000 3.0250250000 -2.9162840000
H -1.8591710000 4.7955810000 -1.4262730000
H -0.0583480000 0.9292760000 -1.9573860000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.307711 (Hartree/Particle)
Thermal correction to Energy= 0.328886
Thermal correction to Enthalpy= 0.329831
Thermal correction to Gibbs (Free) Energy= 0.253713
Sum of electronic and zero-point Energies= -1133.098654
Sum of electronic and thermal Energies= -1133.077479
Sum of electronic and thermal Enthalpies= -1133.076535
Sum of electronic and thermal (Free) Energies= -1133.152653

6a

cRT

C -2.0686570000 0.3817080000 1.2102870000
C -0.8308540000 0.6199370000 0.8451520000
C 0.3924230000 0.8766140000 0.4110460000
C 1.3748420000 -0.2353700000 0.4589770000
C 1.3463810000 -1.2615150000 1.5124410000
C 0.9089180000 -1.0310150000 2.7572600000
H 1.7940480000 -2.2104790000 1.2388250000
C 0.7807330000 2.2394850000 -0.2267740000
H -2.3402760000 0.6088210000 2.2428270000
C -3.1490520000 -0.1695430000 0.3705600000
O 2.2420150000 -0.2807220000 -0.4466310000
C -0.3034930000 3.2851140000 0.0944110000
C 0.8945910000 2.0978440000 -1.7630180000
C 2.1239590000 2.7234770000 0.3643660000
C -4.4312450000 -0.3144610000 0.9232080000
C -2.9398310000 -0.5570420000 -0.9642720000
C -3.9875970000 -1.0711210000 -1.7215060000
H -1.9509910000 -0.4571060000 -1.4035090000
C -5.2620700000 -1.2090620000 -1.1623500000
H -3.8101560000 -1.3677760000 -2.7515500000
C -5.4800390000 -0.8292170000 0.1622970000
H -4.6042030000 -0.0196420000 1.9555770000
H -6.0776200000 -1.6115790000 -1.7564900000
H -6.4663770000 -0.9339130000 0.6057880000
B 3.5368640000 -1.3561430000 -0.5585510000
F 4.1277530000 -0.9386910000 -1.7020530000
F 2.9438040000 -2.5906930000 -0.6224560000
F 4.2305030000 -1.1230660000 0.5929810000
H 2.9448860000 2.0377840000 0.1413230000
H 2.0566170000 2.8439000000 1.4523770000
H 2.3789700000 3.6999260000 -0.0629200000
H -0.0551870000 1.7602110000 -2.1941380000
H 1.6772590000 1.3940310000 -2.0504100000
H 1.1318370000 3.0750990000 -2.2006030000
H -1.2745450000 3.0087750000 -0.3289900000
H -0.0131160000 4.2516700000 -0.3314930000
H -0.4298430000 3.4177110000 1.1751360000
H 0.9621700000 -1.8075670000 3.5148330000
H 0.5234770000 -0.0663160000 3.0704630000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309328 (Hartree/Particle)
Thermal correction to Energy= 0.330987
Thermal correction to Enthalpy= 0.331931
Thermal correction to Gibbs (Free) Energy= 0.256326
Sum of electronic and zero-point Energies= -1019.961920
Sum of electronic and thermal Energies= -1019.940261
Sum of electronic and thermal Enthalpies= -1019.939317
Sum of electronic and thermal (Free) Energies= -1020.014922

cTS

C -1.9247050000 -0.8176650000 1.1617940000
C -0.6481640000 -0.4756190000 0.9583630000
H -2.1588160000 -1.3778790000 2.0667600000
C -3.0537310000 -0.5847340000 0.2575460000
C 0.3684510000 0.3231570000 0.5436700000
C -4.3546100000 -0.8633340000 0.7169250000
C -2.8901100000 -0.1055240000 -1.0563910000
C 1.5680250000 -0.4250030000 0.1631530000
C 0.3331670000 1.8609520000 0.5557800000
C -5.4599270000 -0.6447460000 -0.1012330000
H -4.4933260000 -1.2447900000 1.7256820000
C -3.9964840000 0.1079000000 -1.8721770000
H -1.8905670000 0.0781110000 -1.4386420000
C 1.4559940000 -1.8081630000 0.5118140000
O 2.5284700000 0.1131590000 -0.4767220000
C -0.9731470000 2.3924660000 1.1726580000
C 0.4476180000 2.3691430000 -0.9040590000
C 1.5257210000 2.3925100000 1.3867820000

C -5.2851670000 -0.1567240000 -1.3978910000
H -6.4574510000 -0.8592540000 0.2717050000
H -3.8538520000 0.4735710000 -2.8851170000
C 0.5293280000 -2.1254250000 1.4878640000
H 1.9481850000 -2.5504140000 -0.1066750000
B 3.8879650000 -0.7168700000 -0.7436590000
H -1.8555410000 2.0750910000 0.6085170000
H -0.9511330000 3.4876510000 1.1697740000
H -1.0941330000 2.0630970000 2.2104580000
H -0.4128010000 2.0488750000 -1.5025830000
H 1.3614270000 2.0128990000 -1.3832770000
H 0.4629320000 3.4653130000 -0.9009470000
H 2.4847860000 2.0780520000 0.9704730000
H 1.4650290000 2.0479770000 2.4259250000
H 1.5000960000 3.4881430000 1.3964520000
H -6.1462920000 0.0088460000 -2.0389550000
H 0.1003810000 -3.1268590000 1.5208450000
H 0.4996920000 -1.6051000000 2.4417970000
F 4.7290690000 0.2060350000 -1.2820080000
F 3.5225330000 -1.7345900000 -1.6053910000
F 4.2614690000 -1.1892380000 0.4965660000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309254 (Hartree/Particle)
Thermal correction to Energy= 0.329577
Thermal correction to Enthalpy= 0.330521
Thermal correction to Gibbs (Free) Energy= 0.259470
Sum of electronic and zero-point Energies= -1019.938022
Sum of electronic and thermal Energies= -1019.917700
Sum of electronic and thermal Enthalpies= -1019.916756
Sum of electronic and thermal (Free) Energies= -1019.987806

cPT

C 1.8756630000 1.4991760000 0.5235370000
C 0.5272360000 1.2526470000 0.4671610000
C -0.2921000000 0.0937550000 0.2877120000
C -1.6016430000 0.5346390000 -0.1727230000
C -1.6683940000 1.9234160000 -0.0342880000
C -0.4077400000 2.4673390000 0.4947040000
C -0.0805420000 -1.3460800000 0.7280700000
C 3.0069130000 0.7457360000 0.0127400000
O -2.5051030000 -0.2850470000 -0.6022800000
C 1.2640100000 -1.6306530000 1.4212860000
C -0.2583240000 -2.3147190000 -0.4724610000
C -1.1986170000 -1.6340070000 1.7865760000
C 4.2886540000 0.9756870000 0.5563090000
C 2.8882660000 -0.1340930000 -1.0839620000
C 4.0056070000 -0.7926200000 -1.5866840000
H 1.9203660000 -0.2644910000 -1.5572000000
C 5.2615380000 -0.5862260000 -1.0080410000
H 3.9009180000 -1.4579070000 -2.4387450000
C 5.4001370000 0.3010150000 0.0641520000
H 4.3982180000 1.6735520000 1.3826420000
H 6.1329520000 -1.0998360000 -1.4039760000
H 6.3770950000 0.4728320000 0.5064360000
B -4.0414900000 -0.0056600000 -0.4829950000
F -4.3408310000 -0.2274360000 0.8528770000
F -4.6278500000 -0.8998540000 -1.3359100000
F -4.2687470000 1.3217500000 -0.8465450000
H 2.1416900000 2.4878990000 0.9019680000
H -2.5471270000 2.5007520000 -0.2873630000
H -0.5076250000 2.8061700000 1.5388680000
H -0.0394330000 3.3326770000 -0.0754060000
H -1.0244390000 -1.0432740000 2.6932930000
H -1.1421850000 -2.6934110000 2.0603700000
H -2.2030810000 -1.4231550000 1.4189650000
H 1.4805090000 -0.9019040000 2.2100520000
H 2.1057390000 -1.6489590000 0.7280590000
H 1.2073400000 -2.6181440000 1.8916850000
H -0.1735530000 -3.3442240000 -0.1064760000
H 0.5261720000 -2.1617110000 -1.2223120000
H -1.2324120000 -2.1884110000 -0.9459730000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311892 (Hartree/Particle)
Thermal correction to Energy= 0.331906
Thermal correction to Enthalpy= 0.332850
Thermal correction to Gibbs (Free) Energy= 0.262569
Sum of electronic and zero-point Energies= -1019.966199
Sum of electronic and thermal Energies= -1019.946185
Sum of electronic and thermal Enthalpies= -1019.945241
Sum of electronic and thermal (Free) Energies= -1020.015522

ccRT

C 1.9453590000 0.2020990000 -1.2612690000
C 0.7751420000 0.4425880000 -0.7186750000
C 3.1980520000 -0.1317080000 -0.5590540000
H 2.0009340000 0.2320530000 -2.3512910000
C -0.4204790000 0.7283860000 -0.2288580000
C 4.2993670000 -0.5800570000 -1.3057840000
C 3.3319030000 -0.0148380000 0.8358850000
C -1.3963650000 -0.3851420000 -0.1230110000
C -0.8448330000 2.1831070000 0.1161430000
C 5.4967930000 -0.9163580000 -0.6762900000
H 4.2107990000 -0.6688180000 -2.3858070000
C 4.5280810000 -0.3523540000 1.4628810000
H 2.4988540000 0.3601710000 1.4248490000
C -0.9866490000 -1.7875040000 0.0512490000
O -2.6139610000 -0.0934050000 -0.2083530000
C 0.3986320000 3.0920380000 0.1421920000
C -1.5059800000 2.2146960000 1.5125900000
C -1.8253810000 2.7214740000 -0.9527210000
C 5.6148970000 -0.8064880000 0.7100260000
H 6.3377560000 -1.2638260000 -1.2699760000
H 4.6161730000 -0.2536630000 2.5413660000
C 0.1219640000 -2.1753540000 0.6947640000
H -1.7062510000 -2.5137940000 -0.3103300000
B -3.9288810000 -1.1318680000 -0.0194800000
H 0.8928990000 3.1352340000 -0.8336850000
H 1.1354970000 2.7532630000 0.8797580000
H 0.0977010000 4.1100950000 0.4120510000
H -1.7688500000 3.2478900000 1.7667850000
H -0.8182570000 1.8471420000 2.2838770000
H -2.4205470000 1.6188210000 1.5500780000
H -1.3680740000 2.6957030000 -1.9486990000
H -2.0719260000 3.7653690000 -0.7242500000
H -2.7531880000 2.1483120000 -0.9809260000
H 6.5483010000 -1.0663970000 1.2011620000
H 0.8295830000 -1.4770140000 1.1283630000
H 0.3365370000 -3.2313540000 0.8315490000
F -4.9638070000 -0.2777980000 -0.1965520000
F -3.7636320000 -1.6164110000 1.2450610000
F -3.7642120000 -2.0658030000 -1.0097370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309378 (Hartree/Particle)
Thermal correction to Energy= 0.330986
Thermal correction to Enthalpy= 0.331930
Thermal correction to Gibbs (Free) Energy= 0.256900
Sum of electronic and zero-point Energies= -1019.962042
Sum of electronic and thermal Energies= -1019.940434
Sum of electronic and thermal Enthalpies= -1019.939490
Sum of electronic and thermal (Free) Energies= -1020.014520

ccTS

C 1.8445950000 0.3179720000 -0.8677450000
C 0.6291270000 0.0463570000 -0.3745070000
C 3.1342370000 -0.2414880000 -0.4592940000
H 1.8720840000 0.9948520000 -1.7243560000
C -0.6306080000 0.4138190000 -0.0197140000
C 4.1972810000 -0.2574310000 -1.3821400000
C 3.3644530000 -0.7382030000 0.8387280000
C -1.5999980000 -0.6754860000 -0.1184410000
C -1.0183980000 1.8121960000 0.4876950000
C 5.4372780000 -0.7838280000 -1.0314660000
H 4.0381410000 0.1356350000 -2.3832300000
C 4.6053930000 -1.2655420000 1.1862320000
H 2.5796050000 -0.6712100000 1.5867060000
C -0.9617910000 -1.9167790000 -0.4415760000
O -2.8548350000 -0.4816910000 -0.0279990000
C 0.2100630000 2.7293510000 0.6277100000
C -1.7077320000 1.6922640000 1.8673430000
C -1.9957310000 2.4416940000 -0.5383100000
C 5.6440210000 -1.2955360000 0.2520710000
H 6.2438120000 -0.7944270000 -1.7591290000
H 4.7676740000 -1.6394740000 2.1932390000
C 0.3842650000 -2.0144150000 -0.1513970000

H -1.4930220000 -2.6333820000 -1.0584550000
B -3.8675490000 -1.7404600000 -0.0163560000
H 0.7140310000 2.8912400000 -0.3310870000
H 0.9442320000 2.3256020000 1.3333220000
H -0.1129580000 3.7068670000 1.0017290000
H -1.9937360000 2.6902040000 2.2190300000
H -1.0269890000 1.2588310000 2.6097180000
H -2.6084830000 1.0772680000 1.8192490000
H -1.5178050000 2.5553490000 -1.5183360000
H -2.2895730000 3.4385320000 -0.1892670000
H -2.8973150000 1.8380830000 -0.6571000000
H 6.6128130000 -1.7023590000 0.5274470000
H 0.7783570000 -1.7737190000 0.8322970000
H 1.0139200000 -2.7054410000 -0.7101730000
F -5.0715540000 -1.1833310000 0.2810310000
F -3.3653350000 -2.5872090000 0.9492990000
F -3.7799680000 -2.2807050000 -1.2857690000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.308860 (Hartree/Particle)
Thermal correction to Energy= 0.329237
Thermal correction to Enthalpy= 0.330181
Thermal correction to Gibbs (Free) Energy= 0.258933
Sum of electronic and zero-point Energies= -1019.936403
Sum of electronic and thermal Energies= -1019.916026
Sum of electronic and thermal Enthalpies= -1019.915081
Sum of electronic and thermal (Free) Energies= -1019.986330

ccPT

C 1.9429290000 0.5196740000 0.0034660000
C 0.6853740000 -0.0320370000 0.0471010000
C -0.5709740000 0.6702830000 0.0279650000
C -1.6453740000 -0.3067140000 -0.0293220000
C -1.0803830000 -1.5807180000 -0.0337550000
C 0.3908320000 -1.5187560000 0.0525590000
C -0.9020740000 2.1548680000 0.0764150000
O -2.9047510000 0.0011500000 -0.0720470000
C 0.2807130000 3.1387700000 0.1569870000
C -1.7848090000 2.3939430000 1.3385600000
C -1.7167700000 2.5075590000 -1.2030160000
H -1.6582270000 -2.4927030000 -0.0894680000
C 3.2656480000 -0.0852860000 0.0051380000
H 1.9893270000 1.5954230000 -0.0772720000
C 4.3488460000 0.7843160000 -0.2662360000
C 5.6600750000 0.3246160000 -0.3022270000
C 5.9304510000 -1.0223070000 -0.0532780000
C 4.8786230000 -1.8988110000 0.2333930000
C 3.5662690000 -1.4429550000 0.2632740000
H 4.1442230000 1.8344240000 -0.4584710000
H 6.4696860000 1.0149630000 -0.5198370000
H 6.9531310000 -1.3876680000 -0.0750710000
H 5.0854220000 -2.9448790000 0.4399660000
H 2.7804500000 -2.1449090000 0.5059170000
B -3.9702420000 -1.1492270000 -0.0692850000
F -5.1773480000 -0.5099090000 -0.1062840000
F -3.7524760000 -1.8762100000 1.0953990000
F -3.7112110000 -1.9272930000 -1.1929700000
H -1.1048780000 2.3713660000 -2.1022730000
H -2.0107110000 3.5619950000 -1.1503250000
H -2.6161120000 1.8979450000 -1.2887620000
H -2.0895060000 3.4464680000 1.3557820000
H -1.2162820000 2.1911390000 2.2534980000
H -2.6798910000 1.7723910000 1.3295210000
H 0.9056520000 3.1227470000 -0.7428210000
H 0.9085860000 2.9745840000 1.0393840000
H -0.1268680000 4.1519410000 0.2382360000
H 0.7470080000 -2.0007760000 0.9760460000
H 0.8812670000 -2.0454860000 -0.7787180000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.312678 (Hartree/Particle)
Thermal correction to Energy= 0.332748
Thermal correction to Enthalpy= 0.333693
Thermal correction to Gibbs (Free) Energy= 0.261752
Sum of electronic and zero-point Energies= -1019.976123
Sum of electronic and thermal Energies= -1019.956052
Sum of electronic and thermal Enthalpies= -1019.955108
Sum of electronic and thermal (Free) Energies= -1020.027049

6b

cRT

C -2.1077910000 0.1995950000 -1.1480210000
C -0.8836700000 -0.2306050000 -0.9453510000
C 0.3238730000 -0.7024380000 -0.6920970000
C 1.3212910000 0.2437600000 -0.1204810000
C 1.4175600000 1.6363740000 -0.5470490000
C 1.0044630000 2.0820700000 -1.7484030000
H 1.9320940000 2.2950580000 0.1445050000
C 0.6981040000 -2.1992200000 -0.8766440000
H -2.3559960000 0.5633060000 -2.1469630000
C -3.2031730000 0.2463170000 -0.1609340000
O 2.0872890000 -0.2134420000 0.7658480000
C -0.3626340000 -2.8892820000 -1.7542280000
C 0.7508950000 -2.9135130000 0.4944630000
C 2.0691800000 -2.3010540000 -1.5826570000
C -4.4700590000 0.6896820000 -0.5720020000
C -3.0230300000 -0.1359100000 1.1796990000
C -4.0837190000 -0.0780420000 2.0781230000
H -2.0461510000 -0.4744480000 1.5140410000
C -5.3427460000 0.3625530000 1.6577070000
H -3.9283800000 -0.3755380000 3.1115240000
C -5.5319600000 0.7463490000 0.3297820000
H -4.6209040000 0.9894000000 -1.6065170000
H -6.1684350000 0.4070550000 2.3623080000
H -6.5060960000 1.0911420000 -0.0060760000
B 3.4385280000 0.5196070000 1.4162480000
F 3.8431560000 -0.4074610000 2.3181840000
F 2.9849760000 1.6960610000 1.9605960000
F 4.2483570000 0.6807690000 0.3266710000
H 2.8701980000 -1.8348670000 -1.0030570000
H 2.0390360000 -1.8304800000 -2.5729810000
H 2.3296870000 -3.3561420000 -1.7240880000
H -0.2165500000 -2.8451770000 1.0055820000
H 1.5179390000 -2.4904390000 1.1447910000
H 0.9744530000 -3.9763150000 0.3410820000
H -1.3519900000 -2.8722660000 -1.2856790000
H -0.0813150000 -3.9365960000 -1.9095650000
H -0.4449590000 -2.4130290000 -2.7380880000
C 1.1524810000 3.4917380000 -2.2186990000
H 0.5550390000 1.3828030000 -2.4504810000
H 1.6147930000 4.1311690000 -1.4620560000
H 0.1718260000 3.9103350000 -2.4832000000
H 1.7619410000 3.5299630000 -3.1314200000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337553 (Hartree/Particle)
Thermal correction to Energy= 0.360828
Thermal correction to Enthalpy= 0.361772
Thermal correction to Gibbs (Free) Energy= 0.281925
Sum of electronic and zero-point Energies= -1059.257359
Sum of electronic and thermal Energies= -1059.234085
Sum of electronic and thermal Enthalpies= -1059.233140
Sum of electronic and thermal (Free) Energies= -1059.312987

cTS

C -1.8775510000 0.9520000000 -0.8876950000
C -0.6029400000 0.5512300000 -0.8065770000
C -2.9936820000 0.5399270000 -0.0336360000
H -2.1171440000 1.7224850000 -1.6206890000
C 0.3656080000 -0.3846980000 -0.5984030000
C -4.2975070000 0.9350030000 -0.3882500000
C -2.8155650000 -0.2215710000 1.1375820000
C 1.6073230000 0.2038160000 -0.1047220000
C 0.2463500000 -1.8769530000 -0.9427840000
C -5.3914700000 0.5563810000 0.3854790000
H -4.4478000000 1.5335840000 -1.2835670000
C -3.9103680000 -0.5940130000 1.9108030000
H -1.8127630000 -0.4994400000 1.4471820000
C 1.5651440000 1.6255770000 -0.1681730000
O 2.5513160000 -0.5031640000 0.3872390000
C -1.0937860000 -2.2007000000 -1.6270570000
C 0.3594400000 -2.6974520000 0.3678790000
C 1.3980240000 -2.2700050000 -1.9000420000
C -5.2023040000 -0.2110190000 1.5367870000
H -6.3913660000 0.8638360000 0.0923910000
H -3.7557930000 -1.1773360000 2.8141290000

C 0.6237340000 2.1900110000 -1.0291120000
H 2.1323070000 2.2092340000 0.5492140000
B 3.9475340000 0.1856000000 0.7708000000
H -1.2146440000 -1.6448930000 -2.5633910000
H -1.9508770000 -1.9779680000 -0.9846310000
H -1.1246670000 -3.2692770000 -1.8663350000
H 0.3240700000 -3.7658960000 0.1247980000
H -0.4758710000 -2.4808600000 1.0433250000
H 1.2963050000 -2.4924890000 0.8893620000
H 1.3387450000 -1.7055230000 -2.8382250000
H 1.3168710000 -3.3350280000 -2.1457430000
H 2.3776590000 -2.0970480000 -1.4502530000
H -6.0543260000 -0.5017590000 2.1446240000
H 0.6022790000 1.8513450000 -2.0646280000
C 0.1227030000 3.5975620000 -0.8360040000
F 4.3323440000 0.8741080000 -0.3630060000
F 4.7523930000 -0.8614910000 1.1006280000
F 3.6598870000 1.0388610000 1.8233800000
H -0.8526930000 3.7451620000 -1.3099050000
H 0.8191030000 4.2988190000 -1.3144580000
H 0.0419750000 3.8620430000 0.2216900000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337326 (Hartree/Particle)
Thermal correction to Energy= 0.359297
Thermal correction to Enthalpy= 0.360242
Thermal correction to Gibbs (Free) Energy= 0.285688
Sum of electronic and zero-point Energies= -1059.230880
Sum of electronic and thermal Energies= -1059.208909
Sum of electronic and thermal Enthalpies= -1059.207965
Sum of electronic and thermal (Free) Energies= -1059.282519

cPT

C 1.8179440000 1.2893850000 0.6291080000
C 0.4783270000 1.0025200000 0.6112610000
C -0.2889160000 -0.1905990000 0.4099400000
C -1.6303720000 0.1965020000 0.0133530000
C -1.7569100000 1.5744770000 0.2032990000
C -0.5215910000 2.1782280000 0.7387000000
C 0.0235850000 -1.6374280000 0.7677140000
C 2.9471310000 0.6028830000 0.0231000000
O -2.5288540000 -0.6408030000 -0.3960320000
C 1.3943140000 -1.8703960000 1.4286280000
C -0.1106460000 -2.5372980000 -0.4910230000
C -1.0561570000 -2.0734290000 1.8102520000
C 4.2426930000 0.8172650000 0.5383830000
C 2.8061730000 -0.1897550000 -1.1352670000
C 3.9170070000 -0.7831760000 -1.7264890000
H 1.8246940000 -0.3023290000 -1.5843140000
C 5.1887740000 -0.5967040000 -1.1767840000
H 3.7939490000 -1.3811230000 -2.6248420000
C 5.3483760000 0.2069510000 -0.0434510000
H 4.3690320000 1.4501890000 1.4132440000
H 6.0548980000 -1.0593320000 -1.6412390000
H 6.3370670000 0.3647400000 0.3776550000
B -4.0026060000 -0.1340970000 -0.5947640000
F -4.3955260000 0.3717690000 0.6383010000
F -4.7032700000 -1.2368430000 -0.9929220000
F -3.9496680000 0.8737980000 -1.5516030000
H 2.0762460000 2.2610730000 1.0499800000
H -2.6574740000 2.1290410000 -0.0255580000
H -0.6433490000 2.3482840000 1.8230530000
C -0.1551260000 3.5203830000 0.0815680000
H 0.0651230000 3.3912470000 -0.9827660000
H 0.7086950000 3.9902280000 0.5612380000
H -0.9975110000 4.2138610000 0.1734790000
H 1.5649350000 -1.1850740000 2.2661700000
H 2.2263860000 -1.7762850000 0.7308230000
H 1.4167300000 -2.8903060000 1.8272710000
H -0.9669200000 -1.4852490000 2.7306860000
H -0.8832940000 -3.1248160000 2.0644590000
H -2.0687610000 -1.9719470000 1.4207070000
H 0.0168340000 -3.5834670000 -0.1902480000
H 0.6656630000 -2.3046650000 -1.2277920000
H -1.0905480000 -2.4245390000 -0.9576680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.340027 (Hartree/Particle)
Thermal correction to Energy= 0.361702
Thermal correction to Enthalpy= 0.362647
Thermal correction to Gibbs (Free) Energy= 0.288475
Sum of electronic and zero-point Energies= -1059.251733
Sum of electronic and thermal Energies= -1059.230057
Sum of electronic and thermal Enthalpies= -1059.229113
Sum of electronic and thermal (Free) Energies= -1059.303284

ccRT

C 1.8975840000 0.5353030000 -1.2899550000
C 0.7316350000 0.7079790000 -0.7115270000
C 3.1660250000 0.1633570000 -0.6362140000
H 1.9375460000 0.6603570000 -2.3738530000
C -0.4639080000 0.9172980000 -0.1886050000
C 4.2570780000 -0.2205430000 -1.4326360000
C 3.3259140000 0.1808000000 0.7608500000
C -1.4147550000 -0.2280460000 -0.1796340000
C -0.9251570000 2.3198860000 0.2950960000
C 5.4683630000 -0.5916490000 -0.8509180000
H 4.1493240000 -0.2312990000 -2.5145410000
C 4.5359130000 -0.1914170000 1.3402830000
H 2.5022690000 0.5084890000 1.3898280000
C -0.9837900000 -1.6161740000 -0.0367480000
O -2.6328080000 0.0505480000 -0.3251290000
C 0.2974590000 3.2469690000 0.4311790000
C -1.6036730000 2.1923680000 1.6776090000
C -1.9055480000 2.9440600000 -0.7262340000
C 5.6117130000 -0.5815190000 0.5374050000
H 6.3006970000 -0.8877380000 -1.4834300000
H 4.6438100000 -0.1683810000 2.4213120000
C 0.1457970000 -2.0016330000 0.5853680000
H -1.6930470000 -2.3517660000 -0.4012380000
B -3.9332930000 -0.9882710000 -0.1962780000
H 0.8034660000 3.3974890000 -0.5279030000
H 1.0315160000 2.8504360000 1.1423590000
H -0.0283460000 4.2267940000 0.7969390000
H -1.9054760000 3.1858910000 2.0283900000
H -0.9128160000 1.7735100000 2.4195160000
H -2.4973360000 1.5648110000 1.6433310000
H -1.4367420000 3.0281050000 -1.7136110000
H -2.1765620000 3.9543730000 -0.3964730000
H -2.8196870000 2.3571050000 -0.8247780000
H 6.5561280000 -0.8678080000 0.9914840000
H 0.8119140000 -1.2529570000 1.0077100000
C 0.5551280000 -3.4252130000 0.7759690000
F -4.9709630000 -0.1535110000 -0.4488360000
F -3.8407280000 -1.4476040000 1.0875340000
F -3.7160200000 -1.9483290000 -1.1539950000
H -0.1545640000 -4.1223090000 0.3224340000
H 0.6429550000 -3.6592230000 1.8453670000
H 1.5486080000 -3.5948690000 0.3395320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337604 (Hartree/Particle)
Thermal correction to Energy= 0.360824
Thermal correction to Enthalpy= 0.361769
Thermal correction to Gibbs (Free) Energy= 0.282801
Sum of electronic and zero-point Energies= -1059.257468
Sum of electronic and thermal Energies= -1059.234248
Sum of electronic and thermal Enthalpies= -1059.233304
Sum of electronic and thermal (Free) Energies= -1059.312272

ccTS

C -1.8034710000 0.5203720000 1.0306590000
C -0.5858320000 0.3062930000 0.5034460000
C -3.0950210000 0.0307060000 0.5536250000
H -1.8311760000 1.0840980000 1.9653860000
C 0.6526080000 0.7946960000 0.2127750000
C -4.1660320000 -0.0860750000 1.4618090000
C -3.3261530000 -0.2908350000 -0.7996780000
C 1.6652320000 -0.2511560000 0.1232520000
C 0.9740860000 2.2707530000 -0.0647480000
C -5.4127180000 -0.5390300000 1.0400740000
H -4.0070630000 0.1721370000 2.5058700000
C -4.5739880000 -0.7449390000 -1.2180930000
H -2.5338970000 -0.1439130000 -1.5280120000
C 1.0831880000 -1.5452130000 0.2394530000
O 2.9140070000 0.0074210000 0.0491100000
C -0.2876520000 3.1523020000 -0.0419300000

C 1.6450680000 2.4035950000 -1.4526420000
C 1.9452840000 2.7640470000 1.0394030000
C -5.6198640000 -0.8751680000 -0.3004080000
H -6.2245800000 -0.6286230000 1.7562620000
H -4.7362990000 -0.9821700000 -2.2657560000
C -0.2827480000 -1.6576680000 -0.0144860000
H 1.6642570000 -2.3466960000 0.6835590000
B 3.9654680000 -1.1800760000 -0.1913630000
H -0.7785850000 3.1440900000 0.9369370000
H -1.0208950000 2.8386050000 -0.7927560000
H -0.0049240000 4.1876900000 -0.2610080000
H 1.8890860000 3.4557170000 -1.6397400000
H 0.9682190000 2.0708950000 -2.2486950000
H 2.5675350000 1.8231420000 -1.5140600000
H 1.4802710000 2.6989950000 2.0300910000
H 2.1962050000 3.8149610000 0.8534330000
H 2.8698720000 2.1841840000 1.0484220000
H -6.5942910000 -1.2232500000 -0.6308790000
H -0.6659960000 -1.2926060000 -0.9674600000
C -1.0933940000 -2.7772950000 0.5832960000
F 5.1487700000 -0.5365240000 -0.3881020000
F 3.4906940000 -1.8634590000 -1.2935010000
F 3.9183650000 -1.9509170000 0.9582100000
H -0.7069090000 -3.0812050000 1.5599070000
H -1.0635410000 -3.6470620000 -0.0863790000
H -2.1433820000 -2.4915820000 0.6898710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.337032 (Hartree/Particle)
Thermal correction to Energy= 0.359001
Thermal correction to Enthalpy= 0.359946
Thermal correction to Gibbs (Free) Energy= 0.285389
Sum of electronic and zero-point Energies= -1059.229233
Sum of electronic and thermal Energies= -1059.207263
Sum of electronic and thermal Enthalpies= -1059.206319
Sum of electronic and thermal (Free) Energies= -1059.280875

ccPT

C -1.8789740000 0.6728130000 0.0141530000
C -0.6348070000 0.0890730000 0.0065210000
C 0.6305500000 0.7765310000 0.0088860000
C 1.6914650000 -0.2132430000 0.0032600000
C 1.1073180000 -1.4782680000 0.0322620000
C -0.3672110000 -1.4139790000 0.0413310000
C 0.9832010000 2.2582050000 -0.0225470000
O 2.9565200000 0.0729740000 -0.0167950000
C -0.1828340000 3.2652060000 -0.0125150000
C 1.8057140000 2.5177740000 -1.3198760000
C 1.8661610000 2.5630080000 1.2241220000
H 1.6754990000 -2.3973720000 0.0837880000
C -3.2099050000 0.0951360000 -0.0946040000
H -1.9078370000 1.7436380000 0.1517550000
C -4.2844340000 0.8720050000 0.3992360000
C -5.5941710000 0.4112080000 0.3463060000
C -5.8730950000 -0.8301550000 -0.2321140000
C -4.8321820000 -1.5995980000 -0.7589140000
C -3.5183410000 -1.1469590000 -0.6938180000
H -4.0725590000 1.8411970000 0.8436030000
H -6.3988500000 1.0211070000 0.7463560000
H -6.8968960000 -1.1889380000 -0.2866300000
H -5.0469610000 -2.5524680000 -1.2338780000
H -2.7352650000 -1.7405700000 -1.1485750000
B 3.9991120000 -1.0949270000 -0.1011230000
F 5.2170000000 -0.4768100000 -0.1423290000
F 3.6891290000 -1.8077750000 -1.2538510000
F 3.8044890000 -1.8788430000 1.0316410000
H 1.2956110000 2.4162440000 2.1486270000
H 2.1784010000 3.6126270000 1.1828350000
H 2.7564480000 1.9352140000 1.2517740000
H 2.1234670000 3.5666400000 -1.3280000000
H 1.1904340000 2.3437450000 -2.2101910000
H 2.6917430000 1.8851160000 -1.3697770000
H -0.7790920000 3.2121810000 0.9052870000
H -0.8414020000 3.1602940000 -0.8812650000
H 0.2417780000 4.2738260000 -0.0543490000
H -0.7526490000 -1.8949770000 -0.8709830000
C -0.9555490000 -2.1496950000 1.2694220000
H -0.5947230000 -1.6913470000 2.1952750000
H -0.6393220000 -3.1976150000 1.2618040000
H -2.0485520000 -2.1212290000 1.2667030000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341080 (Hartree/Particle)
Thermal correction to Energy= 0.362569
Thermal correction to Enthalpy= 0.363513
Thermal correction to Gibbs (Free) Energy= 0.289438
Sum of electronic and zero-point Energies= -1059.260913
Sum of electronic and thermal Energies= -1059.239424
Sum of electronic and thermal Enthalpies= -1059.238480
Sum of electronic and thermal (Free) Energies= -1059.312555

6c

c/s RT

C 2.1326490000 0.5013060000 0.8719270000
C 0.9586160000 -0.0868820000 0.8841230000
H 2.2881120000 1.3311670000 1.5639020000
C 3.2831230000 0.1610700000 0.0133890000
C -0.1929740000 -0.7340900000 0.8739530000
C 4.4847550000 0.8685260000 0.1752000000
C 3.2186190000 -0.8465700000 -0.9645570000
C -1.2174480000 -0.2878850000 -0.1098090000
C -0.4672070000 -1.9750960000 1.7677500000
C 5.5955570000 0.5758450000 -0.6150820000
H 4.5460240000 1.6512910000 0.9277460000
C 4.3278950000 -1.1366640000 -1.7525660000
H 2.2930010000 -1.3978560000 -1.1059520000
C -1.4296530000 1.1181550000 -0.4379640000
O -1.8997360000 -1.1895710000 -0.6612710000
C 0.5871970000 -2.0445680000 2.8879910000
C -0.3865750000 -3.2715540000 0.9277290000
C -1.8664500000 -1.8441130000 2.4107460000
C 5.5212560000 -0.4277040000 -1.5814490000
H 6.5179320000 1.1329290000 -0.4753370000
H 4.2619120000 -1.9174620000 -2.5052740000
C -1.1355000000 2.1354980000 0.3935640000
H -1.9348640000 1.2989700000 -1.3809740000
B -3.2468820000 -0.9887130000 -1.6219600000
H 0.5757390000 -1.1421320000 3.5101190000
H 1.5987690000 -2.1671620000 2.4875380000
H 0.3747550000 -2.9025440000 3.5352300000
H -0.5413810000 -4.1378530000 1.5824240000
H 0.6021010000 -3.3738670000 0.4651960000
H -1.1422000000 -3.2947700000 0.1411110000
H -1.9302170000 -0.9463990000 3.0377250000
H -2.0562970000 -2.7118730000 3.0526800000
H -2.6634340000 -1.8012620000 1.6639060000
H 6.3851630000 -0.6565960000 -2.1990970000
C -1.4104630000 3.5820560000 0.1039540000
H -0.6951510000 1.9228990000 1.3674690000
F -4.1252180000 -0.3523850000 -0.7888380000
F -2.8232380000 -0.2248350000 -2.6819650000
F -3.5555760000 -2.2719580000 -1.9311380000
C -2.4463890000 4.1366000000 1.1034770000
H -1.8278790000 3.6604360000 -0.9078450000
C -0.0994570000 4.3925440000 0.1584750000
H -3.3906860000 3.5863070000 1.0432130000
H -2.6497720000 5.1919190000 0.8899980000
H -2.0765740000 4.0678050000 2.1341070000
H 0.3549820000 4.3407370000 1.1559190000
H -0.2977650000 5.4470720000 -0.0631900000
H 0.6310000000 4.0221190000 -0.5683080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394556 (Hartree/Particle)
Thermal correction to Energy= 0.420587
Thermal correction to Enthalpy= 0.421531
Thermal correction to Gibbs (Free) Energy= 0.334838
Sum of electronic and zero-point Energies= -1137.828526
Sum of electronic and thermal Energies= -1137.802495
Sum of electronic and thermal Enthalpies= -1137.801551
Sum of electronic and thermal (Free) Energies= -1137.888243

c/s TS

C 1.9013330000 0.7271120000 0.6557520000
C 0.6207040000 0.3258400000 0.5958870000
H 2.1264520000 1.6011990000 1.2620150000

C 3.0357770000 0.1754680000 -0.0851500000
C -0.2877230000 -0.6928750000 0.5523620000
C 4.3359780000 0.5934460000 0.2593700000
C 2.8811240000 -0.7399020000 -1.1449200000
C -1.5529310000 -0.2756050000 -0.0381220000
C -0.0983060000 -2.0898460000 1.1638290000
C 5.4470480000 0.0875210000 -0.4097280000
H 4.4686530000 1.3102450000 1.0662450000
C 3.9933840000 -1.2391600000 -1.8145610000
H 1.8832120000 -1.0378290000 -1.4514430000
C -1.5893340000 1.1297530000 -0.2224060000
O -2.4573620000 -1.1099200000 -0.3921680000
C 1.2411080000 -2.2239350000 1.9097250000
C -0.1525620000 -3.1400920000 0.0242750000
C -1.2461900000 -2.3582460000 2.1688520000
C 5.2801190000 -0.8319580000 -1.4477570000
H 6.4431910000 0.4141050000 -0.1246980000
H 3.8572680000 -1.9406330000 -2.6328120000
C -0.6629820000 1.8994600000 0.4947740000
H -2.2082270000 1.5464650000 -1.0096100000
B -3.8844750000 -0.5768930000 -0.8734740000
H 1.3249530000 -1.4972370000 2.7252720000
H 2.1007560000 -2.0949670000 1.2463820000
H 1.3059310000 -3.2259520000 2.3478200000
H -0.0745570000 -4.1434420000 0.4591750000
H 0.6841800000 -3.0115180000 -0.6714530000
H -1.0886300000 -3.0774460000 -0.5338690000
H -1.2279310000 -1.6301190000 2.9885210000
H -1.1179090000 -3.3553790000 2.6053320000
H -2.2256710000 -2.3186540000 1.6888130000
H 6.1459650000 -1.2217900000 -1.9752940000
C -0.3661400000 3.3156960000 0.0133960000
H -0.6359250000 1.7989400000 1.5820670000
F -4.3120670000 0.2739790000 0.1287840000
F -3.6494700000 0.1014550000 -2.0596290000
F -4.6320550000 -1.7066560000 -1.0143440000
C -1.5742030000 4.2000360000 0.4045380000
H -0.2992780000 3.2969320000 -1.0816710000
C 0.9294340000 3.9281690000 0.5667910000
H -2.5125390000 3.8141020000 -0.0048380000
H -1.4278210000 5.2182590000 0.0271600000
H -1.6810250000 4.2566830000 1.4947230000
H 0.9763720000 3.8465330000 1.6608360000
H 0.9722760000 4.9940280000 0.3182060000
H 1.8200710000 3.4569930000 0.1431130000

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Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394725 (Hartree/Particle)
Thermal correction to Energy= 0.419220
Thermal correction to Enthalpy= 0.420165
Thermal correction to Gibbs (Free) Energy= 0.339695
Sum of electronic and zero-point Energies= -1137.797546
Sum of electronic and thermal Energies= -1137.773050
Sum of electronic and thermal Enthalpies= -1137.772106
Sum of electronic and thermal (Free) Energies= -1137.852576

c/s PT

C 1.8122960000 1.0441450000 0.5011510000
C 0.4910830000 0.6974950000 0.5849120000
C -0.1930170000 -0.5636520000 0.4969350000
C -1.5630120000 -0.3073710000 0.1085410000
C -1.7964100000 1.0611460000 0.2509350000
C -0.5916890000 1.8058550000 0.6767870000
C 0.2286290000 -1.9491530000 0.9707320000
C 2.9335150000 0.3454890000 -0.1099500000
O -2.4078910000 -1.2288140000 -0.2322300000
C 1.6201170000 -2.0278390000 1.6249840000
C 0.1395800000 -2.9657550000 -0.2000230000
C -0.8062050000 -2.3653280000 2.0660430000
C 4.2448340000 0.6218200000 0.3299160000
C 2.7610440000 -0.5236170000 -1.2071140000
C 3.8589440000 -1.1322030000 -1.8081920000
H 1.7641390000 -0.6842200000 -1.6044660000
C 5.1485150000 -0.8831620000 -1.3304260000
H 3.7105790000 -1.7903410000 -2.6594520000
C 5.3382010000 -0.0019300000 -0.2609670000
H 4.3943870000 1.3133960000 1.1553320000
H 6.0043590000 -1.3573440000 -1.8022650000
H 6.3404610000 0.2047700000 0.1031890000
B -3.8523090000 -0.7978570000 -0.6687120000
F -4.4200520000 -0.1646860000 0.4327510000
F -4.4771410000 -1.9597400000 -1.0215820000
F -3.6880390000 0.0965530000 -1.7213260000
H 2.0530350000 2.0573440000 0.8162550000
H -2.7713540000 1.5038210000 0.1104140000
H -0.6928880000 2.0257820000 1.7549210000
C -0.3369380000 3.1683200000 -0.0575330000
C -1.6167050000 3.7653640000 -0.6683550000
H 0.3530400000 2.9652400000 -0.8861750000
C 0.3104750000 4.2000420000 0.8820140000
H -0.3823970000 4.4710920000 1.6890120000
H 0.5586210000 5.1170130000 0.3365520000
H 1.2311790000 3.8377310000 1.3528180000
H -2.0624910000 3.1062170000 -1.4199110000
H -1.3830320000 4.7178490000 -1.1567400000
H -2.3747600000 3.9671960000 0.0986380000
H -0.7550340000 -1.6893690000 2.9272320000
H -0.5532040000 -3.3729060000 2.4132050000
H -1.8261080000 -2.3762340000 1.6817520000
H 0.3312440000 -3.9709090000 0.1926730000
H 0.8955260000 -2.7555950000 -0.9634840000
H -0.8486980000 -2.9538390000 -0.6626930000
H 1.7525250000 -1.2598970000 2.3950450000
H 2.4350000000 -1.9401910000 0.9064860000
H 1.7180880000 -3.0039550000 2.1121400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.396918 (Hartree/Particle)
Thermal correction to Energy= 0.421325
Thermal correction to Enthalpy= 0.422270
Thermal correction to Gibbs (Free) Energy= 0.341734
Sum of electronic and zero-point Energies= -1137.816176
Sum of electronic and thermal Energies= -1137.791768
Sum of electronic and thermal Enthalpies= -1137.790824
Sum of electronic and thermal (Free) Energies= -1137.871360

cc/s RT

C -1.6962100000 -1.1971690000 -1.2726680000
C -0.5280290000 -1.1901800000 -0.6730250000
C -2.9995640000 -0.8392600000 -0.6833410000
H -1.7110320000 -1.4809090000 -2.3269060000
C 0.6735900000 -1.2316530000 -0.1251430000
C -4.1064060000 -0.6647220000 -1.5297260000
C -3.1777660000 -0.6677270000 0.7011140000
C 1.5393820000 -0.0307060000 -0.2830040000
C 1.2312040000 -2.5108610000 0.5584960000
C -5.3517890000 -0.3127630000 -1.0114560000
H -3.9843730000 -0.8019720000 -2.6014120000
C -4.4220350000 -0.3148310000 1.2172000000
H -2.3394390000 -0.8325570000 1.3728880000
C 1.0129740000 1.3301800000 -0.3251410000
O 2.7744130000 -0.2418130000 -0.3997070000
C 0.0779740000 -3.4945830000 0.8326100000
C 1.8865360000 -2.1316550000 1.9056540000
C 2.2631720000 -3.2057130000 -0.3613250000
C -5.5139700000 -0.1331660000 0.3631170000
H -6.1958630000 -0.1798030000 -1.6825450000
H -4.5436270000 -0.1909520000 2.2899190000
C -0.1415520000 1.7206030000 0.2469470000
H 1.6742750000 2.0572430000 -0.7848410000
B 3.9995030000 0.8885360000 -0.4140160000
H -0.4075060000 -3.8213110000 -0.0926270000
H -0.6889410000 -3.0523430000 1.4792440000
H 0.4709290000 -4.3833820000 1.3382310000
H 2.2586940000 -3.0375190000 2.3977470000
H 1.1599540000 -1.6616260000 2.5796870000
H 2.7310950000 -1.4504370000 1.7776000000
H 1.8109060000 -3.4667030000 -1.3252290000
H 2.6021890000 -4.1348680000 0.1127080000
H 3.1340630000 -2.5753980000 -0.5459120000
H -6.4846630000 0.1382510000 0.7682590000
H -0.7630900000 0.9928980000 0.7668310000
C -0.6453710000 3.1344460000 0.2664840000
F 5.0928200000 0.1005590000 -0.5626000000
F 3.8729290000 1.5022320000 0.8011610000
F 3.7229840000 1.7019360000 -1.4856740000
C -2.0260650000 3.2179600000 -0.4166390000
H 0.0606340000 3.7623580000 -0.2917410000

C -0.7150760000 3.6516450000 1.7181820000
H -1.9759760000 2.8887220000 -1.4596820000
H -2.3905140000 4.2513380000 -0.4015570000
H -2.7621160000 2.5913070000 0.1005900000
H -1.4052180000 3.0466890000 2.3192890000
H -1.0763220000 4.6860300000 1.7332260000
H 0.2685400000 3.6251620000 2.1979940000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394663 (Hartree/Particle)
Thermal correction to Energy= 0.420624
Thermal correction to Enthalpy= 0.421568
Thermal correction to Gibbs (Free) Energy= 0.335736
Sum of electronic and zero-point Energies= -1137.828603
Sum of electronic and thermal Energies= -1137.802642
Sum of electronic and thermal Enthalpies= -1137.801698
Sum of electronic and thermal (Free) Energies= -1137.887530

cc/s TS

C 1.7326980000 0.9027220000 -0.8900710000
C 0.4819160000 0.5578860000 -0.5079790000
C 2.9956200000 0.5842960000 -0.2382290000
H 1.8158970000 1.4857810000 -1.8090980000
C -0.7640370000 1.0654530000 -0.2758120000
C 4.1958220000 0.6689730000 -0.9723130000
C 3.0688790000 0.2554480000 1.1316270000
C -1.7821290000 0.0314460000 -0.1531110000
C -1.0962330000 2.5505790000 -0.0557970000
C 5.4195820000 0.3927190000 -0.3717160000
H 4.1562320000 0.9402440000 -2.0244540000
C 4.2949980000 -0.0204740000 1.7300140000
H 2.1639920000 0.2578650000 1.7320970000
C -1.2099810000 -1.2611300000 -0.2446500000
O -3.0310000000 0.2953240000 -0.0614680000
C 0.1455920000 3.4570250000 -0.1290420000
C -1.7523280000 2.7316970000 1.3344980000
C -2.0867360000 2.9879430000 -1.1671350000
C 5.4730230000 0.0395540000 0.9799620000
H 6.3338450000 0.4543270000 -0.9550820000
H 4.3349490000 -0.2664220000 2.7874110000
C 0.1718470000 -1.3921240000 -0.0552980000
H -1.8138970000 -2.0684190000 -0.6456920000
B -4.0742930000 -0.8770340000 0.2451620000
H 0.6180430000 3.4303610000 -1.1166940000
H 0.8983770000 3.1887100000 0.6196030000
H -0.1584920000 4.4925390000 0.0592180000
H -2.0100640000 3.7871490000 1.4803370000
H -1.0597750000 2.4431250000 2.1343060000
H -2.6647490000 2.1409260000 1.4328880000
H -1.6330340000 2.8852410000 -2.1599540000
H -2.3446890000 4.0436190000 -1.0224270000
H -3.0059330000 2.4007380000 -1.1402720000
H 6.4292140000 -0.1705240000 1.4505740000
H 0.6041290000 -1.0975380000 0.9038990000
C 0.8206890000 -2.6358740000 -0.6692480000
F -5.2520480000 -0.2258880000 0.4551630000
F -3.5730240000 -1.5297870000 1.3556900000
F -4.0643560000 -1.6876280000 -0.8789300000
C 2.3112850000 -2.5329460000 -1.0136670000
H 0.2802620000 -2.8531180000 -1.5993960000
C 0.5817600000 -3.8127060000 0.3046780000
H 2.5048460000 -1.7615510000 -1.7631900000
H 2.6511900000 -3.4910970000 -1.4225500000
H 2.9213860000 -2.3128910000 -0.1319210000
H 1.1029740000 -3.6450680000 1.2553750000
H 0.9674720000 -4.7417890000 -0.1299710000
H -0.4814600000 -3.9528200000 0.5233700000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394343 (Hartree/Particle)
Thermal correction to Energy= 0.418801
Thermal correction to Enthalpy= 0.419745
Thermal correction to Gibbs (Free) Energy= 0.339514
Sum of electronic and zero-point Energies= -1137.791492
Sum of electronic and thermal Energies= -1137.767034
Sum of electronic and thermal Enthalpies= -1137.766090
Sum of electronic and thermal (Free) Energies= -1137.846321

cc/s PT

C -1.8007140000 0.9706350000 -0.0979890000
C -0.5800220000 0.3539970000 -0.0459160000
C 0.6991280000 1.0326720000 0.0002730000
C 1.7240740000 0.0793770000 -0.3587310000
C 1.1123000000 -1.1568250000 -0.5624930000
C -0.3001690000 -1.1469220000 -0.1415370000
C 1.0752960000 2.4667800000 0.3408900000
O 2.9922580000 0.3486730000 -0.4599290000
C -0.0675050000 3.4145460000 0.7535510000
C 1.7949660000 3.0907990000 -0.8890040000
C 2.0677870000 2.3983950000 1.5423890000
H 1.6496730000 -2.0272750000 -0.9108200000
C -3.1368820000 0.4279450000 -0.3387100000
H -1.8078520000 2.0423430000 0.0441890000
C -4.2248000000 1.0934600000 0.2687300000
C -5.5298700000 0.6467190000 0.0942620000
C -5.7871690000 -0.4537370000 -0.7281180000
C -4.7297450000 -1.0948910000 -1.3772000000
C -3.4199100000 -0.6624550000 -1.1869120000
H -4.0302030000 1.9563140000 0.9008840000
H -6.3480450000 1.1622890000 0.5888610000
H -6.8070280000 -0.7964020000 -0.8777730000
H -4.9266230000 -1.9283870000 -2.0454120000
H -2.6207610000 -1.1390100000 -1.7416870000
B 3.9863330000 -0.8563840000 -0.5055600000
F 5.2303230000 -0.3017220000 -0.4135340000
F 3.7563680000 -1.5318220000 -1.6998170000
F 3.6555770000 -1.6681890000 0.5852340000
H 1.5692600000 2.0051290000 2.4358400000
H 2.4119880000 3.4143100000 1.7667100000
H 2.9354450000 1.7788440000 1.3165350000
H 2.1225470000 4.1036930000 -0.6283630000
H 1.1110470000 3.1653170000 -1.7424190000
H 2.6673080000 2.5061680000 -1.1826930000
H -0.6634700000 3.0196260000 1.5833990000
H -0.7310050000 3.6665180000 -0.0807340000
H 0.3774410000 4.3556850000 1.0936010000
H -0.9409330000 -1.6819860000 -0.8494720000
C -0.4349110000 -1.8758450000 1.2653940000
C -1.8931920000 -2.0991490000 1.6787070000
H 0.0351550000 -1.1956670000 1.9885410000
C 0.3500700000 -3.1981620000 1.2855510000
H -2.4547210000 -1.1646490000 1.7557310000
H -1.9238000000 -2.5895360000 2.6585590000
H -2.4166940000 -2.7500810000 0.9680220000
H 0.0180280000 -3.8731770000 0.4857570000
H 0.1841770000 -3.7125340000 2.2385860000
H 1.4265330000 -3.0334410000 1.1756180000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.398155 (Hartree/Particle)
Thermal correction to Energy= 0.422205
Thermal correction to Enthalpy= 0.423149
Thermal correction to Gibbs (Free) Energy= 0.344094
Sum of electronic and zero-point Energies= -1137.824833
Sum of electronic and thermal Energies= -1137.800783
Sum of electronic and thermal Enthalpies= -1137.799839
Sum of electronic and thermal (Free) Energies= -1137.878893

c/d RT

C -2.1849480000 0.5762710000 -0.9757820000
C -1.0630070000 -0.1039680000 -0.9233010000
H -2.2890300000 1.3168010000 -1.7711010000
C -3.3388510000 0.4496510000 -0.0653120000
C 0.0321820000 -0.8385280000 -0.8407460000
C -4.4833590000 1.2259120000 -0.3062720000
C -3.3326090000 -0.4205610000 1.0385630000
C 1.1105990000 -0.3529540000 0.0630360000
C 0.1808070000 -2.2059040000 -1.5633380000
C -5.5954360000 1.1337090000 0.5297120000
H -4.4991150000 1.9038970000 -1.1565020000
C -4.4430150000 -0.5106480000 1.8719200000
H -2.4510180000 -1.0223960000 1.2416950000
C 1.4317750000 1.0625240000 0.2141190000
O 1.7399260000 -1.2287230000 0.7117570000
C -0.9031550000 -2.3336260000 -2.6498860000
C 0.0138010000 -3.3674260000 -0.5554380000
C 1.5693940000 -2.2821770000 -2.2373100000

C -5.5794120000 0.2651410000 1.6214250000
H -6.4732060000 1.7413930000 0.3275120000
H -4.4223250000 -1.1869300000 2.7220860000
C 1.2052550000 1.9829610000 -0.7425660000
H 1.9579940000 1.3143590000 1.1270280000
B 3.1049070000 -1.0015940000 1.6376350000
H -0.8324730000 -1.5263440000 -3.3880550000
H -1.9112450000 -2.3151540000 -2.2231990000
H -0.7783980000 -3.2850750000 -3.1784140000
H 0.0817440000 -4.3232480000 -1.0891370000
H -0.9688490000 -3.3234290000 -0.0713280000
H 0.7833030000 -3.3490620000 0.2177550000
H 1.6939480000 -1.4816610000 -2.9767010000
H 1.6681090000 -3.2386050000 -2.7632840000
H 2.3852770000 -2.2141880000 -1.5132470000
H -6.4443520000 0.1926030000 2.2747510000
C 1.5882040000 3.4358570000 -0.6846500000
H 0.7411530000 1.6673360000 -1.6758120000
F 4.0120530000 -0.5076440000 0.7407510000
F 2.7330440000 -0.1048050000 2.6099500000
F 3.3459650000 -2.2589880000 2.0835080000
C 2.1873110000 3.8846310000 0.6525610000
H 0.6527740000 3.9968400000 -0.8509700000
C 2.5247620000 3.7696480000 -1.8680820000
H 1.5081770000 3.6840940000 1.4879750000
H 2.3867390000 4.9611940000 0.6325390000
H 3.1351490000 3.3732510000 0.8553440000
H 3.4805000000 3.2441600000 -1.7644390000
H 2.7280730000 4.8454120000 -1.8979120000
H 2.0817800000 3.4823550000 -2.8286240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394697 (Hartree/Particle)
Thermal correction to Energy= 0.420603
Thermal correction to Enthalpy= 0.421547
Thermal correction to Gibbs (Free) Energy= 0.335219
Sum of electronic and zero-point Energies= -1137.827623
Sum of electronic and thermal Energies= -1137.801717
Sum of electronic and thermal Enthalpies= -1137.800772
Sum of electronic and thermal (Free) Energies= -1137.887100

c/d TS

C -1.9002940000 0.6432210000 -0.8444980000
C -0.6423850000 0.1946150000 -0.7519830000
H -2.0921470000 1.4642040000 -1.5355180000
C -3.0539850000 0.2207850000 -0.0464990000
C 0.2850860000 -0.7874480000 -0.5702290000
C -4.3338280000 0.6776200000 -0.4140420000
C -2.9343120000 -0.6093740000 1.0848800000
C 1.5306290000 -0.2740190000 -0.0089230000
C 0.1243810000 -2.2517370000 -1.0059380000
C -5.4613050000 0.2933850000 0.3070350000
H -4.4388810000 1.3292860000 -1.2781900000
C -4.0624690000 -0.9871960000 1.8059190000
H -1.9502060000 -0.9371050000 1.4055960000
C 1.5418930000 1.1488820000 0.0085870000
O 2.4349930000 -1.0427040000 0.4671820000
C -1.2048240000 -2.4861680000 -1.7456780000
C 0.1692570000 -3.1509380000 0.2563000000
C 1.2901090000 -2.6300580000 -1.9520210000
C -5.3302050000 -0.5418120000 1.4185710000
H -6.4420400000 0.6493370000 0.0042070000
H -3.9527570000 -1.6240340000 2.6791780000
C 0.6469430000 1.7975540000 -0.8441320000
H 2.1163810000 1.6618680000 0.7715750000
B 3.8424440000 -0.4308530000 0.9223970000
H -1.2779890000 -1.8727310000 -2.6504420000
H -2.0727300000 -2.2702710000 -1.1155710000
H -1.2654770000 -3.5371690000 -2.0486840000
H 0.1046760000 -4.2014760000 -0.0505900000
H -0.6783680000 -2.9441530000 0.9193990000
H 1.0962860000 -3.0106140000 0.8154330000
H 1.2787370000 -2.0101030000 -2.8563860000
H 1.1796720000 -3.6753590000 -2.2625400000
H 2.2610520000 -2.5190400000 -1.4653450000
H -6.2083770000 -0.8371300000 1.9856240000
C 0.1848040000 3.2239340000 -0.6156740000
H 0.6508540000 1.5132140000 -1.8970770000
F 4.2881770000 0.2980700000 -0.1632210000
F 3.5593030000 0.3812400000 2.0095330000
F 4.5977650000 -1.5234280000 1.2216270000
C -0.1035710000 3.5466720000 0.8564150000
H -0.7465640000 3.3527060000 -1.1850330000
C 1.2214060000 4.1962480000 -1.2227070000
H -0.8315910000 2.8475480000 1.2816700000
H -0.5093250000 4.5597100000 0.9504630000
H 0.8064810000 3.4996990000 1.4645980000
H 2.1801880000 4.1252070000 -0.6976930000
H 0.8625650000 5.2279450000 -1.1383480000
H 1.4018970000 3.9858210000 -2.2827910000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394444 (Hartree/Particle)
Thermal correction to Energy= 0.419062
Thermal correction to Enthalpy= 0.420007
Thermal correction to Gibbs (Free) Energy= 0.339435
Sum of electronic and zero-point Energies= -1137.801381
Sum of electronic and thermal Energies= -1137.776762
Sum of electronic and thermal Enthalpies= -1137.775818
Sum of electronic and thermal (Free) Energies= -1137.856390

c/d PT

C 1.7947250000 1.0587700000 0.7189860000
C 0.4879570000 0.6472510000 0.7512470000
C -0.1668250000 -0.6149760000 0.5472670000
C -1.5633700000 -0.3521820000 0.2635010000
C -1.8298470000 0.9683820000 0.6221540000
C -0.6081580000 1.7084830000 0.9918930000
C 0.3084470000 -2.0396400000 0.8028670000
C 2.9627590000 0.4972720000 0.0590250000
O -2.3982880000 -1.2354370000 -0.1876610000
C 1.7181330000 -2.1641360000 1.4091930000
C 0.2206000000 -2.8677050000 -0.5087760000
C -0.6813450000 -2.6569670000 1.8419960000
C 4.2495080000 0.8019750000 0.5500760000
C 2.8568250000 -0.2524210000 -1.1311540000
C 3.9971040000 -0.7188160000 -1.7782420000
H 1.8759590000 -0.4300950000 -1.5599500000
C 5.2634150000 -0.4466360000 -1.2528570000
H 3.8995290000 -1.2842360000 -2.7004840000
C 5.3860870000 0.3170080000 -0.0875540000
H 4.3464930000 1.4048450000 1.4495530000
H 6.1523100000 -0.8104560000 -1.7602360000
H 6.3694490000 0.5421610000 0.3150680000
B -3.7855460000 -0.7247730000 -0.7148680000
F -4.4646990000 -0.2026340000 0.3819300000
F -4.3837700000 -1.8223740000 -1.2632520000
F -3.4950920000 0.2785120000 -1.6380230000
H 1.9729980000 2.0464720000 1.1451450000
H -2.8262070000 1.3884050000 0.6034060000
H -0.5991300000 1.9132390000 2.0769110000
C -0.4887300000 3.0800610000 0.2560290000
C -0.5819860000 2.9183850000 -1.2693890000
H 0.4945020000 3.5021850000 0.5035670000
C -1.5463140000 4.0655540000 0.7781720000
H -2.5628130000 3.7379520000 0.5325520000
H -1.4028850000 5.0509180000 0.3215850000
H -1.4840740000 4.1884320000 1.8662510000
H 0.2166170000 2.2756750000 -1.6566050000
H -0.4929610000 3.8922030000 -1.7632840000
H -1.5399050000 2.4741380000 -1.5651500000
H -0.6325550000 -2.1167870000 2.7943920000
H -0.3838510000 -3.6945910000 2.0276110000
H -1.7097980000 -2.6501350000 1.4811530000
H 0.4601150000 -3.9128020000 -0.2811860000
H 0.9433690000 -2.5131860000 -1.2507490000
H -0.7816460000 -2.8238310000 -0.9386810000
H 1.8456770000 -1.5107590000 2.2794280000
H 2.5115850000 -1.9457590000 0.6949450000
H 1.8593990000 -3.1961340000 1.7478880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397023 (Hartree/Particle)
Thermal correction to Energy= 0.421363
Thermal correction to Enthalpy= 0.422307
Thermal correction to Gibbs (Free) Energy= 0.342673
Sum of electronic and zero-point Energies= -1137.821306
Sum of electronic and thermal Energies= -1137.796966

Sum of electronic and thermal Enthalpies= -1137.796022
Sum of electronic and thermal (Free) Energies= -1137.875656

cc/d RT

C -1.7932410000 -1.0022210000 -1.2868240000
C -0.6234180000 -1.1088450000 -0.7001330000
C -3.0806300000 -0.6710460000 -0.6488950000
H -1.8223580000 -1.1588030000 -2.3670090000
C 0.5769070000 -1.2644120000 -0.1698980000
C -4.1845340000 -0.3617910000 -1.4598330000
C -3.2467840000 -0.6571220000 0.7476060000
C 1.4928960000 -0.0912940000 -0.1931050000
C 1.0801140000 -2.6394370000 0.3512440000
C -5.4151130000 -0.0322600000 -0.8936430000
H -4.0718440000 -0.3763080000 -2.5411880000
C -4.4762920000 -0.3265080000 1.3116940000
H -2.4113430000 -0.9263470000 1.3885450000
C 1.0296290000 1.2891360000 -0.0880440000
O 2.7191250000 -0.3409970000 -0.3296500000
C -0.1140930000 -3.5986190000 0.5149810000
C 1.7556590000 -2.4544000000 1.7286510000
C 2.0775560000 -3.2624160000 -0.6541500000
C -5.5652320000 -0.0101460000 0.4937720000
H -6.2570880000 0.2064080000 -1.5375480000
H -4.5888700000 -0.3250810000 2.3925100000
C -0.1006040000 1.6656430000 0.5396370000
H 1.7261520000 2.0235530000 -0.4738270000
B 3.9836090000 0.7401280000 -0.2437790000
H -0.6160490000 -3.7911770000 -0.4386510000
H -0.8592060000 -3.2046160000 1.2160120000
H 0.2414130000 -4.5575450000 0.9075020000
H 2.0841620000 -3.4291040000 2.1071860000
H 1.0543250000 -2.0330750000 2.4592410000
H 2.6321330000 -1.8045040000 1.6748250000
H 1.6106120000 -3.3870060000 -1.6381330000
H 2.3782400000 -4.2550610000 -0.2974800000
H 2.9740220000 -2.6518840000 -0.7700310000
H -6.5244600000 0.2436640000 0.9359340000
H -0.7462080000 0.9048740000 0.9745490000
C -0.5726120000 3.0807670000 0.7347060000
F 5.0500510000 -0.0739250000 -0.4397050000
F 3.8664860000 1.2694910000 1.0118360000
F 3.7484460000 1.6403050000 -1.2544650000
C 0.3835720000 4.1519330000 0.1992110000
H -0.6673760000 3.2163990000 1.8249550000
C -1.9926340000 3.2372650000 0.1430570000
H 1.3786830000 4.0686410000 0.6481830000
H -0.0066580000 5.1497710000 0.4255970000
H 0.4950000000 4.0779080000 -0.8889420000
H -1.9728670000 3.1215120000 -0.9464820000
H -2.3866900000 4.2333390000 0.3720250000
H -2.6864880000 2.4935670000 0.5491250000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394851 (Hartree/Particle)
Thermal correction to Energy= 0.420667
Thermal correction to Enthalpy= 0.421612
Thermal correction to Gibbs (Free) Energy= 0.336415
Sum of electronic and zero-point Energies= -1137.827568
Sum of electronic and thermal Energies= -1137.801751
Sum of electronic and thermal Enthalpies= -1137.800807
Sum of electronic and thermal (Free) Energies= -1137.886004

cc/d TS

C 1.6709580000 0.8533110000 -0.8752070000
C 0.4357810000 0.5476630000 -0.4286830000
C 2.9523030000 0.5807890000 -0.2326580000
H 1.7277770000 1.3391970000 -1.8513180000
C -0.8351080000 1.0098900000 -0.2487550000
C 4.1201930000 0.4895560000 -1.0156550000
C 3.0715440000 0.4709830000 1.1679200000
C -1.8052420000 -0.0614920000 -0.0717780000
C -1.2329700000 2.4905390000 -0.1451440000
C 5.3574940000 0.2552170000 -0.4230910000
H 4.0458800000 0.5934200000 -2.0954000000
C 4.3113420000 0.2421640000 1.7580830000
H 2.1915380000 0.6025570000 1.7908330000
C -1.1705270000 -1.3305820000 -0.0456500000
O -3.0663170000 0.1492260000 -0.0329410000
C -0.0221160000 3.4348660000 -0.2512160000
C -1.9358730000 2.7428740000 1.2104340000
C -2.2070690000 2.8056590000 -1.3107270000
C 5.4565370000 0.1261410000 0.9653250000
H 6.2466760000 0.1776330000 -1.0422400000
H 4.3875740000 0.1668600000 2.8391030000
C 0.2068120000 -1.3740820000 0.2002630000
H -1.7259930000 -2.1993150000 -0.3825920000
B -4.0692750000 -1.0446260000 0.3289880000
H 0.4839440000 3.3497530000 -1.2187100000
H 0.7148700000 3.2505080000 0.5376710000
H -0.3671340000 4.4698050000 -0.1515180000
H -2.2379650000 3.7947270000 1.2733890000
H -1.2568650000 2.5393870000 2.0471640000
H -2.8274480000 2.1239800000 1.3263300000
H -1.7208990000 2.6526110000 -2.2814350000
H -2.5121790000 3.8568630000 -1.2490220000
H -3.1018410000 2.1826800000 -1.2656370000
H 6.4236270000 -0.0482120000 1.4282050000
H 0.5851300000 -0.9478120000 1.1314630000
C 0.9851720000 -2.5833080000 -0.3268020000
F -5.2823470000 -0.4350570000 0.4369490000
F -3.5867690000 -1.5786540000 1.5080260000
F -3.9744910000 -1.9414320000 -0.7233860000
C 1.2982170000 -2.4873990000 -1.8328750000
H 0.2779490000 -3.4188710000 -0.2128580000
C 2.2325550000 -2.9355560000 0.4948920000
H 0.4043640000 -2.2274780000 -2.4099460000
H 1.6686210000 -3.4509470000 -2.1995600000
H 2.0673030000 -1.7343790000 -2.0310020000
H 3.0252840000 -2.1922660000 0.3754450000
H 2.6311360000 -3.9033400000 0.1709790000
H 1.9980250000 -3.0151440000 1.5628770000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394044 (Hartree/Particle)
Thermal correction to Energy= 0.418651
Thermal correction to Enthalpy= 0.419596
Thermal correction to Gibbs (Free) Energy= 0.339050
Sum of electronic and zero-point Energies= -1137.793559
Sum of electronic and thermal Energies= -1137.768951
Sum of electronic and thermal Enthalpies= -1137.768007
Sum of electronic and thermal (Free) Energies= -1137.848553

cc/d PT

C -1.7918720000 0.8992200000 -0.0721110000
C -0.5742150000 0.2712870000 -0.0970940000
C 0.7088200000 0.9410560000 -0.0841560000
C 1.7198920000 -0.0206920000 -0.4627990000
C 1.1002770000 -1.2557240000 -0.6439550000
C -0.3222630000 -1.2269420000 -0.2624540000
C 1.1065390000 2.3751660000 0.2355060000
O 2.9882410000 0.2455760000 -0.5786810000
C -0.0149720000 3.3435470000 0.6584110000
C 1.8058250000 2.9780550000 -1.0168390000
C 2.1221180000 2.3126800000 1.4181650000
H 1.6409430000 -2.1480650000 -0.9331920000
C -3.1378160000 0.3839370000 -0.3136420000
H -1.7871680000 1.9582370000 0.1439560000
C -4.2054270000 1.0018180000 0.3741910000
C -5.5176420000 0.5796390000 0.1924830000
C -5.8026300000 -0.4428970000 -0.7168880000
C -4.7659600000 -1.0316930000 -1.4446200000
C -3.4485660000 -0.6265280000 -1.2468290000
H -3.9891550000 1.8056980000 1.0734590000
H -6.3201980000 1.0548400000 0.7491460000
H -6.8285430000 -0.7642620000 -0.8722680000
H -4.9853380000 -1.8017000000 -2.1787270000
H -2.6647940000 -1.0580440000 -1.8580970000
B 3.9924840000 -0.9446120000 -0.4820300000
F 5.2319110000 -0.3715780000 -0.4630120000
F 3.7728660000 -1.7681640000 -1.5830330000
F 3.6687110000 -1.6139310000 0.7030270000
H 1.6363660000 1.9395040000 2.3269600000
H 2.4825250000 3.3278750000 1.6192400000
H 2.9774980000 1.6789170000 1.1862240000
H 2.1493040000 3.9901930000 -0.7743720000
H 1.1039980000 3.0510980000 -1.8558490000

H 2.6657460000 2.3817430000 -1.3228230000
H -0.5802240000 2.9823180000 1.5244780000
H -0.7082280000 3.5723920000 -0.1582260000
H 0.4486620000 4.2917300000 0.9505600000
H -0.9528240000 -1.6798200000 -1.0357560000
C -0.5131500000 -2.1180630000 1.0413920000
C 0.3765160000 -1.6672650000 2.2086610000
H -0.1692030000 -3.1132780000 0.7274800000
C -1.9762820000 -2.2560430000 1.4760900000
H 1.4402000000 -1.6903910000 1.9528800000
H 0.2194200000 -2.3326860000 3.0648870000
H 0.1238070000 -0.6508870000 2.5363420000
H -2.3771790000 -1.3112180000 1.8578020000
H -2.0467180000 -2.9951720000 2.2824160000
H -2.6237700000 -2.5908630000 0.6591750000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.398128 (Hartree/Particle)
Thermal correction to Energy= 0.422155
Thermal correction to Enthalpy= 0.423099
Thermal correction to Gibbs (Free) Energy= 0.344224
Sum of electronic and zero-point Energies= -1137.825481
Sum of electronic and thermal Energies= -1137.801455
Sum of electronic and thermal Enthalpies= -1137.800511
Sum of electronic and thermal (Free) Energies= -1137.879385

c/u RT

C -2.1591810000 0.2729060000 -0.9662580000
C -0.9732640000 -0.2887920000 -0.9172080000
H -2.3652810000 0.9435780000 -1.8025300000
C -3.2611660000 0.0972280000 -0.0012800000
C 0.1925760000 -0.9046380000 -0.8334890000
C -4.4850830000 0.7409870000 -0.2425210000
C -3.1286720000 -0.6911240000 1.1549340000
C 1.2475130000 -0.2550560000 -0.0081170000
C 0.4536370000 -2.2967810000 -1.4721190000
C -5.5515240000 0.5989240000 0.6443930000
H -4.5988270000 1.3547150000 -1.1331390000
C -4.1937700000 -0.8311300000 2.0390040000
H -2.1849480000 -1.1897790000 1.3584490000
C 1.4371050000 1.1915630000 0.0309230000
O 1.9784230000 -1.0183080000 0.6750930000
C -0.6475490000 -2.6032370000 -2.5042080000
C 0.4379830000 -3.3981880000 -0.3860680000
C 1.8197200000 -2.2818880000 -2.1944690000
C -5.4098700000 -0.1876180000 1.7879780000
H -6.4920260000 1.1037280000 0.4412200000
H -4.0753220000 -1.4428180000 2.9291590000
C 1.0914550000 2.0147900000 -0.9771950000
H 1.9709800000 1.5560980000 0.9001370000
B 3.3435330000 -0.5964090000 1.5313130000
H -0.6826650000 -1.8446240000 -3.2946810000
H -1.6376370000 -2.6546360000 -2.0397540000
H -0.4456600000 -3.5714630000 -2.9752980000
H 0.5836420000 -4.3766700000 -0.8597910000
H -0.5273030000 -3.4180760000 0.1332770000
H 1.2271920000 -3.2522810000 0.3529770000
H 1.8384110000 -1.5255170000 -2.9885640000
H 1.9970530000 -3.2577000000 -2.6608100000
H 2.6481030000 -2.0845350000 -1.5092960000
H -6.2391300000 -0.2987250000 2.4809440000
C 1.3152510000 3.5011490000 -1.0266620000
H 0.6189960000 1.5917830000 -1.8625080000
F 4.1685130000 -0.0809110000 0.5697000000
F 2.9148900000 0.3259600000 2.4549350000
F 3.7213150000 -1.7905410000 2.0499640000
C -0.0324020000 4.2124530000 -1.2867500000
H 1.9453960000 3.6815230000 -1.9133670000
C 2.0316270000 4.0797290000 0.1982380000
H -0.5264930000 3.8269470000 -2.1862360000
H 0.1278490000 5.2869670000 -1.4251010000
H -0.7136960000 4.0760190000 -0.4393510000
H 1.4359600000 3.9434980000 1.1084330000
H 2.1949190000 5.1543240000 0.0651750000
H 3.0066610000 3.6079190000 0.3571830000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394755 (Hartree/Particle)
Thermal correction to Energy= 0.420640
Thermal correction to Enthalpy= 0.421584
Thermal correction to Gibbs (Free) Energy= 0.335517
Sum of electronic and zero-point Energies= -1137.827448
Sum of electronic and thermal Energies= -1137.801564
Sum of electronic and thermal Enthalpies= -1137.800619
Sum of electronic and thermal (Free) Energies= -1137.886686

c/u TS

C -1.8735880000 0.5438930000 -0.7792360000
C -0.5724450000 0.2262370000 -0.7110620000
H -2.1625350000 1.3492890000 -1.4515200000
C -2.9614010000 -0.0164230000 0.0252920000
C 0.4269440000 -0.6908760000 -0.5761400000
C -4.2895690000 0.2972660000 -0.3218050000
C -2.7342790000 -0.8410120000 1.1444880000
C 1.6417850000 -0.1092440000 -0.0150140000
C 0.3704370000 -2.1457410000 -1.0678660000
C -5.3570440000 -0.2221160000 0.4056270000
H -4.4786220000 0.9435930000 -1.1756070000
C -3.8032910000 -1.3540190000 1.8719230000
H -1.7153680000 -1.0575320000 1.4502970000
C 1.5563170000 1.3067830000 0.0448560000
O 2.6079280000 -0.8282800000 0.4173790000
C -0.9470830000 -2.4565670000 -1.8002040000
C 0.5052500000 -3.0875630000 0.1564180000
C 1.5465580000 -2.3945570000 -2.0440800000
C -5.1180390000 -1.0511040000 1.5039010000
H -6.3755550000 0.0235570000 0.1184340000
H -3.6114960000 -1.9846240000 2.7354530000
C 0.5862240000 1.9254220000 -0.7509710000
H 2.1299820000 1.8427340000 0.7933080000
B 3.9803820000 -0.1391420000 0.8647730000
H -1.0844040000 -1.8140480000 -2.6768820000
H -1.8195480000 -2.3401170000 -1.1507870000
H -0.9262430000 -3.4953450000 -2.1474990000
H 0.5187810000 -4.1268560000 -0.1923390000
H -0.3460360000 -2.9748090000 0.8371630000
H 1.4269120000 -2.8965970000 0.7092810000
H 1.4718930000 -1.7426790000 -2.9226160000
H 1.5119500000 -3.4324170000 -2.3946750000
H 2.5139580000 -2.2271650000 -1.5668000000
H -5.9500010000 -1.4514200000 2.0762050000
C 0.0928080000 3.3258430000 -0.4053800000
H 0.5749700000 1.6961160000 -1.8171680000
F 4.3619640000 0.6399160000 -0.2102450000
F 3.6665040000 0.6294480000 1.9752480000
F 4.8077820000 -1.1884600000 1.1275680000
C -0.7655820000 3.9562490000 -1.5122600000
H 1.0173240000 3.9223300000 -0.3396940000
C -0.5914850000 3.4030840000 0.9711300000
H -0.2721720000 3.8948050000 -2.4892490000
H -0.9454220000 5.0147900000 -1.2970650000
H -1.7457250000 3.4729260000 -1.5945340000
H -1.5371220000 2.8506580000 0.9742750000
H -0.8070280000 4.4455310000 1.2290830000
H 0.0448140000 2.9877740000 1.7591960000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394285 (Hartree/Particle)
Thermal correction to Energy= 0.418935
Thermal correction to Enthalpy= 0.419879
Thermal correction to Gibbs (Free) Energy= 0.339253
Sum of electronic and zero-point Energies= -1137.798795
Sum of electronic and thermal Energies= -1137.774145
Sum of electronic and thermal Enthalpies= -1137.773201
Sum of electronic and thermal (Free) Energies= -1137.853827

c/u PT

C -1.7927280000 0.9001080000 -0.7672760000
C -0.4508180000 0.6102110000 -0.7829650000
C 0.2982640000 -0.5946190000 -0.5605150000
C 1.6811890000 -0.2269120000 -0.3301390000
C 1.8421750000 1.0904140000 -0.7515370000
C 0.5579720000 1.7467150000 -1.0627970000
C -0.0757120000 -2.0594050000 -0.7601110000
C -2.8945260000 0.2685860000 -0.0606330000
O 2.5886470000 -1.0314070000 0.1296130000
C -1.4837180000 -2.3140590000 -1.3288670000

C 0.1006880000 -2.8304400000 0.5773140000
C 0.9349520000 -2.6390130000 -1.8006420000
C -4.2100770000 0.4203740000 -0.5473740000
C -2.7039100000 -0.3983940000 1.1680890000
C -3.7868170000 -0.9347370000 1.8578900000
H -1.7056880000 -0.4566690000 1.5896480000
C -5.0789260000 -0.8154100000 1.3381860000
H -3.6256370000 -1.4350820000 2.8083630000
C -5.2874120000 -0.1342930000 0.1342890000
H -4.3742110000 0.9587440000 -1.4775040000
H -5.9231620000 -1.2333300000 1.8790630000
H -6.2922410000 -0.0279370000 -0.2641970000
B 3.9155840000 -0.3930300000 0.6697150000
F 4.5652490000 0.1784610000 -0.4199320000
F 4.6013320000 -1.4261340000 1.2406250000
F 3.5193160000 0.5880320000 1.5796820000
H -2.0679370000 1.8307840000 -1.2589880000
H 2.8044950000 1.5855910000 -0.7800030000
H 0.4801860000 1.9763400000 -2.1391300000
C 0.4725850000 3.1040640000 -0.2815340000
C -0.7016590000 4.0098210000 -0.6819280000
H 1.3891170000 3.6311480000 -0.5846730000
C 0.5420340000 2.9053440000 1.2414240000
H -0.3476010000 2.3829600000 1.6141890000
H 0.5871170000 3.8764800000 1.7467770000
H 1.4264140000 2.3303810000 1.5366130000
H -0.8215510000 4.0731280000 -1.7708680000
H -0.5289150000 5.0263160000 -0.3109690000
H -1.6489330000 3.6698790000 -0.2487900000
H 0.8253110000 -2.1383250000 -2.7694610000
H 0.7121460000 -3.7017760000 -1.9436370000
H 1.9676340000 -2.5436690000 -1.4655930000
H -0.0654610000 -3.8978960000 0.3919130000
H -0.6310100000 -2.5026420000 1.3228640000
H 1.1056350000 -2.6977400000 0.9819140000
H -1.6837890000 -1.6981080000 -2.2126320000
H -2.2767020000 -2.1423810000 -0.6017170000
H -1.5467140000 -3.3631470000 -1.6372820000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397316 (Hartree/Particle)
Thermal correction to Energy= 0.421498
Thermal correction to Enthalpy= 0.422442
Thermal correction to Gibbs (Free) Energy= 0.343473
Sum of electronic and zero-point Energies= -1137.818300
Sum of electronic and thermal Energies= -1137.794118
Sum of electronic and thermal Enthalpies= -1137.793173
Sum of electronic and thermal (Free) Energies= -1137.872143

cc/u RT

C -1.8506640000 -1.0968390000 -1.3045100000
C -0.6877960000 -1.1856160000 -0.7016200000
C -3.1278180000 -0.6636850000 -0.7077770000
H -1.8807990000 -1.3501060000 -2.3661140000
C 0.5046860000 -1.3169310000 -0.1468240000
C -4.2164700000 -0.3884710000 -1.5510400000
C -3.2982200000 -0.5170290000 0.6804790000
C 1.4408650000 -0.1654920000 -0.2621870000
C 0.9745620000 -2.6480510000 0.5022050000
C -5.4357250000 0.0362590000 -1.0252890000
H -4.1005820000 -0.5049410000 -2.6258730000
C -4.5162120000 -0.0914590000 1.2038120000
H -2.4762270000 -0.7591020000 1.3490510000
C 0.9908840000 1.2225330000 -0.3126830000
O 2.6665990000 -0.4416740000 -0.3395480000
C -0.2386450000 -3.5705320000 0.7262730000
C 1.6292040000 -2.3541100000 1.8707430000
C 1.9785980000 -3.3718810000 -0.4261430000
C -5.5895990000 0.1894040000 0.3534390000
H -6.2660250000 0.2464450000 -1.6938410000
H -4.6323300000 0.0122830000 2.2792660000
C -0.1491000000 1.6681270000 0.2482660000
H 1.6971760000 1.9065050000 -0.7678690000
B 3.9397280000 0.6315860000 -0.3297730000
H -0.7276090000 -3.8370240000 -0.2163010000
H -0.9887160000 -3.1056510000 1.3767630000
H 0.0935840000 -4.4973000000 1.2066220000
H 1.9336310000 -3.2971530000 2.3390100000
H 0.9228090000 -1.8591260000 2.5483410000
H 2.5178860000 -1.7258040000 1.7767800000
H 1.5267520000 -3.5755430000 -1.4039690000
H 2.2568360000 -4.3336640000 0.0216190000
H 2.8869090000 -2.7873020000 -0.5782170000
H -6.5401970000 0.5175330000 0.7642630000
H -0.7987950000 0.9632540000 0.7634530000
C -0.6188850000 3.0960410000 0.2871630000
F 5.0025090000 -0.2066210000 -0.4100290000
F 3.7946250000 1.2898450000 0.8602850000
F 3.7422290000 1.4238190000 -1.4347290000
C -0.8207320000 3.5327970000 1.7557250000
H -1.6170380000 3.0903060000 -0.1822780000
C 0.2702980000 4.0820880000 -0.4778800000
H -1.4906080000 2.8499380000 2.2906720000
H -1.2590110000 4.5357500000 1.7954640000
H 0.1368230000 3.5573630000 2.2877370000
H 1.2718430000 4.1397220000 -0.0365740000
H -0.1669220000 5.0856100000 -0.4456730000
H 0.3795120000 3.7971590000 -1.5297340000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394766 (Hartree/Particle)
Thermal correction to Energy= 0.420618
Thermal correction to Enthalpy= 0.421562
Thermal correction to Gibbs (Free) Energy= 0.336061
Sum of electronic and zero-point Energies= -1137.827687
Sum of electronic and thermal Energies= -1137.801835
Sum of electronic and thermal Enthalpies= -1137.800891
Sum of electronic and thermal (Free) Energies= -1137.886392

cc/u TS

C 1.7324010000 0.9767860000 -0.8539070000
C 0.5033960000 0.7087170000 -0.3790720000
C 3.0249590000 0.6126080000 -0.2778870000
H 1.7757530000 1.4877600000 -1.8179700000
C -0.7765540000 1.1332650000 -0.1833700000
C 4.1539980000 0.5259450000 -1.1162230000
C 3.1975540000 0.3889110000 1.1036140000
C -1.7265710000 0.0322710000 -0.0783400000
C -1.2019220000 2.5995770000 -0.0138120000
C 5.4029930000 0.1952300000 -0.5987330000
H 4.0394250000 0.7105020000 -2.1815130000
C 4.4479750000 0.0567820000 1.6179960000
H 2.3540020000 0.5160130000 1.7759190000
C -1.0635530000 -1.2264760000 -0.0873270000
O -2.9918050000 0.2147530000 -0.0780560000
C 0.0020440000 3.5585960000 -0.0326690000
C -1.9488810000 2.7705470000 1.3304200000
C -2.1448400000 2.9627570000 -1.1904950000
C 5.5536570000 -0.0457450000 0.7694820000
H 6.2607260000 0.1269990000 -1.2618710000
H 4.5642300000 -0.1061620000 2.6857950000
C 0.2923260000 -1.2401710000 0.2384320000
H -1.5803400000 -2.0830570000 -0.5056010000
B -3.9782480000 -1.0185970000 0.1890670000
H 0.5408030000 3.5251110000 -0.9855160000
H 0.7149170000 3.3381160000 0.7691830000
H -0.3551990000 4.5844690000 0.1087020000
H -2.2670140000 3.8137720000 1.4401660000
H -1.2934760000 2.5302500000 2.1761260000
H -2.8352580000 2.1357390000 1.3849010000
H -1.6273510000 2.8691580000 -2.1524890000
H -2.4691490000 4.0044560000 -1.0824420000
H -3.0301740000 2.3247280000 -1.2063180000
H 6.5294990000 -0.2980800000 1.1744150000
H 0.5951900000 -0.7964820000 1.1882350000
C 1.2200480000 -2.3463760000 -0.2258620000
F -5.2084150000 -0.4429140000 0.2842730000
F -3.5227050000 -1.6003280000 1.3561450000
F -3.8247650000 -1.8582780000 -0.9027050000
C 1.1424750000 -3.5248250000 0.7705840000
H 2.2396190000 -1.9456830000 -0.1725210000
C 0.9568290000 -2.8038510000 -1.6669450000
H 1.3747300000 -3.2051310000 1.7926590000
H 1.8606870000 -4.3027010000 0.4886940000
H 0.1418050000 -3.9711400000 0.7763570000
H -0.0220830000 -3.2850560000 -1.7698190000
H 1.7142650000 -3.5322910000 -1.9760540000
H 0.9930360000 -1.9599330000 -2.3646520000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394085 (Hartree/Particle)
Thermal correction to Energy= 0.418755
Thermal correction to Enthalpy= 0.419700
Thermal correction to Gibbs (Free) Energy= 0.338817
Sum of electronic and zero-point Energies= -1137.799425
Sum of electronic and thermal Energies= -1137.774755
Sum of electronic and thermal Enthalpies= -1137.773811
Sum of electronic and thermal (Free) Energies= -1137.854694

cc/u PT

C -1.8334650000 0.9538010000 -0.0963910000
C -0.5972120000 0.3730380000 -0.2400690000
C 0.6729630000 1.0550150000 -0.1662700000
C 1.7213540000 0.0841850000 -0.3986970000
C 1.1266280000 -1.1424340000 -0.6823390000
C -0.3329190000 -1.1089780000 -0.4890330000
C 1.0398570000 2.5120590000 0.0862410000
O 2.9955090000 0.3391640000 -0.3451890000
C -0.1143340000 3.5141230000 0.2800300000
C 1.8779530000 3.0069370000 -1.1295310000
C 1.9153790000 2.5579310000 1.3743910000
H 1.6970720000 -2.0190720000 -0.9578350000
C -3.1818430000 0.4101930000 -0.1862550000
H -1.8398060000 2.0043170000 0.1529040000
C -4.2095260000 1.1761330000 0.4134420000
C -5.5335060000 0.7544460000 0.3960490000
C -5.8762360000 -0.4363680000 -0.2493050000
C -4.8837670000 -1.1938190000 -0.8774310000
C -3.5558980000 -0.7805820000 -0.8490340000
H -3.9492940000 2.1067770000 0.9113130000
H -6.2991610000 1.3562680000 0.8768410000
H -6.9111640000 -0.7652050000 -0.2754940000
H -5.1478450000 -2.1077570000 -1.4015960000
H -2.8153750000 -1.3676120000 -1.3763670000
B 3.9704030000 -0.8702300000 -0.1780500000
F 5.1971310000 -0.3146380000 0.0483570000
F 3.9016530000 -1.6217600000 -1.3478130000
F 3.4820600000 -1.6065200000 0.9057460000
H 1.3361810000 2.2393190000 2.2487490000
H 2.2376730000 3.5922600000 1.5406020000
H 2.7991530000 1.9266050000 1.2845220000
H 2.2094360000 4.0327000000 -0.9324940000
H 1.2695140000 3.0176710000 -2.0413810000
H 2.7569070000 2.3838500000 -1.2948270000
H -0.7140970000 3.3009470000 1.1716530000
H -0.7713550000 3.5782380000 -0.5940930000
H 0.3221930000 4.5081580000 0.4241730000
H -0.8399060000 -1.4475100000 -1.4040540000
C -0.7806200000 -2.0706170000 0.6777720000
C -0.6332960000 -3.5375430000 0.2485020000
H -1.8468970000 -1.8760880000 0.8452660000
C -0.0254780000 -1.7942800000 1.9869580000
H -1.1788920000 -3.7471080000 -0.6800660000
H -1.0324240000 -4.1990810000 1.0253070000
H 0.4163730000 -3.8113580000 0.0941860000
H 1.0500740000 -1.9747720000 1.8834850000
H -0.4076820000 -2.4475800000 2.7792640000
H -0.1605600000 -0.7593180000 2.3209240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.398277 (Hartree/Particle)
Thermal correction to Energy= 0.422346
Thermal correction to Enthalpy= 0.423291
Thermal correction to Gibbs (Free) Energy= 0.344139
Sum of electronic and zero-point Energies= -1137.831048
Sum of electronic and thermal Energies= -1137.806979
Sum of electronic and thermal Enthalpies= -1137.806035
Sum of electronic and thermal (Free) Energies= -1137.885187

6d

cRT

C -1.9547000000 -1.3517020000 0.8108270000
C -1.3120570000 -0.2074680000 0.8745170000
C -0.7123260000 0.9668200000 0.9061820000
C 0.3896660000 1.2056900000 -0.0705220000
C 1.4338430000 0.2360800000 -0.3331700000
C 1.7263520000 -0.7958280000 0.4971700000
H 2.0220720000 0.4387400000 -1.2199180000
C -1.1548080000 2.1260480000 1.8415630000
H -1.6216540000 -2.1576400000 1.4675840000
C -3.0970680000 -1.6743050000 -0.0650740000
O 0.3673540000 2.3177710000 -0.6660130000
C -2.0248820000 1.5617690000 2.9796890000
C -1.9800600000 3.1686670000 1.0514340000
C 0.0978470000 2.7938230000 2.4535910000
C -3.6954680000 -2.9401460000 0.0354060000
C -3.6079130000 -0.7582960000 -1.0010060000
C -4.6880280000 -1.1021650000 -1.8076570000
H -3.1504130000 0.2228250000 -1.0947930000
C -5.2786690000 -2.3651510000 -1.6975850000
H -5.0704300000 -0.3834520000 -2.5272880000
C -4.7782770000 -3.2827950000 -0.7734620000
H -3.3075680000 -3.6579640000 0.7545290000
H -6.1215640000 -2.6303370000 -2.3296430000
H -5.2293930000 -4.2670450000 -0.6813250000
B 1.5869130000 3.0394530000 -1.5137420000
F 0.9840090000 4.1634930000 -1.9758930000
F 1.9566320000 2.1463140000 -2.4944580000
F 2.5428290000 3.2353290000 -0.5518430000
H 0.7632410000 3.2098150000 1.6919520000
H 0.6698910000 2.0791890000 3.0580480000
H -0.2100390000 3.6137270000 3.1124840000
H -2.8708400000 2.7057160000 0.6109660000
H -1.3967430000 3.6273660000 0.2515600000
H -2.3150240000 3.9593070000 1.7340280000
H -2.9407460000 1.0980690000 2.5990100000
H -2.3138970000 2.3741110000 3.6556530000
H -1.4833390000 0.8110790000 3.5669240000
C 2.7813370000 -1.7836920000 0.3186700000
H 1.1408330000 -0.9067180000 1.4066120000
C 3.6391200000 -1.8007340000 -0.8009310000
C 2.9512880000 -2.7700350000 1.3100450000
C 4.6260080000 -2.7718110000 -0.9175480000
C 3.9401080000 -3.7424720000 1.1912940000
C 4.7800240000 -3.7453660000 0.0761080000
H 2.2978230000 -2.7654940000 2.1792140000
H 3.5337400000 -1.0500640000 -1.5775560000
H 4.0568190000 -4.4949530000 1.9658640000
H 5.2805030000 -2.7719250000 -1.7843350000
H 5.5540890000 -4.5015940000 -0.0202670000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.391166 (Hartree/Particle)
Thermal correction to Energy= 0.417383
Thermal correction to Enthalpy= 0.418327
Thermal correction to Gibbs (Free) Energy= 0.330647
Sum of electronic and zero-point Energies= -1250.946713
Sum of electronic and thermal Energies= -1250.920497
Sum of electronic and thermal Enthalpies= -1250.919553
Sum of electronic and thermal (Free) Energies= -1251.007232

cTS

C 1.7712490000 -0.3336720000 0.7323530000
C 0.4331830000 -0.3781790000 0.6952410000
C 2.7099710000 -1.1392460000 -0.0498010000
H 2.2284740000 0.4458290000 1.3419860000
C -0.7519130000 -1.0450580000 0.5693300000
C 4.0805890000 -1.0734790000 0.2659150000
C 2.3038550000 -1.9627560000 -1.1178650000
C -1.8017020000 -0.1985370000 0.0121210000
C -1.0308760000 -2.4694110000 1.0707290000
C 5.0111440000 -1.8308680000 -0.4403450000
H 4.4089110000 -0.4298460000 1.0783840000
C 3.2369400000 -2.7137980000 -1.8251650000
H 1.2565780000 -1.9904230000 -1.4024280000
C -1.4003910000 1.1611230000 -0.0284960000
O -2.9066350000 -0.6784380000 -0.4248260000
C 0.1847790000 -3.0705250000 1.7983810000
C -1.3904540000 -3.3623050000 -0.1450580000
C -2.2267930000 -2.4317130000 2.0541160000
C 4.5926980000 -2.6554060000 -1.4870360000
H 6.0637410000 -1.7740300000 -0.1775450000
H 2.9082450000 -3.3400620000 -2.6497540000
C -0.2980770000 1.5133840000 0.7734210000

H -1.8602990000 1.8416100000 -0.7350040000
B -4.0869510000 0.3029600000 -0.8606940000
H 0.4714920000 -2.4715240000 2.6697350000
H 1.0566940000 -3.1601010000 1.1438920000
H -0.0709990000 -4.0749980000 2.1529610000
H -1.6420580000 -4.3674720000 0.2131420000
H -0.5421940000 -3.4557280000 -0.8324740000
H -2.2467240000 -2.9654860000 -0.6934970000
H -1.9962940000 -1.8118500000 2.9287470000
H -2.4342370000 -3.4473680000 2.4100870000
H -3.1305260000 -2.0439310000 1.5801030000
H 5.3186480000 -3.2417070000 -2.0431570000
H -0.3554750000 1.2901490000 1.8391540000
C 0.5697930000 2.6638600000 0.4661090000
F -4.2995290000 1.1241970000 0.2298530000
F -5.1237630000 -0.5315350000 -1.1527410000
F -3.6036930000 1.0096780000 -1.9526320000
C 0.7723440000 3.0973850000 -0.8561000000
C 1.2210600000 3.3438590000 1.5093810000
C 1.5872740000 4.1937510000 -1.1217780000
H 0.2938910000 2.5654790000 -1.6737570000
C 2.0390720000 4.4401510000 1.2427310000
H 1.0678520000 3.0193500000 2.5364370000
C 2.2219040000 4.8677610000 -0.0737840000
H 1.7332300000 4.5214430000 -2.1470440000
H 2.5285110000 4.9624350000 2.0598550000
H 2.8593360000 5.7219520000 -0.2844580000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.390681 (Hartree/Particle)
Thermal correction to Energy= 0.415631
Thermal correction to Enthalpy= 0.416575
Thermal correction to Gibbs (Free) Energy= 0.334252
Sum of electronic and zero-point Energies= -1250.919933
Sum of electronic and thermal Energies= -1250.894984
Sum of electronic and thermal Enthalpies= -1250.894039
Sum of electronic and thermal (Free) Energies= -1250.976363

cPT

C 1.7915660000 0.4421830000 0.7456330000
C 0.4745540000 0.0842260000 0.8424410000
C -0.2611520000 -1.1213710000 0.5980840000
C -1.6434430000 -0.7612330000 0.3470830000
C -1.8300440000 0.5473430000 0.7890120000
C -0.5637210000 1.1871890000 1.2002810000
C 0.1348520000 -2.5795990000 0.7835880000
C 2.8910150000 -0.1529780000 0.0022690000
O -2.5285370000 -1.5669070000 -0.1495970000
C 1.5465920000 -2.8012890000 1.3556590000
C -0.0220630000 -3.3473830000 -0.5580510000
C -0.8729100000 -3.1818280000 1.8137510000
C 4.2155570000 0.0672080000 0.4342370000
C 2.6840550000 -0.8549920000 -1.2031290000
C 3.7629230000 -1.3600290000 -1.9226220000
H 1.6751360000 -0.9607030000 -1.5880340000
C 5.0671040000 -1.1739980000 -1.4557420000
H 3.5880330000 -1.8870370000 -2.8561470000
C 5.2901370000 -0.4566360000 -0.2760780000
H 4.3905140000 0.6348110000 1.3447040000
H 5.9079270000 -1.5678470000 -2.0195420000
H 6.3034560000 -0.2971720000 0.0811360000
B -3.8351140000 -0.9255190000 -0.7409300000
F -4.5354190000 -0.3740880000 0.3260940000
F -4.4871150000 -1.9536870000 -1.3579470000
F -3.3983630000 0.0690330000 -1.6162680000
H 2.0329610000 1.4122840000 1.1805710000
H -2.7944840000 1.0376670000 0.8054900000
H -0.5211920000 1.2791130000 2.2985660000
C -0.3691930000 2.5696410000 0.5975960000
C -0.8089180000 2.8359700000 -0.7079910000
C 0.2378380000 3.5936610000 1.3343950000
H -0.7837060000 -2.6823840000 2.7852580000
H -0.6305220000 -4.2404460000 1.9557790000
H -1.9038460000 -3.1051460000 1.4672560000
H 0.1528770000 -4.4135070000 -0.3733970000
H 0.7132570000 -3.0109510000 -1.2955780000
H -1.0245690000 -3.2232430000 -0.9711950000
H 1.7176680000 -2.2027770000 2.2573650000
H 2.3364020000 -2.5773540000 0.6387090000
H 1.6469930000 -3.8557000000 1.6347020000
C -0.6274490000 4.1009030000 -1.2654400000
C -0.0057260000 5.1128560000 -0.5297530000
C 0.4243500000 4.8581630000 0.7731450000
H 0.5571440000 3.4052320000 2.3578060000
H 0.1332490000 6.0979010000 -0.9666780000
H 0.8952890000 5.6443890000 1.3570220000
H -1.3174390000 2.0587290000 -1.2750120000
H -0.9787560000 4.2976250000 -2.2744790000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.393067 (Hartree/Particle)
Thermal correction to Energy= 0.417841
Thermal correction to Enthalpy= 0.418785
Thermal correction to Gibbs (Free) Energy= 0.337037
Sum of electronic and zero-point Energies= -1250.935412
Sum of electronic and thermal Energies= -1250.910639
Sum of electronic and thermal Enthalpies= -1250.909695
Sum of electronic and thermal (Free) Energies= -1250.991442

cRTccRT TS

C -2.3519730000 0.0377130000 -1.1200700000
C -1.3065390000 -0.7285470000 -0.9060300000
C -0.3208840000 -1.5846670000 -0.7062230000
C 1.0059250000 -1.1206610000 -0.2030360000
C 1.5254730000 0.2402430000 -0.1974110000
C 0.8692250000 1.4044390000 -0.4183110000
H 2.5849290000 0.2624340000 0.0243470000
C -0.5594900000 -3.1095790000 -0.9566790000
H -2.4812210000 0.4353750000 -2.1294540000
C -3.3725520000 0.4428820000 -0.1351240000
O 1.7588580000 -2.0413490000 0.2230510000
C -1.9508060000 -3.3212900000 -1.5856520000
C -0.5103660000 -3.8995100000 0.3734190000
C 0.4984700000 -3.6522880000 -1.9457510000
C -4.4392190000 1.2539490000 -0.5543130000
C -3.3140080000 0.0452010000 1.2121520000
C -4.2986490000 0.4470370000 2.1091940000
H -2.4911050000 -0.5781180000 1.5514260000
C -5.3584940000 1.2528060000 1.6808420000
H -4.2394630000 0.1322320000 3.1474140000
C -5.4253090000 1.6545240000 0.3462910000
H -4.4949960000 1.5670970000 -1.5943420000
H -6.1253470000 1.5647510000 2.3842550000
H -6.2450910000 2.2803110000 0.0043090000
B 3.1886660000 -1.9354520000 1.0552190000
F 3.4523890000 -3.2463930000 1.2896770000
F 2.8776680000 -1.1901750000 2.1583700000
F 4.0642350000 -1.3138440000 0.1958410000
H 1.5096090000 -3.5973900000 -1.5395250000
H 0.4689880000 -3.1021880000 -2.8940420000
H 0.2802980000 -4.7040910000 -2.1647830000
H -1.2392210000 -3.5026030000 1.0901260000
H 0.4788620000 -3.8772720000 0.8309280000
H -0.7743040000 -4.9458930000 0.1776020000
H -2.7565070000 -2.9885880000 -0.9229260000
H -2.0959690000 -4.3893270000 -1.7799310000
H -2.0538870000 -2.7900760000 -2.5385030000
C 1.4641510000 2.7358580000 -0.3791440000
H -0.1925850000 1.3879590000 -0.6346080000
C 2.8196450000 2.9721850000 -0.0677870000
C 0.6400320000 3.8415230000 -0.6680260000
C 3.3242740000 4.2668450000 -0.0559940000
C 1.1476760000 5.1376450000 -0.6558210000
C 2.4926700000 5.3533260000 -0.3505210000
H -0.4081140000 3.6728180000 -0.9031900000
H 3.4771510000 2.1428390000 0.1722560000
H 0.4965170000 5.9772070000 -0.8819040000
H 4.3697720000 4.4333350000 0.1869960000
H 2.8933520000 6.3631510000 -0.3379840000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.390934 (Hartree/Particle)
Thermal correction to Energy= 0.416416
Thermal correction to Enthalpy= 0.417360
Thermal correction to Gibbs (Free) Energy= 0.332357
Sum of electronic and zero-point Energies= -1250.941121
Sum of electronic and thermal Energies= -1250.915639
Sum of electronic and thermal Enthalpies= -1250.914695

Sum of electronic and thermal (Free) Energies= -1250.999698

ccRT

C -1.1264280000 -2.0530500000 -1.3166840000
C -0.0069380000 -1.7505180000 -0.6991430000
C 1.1481120000 -1.4762330000 -0.1240900000
C 1.7117960000 -0.1056660000 -0.3000980000
C 0.9142400000 1.1036100000 -0.2888460000
C -0.3531700000 1.1892400000 0.1862340000
H 1.4410420000 1.9785370000 -0.6497170000
C 1.9810320000 -2.5458300000 0.6375540000
H -1.0546050000 -2.3640070000 -2.3606900000
C -2.4881420000 -1.9967810000 -0.7524760000
O 2.9607410000 -0.0496320000 -0.4726450000
C 1.0898330000 -3.7601450000 0.9589860000
C 2.4946000000 -1.9425530000 1.9651550000
C 3.1702140000 -3.0241330000 -0.2290300000
C -3.5912770000 -2.0824000000 -1.6171070000
C -2.7253250000 -1.8657780000 0.6278660000
C -4.0265050000 -1.8037990000 1.1216340000
H -1.8834250000 -1.8377710000 1.3147150000
C -5.1161660000 -1.8777810000 0.2487190000
H -4.1914100000 -1.7117770000 2.1919170000
C -4.8928920000 -2.0208030000 -1.1216020000
H -3.4228210000 -2.1921010000 -2.6856280000
H -6.1301860000 -1.8346490000 0.6360680000
H -5.7331560000 -2.0860010000 -1.8073590000
B 3.9683500000 1.2520680000 -0.3580610000
F 5.1550280000 0.7228900000 -0.7503310000
F 3.8790180000 1.5812790000 0.9683820000
F 3.4664020000 2.2128430000 -1.2075840000
H 3.8731910000 -2.2171310000 -0.4387150000
H 2.8159720000 -3.4334510000 -1.1823310000
H 3.7049980000 -3.8217950000 0.3009910000
H 1.6592450000 -1.6478010000 2.6122370000
H 3.1327530000 -1.0691660000 1.8081190000
H 3.0823810000 -2.6946140000 2.5039030000
H 0.2264050000 -3.4795210000 1.5734490000
H 1.6719810000 -4.5009730000 1.5179570000
H 0.7158300000 -4.2425620000 0.0501070000
C -1.1747670000 2.3911670000 0.2395690000
H -0.8267200000 0.2941610000 0.5797780000
C -0.6968170000 3.6669340000 -0.1267150000
C -2.5087760000 2.2716880000 0.6772630000
C -1.5295850000 4.7770460000 -0.0585370000
C -3.3419330000 3.3852130000 0.7399870000
C -2.8540410000 4.6406990000 0.3729450000
H -2.8896480000 1.2922470000 0.9554460000
H 0.3309590000 3.7898590000 -0.4529840000
H -4.3692720000 3.2746290000 1.0750850000
H -1.1471900000 5.7542270000 -0.3390430000
H -3.5004330000 5.5125100000 0.4244660000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.391331 (Hartree/Particle)
Thermal correction to Energy= 0.417470
Thermal correction to Enthalpy= 0.418414
Thermal correction to Gibbs (Free) Energy= 0.331559
Sum of electronic and zero-point Energies= -1250.946952
Sum of electronic and thermal Energies= -1250.920812
Sum of electronic and thermal Enthalpies= -1250.919868
Sum of electronic and thermal (Free) Energies= -1251.006724

ccTS

C -1.1846590000 -1.4640370000 -0.8973340000
C -0.0250890000 -0.9926430000 -0.4014340000
C -2.4960460000 -1.4699630000 -0.2571710000
H -1.1584160000 -1.8397260000 -1.9221250000
C 1.3216760000 -1.1697630000 -0.2818340000
C -3.6581030000 -1.4761780000 -1.0530700000
C -2.6409340000 -1.5366690000 1.1434140000
C 2.0351890000 0.0743270000 -0.0150160000
C 2.0405850000 -2.5259200000 -0.3354210000
C -4.9205170000 -1.5105010000 -0.4692710000
H -3.5606060000 -1.4403050000 -2.1351670000
C -3.9055270000 -1.5769730000 1.7248570000
H -1.7553560000 -1.6032490000 1.7691130000
C 1.1372330000 1.1540980000 0.1734580000
O 3.3130300000 0.1495650000 -0.0419220000
C 1.0595010000 -3.7004340000 -0.5004460000
C 2.8475230000 -2.7356620000 0.9682670000
C 3.0017650000 -2.5083120000 -1.5530760000
C -5.0488210000 -1.5572880000 0.9217780000
H -5.8063140000 -1.5051220000 -1.0980940000
H -4.0000080000 -1.6411630000 2.8053740000
C -0.2030890000 0.8337730000 0.4599580000
H 1.4616870000 2.1643360000 -0.0458540000
B 4.0490370000 1.4941060000 0.4108010000
H 0.4977310000 -3.6399310000 -1.4385580000
H 0.3406270000 -3.7544330000 0.3241640000
H 1.6244680000 -4.6388530000 -0.5147180000
H 3.3764970000 -3.6944760000 0.9182070000
H 2.1825080000 -2.7657930000 1.8396880000
H 3.5852950000 -1.9456000000 1.1195230000
H 2.4468060000 -2.3822250000 -2.4901940000
H 3.5341000000 -3.4654440000 -1.6032110000
H 3.7375300000 -1.7065670000 -1.4713130000
H -6.0345390000 -1.5949430000 1.3768400000
H -0.4113290000 0.2487450000 1.3570760000
C -1.2888400000 1.7566890000 0.0761980000
F 5.3723580000 1.1700940000 0.3882680000
F 3.5485470000 1.7787820000 1.6661840000
F 3.6834990000 2.4520070000 -0.5226680000
C -1.2146740000 2.4869660000 -1.1235290000
C -2.4013420000 1.9416450000 0.9131780000
C -2.2187920000 3.3872570000 -1.4671900000
H -0.3673600000 2.3378190000 -1.7874600000
C -3.4043750000 2.8461720000 0.5710590000
H -2.4720550000 1.3818260000 1.8410750000
C -3.3151640000 3.5703960000 -0.6192780000
H -2.1489670000 3.9455610000 -2.3964350000
H -4.2537160000 2.9871010000 1.2334440000
H -4.0984450000 4.2738400000 -0.8880950000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.390238 (Hartree/Particle)
Thermal correction to Energy= 0.415193
Thermal correction to Enthalpy= 0.416137
Thermal correction to Gibbs (Free) Energy= 0.333895
Sum of electronic and zero-point Energies= -1250.915994
Sum of electronic and thermal Energies= -1250.891039
Sum of electronic and thermal Enthalpies= -1250.890095
Sum of electronic and thermal (Free) Energies= -1250.972337

ccPT

C -1.3379160000 1.5614390000 0.0070320000
C -0.2129360000 0.7985160000 -0.1998670000
C 1.1433020000 1.1850780000 0.0790040000
C 2.0136570000 0.0539700000 -0.1850990000
C 1.2289720000 -1.0041420000 -0.6390870000
C -0.2064430000 -0.6455300000 -0.7127370000
C 1.7473270000 2.5146040000 0.5135810000
O 3.3002160000 0.0718970000 -0.0227370000
C 0.7776810000 3.6879880000 0.7528770000
C 2.7402490000 2.9611680000 -0.6013000000
C 2.5265910000 2.2766380000 1.8405680000
H 1.6173780000 -1.9846120000 -0.8775700000
C -2.7321110000 1.3127240000 -0.3121280000
H -1.1955490000 2.4904620000 0.5394920000
C -3.6964790000 2.0400310000 0.4253550000
C -5.0563100000 1.8718090000 0.1983850000
C -5.4916860000 0.9925480000 -0.7974030000
C -4.5563590000 0.2908720000 -1.5624420000
C -3.1947030000 0.4452640000 -1.3258780000
H -3.3600910000 2.7291880000 1.1958720000
H -5.7772160000 2.4301140000 0.7884050000
H -6.5538970000 0.8668060000 -0.9869730000
H -4.8905840000 -0.3736270000 -2.3538400000
H -2.4882860000 -0.0746410000 -1.9590940000
B 4.1429660000 -1.1737340000 -0.4704760000
F 5.4403470000 -0.8283780000 -0.2149150000
F 3.8645080000 -1.3603910000 -1.8195440000
F 3.6885250000 -2.2498100000 0.2831800000
H 1.8413490000 1.9879600000 2.6463250000
H 3.0145650000 3.2134660000 2.1325090000
H 3.2888580000 1.5059110000 1.7282700000
H 3.2363440000 3.8831910000 -0.2775600000

H 2.2051470000 3.1745490000 -1.5338150000
H 3.5016290000 2.2051250000 -0.7920020000
H 0.1095820000 3.5176580000 1.6045180000
H 0.1816020000 3.9332560000 -0.1323820000
H 1.3735820000 4.5743710000 0.9949550000
H -0.5223060000 -0.6613040000 -1.7672160000
C -1.0518210000 -1.6609590000 0.0573210000
C -1.0130130000 -1.7055380000 1.4573350000
C -1.8054040000 -2.6195700000 -0.6291820000
C -1.7339270000 -2.6729070000 2.1543500000
C -2.4916010000 -3.6203720000 1.4612990000
C -2.5223040000 -3.5940980000 0.0672210000
H -0.4142080000 -0.9811790000 2.0030760000
H -1.6964580000 -2.6930250000 3.2400080000
H -3.0488750000 -4.3775360000 2.0057530000
H -1.8263090000 -2.6110600000 -1.7168540000
H -3.1018220000 -4.3315730000 -0.4813050000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.393595 (Hartree/Particle)
Thermal correction to Energy= 0.418350
Thermal correction to Enthalpy= 0.419295
Thermal correction to Gibbs (Free) Energy= 0.336559
Sum of electronic and zero-point Energies= -1250.942031
Sum of electronic and thermal Energies= -1250.917276
Sum of electronic and thermal Enthalpies= -1250.916331
Sum of electronic and thermal (Free) Energies= -1250.999067

RB3LYP/6-311G(d)

1a

cRT

C 3.5888110000 -0.1563870000 -0.0610770000
C 2.3832110000 0.2819510000 -0.2708530000
C 1.1835630000 0.8069260000 -0.4439280000
C -0.0342640000 0.0117820000 -0.1962630000
C -0.0444810000 -1.4577200000 -0.1838650000
C 0.7223050000 -2.2122300000 -0.9742470000
H -0.7970450000 -1.9055510000 0.4537050000
C 0.9860560000 2.2721580000 -0.7780340000
O -1.0782420000 0.6664910000 0.0168390000
H 1.9448770000 2.7631280000 -0.9403970000
H 0.4577500000 2.7789260000 0.0320000000
H 0.3736540000 2.3836610000 -1.6762330000
B -2.6278900000 0.0420610000 0.2870930000
F -3.3597530000 1.1716480000 0.4247490000
F -2.4831270000 -0.7073110000 1.4290770000
F -2.8755720000 -0.6964660000 -0.8358940000
C 4.3081210000 -0.1203020000 1.2651360000
H 4.1272320000 -0.5965390000 -0.9010980000
H 3.6988410000 0.3407800000 2.0424740000
H 5.2419860000 0.4425860000 1.1762300000
H 4.5689910000 -1.1332820000 1.5856110000
H 1.4268850000 -1.7912630000 -1.6809490000
H 0.6283660000 -3.2925830000 -0.9641320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169768 (Hartree/Particle)
Thermal correction to Energy= 0.184595
Thermal correction to Enthalpy= 0.185539
Thermal correction to Gibbs (Free) Energy= 0.126998
Sum of electronic and zero-point Energies= -710.612266
Sum of electronic and thermal Energies= -710.597439
Sum of electronic and thermal Enthalpies= -710.596495
Sum of electronic and thermal (Free) Energies= -710.655036

cTS

C 3.4599240000 -0.4284020000 -0.0579750000
C 2.1885840000 -0.1436790000 -0.2850310000
C 1.1248020000 0.6990080000 -0.3249080000
C -0.1586240000 0.0682880000 -0.1105450000
C -0.0268700000 -1.3562510000 -0.0643120000
C 1.0923380000 -1.8901150000 -0.6703800000
C 1.2028980000 2.1653310000 -0.6351940000
O -1.2038650000 0.7632420000 0.0736920000
H 0.7464290000 2.7273950000 0.1850610000
H 0.6225030000 2.4045890000 -1.5303780000
H 2.2294320000 2.5035870000 -0.7702510000
H -0.6874310000 -1.9348120000 0.5698290000
B -2.6389380000 0.0460540000 0.1854440000
F -2.7272930000 -0.7557470000 -0.9395400000
F -3.5315400000 1.0726570000 0.2235180000
F -2.5782060000 -0.7062510000 1.3495490000
H 3.9329890000 -1.2181310000 -0.6378700000
C 4.2985650000 0.2227540000 1.0082130000
H 3.7581600000 1.0136640000 1.5283530000
H 5.2052840000 0.6489770000 0.5663630000
H 4.6231020000 -0.5156090000 1.7487370000
H 1.4647980000 -2.8623050000 -0.3546840000
H 1.3739910000 -1.6210960000 -1.6828740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169165 (Hartree/Particle)
Thermal correction to Energy= 0.182863
Thermal correction to Enthalpy= 0.183807
Thermal correction to Gibbs (Free) Energy= 0.128075
Sum of electronic and zero-point Energies= -710.585080
Sum of electronic and thermal Energies= -710.571382
Sum of electronic and thermal Enthalpies= -710.570438
Sum of electronic and thermal (Free) Energies= -710.626170

cPT

C 3.4251180000 -0.5486610000 0.0000000000
C 2.0687330000 -0.5452910000 0.0000000000
C 1.1313230000 0.5358590000 0.0000000000
C -0.2067690000 0.0255980000 0.0000000000
C -0.1286580000 -1.3751040000 0.0000000000
C 1.2702150000 -1.8344040000 0.0000000000
C 1.3745280000 2.0014470000 0.0000000000
O -1.2412700000 0.7925350000 0.0000000000
H 1.9460500000 2.3109650000 0.8809610000
H 0.4212310000 2.5278030000 0.0000000000
H 1.9460500000 2.3109650000 -0.8809610000
H -0.9928470000 -2.0236870000 0.0000000000
B -2.6605370000 0.1352240000 0.0000000000
F -2.7204240000 -0.6614520000 -1.1454750000
F -3.5515180000 1.1707710000 0.0000000000
F -2.7204240000 -0.6614520000 1.1454750000
H 3.8933800000 -1.5327260000 0.0000000000
C 4.3883530000 0.5869200000 0.0000000000
H 3.9254740000 1.5692400000 0.0000000000
H 5.0471690000 0.5149300000 -0.8736280000
H 5.0471690000 0.5149300000 0.8736290000
H 1.4967050000 -2.4589020000 0.8763190000
H 1.4967050000 -2.4589020000 -0.8763190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171711 (Hartree/Particle)
Thermal correction to Energy= 0.185221
Thermal correction to Enthalpy= 0.186165
Thermal correction to Gibbs (Free) Energy= 0.130323
Sum of electronic and zero-point Energies= -710.628008
Sum of electronic and thermal Energies= -710.614498
Sum of electronic and thermal Enthalpies= -710.613554
Sum of electronic and thermal (Free) Energies= -710.669396

ccRT

C -3.5047950000 0.1318160000 0.7103880000
C -2.3218040000 0.4913300000 0.3097480000
C -1.1350430000 0.9375900000 -0.0608610000
C 0.0568490000 0.0721600000 0.0154240000
C -0.0177010000 -1.3940870000 0.0882220000
C -0.9445270000 -2.1255580000 -0.5343520000
H 0.8013730000 -1.8674660000 0.6160240000
C -0.9053650000 2.3827380000 -0.4554590000
O 1.1590260000 0.6628960000 0.0286290000
H -1.8469140000 2.9301380000 -0.4794470000
H -0.4333120000 2.4441450000 -1.4390730000
H -0.2292310000 2.8665260000 0.2523640000
B 2.6923100000 -0.0533090000 0.0628800000
F 3.5026790000 1.0295600000 0.0297570000
F 2.7021580000 -0.8404260000 -1.0544860000
F 2.6982260000 -0.7563170000 1.2427020000
C -4.5864790000 -0.4645650000 -0.1547680000
H -3.7344060000 0.2577990000 1.7692510000

H -4.8377690000 -1.4733100000 0.1873050000
H -4.2878810000 -0.5180460000 -1.2021970000
H -5.4991980000 0.1346680000 -0.0902170000
H -1.7288170000 -1.6863290000 -1.1385940000
H -0.9119740000 -3.2086370000 -0.4906620000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169731 (Hartree/Particle)
Thermal correction to Energy= 0.184564
Thermal correction to Enthalpy= 0.185508
Thermal correction to Gibbs (Free) Energy= 0.126985
Sum of electronic and zero-point Energies= -710.612204
Sum of electronic and thermal Energies= -710.597372
Sum of electronic and thermal Enthalpies= -710.596427
Sum of electronic and thermal (Free) Energies= -710.654950

ccTS

C -3.4280640000 0.1865730000 0.5076140000
C -2.1661570000 0.2769380000 0.1216190000
C -1.0125550000 0.9836390000 -0.0206280000
C 0.1952600000 0.1937070000 0.0277080000
C -0.1118750000 -1.2039940000 0.0630370000
C -1.3459730000 -1.5759240000 -0.4318350000
H 0.5319120000 -1.8802210000 0.6123070000
C -0.9385440000 2.4611530000 -0.2694310000
O 1.3358740000 0.7448280000 0.1032340000
H -1.9198540000 2.9327080000 -0.2423050000
H -0.4626040000 2.6715740000 -1.2313370000
H -0.3000210000 2.9169150000 0.4932530000
B 2.6663740000 -0.1536080000 0.0332770000
F 3.6854680000 0.7465300000 -0.0218070000
F 2.5164800000 -0.9275240000 -1.1055160000
F 2.6433680000 -0.9265840000 1.1852540000
C -4.5055670000 -0.6861590000 -0.0638020000
H -3.7059740000 0.7885060000 1.3751370000
H -4.1660480000 -1.2586560000 -0.9271100000
H -5.3563800000 -0.0734480000 -0.3787870000
H -4.8840110000 -1.3839520000 0.6900990000
H -1.6844150000 -1.2425990000 -1.4066620000
H -1.7984510000 -2.5088060000 -0.1039240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169065 (Hartree/Particle)
Thermal correction to Energy= 0.182749
Thermal correction to Enthalpy= 0.183693
Thermal correction to Gibbs (Free) Energy= 0.128033
Sum of electronic and zero-point Energies= -710.584190
Sum of electronic and thermal Energies= -710.570506
Sum of electronic and thermal Enthalpies= -710.569562
Sum of electronic and thermal (Free) Energies= -710.625222

cPT

C 3.4091940000 0.3164890000 0.0000010000
C 2.0991660000 -0.0241760000 0.0000000000
C 0.9962790000 0.8848360000 0.0000000000
C -0.2400360000 0.1658710000 0.0000000000
C 0.0701070000 -1.1986530000 0.0000000000
C 1.5323920000 -1.4280390000 0.0000000000
C 1.0126340000 2.3627750000 0.0000000000
O -1.3820910000 0.7642520000 0.0000000000
H 2.0102240000 2.7997290000 0.0000000000
H 0.4535920000 2.7295670000 0.8680940000
H 0.4535920000 2.7295670000 -0.8680940000
H -0.6727220000 -1.9833880000 0.0000000000
B -2.6774040000 -0.1097250000 0.0000000000
F -3.7232850000 0.7699770000 -0.0000010000
F -2.6108490000 -0.9062970000 1.1455810000
F -2.6108480000 -0.9062970000 -1.1455820000
C 4.5647340000 -0.6223220000 0.0000010000
H 3.6618240000 1.3743780000 0.0000010000
H 4.2680020000 -1.6710810000 0.0000010000
H 5.2010240000 -0.4427110000 0.8744880000
H 5.2010250000 -0.4427110000 -0.8744860000
H 1.8526010000 -2.0079380000 0.8766070000
H 1.8526010000 -2.0079380000 -0.8766060000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171565 (Hartree/Particle)
Thermal correction to Energy= 0.185113
Thermal correction to Enthalpy= 0.186057
Thermal correction to Gibbs (Free) Energy= 0.130364
Sum of electronic and zero-point Energies= -710.632601
Sum of electronic and thermal Energies= -710.619053
Sum of electronic and thermal Enthalpies= -710.618109
Sum of electronic and thermal (Free) Energies= -710.673802

RB3LYP/6-31+G(d,p)

1a

cRT

C 3.5938590000 -0.1442280000 -0.0626850000
C 2.3785060000 0.2830540000 -0.2728930000
C 1.1694530000 0.8018630000 -0.4495250000
C -0.0380790000 -0.0054750000 -0.1999640000
C -0.0469780000 -1.4745000000 -0.1787530000
C 0.7365070000 -2.2345480000 -0.9575090000
H -0.8112380000 -1.9219300000 0.4481350000
C 0.9631100000 2.2664470000 -0.7926730000
O -1.0942270000 0.6511770000 0.0077700000
H 1.9229090000 2.7537950000 -0.9705350000
H 0.4440600000 2.7780550000 0.0231050000
H 0.3378950000 2.3671270000 -1.6854160000
B -2.5962550000 0.0553050000 0.2850080000
F -3.3527950000 1.1843480000 0.3954870000
F -2.4779050000 -0.6721540000 1.4551580000
F -2.8767430000 -0.7246760000 -0.8160810000
C 4.3177300000 -0.0906890000 1.2634170000
H 4.1327250000 -0.5857530000 -0.9031660000
H 3.7028050000 0.3714070000 2.0384010000
H 5.2460590000 0.4826440000 1.1630580000
H 4.5892070000 -1.1013120000 1.5883220000
H 1.4494420000 -1.8131110000 -1.6574170000
H 0.6435650000 -3.3160750000 -0.9392510000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169851 (Hartree/Particle)
Thermal correction to Energy= 0.184613
Thermal correction to Enthalpy= 0.185557
Thermal correction to Gibbs (Free) Energy= 0.127197
Sum of electronic and zero-point Energies= -710.480255
Sum of electronic and thermal Energies= -710.465493
Sum of electronic and thermal Enthalpies= -710.464549
Sum of electronic and thermal (Free) Energies= -710.522910

cTS

C 3.4761340000 -0.4154530000 -0.0512630000
C 2.1987180000 -0.1394510000 -0.2829330000
C 1.1230290000 0.6954830000 -0.3311240000
C -0.1534320000 0.0492920000 -0.1169900000
C -0.0192400000 -1.3758040000 -0.0683460000
C 1.1051790000 -1.9104540000 -0.6717070000
C 1.1907890000 2.1620420000 -0.6555410000
O -1.2104050000 0.7429080000 0.0658030000
H 0.7270800000 2.7272970000 0.1609060000
H 0.6105310000 2.3863480000 -1.5569330000
H 2.2186180000 2.5016040000 -0.7903210000
H -0.6886860000 -1.9596280000 0.5551930000
B -2.6305430000 0.0560080000 0.1881740000
F -2.7589730000 -0.7581580000 -0.9338220000
F -3.5217010000 1.0949660000 0.2284660000
F -2.5898440000 -0.6973790000 1.3607570000
H 3.9554310000 -1.2051230000 -0.6280650000
C 4.3065140000 0.2450940000 1.0193740000
H 3.7579940000 1.0408560000 1.5273990000
H 5.2172740000 0.6670830000 0.5778770000
H 4.6232260000 -0.4909990000 1.7681550000
H 1.4774140000 -2.8827680000 -0.3522140000
H 1.4055930000 -1.6273460000 -1.6767260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169043 (Hartree/Particle)
Thermal correction to Energy= 0.182786
Thermal correction to Enthalpy= 0.183730
Thermal correction to Gibbs (Free) Energy= 0.127811
Sum of electronic and zero-point Energies= -710.455156

Sum of electronic and thermal Energies= -710.441413
Sum of electronic and thermal Enthalpies= -710.440469
Sum of electronic and thermal (Free) Energies= -710.496388

cPT

C 3.4401880000 -0.5389030000 0.0000000000
C 2.0787610000 -0.5459790000 0.0000000000
C 1.1325070000 0.5327730000 0.0000000000
C -0.2017970000 0.0077280000 0.0000000000
C -0.1168510000 -1.3929790000 0.0000000000
C 1.2885140000 -1.8430360000 0.0000000000
C 1.3683470000 2.0015700000 0.0000000000
O -1.2477060000 0.7729990000 0.0000000000
H 1.9403370000 2.3101570000 0.8831830000
H 0.4098850000 2.5234630000 0.0000000000
H 1.9403370000 2.3101570000 -0.8831830000
H -0.9790730000 -2.0477920000 0.0000000000
B -2.6581100000 0.1411990000 0.0000000000
F -2.7468520000 -0.6593470000 -1.1492100000
F -3.5443420000 1.1912390000 0.0000000000
F -2.7468530000 -0.6593470000 1.1492090000
H 3.9143160000 -1.5214080000 0.0000000000
C 4.3964690000 0.6053800000 0.0000000000
H 3.9233490000 1.5847630000 0.0000000000
H 5.0552390000 0.5349430000 -0.8759120000
H 5.0552390000 0.5349430000 0.8759130000
H 1.5190870000 -2.4657220000 0.8785140000
H 1.5190870000 -2.4657220000 -0.8785140000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171584 (Hartree/Particle)
Thermal correction to Energy= 0.185089
Thermal correction to Enthalpy= 0.186033
Thermal correction to Gibbs (Free) Energy= 0.130375
Sum of electronic and zero-point Energies= -710.500188
Sum of electronic and thermal Energies= -710.486684
Sum of electronic and thermal Enthalpies= -710.485739
Sum of electronic and thermal (Free) Energies= -710.541398

ccRT

C -3.5063260000 0.1468650000 0.7116580000
C -2.3166560000 0.4949590000 0.3032460000
C -1.1202800000 0.9359270000 -0.0664610000
C 0.0593480000 0.0564800000 0.0092610000
C -0.0180810000 -1.4093070000 0.0802060000
C -0.9608270000 -2.1384230000 -0.5340170000
H 0.8092610000 -1.8887940000 0.5930390000
C -0.8809130000 2.3819120000 -0.4618410000
O 1.1737680000 0.6461740000 0.0215770000
H -1.8252740000 2.9270260000 -0.4988290000
H -0.3942360000 2.4376270000 -1.4405740000
H -0.2134070000 2.8656110000 0.2573850000
B 2.6615680000 -0.0414670000 0.0666700000
F 3.4938920000 1.0372930000 0.0147840000
F 2.7058010000 -0.8611620000 -1.0405440000
F 2.6955360000 -0.7348980000 1.2625360000
C -4.5991440000 -0.4443250000 -0.1472360000
H -3.7282190000 0.2822550000 1.7722890000
H -4.8644260000 -1.4457750000 0.2107470000
H -4.2984130000 -0.5143820000 -1.1950570000
H -5.5018940000 0.1734420000 -0.0874950000
H -1.7507330000 -1.6919550000 -1.1277240000
H -0.9304260000 -3.2227350000 -0.4896270000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169814 (Hartree/Particle)
Thermal correction to Energy= 0.184581
Thermal correction to Enthalpy= 0.185525
Thermal correction to Gibbs (Free) Energy= 0.127184
Sum of electronic and zero-point Energies= -710.480222
Sum of electronic and thermal Energies= -710.465455
Sum of electronic and thermal Enthalpies= -710.464510
Sum of electronic and thermal (Free) Energies= -710.522851

ccTS

C -3.4393170000 0.1979960000 0.5150380000
C -2.1740100000 0.2814710000 0.1226310000
C -1.0105300000 0.9805930000 -0.0237010000
C 0.1884370000 0.1759100000 0.0225130000
C -0.1211970000 -1.2222030000 0.0534830000
C -1.3598340000 -1.5916810000 -0.4411510000
H 0.5286620000 -1.9071070000 0.5889150000
C -0.9271120000 2.4591230000 -0.2794280000
O 1.3401040000 0.7239940000 0.0993350000
H -1.9104300000 2.9306370000 -0.2618410000
H -0.4416950000 2.6607790000 -1.2405010000
H -0.2922620000 2.9145160000 0.4892860000
B 2.6615020000 -0.1425750000 0.0378510000
F 3.6809370000 0.7704380000 -0.0074160000
F 2.5509240000 -0.9262870000 -1.1082320000
F 2.6578020000 -0.9270440000 1.1906790000
C -4.5260010000 -0.6678420000 -0.0553230000
H -3.7075670000 0.8010110000 1.3864200000
H -4.9112320000 -1.3588180000 0.7037990000
H -4.1870750000 -1.2464330000 -0.9171620000
H -5.3696400000 -0.0438850000 -0.3736610000
H -1.7136470000 -1.2383040000 -1.4052780000
H -1.8130360000 -2.5256340000 -0.1135610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.168949 (Hartree/Particle)
Thermal correction to Energy= 0.182671
Thermal correction to Enthalpy= 0.183615
Thermal correction to Gibbs (Free) Energy= 0.127794
Sum of electronic and zero-point Energies= -710.454324
Sum of electronic and thermal Energies= -710.440602
Sum of electronic and thermal Enthalpies= -710.439657
Sum of electronic and thermal (Free) Energies= -710.49547

ccPT

C 3.4200670000 0.3259860000 0.0000010000
C 2.1080420000 -0.0263200000 0.0000000000
C 0.9978780000 0.8802980000 0.0000000000
C -0.2332370000 0.1488460000 0.0000000000
C 0.0825710000 -1.2149030000 0.0000000000
C 1.5495950000 -1.4356220000 0.0000000000
C 1.0101550000 2.3601980000 0.0000000000
O -1.3857650000 0.7446910000 0.0000000000
H 2.0100260000 2.7955640000 0.0000000000
H 0.4488550000 2.7237740000 0.8703830000
H 0.4488550000 2.7237740000 -0.8703820000
H -0.6579100000 -2.0047820000 0.0000000000
B -2.6781720000 -0.1009010000 0.0000000000
F -3.7197930000 0.7959760000 -0.0000010000
F -2.6408120000 -0.9057600000 1.1493550000
F -2.6408120000 -0.9057600000 -1.1493560000
C 4.5829230000 -0.6070740000 0.0000010000
H 3.6627900000 1.3873460000 0.0000010000
H 4.2887010000 -1.6583920000 0.0000010000
H 5.2171060000 -0.4210670000 0.8767900000
H 5.2171070000 -0.4210670000 -0.8767880000
H 1.8731150000 -2.0133670000 0.8787440000
H 1.8731150000 -2.0133670000 -0.8787440000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171488 (Hartree/Particle)
Thermal correction to Energy= 0.185011
Thermal correction to Enthalpy= 0.185955
Thermal correction to Gibbs (Free) Energy= 0.130475
Sum of electronic and zero-point Energies= -710.504998
Sum of electronic and thermal Energies= -710.491475
Sum of electronic and thermal Enthalpies= -710.490530
Sum of electronic and thermal (Free) Energies= -710.546010

6d

cRT

C -1.8565640000 -1.3983090000 0.8536910000
C -1.2794430000 -0.2198800000 0.9246820000
C -0.7510850000 0.9904710000 0.9672010000
C 0.3588700000 1.2734860000 0.0148780000
C 1.4237180000 0.3319880000 -0.2605550000
C 1.7615960000 -0.6873930000 0.5705770000
H 1.9993480000 0.5425450000 -1.1532320000
C -1.3192890000 2.1250060000 1.8667570000

H -1.5061920000 -2.1721580000 1.5389780000
C -2.9429910000 -1.7970100000 -0.0634900000
O 0.3172660000 2.3995210000 -0.5654310000
C -2.1625140000 1.5057200000 2.9981300000
C -2.2186580000 3.0680910000 1.0326020000
C -0.1542230000 2.9218850000 2.4958370000
C -3.5011280000 -3.0802130000 0.0618350000
C -3.4377850000 -0.9390590000 -1.0625220000
C -4.4658300000 -1.3553100000 -1.9051710000
H -3.0108040000 0.0525810000 -1.1800950000
C -5.0183790000 -2.6344670000 -1.7692770000
H -4.8351570000 -0.6821250000 -2.6731900000
C -4.5319490000 -3.4954690000 -0.7831030000
H -3.1251910000 -3.7542330000 0.8274280000
H -5.8187880000 -2.9557720000 -2.4289780000
H -4.9523840000 -4.4905670000 -0.6709860000
B 1.4009710000 3.0181020000 -1.5913230000
F 0.8876960000 4.2529190000 -1.8779000000
F 1.4336700000 2.1538530000 -2.6746470000
F 2.5950400000 3.0454560000 -0.8936780000
H 0.4532540000 3.4291860000 1.7430780000
H 0.4978330000 2.2704390000 3.0891460000
H -0.5584280000 3.6869340000 3.1671970000
H -3.0594540000 2.5174480000 0.5971410000
H -1.6637820000 3.5503040000 0.2266680000
H -2.6286060000 3.8480940000 1.6845550000
H -3.0219940000 0.9517510000 2.6090290000
H -2.5415690000 2.3031680000 3.6455400000
H -1.5686780000 0.8235450000 3.6166260000
C 2.8455840000 -1.6416530000 0.3777870000
H 1.1978440000 -0.8107080000 1.4917140000
C 3.6802070000 -1.6415830000 -0.7607820000
C 3.0683900000 -2.6132220000 1.3752960000
C 4.6960420000 -2.5827040000 -0.8897410000
C 4.0867100000 -3.5554200000 1.2441470000
C 4.9030530000 -3.5421340000 0.1100580000
H 2.4350500000 -2.6216050000 2.2586610000
H 3.5364330000 -0.9034090000 -1.5425730000
H 4.2444110000 -4.2956500000 2.0225430000
H 5.3314580000 -2.5699880000 -1.7699080000
H 5.6987640000 -4.2734420000 0.0037390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.388878 (Hartree/Particle)
Thermal correction to Energy= 0.415194
Thermal correction to Enthalpy= 0.416138
Thermal correction to Gibbs (Free) Energy= 0.328383
Sum of electronic and zero-point Energies= -1251.039778
Sum of electronic and thermal Energies= -1251.013462
Sum of electronic and thermal Enthalpies= -1251.012518
Sum of electronic and thermal (Free) Energies= -1251.100272

cTS

C 1.7698470000 -0.3842930000 0.7382880000
C 0.4309970000 -0.3903420000 0.7143510000
C 2.6771790000 -1.2134740000 -0.0580850000
H 2.2543870000 0.3776640000 1.3483930000
C -0.7787070000 -1.0130650000 0.5973760000
C 4.0528240000 -1.1907460000 0.2468200000
C 2.2366400000 -2.0174740000 -1.1282520000
C -1.7974790000 -0.1304850000 0.0401060000
C -1.1058670000 -2.4245110000 1.1102200000
C 4.9550570000 -1.9722050000 -0.4729540000
H 4.4082780000 -0.5622810000 1.0591270000
C 3.1415950000 -2.7911040000 -1.8503380000
H 1.1868270000 -2.0163160000 -1.4027950000
C -1.3608490000 1.2153140000 -0.0014620000
O -2.9190740000 -0.5860980000 -0.3944040000
C 0.0942840000 -3.0602770000 1.8359700000
C -1.5015010000 -3.3167240000 -0.0960300000
C -2.2944170000 -2.3384100000 2.1006910000
C 4.5025940000 -2.7766220000 -1.5230420000
H 6.0105170000 -1.9495320000 -0.2187590000
H 2.7875590000 -3.4005440000 -2.6763950000
C -0.2411290000 1.5376030000 0.7909090000
H -1.8142370000 1.9201340000 -0.6889750000
B -4.0643000000 0.3589690000 -0.8903330000
H 0.4036490000 -2.4671010000 2.7027470000
H 0.9590420000 -3.1823200000 1.1783860000
H -0.1924800000 -4.0534250000 2.1961710000
H -1.7720600000 -4.3113840000 0.2750710000
H -0.6646060000 -3.4364950000 -0.7917450000
H -2.3548420000 -2.9061360000 -0.6377120000
H -2.0413940000 -1.7131770000 2.9643850000
H -2.5260310000 -3.3424170000 2.4721290000
H -3.1911780000 -1.9351040000 1.6274740000
H 5.2052900000 -3.3801830000 -2.0894820000
H -0.2900080000 1.3066100000 1.8549700000
C 0.6567160000 2.6613830000 0.4747380000
F -4.3187910000 1.2560570000 0.1465910000
F -5.1190950000 -0.4781760000 -1.1638110000
F -3.5762550000 1.0213950000 -2.0202670000
C 0.8651180000 3.0843930000 -0.8512090000
C 1.3305700000 3.3283340000 1.5138570000
C 1.7095900000 4.1581030000 -1.1248560000
H 0.3698190000 2.5640740000 -1.6658790000
C 2.1770320000 4.4026200000 1.2393440000
H 1.1735320000 3.0127810000 2.5426300000
C 2.3667470000 4.8198430000 -0.0811430000
H 1.8602260000 4.4773850000 -2.1515620000
H 2.6825890000 4.9154510000 2.0519740000
H 3.0254280000 5.6556130000 -0.2976810000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.388471 (Hartree/Particle)
Thermal correction to Energy= 0.413537
Thermal correction to Enthalpy= 0.414481
Thermal correction to Gibbs (Free) Energy= 0.331844
Sum of electronic and zero-point Energies= -1251.014393
Sum of electronic and thermal Energies= -1250.989327
Sum of electronic and thermal Enthalpies= -1250.988382
Sum of electronic and thermal (Free) Energies= -1251.071019

cPT

C -1.8204300000 0.1332630000 -0.7228520000
C -0.4540800000 0.0364980000 -0.7283710000
C 0.4868150000 -1.0109990000 -0.4722210000
C 1.7574810000 -0.3998250000 -0.1266040000
C 1.6875580000 0.9608990000 -0.4221590000
C 0.3699200000 1.3371500000 -0.9780210000
C 0.3902140000 -2.5070170000 -0.7408980000
C -2.8293030000 -0.6666610000 -0.0475660000
O 2.7685230000 -1.0752220000 0.3306930000
C -0.9382140000 -2.9684640000 -1.3683370000
C 0.6571840000 -3.3037270000 0.5669860000
C 1.5180260000 -2.8462070000 -1.7693430000
C -4.1521020000 -0.6639160000 -0.5416010000
C -2.5588880000 -1.3633670000 1.1495310000
C -3.5661430000 -2.0704890000 1.8009810000
H -1.5650050000 -1.3134660000 1.5811230000
C -4.8612550000 -2.0973330000 1.2723470000
H -3.3456110000 -2.5907650000 2.7280470000
C -5.1514920000 -1.3903810000 0.0993670000
H -4.3822130000 -0.1036750000 -1.4438200000
H -5.6450950000 -2.6490610000 1.7823620000
H -6.1590020000 -1.3969000000 -0.3051120000
B 4.1163730000 -0.3806410000 0.6240560000
F 4.5477350000 0.2081290000 -0.5733870000
F 4.9564250000 -1.3788240000 1.0660580000
F 3.8761200000 0.6035320000 1.5921370000
H -2.2150330000 1.0411920000 -1.1786780000
H 2.5041540000 1.6564020000 -0.2769310000
H 0.4527950000 1.4048750000 -2.0759010000
C -0.1884350000 2.6536320000 -0.4689590000
C -0.1683060000 2.9563440000 0.9013680000
C -0.7236030000 3.5912110000 -1.3616430000
H 1.3556130000 -2.3166540000 -2.7143020000
H 1.4801400000 -3.9205510000 -1.9755300000
H 2.5094300000 -2.6017240000 -1.3897120000
H 0.6732670000 -4.3717970000 0.3252400000
H -0.1379350000 -3.1389690000 1.3002670000
H 1.6151340000 -3.0326210000 1.0124520000
H -1.1990110000 -2.3763540000 -2.2516220000
H -1.7738580000 -2.9342870000 -0.6704750000
H -0.8248980000 -4.0083420000 -1.6901750000
C -0.6810590000 4.1673410000 1.3666690000
C -1.2200530000 5.0946420000 0.4685210000
C -1.2388040000 4.8052550000 -0.8973210000

H -0.7285100000 3.3774690000 -2.4281990000
H -1.6153450000 6.0386220000 0.8316480000
H -1.6453830000 5.5240760000 -1.6026710000
H 0.2576040000 2.2447540000 1.6044930000
H -0.6539970000 4.3901490000 2.4291540000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.390584 (Hartree/Particle)
Thermal correction to Energy= 0.415590
Thermal correction to Enthalpy= 0.416534
Thermal correction to Gibbs (Free) Energy= 0.333902
Sum of electronic and zero-point Energies= -1251.031121
Sum of electronic and thermal Energies= -1251.006115
Sum of electronic and thermal Enthalpies= -1251.005170
Sum of electronic and thermal (Free) Energies= -1251.087803

ccRT

C -1.1082310000 -1.9876200000 -1.3008500000
C 0.0012980000 -1.7155450000 -0.6516170000
C 1.1596530000 -1.4817450000 -0.0595630000
C 1.7307160000 -0.1116520000 -0.1869230000
C 0.9357080000 1.0983460000 -0.2032070000
C -0.3383210000 1.1958990000 0.2559750000
H 1.4633250000 1.9732720000 -0.5615150000
C 1.9763680000 -2.6113320000 0.6329590000
H -1.0111850000 -2.2476000000 -2.3564990000
C -2.4815850000 -1.9619560000 -0.7607840000
O 2.9919090000 -0.0533050000 -0.3052600000
C 1.0480630000 -3.8034310000 0.9385460000
C 2.5641400000 -2.0932730000 1.9652280000
C 3.1114300000 -3.0959960000 -0.3005130000
C -3.5674010000 -2.0086310000 -1.6520010000
C -2.7470170000 -1.9022560000 0.6200510000
C -4.0591430000 -1.8743250000 1.0904880000
H -1.9210090000 -1.9013870000 1.3257040000
C -5.1320600000 -1.9093340000 0.1926370000
H -4.2458660000 -1.8375570000 2.1600110000
C -4.8805120000 -1.9789600000 -1.1799870000
H -3.3782080000 -2.0627870000 -2.7208320000
H -6.1532840000 -1.8924180000 0.5612400000
H -5.7062310000 -2.0127210000 -1.8845840000
B 3.9200770000 1.2643230000 -0.3974100000
F 5.1849500000 0.7476630000 -0.4642040000
F 3.6594940000 1.9820210000 0.7563290000
F 3.5209880000 1.9323050000 -1.5443650000
H 3.8229770000 -2.3000140000 -0.5225890000
H 2.7030680000 -3.4728250000 -1.2446980000
H 3.6520090000 -3.9171380000 0.1841500000
H 1.7733260000 -1.7376430000 2.6359230000
H 3.2820590000 -1.2850400000 1.8141100000
H 3.0857620000 -2.9120290000 2.4722740000
H 0.2234900000 -3.5158510000 1.6000930000
H 1.6219910000 -4.5884440000 1.4413660000
H 0.6200010000 -4.2324100000 0.0277300000
C -1.1527490000 2.4044480000 0.2863110000
H -0.8195610000 0.3099740000 0.6601450000
C -0.6683380000 3.6713560000 -0.1057610000
C -2.4884500000 2.3001530000 0.7268500000
C -1.4968970000 4.7874380000 -0.0593200000
C -3.3173710000 3.4196770000 0.7686630000
C -2.8231180000 4.6663530000 0.3760050000
H -2.8739710000 1.3293840000 1.0261510000
H 0.3587550000 3.7854850000 -0.4356850000
H -4.3444720000 3.3206470000 1.1063660000
H -1.1098420000 5.7564810000 -0.3590480000
H -3.4647760000 5.5418620000 0.4103540000
C -3.8112863000 -1.9392437000 -0.2815993000
H -3.4546319000 -2.9480537000 -0.2815993000
H -3.4546135000 -1.4348455000 0.5920522000
H -3.4546135000 -1.4348455000 -1.1552508000
H -4.8812863000 -1.9392305000 -0.2815993000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.389028 (Hartree/Particle)
Thermal correction to Energy= 0.415269
Thermal correction to Enthalpy= 0.416214
Thermal correction to Gibbs (Free) Energy= 0.329371
Sum of electronic and zero-point Energies= -1251.039599
Sum of electronic and thermal Energies= -1251.013358
Sum of electronic and thermal Enthalpies= -1251.012414
Sum of electronic and thermal (Free) Energies= -1251.099257

ccTS

C -1.1890890000 -1.4571430000 -0.8942710000
C -0.0339160000 -0.9944110000 -0.3819910000
C -2.5114560000 -1.4673250000 -0.2745410000
H -1.1462470000 -1.8274880000 -1.9202720000
C 1.3135840000 -1.1672130000 -0.2550770000
C -3.6598770000 -1.4720960000 -1.0920860000
C -2.6809640000 -1.5445310000 1.1232670000
C 2.0212340000 0.0807530000 0.0060930000
C 2.0353090000 -2.5239660000 -0.2976820000
C -4.9338680000 -1.5158210000 -0.5308620000
H -3.5442340000 -1.4280720000 -2.1717080000
C -3.9566180000 -1.5965860000 1.6821440000
H -1.8080340000 -1.6090150000 1.7659960000
C 1.1293640000 1.1604870000 0.2021880000
O 3.3041920000 0.1485540000 -0.0298040000
C 1.0523270000 -3.6998280000 -0.4496240000
C 2.8450220000 -2.7229610000 1.0069340000
C 2.9935010000 -2.5193330000 -1.5191530000
C -5.0868180000 -1.5753090000 0.8585810000
H -5.8079330000 -1.5085580000 -1.1750210000
H -4.0700050000 -1.6701390000 2.7597570000
C -0.2137030000 0.8443610000 0.4865490000
H 1.4541760000 2.1760850000 0.0063990000
B 4.0834490000 1.4550220000 0.3477160000
H 0.4903870000 -3.6492710000 -1.3873080000
H 0.3357400000 -3.7456550000 0.3766250000
H 1.6173250000 -4.6373470000 -0.4550720000
H 3.3657140000 -3.6858290000 0.9655580000
H 2.1829190000 -2.7383750000 1.8801580000
H 3.5904080000 -1.9387760000 1.1470740000
H 2.4373260000 -2.3933950000 -2.4548090000
H 3.5151890000 -3.4816890000 -1.5645650000
H 3.7384180000 -1.7261010000 -1.4446130000
H -6.0797550000 -1.6212710000 1.2956710000
H -0.4233740000 0.2461100000 1.3738290000
C -1.2963840000 1.7710350000 0.1065700000
F 5.4095260000 1.0972140000 0.3039340000
F 3.6478220000 1.8260870000 1.6187160000
F 3.7379930000 2.4160720000 -0.6056420000
C -1.2253560000 2.5008200000 -1.0950100000
C -2.4027450000 1.9633770000 0.9520760000
C -2.2278890000 3.4072800000 -1.4329090000
H -0.3838910000 2.3482260000 -1.7650800000
C -3.4031690000 2.8754910000 0.6168040000
H -2.4695140000 1.4068410000 1.8819440000
C -3.3182080000 3.5981570000 -0.5764770000
H -2.1610250000 3.9646250000 -2.3623420000
H -4.2458590000 3.0233670000 1.2853150000
H -4.0982720000 4.3063940000 -0.8398880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.388032 (Hartree/Particle)
Thermal correction to Energy= 0.413111
Thermal correction to Enthalpy= 0.414055
Thermal correction to Gibbs (Free) Energy= 0.331448
Sum of electronic and zero-point Energies= -1251.010386
Sum of electronic and thermal Energies= -1250.985307
Sum of electronic and thermal Enthalpies= -1250.984363
Sum of electronic and thermal (Free) Energies= -1251.06697

ccPT

C 1.3354290000 -1.5655700000 0.0123300000
C 0.2155230000 -0.7958790000 -0.2028560000
C -1.1451200000 -1.1820290000 0.0629920000
C -2.0044920000 -0.0418720000 -0.1959530000
C -1.2188390000 1.0133630000 -0.6454470000
C 0.2169180000 0.6472870000 -0.7165620000
C -1.7571990000 -2.5151790000 0.4750550000
O -3.2960040000 -0.0605390000 -0.0323870000
C -0.7900990000 -3.6947800000 0.6994490000
C -2.7456560000 -2.9428270000 -0.6531120000
C -2.5420940000 -2.2972630000 1.8036800000
H -1.6033900000 1.9933860000 -0.8960580000
C 2.7341040000 -1.3232850000 -0.2942170000

H 1.1821440000 -2.4937280000 0.5426960000
C 3.6890830000 -2.0567420000 0.4516610000
C 5.0530300000 -1.8948060000 0.2358040000
C 5.5011300000 -1.0172740000 -0.7576760000
C 4.5746140000 -0.3103900000 -1.5311130000
C 3.2091650000 -0.4572160000 -1.3046700000
H 3.3439670000 -2.7455410000 1.2180310000
H 5.7661480000 -2.4559700000 0.8316520000
H 6.5649680000 -0.8963060000 -0.9382890000
H 4.9186910000 0.3525150000 -2.3189480000
H 2.5119800000 0.0705130000 -1.9410330000
B -4.1601060000 1.1584960000 -0.4100780000
F -5.4610100000 0.7812510000 -0.1540780000
F -3.9268680000 1.4291270000 -1.7673830000
F -3.7377710000 2.2373210000 0.3783450000
H -1.8610150000 -2.0163300000 2.6146610000
H -3.0242440000 -3.2408980000 2.0800500000
H -3.3099740000 -1.5312640000 1.7022750000
H -3.2359190000 -3.8736250000 -0.3488680000
H -2.2069470000 -3.1342700000 -1.5875630000
H -3.5128580000 -2.1902590000 -0.8312220000
H -0.1282370000 -3.5417230000 1.5581750000
H -0.1912280000 -3.9273880000 -0.1865860000
H -1.3901200000 -4.5822870000 0.9228280000
H 0.5254820000 0.6537070000 -1.7731080000
C 1.0722590000 1.6664270000 0.0379270000
C 1.1029970000 1.6858780000 1.4392690000
C 1.7657670000 2.6579910000 -0.6672910000
C 1.8316190000 2.6626720000 2.1186730000
C 2.5287140000 3.6435850000 1.4065310000
C 2.4904120000 3.6415640000 0.0107840000
H 0.5529290000 0.9372920000 2.0026190000
H 1.8466970000 2.6635670000 3.2045360000
H 3.0908720000 4.4066190000 1.9364580000
H 1.7348730000 2.6685640000 -1.7544340000
H 3.0209820000 4.4040280000 -0.5518950000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.391467 (Hartree/Particle)
Thermal correction to Energy= 0.416308
Thermal correction to Enthalpy= 0.417252
Thermal correction to Gibbs (Free) Energy= 0.334575
Sum of electronic and zero-point Energies= -1251.037637
Sum of electronic and thermal Energies= -1251.012796
Sum of electronic and thermal Enthalpies= -1251.011852
Sum of electronic and thermal (Free) Energies= -1251.094529

RB3LYP/6-311+G(d,p)

1a

cRT

C 3.5854720000 -0.1483640000 -0.0600280000
C 2.3771990000 0.2808550000 -0.2730010000
C 1.1743640000 0.8007390000 -0.4482500000
C -0.0353430000 -0.0015030000 -0.2001850000
C -0.0417690000 -1.4694520000 -0.1795140000
C 0.7304600000 -2.2253610000 -0.9646610000
H -0.7987890000 -1.9159050000 0.4540380000
C 0.9726750000 2.2639300000 -0.7913900000
O -1.0860010000 0.6521570000 0.0052220000
H 1.9324540000 2.7505290000 -0.9600640000
H 0.4469850000 2.7738700000 0.0186710000
H 0.3566350000 2.3650960000 -1.6882960000
B -2.6012380000 0.0534990000 0.2861310000
F -3.3510320000 1.1831720000 0.3871340000
F -2.4786410000 -0.6645920000 1.4580160000
F -2.8736100000 -0.7308370000 -0.8100750000
C 4.3031690000 -0.0975930000 1.2670750000
H 4.1253670000 -0.5896250000 -0.8976090000
H 3.6872060000 0.3645710000 2.0384140000
H 5.2318170000 0.4726420000 1.1714410000
H 4.5705320000 -1.1073830000 1.5919670000
H 1.4357420000 -1.8025360000 -1.6685630000
H 0.6384330000 -3.3051920000 -0.9483740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169080 (Hartree/Particle)
Thermal correction to Energy= 0.183881
Thermal correction to Enthalpy= 0.184825
Thermal correction to Gibbs (Free) Energy= 0.126365
Sum of electronic and zero-point Energies= -710.644781
Sum of electronic and thermal Energies= -710.629980
Sum of electronic and thermal Enthalpies= -710.629036
Sum of electronic and thermal (Free) Energies= -710.687496

cTS

C 3.4652070000 -0.4187230000 -0.0506500000
C 2.1937590000 -0.1405320000 -0.2848210000
C 1.1227060000 0.6936210000 -0.3308360000
C -0.1532840000 0.0514020000 -0.1165200000
C -0.0156120000 -1.3708470000 -0.0686940000
C 1.1091950000 -1.9011680000 -0.6678530000
C 1.1934020000 2.1590470000 -0.6494520000
O -1.2053790000 0.7427620000 0.0655290000
H 0.7236690000 2.7205950000 0.1638710000
H 0.6202080000 2.3853510000 -1.5527290000
H 2.2202430000 2.4991550000 -0.7756860000
H -0.6835070000 -1.9548340000 0.5531470000
B -2.6301450000 0.0550180000 0.1872670000
F -2.7536730000 -0.7581820000 -0.9342870000
F -3.5186910000 1.0922050000 0.2263850000
F -2.5878200000 -0.6986290000 1.3578580000
H 3.9435460000 -1.2089960000 -0.6240360000
C 4.2946170000 0.2438780000 1.0162160000
H 3.7467880000 1.0380750000 1.5232820000
H 5.2030680000 0.6657160000 0.5739090000
H 4.6130530000 -0.4897070000 1.7641120000
H 1.4841060000 -2.8701880000 -0.3471270000
H 1.4043070000 -1.6209590000 -1.6732480000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.168340 (Hartree/Particle)
Thermal correction to Energy= 0.182082
Thermal correction to Enthalpy= 0.183026
Thermal correction to Gibbs (Free) Energy= 0.127111
Sum of electronic and zero-point Energies= -710.618641
Sum of electronic and thermal Energies= -710.604899
Sum of electronic and thermal Enthalpies= -710.603954
Sum of electronic and thermal (Free) Energies= -710.659870

cPT

C 3.4321970000 -0.5395580000 0.0000000000
C 2.0749790000 -0.5452050000 0.0000000000
C 1.1317630000 0.5321640000 0.0000000000
C -0.2012910000 0.0101420000 0.0000000000
C -0.1175750000 -1.3880550000 0.0000000000
C 1.2842990000 -1.8393970000 0.0000000000
C 1.3680170000 1.9987970000 0.0000000000
O -1.2425530000 0.7740680000 0.0000000000
H 1.9398870000 2.3054190000 0.8818000000
H 0.4115560000 2.5204720000 0.0000000000
H 1.9398870000 2.3054190000 -0.8817990000
H -0.9799480000 -2.0399270000 0.0000000000
B -2.6551880000 0.1416930000 0.0000000000
F -2.7403490000 -0.6596520000 -1.1479820000
F -3.5408920000 1.1883750000 0.0000000000
F -2.7403490000 -0.6596520000 1.1479810000
H 3.9053010000 -1.5206970000 0.0000000000
C 4.3876420000 0.6022260000 0.0000000000
H 3.9164760000 1.5803750000 0.0000000000
H 5.0456240000 0.5307550000 -0.8744010000
H 5.0456230000 0.5307550000 0.8744020000
H 1.5130420000 -2.4609440000 0.8775040000
H 1.5130420000 -2.4609440000 -0.8775040000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170830 (Hartree/Particle)
Thermal correction to Energy= 0.184391
Thermal correction to Enthalpy= 0.185336
Thermal correction to Gibbs (Free) Energy= 0.129407
Sum of electronic and zero-point Energies= -710.662359
Sum of electronic and thermal Energies= -710.648798
Sum of electronic and thermal Enthalpies= -710.647854
Sum of electronic and thermal (Free) Energies= -710.703783

ccRT

C -3.4996190000 0.1418680000 0.7109550000
C -2.3153310000 0.4923080000 0.3062540000
C -1.1252170000 0.9340260000 -0.0633770000
C 0.0571810000 0.0602080000 0.0111150000
C -0.0217510000 -1.4042870000 0.0854790000
C -0.9530570000 -2.1323890000 -0.5360570000
H 0.7996380000 -1.8802530000 0.6076910000
C -0.8911030000 2.3784170000 -0.4603450000
O 1.1653500000 0.6477010000 0.0193220000
H -1.8342280000 2.9225720000 -0.4885350000
H -0.4147270000 2.4336880000 -1.4422080000
H -0.2176620000 2.8612820000 0.2510240000
B 2.6671560000 -0.0427650000 0.0656860000
F 3.4906250000 1.0370850000 0.0010620000
F 2.7025660000 -0.8693270000 -1.0328950000
F 2.6998340000 -0.7229660000 1.2655970000
C -4.5877800000 -0.4496260000 -0.1499180000
H -3.7230130000 0.2741020000 1.7698030000
H -4.8473310000 -1.4527900000 0.2020420000
H -4.2873070000 -0.5123720000 -1.1961980000
H -5.4924790000 0.1617910000 -0.0871120000
H -1.7357460000 -1.6872010000 -1.1368090000
H -0.9228880000 -3.2148770000 -0.4912090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169037 (Hartree/Particle)
Thermal correction to Energy= 0.183846
Thermal correction to Enthalpy= 0.184790
Thermal correction to Gibbs (Free) Energy= 0.126336
Sum of electronic and zero-point Energies= -710.644713
Sum of electronic and thermal Energies= -710.629904
Sum of electronic and thermal Enthalpies= -710.628960
Sum of electronic and thermal (Free) Energies= -710.687414

ccTS

C -3.4303020000 0.1954790000 0.5105560000
C -2.1696040000 0.2798440000 0.1194390000
C -1.0101970000 0.9784440000 -0.0241150000
C 0.1888200000 0.1779290000 0.0227690000
C -0.1237460000 -1.2168960000 0.0544490000
C -1.3615220000 -1.5830060000 -0.4360010000
H 0.5244450000 -1.9010520000 0.5891130000
C -0.9294150000 2.4558350000 -0.2741730000
O 1.3353720000 0.7244610000 0.0988560000
H -1.9092760000 2.9291690000 -0.2356810000
H -0.4631480000 2.6599780000 -1.2422640000
H -0.2786140000 2.9051050000 0.4822240000
B 2.6610010000 -0.1434490000 0.0370290000
F 3.6775200000 0.7680860000 -0.0109240000
F 2.5454800000 -0.9274480000 -1.1068100000
F 2.6559300000 -0.9262200000 1.1892320000
C -4.5156100000 -0.6706660000 -0.0558870000
H -3.6995170000 0.8017390000 1.3772660000
H -4.1798080000 -1.2478210000 -0.9173780000
H -5.3599300000 -0.0487470000 -0.3704440000
H -4.8970610000 -1.3606360000 0.7036360000
H -1.7097970000 -1.2340500000 -1.4016340000
H -1.8161930000 -2.5136560000 -0.1065460000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.168240 (Hartree/Particle)
Thermal correction to Energy= 0.181966
Thermal correction to Enthalpy= 0.182910
Thermal correction to Gibbs (Free) Energy= 0.127078
Sum of electronic and zero-point Energies= -710.617680
Sum of electronic and thermal Energies= -710.603954
Sum of electronic and thermal Enthalpies= -710.603010
Sum of electronic and thermal (Free) Energies= -710.658841

ccPT

C 3.4125450000 0.3232000000 0.0000010000
C 2.1041730000 -0.0266820000 0.0000000000
C 0.9973690000 0.8791710000 0.0000000000
C -0.2330710000 0.1507150000 0.0000000000
C 0.0808160000 -1.2106320000 0.0000000000
C 1.5447590000 -1.4332770000 0.0000000000
C 1.0111330000 2.3567460000 0.0000000000
O -1.3807500000 0.7459680000 0.0000000000
H 2.0097390000 2.7906220000 0.0000000000
H 0.4503660000 2.7196950000 0.8689500000
H 0.4503660000 2.7196950000 -0.8689500000
H -0.6603180000 -1.9976130000 0.0000000000
B -2.6752190000 -0.1000810000 0.0000000000
F -3.7157580000 0.7936660000 -0.0000010000
F -2.6343920000 -0.9051780000 1.1481750000
F -2.6343910000 -0.9051780000 -1.1481760000
C 4.5738520000 -0.6079630000 0.0000010000
H 3.6552670000 1.3827840000 0.0000010000
H 4.2816340000 -1.6578440000 0.0000010000
H 5.2070160000 -0.4209370000 0.8752730000
H 5.2070170000 -0.4209370000 -0.8752710000
H 1.8662110000 -2.0101360000 0.8777720000
H 1.8662110000 -2.0101360000 -0.8777710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170802 (Hartree/Particle)
Thermal correction to Energy= 0.184348
Thermal correction to Enthalpy= 0.185293
Thermal correction to Gibbs (Free) Energy= 0.129712
Sum of electronic and zero-point Energies= -710.667145
Sum of electronic and thermal Energies= -710.653599
Sum of electronic and thermal Enthalpies= -710.652654
Sum of electronic and thermal (Free) Energies= -710.708235

RB3LYP/6-31G(d)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)

1a

cRT

C 3.5809170000 -0.1452090000 -0.1071600000
C 2.3646310000 0.2898470000 -0.2724120000
C 1.1520810000 0.8186390000 -0.4082620000
C -0.0391040000 0.0067190000 -0.1629560000
C -0.0342560000 -1.4575140000 -0.1340500000
C 0.7457870000 -2.2142050000 -0.9190930000
H -0.7742830000 -1.9092070000 0.5173860000
C 0.9478670000 2.2927470000 -0.7087870000
O -1.1113970000 0.6562880000 0.0449260000
H 1.9059540000 2.7742680000 -0.9127190000
H 0.4731420000 2.7945840000 0.1406570000
H 0.2914110000 2.4232230000 -1.5754340000
B -2.5674670000 0.0441780000 0.2536680000
F -3.3597430000 1.1546420000 0.3817180000
F -2.5132280000 -0.7197840000 1.4048830000
F -2.8388240000 -0.7013090000 -0.8714440000
C 4.3453890000 -0.1157360000 1.1959540000
H 4.0914270000 -0.5758830000 -0.9705890000
H 3.7575830000 0.3337220000 1.9993610000
H 5.2715550000 0.4570510000 1.0715930000
H 4.6258340000 -1.1337350000 1.4898030000
H 1.4355720000 -1.7916360000 -1.6411930000
H 0.6765970000 -3.2972590000 -0.8824260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171056 (Hartree/Particle)
Thermal correction to Energy= 0.185619
Thermal correction to Enthalpy= 0.186563
Thermal correction to Gibbs (Free) Energy= 0.128795
Sum of electronic and zero-point Energies= -710.436528
Sum of electronic and thermal Energies= -710.421965
Sum of electronic and thermal Enthalpies= -710.421021
Sum of electronic and thermal (Free) Energies= -710.478789

cTS

C 3.4791160000 -0.4004770000 -0.0718050000
C 2.2046870000 -0.1070500000 -0.2729470000
C 1.1127050000 0.7030760000 -0.3143980000
C -0.1467240000 0.0378360000 -0.0935990000
C -0.0120120000 -1.3804650000 -0.0572640000
C 1.1072440000 -1.9155310000 -0.6656410000
C 1.1623320000 2.1731860000 -0.6336210000
O -1.2170180000 0.7285920000 0.1089390000
H 0.7427630000 2.7374150000 0.2076380000
H 0.5482480000 2.4025910000 -1.5112980000
H 2.1845220000 2.5117900000 -0.8094010000

H -0.6738000000 -1.9690520000 0.5684990000
B -2.6069540000 0.0521720000 0.1775000000
F -2.7704640000 -0.6853220000 -0.9862820000
F -3.5031790000 1.0933620000 0.2795080000
F -2.6185710000 -0.7692950000 1.3017190000
H 3.9420790000 -1.1765030000 -0.6791960000
C 4.3338590000 0.2268480000 0.9976330000
H 3.8021490000 1.0111720000 1.5405990000
H 5.2355580000 0.6538260000 0.5417650000
H 4.6648640000 -0.5360160000 1.7130240000
H 1.4852030000 -2.8881480000 -0.3555250000
H 1.4220240000 -1.6099130000 -1.6597540000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170303 (Hartree/Particle)
Thermal correction to Energy= 0.183925
Thermal correction to Enthalpy= 0.184869
Thermal correction to Gibbs (Free) Energy= 0.129197
Sum of electronic and zero-point Energies= -710.416130
Sum of electronic and thermal Energies= -710.402508
Sum of electronic and thermal Enthalpies= -710.401563
Sum of electronic and thermal (Free) Energies= -710.457236

cPT

C 3.4469120000 0.5238010000 -0.0053000000
C 2.0840010000 0.5472290000 0.0001230000
C 1.1349900000 -0.5224130000 0.0051890000
C -0.1946910000 0.0182250000 0.0101390000
C -0.1020910000 1.4080740000 0.0088020000
C 1.3066750000 1.8486530000 0.0012020000
C 1.3675560000 -1.9908790000 0.0056330000
O -1.2544290000 -0.7539840000 0.0149220000
H 1.9430420000 -2.2980440000 -0.8757730000
H 0.4127280000 -2.5188140000 0.0049470000
H 1.9407340000 -2.2972690000 0.8889690000
H -0.9509060000 2.0785270000 0.0144260000
B -2.6409030000 -0.1415540000 -0.0033860000
F -3.5238930000 -1.2071550000 0.0168210000
F -2.7746180000 0.6225370000 -1.1657850000
F -2.7840540000 0.6725550000 1.1242550000
H 1.5389140000 2.4683500000 -0.8786920000
H 1.5473710000 2.4724520000 0.8758670000
C 4.3903530000 -0.6251440000 -0.0059120000
H 3.9168170000 -1.6044070000 0.0019780000
H 5.0446080000 -0.5534570000 -0.8860050000
H 5.0560150000 -0.5449200000 0.8647750000
H 3.9314630000 1.5005170000 -0.0097960000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172637 (Hartree/Particle)
Thermal correction to Energy= 0.186149
Thermal correction to Enthalpy= 0.187094
Thermal correction to Gibbs (Free) Energy= 0.130257
Sum of electronic and zero-point Energies= -710.465732
Sum of electronic and thermal Energies= -710.452219
Sum of electronic and thermal Enthalpies= -710.451275
Sum of electronic and thermal (Free) Energies= -710.508111

ccRT

C -3.5031880000 0.1381800000 0.6854460000
C -2.3085560000 0.4923990000 0.3072010000
C -1.1065270000 0.9437270000 -0.0396880000
C 0.0605580000 0.0671180000 0.0406450000
C -0.0234320000 -1.3924720000 0.1300820000
C -0.9573050000 -2.1234850000 -0.4947790000
H 0.7820510000 -1.8685920000 0.6784230000
C -0.8707610000 2.3952410000 -0.4161900000
O 1.1879250000 0.6536390000 0.0474250000
H -1.8201640000 2.9302600000 -0.4772120000
H -0.3585280000 2.4660610000 -1.3813830000
H -0.2353690000 2.8851980000 0.3288410000
B 2.6197360000 -0.0452870000 0.0440150000
F 3.4868310000 1.0141700000 -0.0091740000
F 2.6570410000 -0.8461030000 -1.0753210000
F 2.7108340000 -0.7632710000 1.2221430000
C -4.5708230000 -0.4564410000 -0.2015430000
H -3.7538190000 0.2688480000 1.7403800000
H -4.8372790000 -1.4593070000 0.1522360000
H -4.2452070000 -0.5238570000 -1.2422050000
H -5.4770650000 0.1581200000 -0.1570290000
H -1.7228430000 -1.6811820000 -1.1226580000
H -0.9460060000 -3.2069870000 -0.4247360000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171088 (Hartree/Particle)
Thermal correction to Energy= 0.185619
Thermal correction to Enthalpy= 0.186563
Thermal correction to Gibbs (Free) Energy= 0.128977
Sum of electronic and zero-point Energies= -710.436538
Sum of electronic and thermal Energies= -710.422008
Sum of electronic and thermal Enthalpies= -710.421064
Sum of electronic and thermal (Free) Energies= -710.478650

ccTS

C -3.4473300000 0.2031500000 0.5093520000
C -2.1793800000 0.3003110000 0.1430460000
C -1.0054670000 0.9759800000 -0.0090750000
C 0.1786620000 0.1598090000 0.0475930000
C -0.1262180000 -1.2324440000 0.0761980000
C -1.3605940000 -1.6107440000 -0.4163970000
H 0.5212320000 -1.9158100000 0.6147570000
C -0.9105380000 2.4533570000 -0.2774380000
O 1.3430900000 0.7082040000 0.1355390000
H -1.8951250000 2.9229370000 -0.2917730000
H -0.4027950000 2.6463060000 -1.2290250000
H -0.3051400000 2.9209220000 0.5081310000
B 2.6347600000 -0.1363430000 0.0273910000
F 3.6607420000 0.7828120000 0.0295320000
F 2.5632760000 -0.8589080000 -1.1552730000
F 2.6771100000 -0.9813730000 1.1331840000
C -4.5201510000 -0.6569730000 -0.0914270000
H -3.7347740000 0.7929920000 1.3837390000
H -4.9068540000 -1.3623470000 0.6538680000
H -4.1696460000 -1.2159890000 -0.9615620000
H -5.3627210000 -0.0260670000 -0.3997590000
H -1.7315160000 -1.2403950000 -1.3679880000
H -1.8152330000 -2.5439080000 -0.0897540000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170205 (Hartree/Particle)
Thermal correction to Energy= 0.183804
Thermal correction to Enthalpy= 0.184748
Thermal correction to Gibbs (Free) Energy= 0.129189
Sum of electronic and zero-point Energies= -710.415373
Sum of electronic and thermal Energies= -710.401774
Sum of electronic and thermal Enthalpies= -710.400830
Sum of electronic and thermal (Free) Energies= -710.456389

ccPT

C 3.4217900000 0.3334150000 0.0000010000
C 2.1116390000 -0.0327850000 0.0000000000
C 1.0030220000 0.8662160000 0.0000000000
C -0.2226950000 0.1221390000 0.0000010000
C 0.0964380000 -1.2308650000 0.0000010000
C 1.5645260000 -1.4434500000 0.0000010000
C 1.0116730000 2.3469780000 0.0000000000
O -1.3882200000 0.7246850000 0.0000010000
H 2.0117090000 2.7816840000 0.0000010000
H 0.4571840000 2.7119950000 0.8743590000
H 0.4571870000 2.7119940000 -0.8743620000
H -0.6296950000 -2.0327160000 0.0000020000
B -2.6630750000 -0.0938910000 -0.0000010000
F -3.6996840000 0.8239310000 0.0000040000
F -2.6789970000 -0.8953630000 1.1453750000
F -2.6790000000 -0.8953540000 -1.1453830000
C 4.5890250000 -0.5863230000 0.0000010000
H 3.6566350000 1.3960880000 0.0000000000
H 4.3091730000 -1.6416030000 0.0000010000
H 5.2200120000 -0.3836160000 0.8763270000
H 5.2200130000 -0.3836160000 -0.8763250000
H 1.8927710000 -2.0195530000 0.8777410000
H 1.8927700000 -2.0195530000 -0.8777390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172700 (Hartree/Particle)
Thermal correction to Energy= 0.186199

Thermal correction to Enthalpy= 0.187143
Thermal correction to Gibbs (Free) Energy= 0.130261
Sum of electronic and zero-point Energies= -710.470600
Sum of electronic and thermal Energies= -710.457101
Sum of electronic and thermal Enthalpies= -710.456157
Sum of electronic and thermal (Free) Energies= -710.513038

6d

cRT

C -1.9139510000 -1.2915170000 0.8279540000
C -1.2813340000 -0.1421340000 0.8685630000
C -0.6935720000 1.0419470000 0.8872900000
C 0.4356840000 1.2509700000 -0.0520190000
C 1.4361650000 0.2484920000 -0.3132790000
C 1.6960350000 -0.7856030000 0.5336050000
H 2.0277830000 0.4069090000 -1.2064590000
C -1.1907440000 2.2130170000 1.7804380000
H -1.5848680000 -2.0704240000 1.5181290000
C -3.0348900000 -1.6526840000 -0.0611440000
O 0.4677780000 2.3845970000 -0.6369860000
C -2.1114210000 1.6597990000 2.8842560000
C -1.9880020000 3.2359690000 0.9380360000
C 0.0223910000 2.8998590000 2.4471290000
C -3.6213900000 -2.9220970000 0.0695540000
C -3.5365760000 -0.7718140000 -1.0358410000
C -4.5974730000 -1.1534700000 -1.8522980000
H -3.0893740000 0.2116370000 -1.1520760000
C -5.1766550000 -2.4196800000 -1.7129220000
H -4.9740890000 -0.4623220000 -2.6012720000
C -4.6847750000 -3.3021640000 -0.7495750000
H -3.2406260000 -3.6113230000 0.8191490000
H -6.0041740000 -2.7142320000 -2.3521010000
H -5.1272560000 -4.2877400000 -0.6344450000
B 1.6480910000 3.0098130000 -1.4791150000
F 1.1350350000 4.2114700000 -1.9007770000
F 1.9277990000 2.1523140000 -2.5307370000
F 2.7050060000 3.1402370000 -0.6023820000
H 0.7166160000 3.3186550000 1.7132650000
H 0.5741490000 2.1955110000 3.0808370000
H -0.3267090000 3.7204710000 3.0840390000
H -2.8488510000 2.7566480000 0.4579500000
H -1.3710220000 3.6946480000 0.1635310000
H -2.3661650000 4.0295260000 1.5938200000
H -3.0074210000 1.1895270000 2.4664720000
H -2.4328070000 2.4810860000 3.5341120000
H -1.5952900000 0.9185980000 3.5048280000
C 2.6937420000 -1.8254810000 0.3563890000
H 1.1302480000 -0.8453450000 1.4593720000
C 3.4982520000 -1.9362080000 -0.7987990000
C 2.8583800000 -2.7732980000 1.3881290000
C 4.4319170000 -2.9587870000 -0.9097770000
C 3.7949450000 -3.7965410000 1.2741840000
C 4.5835940000 -3.8908010000 0.1249070000
H 2.2434670000 -2.6975450000 2.2811210000
H 3.3901640000 -1.2226580000 -1.6091630000
H 3.9104330000 -4.5181460000 2.0772370000
H 5.0449880000 -3.0342650000 -1.8027930000
H 5.3156340000 -4.6878930000 0.0322850000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.391007 (Hartree/Particle)
Thermal correction to Energy= 0.417094
Thermal correction to Enthalpy= 0.418038
Thermal correction to Gibbs (Free) Energy= 0.330573
Sum of electronic and zero-point Energies= -1250.962558
Sum of electronic and thermal Energies= -1250.936472
Sum of electronic and thermal Enthalpies= -1250.935528
Sum of electronic and thermal (Free) Energies= -1251.022992

cTS

C 1.7660640000 -0.3954300000 0.7364730000
C 0.4300630000 -0.4129280000 0.6848810000
C 2.6951370000 -1.2069310000 -0.0498090000
H 2.2303980000 0.3585450000 1.3718670000
C -0.7829240000 -1.0215750000 0.5581520000
C 4.0651110000 -1.1607010000 0.2747900000
C 2.2796640000 -2.0188510000 -1.1238970000
C -1.7911340000 -0.1308070000 0.0013000000
C -1.1123950000 -2.4346710000 1.0677730000
C 4.9875700000 -1.9283370000 -0.4319180000
H 4.3980770000 -0.5263540000 1.0920490000
C 3.2052630000 -2.7795720000 -1.8309990000
H 1.2337390000 -2.0305080000 -1.4145480000
C -1.3616530000 1.2093040000 -0.0312400000
O -2.9214720000 -0.5853810000 -0.4477070000
C 0.0853990000 -3.0696960000 1.7970260000
C -1.4964000000 -3.3265320000 -0.1405250000
C -2.3009920000 -2.3537720000 2.0561960000
C 4.5607330000 -2.7412240000 -1.4852750000
H 6.0395320000 -1.8885200000 -0.1646840000
H 2.8722960000 -3.3972680000 -2.6599670000
C -0.2436190000 1.5366680000 0.7636360000
H -1.8100180000 1.9141890000 -0.7206520000
B -4.0755900000 0.3523210000 -0.8408620000
H 0.3915940000 -2.4747800000 2.6640510000
H 0.9516320000 -3.1888910000 1.1396550000
H -0.2015140000 -4.0641920000 2.1553520000
H -1.7687390000 -4.3232370000 0.2254720000
H -0.6537510000 -3.4414520000 -0.8309570000
H -2.3454530000 -2.9160810000 -0.6901760000
H -2.0466310000 -1.7343790000 2.9239830000
H -2.5380910000 -3.3601440000 2.4194030000
H -3.1955890000 -1.9417230000 1.5846250000
H 5.2806350000 -3.3347170000 -2.0413320000
H -0.2878580000 1.2886950000 1.8242460000
C 0.6526870000 2.6586900000 0.4580910000
F -4.3748060000 1.1447360000 0.2602050000
F -5.1146050000 -0.4877210000 -1.1859720000
F -3.6546990000 1.1322700000 -1.9184460000
C 0.8479810000 3.1082140000 -0.8614410000
C 1.3397730000 3.2997640000 1.5051750000
C 1.6920500000 4.1838610000 -1.1204460000
H 0.3455260000 2.6036600000 -1.6817960000
C 2.1858030000 4.3756610000 1.2437670000
H 1.1941800000 2.9592750000 2.5274700000
C 2.3615290000 4.8200130000 -0.0691230000
H 1.8354100000 4.5241100000 -2.1417410000
H 2.7047320000 4.8675920000 2.0610860000
H 3.0223420000 5.6571870000 -0.2750470000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.390475 (Hartree/Particle)
Thermal correction to Energy= 0.415436
Thermal correction to Enthalpy= 0.416380
Thermal correction to Gibbs (Free) Energy= 0.333738
Sum of electronic and zero-point Energies= -1250.941128
Sum of electronic and thermal Energies= -1250.916167
Sum of electronic and thermal Enthalpies= -1250.915223
Sum of electronic and thermal (Free) Energies= -1250.997865

cPT

C 1.8130400000 0.0415490000 0.7753430000
C 0.4402410000 0.0125040000 0.7038300000
C -0.5320810000 -0.9818640000 0.4012480000
C -1.7735860000 -0.3044310000 0.0553700000
C -1.6470050000 1.0406900000 0.3582910000
C -0.3216750000 1.3491790000 0.9385850000
C -0.5025700000 -2.4865530000 0.6432510000
C 2.8126760000 -0.7630620000 0.1097640000
O -2.8183570000 -0.9370680000 -0.4257760000
C 0.7979550000 -3.0266580000 1.2653000000
C -0.7968730000 -3.2477450000 -0.6775960000
C -1.6416350000 -2.7883750000 1.6688310000
C 4.1245840000 -0.7912170000 0.6350030000
C 2.5528490000 -1.4394890000 -1.1034860000
C 3.5588890000 -2.1583330000 -1.7389140000
H 1.5721740000 -1.3563760000 -1.5601160000
C 4.8399130000 -2.2169340000 -1.1787160000
H 3.3515140000 -2.6621640000 -2.6780230000
C 5.1204440000 -1.5307880000 0.0085780000
H 4.3426000000 -0.2466200000 1.5495380000
H 5.6242450000 -2.7779040000 -1.6782870000
H 6.1187740000 -1.5640460000 0.4339780000
B -4.1668760000 -0.2471580000 -0.5430710000
F -4.5951970000 0.0983650000 0.7385490000
F -5.0061160000 -1.1742990000 -1.1370220000

F -4.0260490000 0.8980690000 -1.3341270000
H 2.2222910000 0.8995420000 1.3086090000
H -2.4154890000 1.7829480000 0.1921060000
H -0.4182320000 1.4214930000 2.0348510000
C 0.3122390000 2.6338050000 0.4341510000
C 0.3996660000 2.8936100000 -0.9417670000
C 0.8072170000 3.5829190000 1.3360110000
H -1.4364190000 -2.3016270000 2.6286820000
H -1.6745110000 -3.8698660000 1.8380320000
H -2.6175720000 -2.4638640000 1.3085970000
H -0.8602820000 -4.3192050000 -0.4572780000
H 0.0081220000 -3.1015630000 -1.4050220000
H -1.7389990000 -2.9263560000 -1.1238210000
H 1.0971000000 -2.4517980000 2.1480970000
H 1.6310330000 -3.0411630000 0.5626290000
H 0.6227760000 -4.0592870000 1.5849670000
C 0.9737620000 4.0769490000 -1.4034310000
C 1.4678770000 5.0187900000 -0.4954490000
C 1.3833750000 4.7695260000 0.8748850000
H 0.7372930000 3.3968680000 2.4052940000
H 1.9138450000 5.9415260000 -0.8559550000
H 1.7609620000 5.4976260000 1.5874020000
H 0.0162400000 2.1648220000 -1.6521140000
H 1.0342250000 4.2656930000 -2.4716710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392672 (Hartree/Particle)
Thermal correction to Energy= 0.417548
Thermal correction to Enthalpy= 0.418492
Thermal correction to Gibbs (Free) Energy= 0.335727
Sum of electronic and zero-point Energies= -1250.959563
Sum of electronic and thermal Energies= -1250.934687
Sum of electronic and thermal Enthalpies= -1250.933743
Sum of electronic and thermal (Free) Energies= -1251.016508

ccRT

C -1.0809810000 -2.0004080000 -1.3122240000
C 0.0293520000 -1.7021600000 -0.6793450000
C 1.1899810000 -1.4467160000 -0.0981560000
C 1.7340680000 -0.0746600000 -0.2401130000
C 0.9187670000 1.1141050000 -0.2634140000
C -0.3415170000 1.1846910000 0.2441250000
H 1.4086130000 1.9928530000 -0.6642260000
C 2.0198010000 -2.5516460000 0.6152110000
H -0.9906410000 -2.2796410000 -2.3637230000
C -2.4497630000 -1.9809300000 -0.7625460000
O 3.0012530000 0.0042710000 -0.3703320000
C 1.1245930000 -3.7771800000 0.8801050000
C 2.5315850000 -2.0159520000 1.9710880000
C 3.2081610000 -2.9965150000 -0.2695170000
C -3.5383630000 -2.0766010000 -1.6451800000
C -2.7055260000 -1.8775620000 0.6170960000
C -4.0142860000 -1.8521360000 1.0943630000
H -1.8751010000 -1.8394950000 1.3171860000
C -5.0907460000 -1.9358280000 0.2050960000
H -4.1950470000 -1.7779860000 2.1631460000
C -4.8476640000 -2.0514310000 -1.1651000000
H -3.3536040000 -2.1662260000 -2.7125820000
H -6.1101840000 -1.9195180000 0.5797420000
H -5.6775400000 -2.1234740000 -1.8624820000
B 3.9079410000 1.2966510000 -0.3474560000
F 5.1695150000 0.7992410000 -0.5628930000
F 3.7434950000 1.8566370000 0.9018190000
F 3.4836090000 2.1328330000 -1.3674920000
H 3.9176540000 -2.1849200000 -0.4377480000
H 2.8545370000 -3.3570210000 -1.2423620000
H 3.7367260000 -3.8212910000 0.2234640000
H 1.6964270000 -1.7295710000 2.6211290000
H 3.1889380000 -1.1506780000 1.8525240000
H 3.1001250000 -2.8010010000 2.4824820000
H 0.2587610000 -3.5195280000 1.5005960000
H 1.7039720000 -4.5405390000 1.4107600000
H 0.7565230000 -4.2199390000 -0.0508940000
C -1.2008780000 2.3561370000 0.2701870000
H -0.7650750000 0.2967840000 0.7044480000
C -0.8198350000 3.6062070000 -0.2645480000
C -2.4781880000 2.2328570000 0.8558430000
C -1.6887850000 4.6887390000 -0.2106010000
C -3.3470910000 3.3191350000 0.9067750000
C -2.9537250000 4.5493860000 0.3746660000
H -2.7854040000 1.2729250000 1.2620570000
H 0.1576830000 3.7304480000 -0.7189410000
H -4.3279070000 3.2077410000 1.3591460000
H -1.3838120000 5.6455460000 -0.6236750000
H -3.6286990000 5.3995180000 0.4141130000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.391113 (Hartree/Particle)
Thermal correction to Energy= 0.417142
Thermal correction to Enthalpy= 0.418086
Thermal correction to Gibbs (Free) Energy= 0.331591
Sum of electronic and zero-point Energies= -1250.962278
Sum of electronic and thermal Energies= -1250.936249
Sum of electronic and thermal Enthalpies= -1250.935305
Sum of electronic and thermal (Free) Energies= -1251.021800

ccTS

C -1.1886590000 -1.4628720000 -0.9050430000
C -0.0287020000 -1.0032910000 -0.4062560000
C -2.5045910000 -1.4756770000 -0.2773280000
H -1.1543750000 -1.8216180000 -1.9358550000
C 1.3167280000 -1.1588860000 -0.2696720000
C -3.6540320000 -1.5020410000 -1.0924040000
C -2.6653810000 -1.5291960000 1.1225490000
C 2.0125170000 0.0963930000 -0.0257680000
C 2.0383870000 -2.5172660000 -0.2920720000
C -4.9241850000 -1.5441680000 -0.5251260000
H -3.5410680000 -1.4783440000 -2.1729660000
C -3.9377320000 -1.5795380000 1.6859010000
H -1.7894070000 -1.5752380000 1.7628570000
C 1.1290380000 1.1718210000 0.1745030000
O 3.3070600000 0.1727240000 -0.0790970000
C 1.0514620000 -3.6922730000 -0.4177010000
C 2.8505360000 -2.6977790000 1.0120140000
C 2.9871270000 -2.5392460000 -1.5184920000
C -5.0697370000 -1.5801460000 0.8652110000
H -5.8013760000 -1.5545730000 -1.1653390000
H -4.0470810000 -1.6319310000 2.7652130000
C -0.2144990000 0.8628050000 0.4688390000
H 1.4514200000 2.1855640000 -0.0292160000
B 4.0688480000 1.4391640000 0.3492020000
H 0.4825530000 -3.6525830000 -1.3521320000
H 0.3412180000 -3.7195260000 0.4154020000
H 1.6141430000 -4.6320510000 -0.4118470000
H 3.3715210000 -3.6616800000 0.9846950000
H 2.1893080000 -2.6977920000 1.8863020000
H 3.5961700000 -1.9105040000 1.1394850000
H 2.4227610000 -2.4347450000 -2.4521490000
H 3.5128650000 -3.5007080000 -1.5471600000
H 3.7295810000 -1.7408290000 -1.4681970000
H -6.0610070000 -1.6235340000 1.3070600000
H -0.4178360000 0.2497030000 1.3477330000
C -1.3011620000 1.7811660000 0.1001100000
F 5.4031370000 1.1048310000 0.2367800000
F 3.7037040000 1.7370790000 1.6556540000
F 3.7150990000 2.4729740000 -0.5180710000
C -1.2317940000 2.5378360000 -1.0853210000
C -2.4175380000 1.9357970000 0.9413100000
C -2.2454620000 3.4337740000 -1.4112120000
H -0.3855630000 2.4079600000 -1.7542460000
C -3.4289020000 2.8376530000 0.6165010000
H -2.4823110000 1.3573520000 1.8577740000
C -3.3449720000 3.5870690000 -0.5595320000
H -2.1834260000 4.0098110000 -2.3298200000
H -4.2809000000 2.9559380000 1.2794580000
H -4.1360670000 4.2861630000 -0.8156050000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.390065 (Hartree/Particle)
Thermal correction to Energy= 0.415001
Thermal correction to Enthalpy= 0.415945
Thermal correction to Gibbs (Free) Energy= 0.333724
Sum of electronic and zero-point Energies= -1250.937578
Sum of electronic and thermal Energies= -1250.912642
Sum of electronic and thermal Enthalpies= -1250.911698
Sum of electronic and thermal (Free) Energies= -1250.993919

ccPT

C -1.3446470000 1.5531120000 0.0187850000
C -0.2183140000 0.7888200000 -0.2062240000
C 1.1333100000 1.1773880000 0.0650950000
C 1.9961700000 0.0378280000 -0.2055450000
C 1.2199210000 -1.0117760000 -0.6574710000
C -0.2172060000 -0.6507230000 -0.7247260000
C 1.7334030000 2.5115670000 0.4919060000
O 3.3007550000 0.0589220000 -0.0363750000
C 0.7596370000 3.6837660000 0.7220130000
C 2.7213130000 2.9581440000 -0.6270680000
C 2.5094310000 2.2883060000 1.8230230000
H 1.5964990000 -1.9931740000 -0.9095610000
C -2.7341160000 1.3117780000 -0.2997220000
H -1.1985150000 2.4693270000 0.5709900000
C -3.6928720000 2.0475080000 0.4410200000
C -5.0533290000 1.8808140000 0.2190240000
C -5.4922390000 1.0003420000 -0.7755480000
C -4.5624580000 0.2938760000 -1.5458910000
C -3.2002910000 0.4421010000 -1.3133250000
H -3.3511140000 2.7377480000 1.2073840000
H -5.7718130000 2.4409670000 0.8094010000
H -6.5551550000 0.8774860000 -0.9616840000
H -4.9027770000 -0.3677140000 -2.3365360000
H -2.4987590000 -0.0782990000 -1.9510490000
B 4.1531260000 -1.1334710000 -0.4275400000
F 5.4548140000 -0.7757230000 -0.1187650000
F 3.9905230000 -1.3701290000 -1.7945310000
F 3.7365930000 -2.2479530000 0.3067670000
H 1.8223240000 2.0015850000 2.6269640000
H 2.9894330000 3.2309440000 2.1081870000
H 3.2775650000 1.5218510000 1.7230170000
H 3.2106810000 3.8851110000 -0.3084360000
H 2.1820290000 3.1624500000 -1.5586590000
H 3.4884580000 2.2081110000 -0.8177900000
H 0.1002970000 3.5229950000 1.5812160000
H 0.1564840000 3.9127810000 -0.1622790000
H 1.3550570000 4.5749770000 0.9461900000
H -0.5305070000 -0.6580860000 -1.7790820000
C -1.0643500000 -1.6688120000 0.0407380000
C -1.0532410000 -1.7001370000 1.4421830000
C -1.7960660000 -2.6399660000 -0.6532260000
C -1.7778810000 -2.6699710000 2.1337520000
C -2.5122530000 -3.6316560000 1.4338270000
C -2.5168310000 -3.6161480000 0.0384340000
H -0.4797140000 -0.9607750000 1.9948760000
H -1.7649840000 -2.6777050000 3.2201200000
H -3.0745650000 -4.3883130000 1.9737130000
H -1.8010720000 -2.6378440000 -1.7406570000
H -3.0814350000 -4.3611750000 -0.5151990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.393689 (Hartree/Particle)
Thermal correction to Energy= 0.418398
Thermal correction to Enthalpy= 0.419342
Thermal correction to Gibbs (Free) Energy= 0.336492
Sum of electronic and zero-point Energies= -1250.967361
Sum of electronic and thermal Energies= -1250.942651
Sum of electronic and thermal Enthalpies= -1250.941707
Sum of electronic and thermal (Free) Energies= -1251.024557

RB3LYP/6-31+G(d,p)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)

6d

cRT

C -1.8565640000 -1.3983090000 0.8536910000
C -1.2794430000 -0.2198800000 0.9246820000
C -0.7510850000 0.9904710000 0.9672010000
C 0.3588700000 1.2734860000 0.0148780000
C 1.4237180000 0.3319880000 -0.2605550000
C 1.7615960000 -0.6873930000 0.5705770000
H 1.9993480000 0.5425450000 -1.1532320000
C -1.3192890000 2.1250060000 1.8667570000
H -1.5061920000 -2.1721580000 1.5389780000
C -2.9429910000 -1.7970100000 -0.0634900000
O 0.3172660000 2.3995210000 -0.5654310000
C -2.1625140000 1.5057200000 2.9981300000
C -2.2186580000 3.0680910000 1.0326020000
C -0.1542230000 2.9218850000 2.4958370000
C -3.5011280000 -3.0802130000 0.0618350000
C -3.4377850000 -0.9390590000 -1.0625220000
C -4.4658300000 -1.3553100000 -1.9051710000
H -3.0108040000 0.0525810000 -1.1800950000
C -5.0183790000 -2.6344670000 -1.7692770000
H -4.8351570000 -0.6821250000 -2.6731900000
C -4.5319490000 -3.4954690000 -0.7831030000
H -3.1251910000 -3.7542330000 0.8274280000
H -5.8187880000 -2.9557720000 -2.4289780000
H -4.9523840000 -4.4905670000 -0.6709860000
B 1.4009710000 3.0181020000 -1.5913230000
F 0.8876960000 4.2529190000 -1.8779000000
F 1.4336700000 2.1538530000 -2.6746470000
F 2.5950400000 3.0454560000 -0.8936780000
H 0.4532540000 3.4291860000 1.7430780000
H 0.4978330000 2.2704390000 3.0891460000
H -0.5584280000 3.6869340000 3.1671970000
H -3.0594540000 2.5174480000 0.5971410000
H -1.6637820000 3.5503040000 0.2266680000
H -2.6286060000 3.8480940000 1.6845550000
H -3.0219940000 0.9517510000 2.6090290000
H -2.5415690000 2.3031680000 3.6455400000
H -1.5686780000 0.8235450000 3.6166260000
C 2.8455840000 -1.6416530000 0.3777870000
H 1.1978440000 -0.8107080000 1.4917140000
C 3.6802070000 -1.6415830000 -0.7607820000
C 3.0683900000 -2.6132220000 1.3752960000
C 4.6960420000 -2.5827040000 -0.8897410000
C 4.0867100000 -3.5554200000 1.2441470000
C 4.9030530000 -3.5421340000 0.1100580000
H 2.4350500000 -2.6216050000 2.2586610000
H 3.5364330000 -0.9034090000 -1.5425730000
H 4.2444110000 -4.2956500000 2.0225430000
H 5.3314580000 -2.5699880000 -1.7699080000
H 5.6987640000 -4.2734420000 0.0037390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.388878 (Hartree/Particle)
Thermal correction to Energy= 0.415194
Thermal correction to Enthalpy= 0.416138
Thermal correction to Gibbs (Free) Energy= 0.328383
Sum of electronic and zero-point Energies= -1251.039778
Sum of electronic and thermal Energies= -1251.013462
Sum of electronic and thermal Enthalpies= -1251.012518
Sum of electronic and thermal (Free) Energies= -1251.100272

cTS

C 1.7698470000 -0.3842930000 0.7382880000
C 0.4309970000 -0.3903420000 0.7143510000
C 2.6771790000 -1.2134740000 -0.0580850000
H 2.2543870000 0.3776640000 1.3483930000
C -0.7787070000 -1.0130650000 0.5973760000
C 4.0528240000 -1.1907460000 0.2468200000
C 2.2366400000 -2.0174740000 -1.1282520000
C -1.7974790000 -0.1304850000 0.0401060000
C -1.1058670000 -2.4245110000 1.1102200000
C 4.9550570000 -1.9722050000 -0.4729540000
H 4.4082780000 -0.5622810000 1.0591270000
C 3.1415950000 -2.7911040000 -1.8503380000
H 1.1868270000 -2.0163160000 -1.4027950000
C -1.3608490000 1.2153140000 -0.0014620000
O -2.9190740000 -0.5860980000 -0.3944040000
C 0.0942840000 -3.0602770000 1.8359700000
C -1.5015010000 -3.3167240000 -0.0960300000
C -2.2944170000 -2.3384100000 2.1006910000
C 4.5025940000 -2.7766220000 -1.5230420000
H 6.0105170000 -1.9495320000 -0.2187590000
H 2.7875590000 -3.4005440000 -2.6763950000
C -0.2411290000 1.5376030000 0.7909090000
H -1.8142370000 1.9201340000 -0.6889750000
B -4.0643000000 0.3589690000 -0.8903330000
H 0.4036490000 -2.4671010000 2.7027470000
H 0.9590420000 -3.1823200000 1.1783860000
H -0.1924800000 -4.0534250000 2.1961710000
H -1.7720600000 -4.3113840000 0.2750710000
H -0.6646060000 -3.4364950000 -0.7917450000
H -2.3548420000 -2.9061360000 -0.6377120000
H -2.0413940000 -1.7131770000 2.9643850000

H -2.5260310000 -3.3424170000 2.4721290000
H -3.1911780000 -1.9351040000 1.6274740000
H 5.2052900000 -3.3801830000 -2.0894820000
H -0.2900080000 1.3066100000 1.8549700000
C 0.6567160000 2.6613830000 0.4747380000
F -4.3187910000 1.2560570000 0.1465910000
F -5.1190950000 -0.4781760000 -1.1638110000
F -3.5762550000 1.0213950000 -2.0202670000
C 0.8651180000 3.0843930000 -0.8512090000
C 1.3305700000 3.3283340000 1.5138570000
C 1.7095900000 4.1581030000 -1.1248560000
H 0.3698190000 2.5640740000 -1.6658790000
C 2.1770320000 4.4026200000 1.2393440000
H 1.1735320000 3.0127810000 2.5426300000
C 2.3667470000 4.8198430000 -0.0811430000
H 1.8602260000 4.4773850000 -2.1515620000
H 2.6825890000 4.9154510000 2.0519740000
H 3.0254280000 5.6556130000 -0.2976810000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.388471 (Hartree/Particle)
Thermal correction to Energy= 0.413537
Thermal correction to Enthalpy= 0.414481
Thermal correction to Gibbs (Free) Energy= 0.331844
Sum of electronic and zero-point Energies= -1251.014393
Sum of electronic and thermal Energies= -1250.989327
Sum of electronic and thermal Enthalpies= -1250.988382
Sum of electronic and thermal (Free) Energies= -1251.071019

cPT

C -1.8204300000 0.1332630000 -0.7228520000
C -0.4540800000 0.0364980000 -0.7283710000
C 0.4868150000 -1.0109990000 -0.4722210000
C 1.7574810000 -0.3998250000 -0.1266040000
C 1.6875580000 0.9608990000 -0.4221590000
C 0.3699200000 1.3371500000 -0.9780210000
C 0.3902140000 -2.5070170000 -0.7408980000
C -2.8293030000 -0.6666610000 -0.0475660000
O 2.7685230000 -1.0752220000 0.3306930000
C -0.9382140000 -2.9684640000 -1.3683370000
C 0.6571840000 -3.3037270000 0.5669860000
C 1.5180260000 -2.8462070000 -1.7693430000
C -4.1521020000 -0.6639160000 -0.5416010000
C -2.5588880000 -1.3633670000 1.1495310000
C -3.5661430000 -2.0704890000 1.8009810000
H -1.5650050000 -1.3134660000 1.5811230000
C -4.8612550000 -2.0973330000 1.2723470000
H -3.3456110000 -2.5907650000 2.7280470000
C -5.1514920000 -1.3903810000 0.0993670000
H -4.3822130000 -0.1036750000 -1.4438200000
H -5.6450950000 -2.6490610000 1.7823620000
H -6.1590020000 -1.3969000000 -0.3051120000
B 4.1163730000 -0.3806410000 0.6240560000
F 4.5477350000 0.2081290000 -0.5733870000
F 4.9564250000 -1.3788240000 1.0660580000
F 3.8761200000 0.6035320000 1.5921370000
H -2.2150330000 1.0411920000 -1.1786780000
H 2.5041540000 1.6564020000 -0.2769310000
H 0.4527950000 1.4048750000 -2.0759010000
C -0.1884350000 2.6536320000 -0.4689590000
C -0.1683060000 2.9563440000 0.9013680000
C -0.7236030000 3.5912110000 -1.3616430000
H 1.3556130000 -2.3166540000 -2.7143020000
H 1.4801400000 -3.9205510000 -1.9755300000
H 2.5094300000 -2.6017240000 -1.3897120000
H 0.6732670000 -4.3717970000 0.3252400000
H -0.1379350000 -3.1389690000 1.3002670000
H 1.6151340000 -3.0326210000 1.0124520000
H -1.1990110000 -2.3763540000 -2.2516220000
H -1.7738580000 -2.9342870000 -0.6704750000
H -0.8248980000 -4.0083420000 -1.6901750000
C -0.6810590000 4.1673410000 1.3666690000
C -1.2200530000 5.0946420000 0.4685210000
C -1.2388040000 4.8052550000 -0.8973210000
H -0.7285100000 3.3774690000 -2.4281990000
H -1.6153450000 6.0386220000 0.8316480000
H -1.6453830000 5.5240760000 -1.6026710000
H 0.2576040000 2.2447540000 1.6044930000
H -0.6539970000 4.3901490000 2.4291540000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.390584 (Hartree/Particle)
Thermal correction to Energy= 0.415590
Thermal correction to Enthalpy= 0.416534
Thermal correction to Gibbs (Free) Energy= 0.333902
Sum of electronic and zero-point Energies= -1251.031121
Sum of electronic and thermal Energies= -1251.006115
Sum of electronic and thermal Enthalpies= -1251.005170
Sum of electronic and thermal (Free) Energies= -1251.087803

ccRT

C -1.1082310000 -1.9876200000 -1.3008500000
C 0.0012980000 -1.7155450000 -0.6516170000
C 1.1596530000 -1.4817450000 -0.0595630000
C 1.7307160000 -0.1116520000 -0.1869230000
C 0.9357080000 1.0983460000 -0.2032070000
C -0.3383210000 1.1958990000 0.2559750000
H 1.4633250000 1.9732720000 -0.5615150000
C 1.9763680000 -2.6113320000 0.6329590000
H -1.0111850000 -2.2476000000 -2.3564990000
C -2.4815850000 -1.9619560000 -0.7607840000
O 2.9919090000 -0.0533050000 -0.3052600000
C 1.0480630000 -3.8034310000 0.9385460000
C 2.5641400000 -2.0932730000 1.9652280000
C 3.1114300000 -3.0959960000 -0.3005130000
C -3.5674010000 -2.0086310000 -1.6520010000
C -2.7470170000 -1.9022560000 0.6200510000
C -4.0591430000 -1.8743250000 1.0904880000
H -1.9210090000 -1.9013870000 1.3257040000
C -5.1320600000 -1.9093340000 0.1926370000
H -4.2458660000 -1.8375570000 2.1600110000
C -4.8805120000 -1.9789600000 -1.1799870000
H -3.3782080000 -2.0627870000 -2.7208320000
H -6.1532840000 -1.8924180000 0.5612400000
H -5.7062310000 -2.0127210000 -1.8845840000
B 3.9200770000 1.2643230000 -0.3974100000
F 5.1849500000 0.7476630000 -0.4642040000
F 3.6594940000 1.9820210000 0.7563290000
F 3.5209880000 1.9323050000 -1.5443650000
H 3.8229770000 -2.3000140000 -0.5225890000
H 2.7030680000 -3.4728250000 -1.2446980000
H 3.6520090000 -3.9171380000 0.1841500000
H 1.7733260000 -1.7376430000 2.6359230000
H 3.2820590000 -1.2850400000 1.8141100000
H 3.0857620000 -2.9120290000 2.4722740000
H 0.2234900000 -3.5158510000 1.6000930000
H 1.6219910000 -4.5884440000 1.4413660000
H 0.6200010000 -4.2324100000 0.0277300000
C -1.1527490000 2.4044480000 0.2863110000
H -0.8195610000 0.3099740000 0.6601450000
C -0.6683380000 3.6713560000 -0.1057610000
C -2.4884500000 2.3001530000 0.7268500000
C -1.4968970000 4.7874380000 -0.0593200000
C -3.3173710000 3.4196770000 0.7686630000
C -2.8231180000 4.6663530000 0.3760050000
H -2.8739710000 1.3293840000 1.0261510000
H 0.3587550000 3.7854850000 -0.4356850000
H -4.3444720000 3.3206470000 1.1063660000
H -1.1098420000 5.7564810000 -0.3590480000
H -3.4647760000 5.5418620000 0.4103540000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.389028 (Hartree/Particle)
Thermal correction to Energy= 0.415269
Thermal correction to Enthalpy= 0.416214
Thermal correction to Gibbs (Free) Energy= 0.329371
Sum of electronic and zero-point Energies= -1251.039599
Sum of electronic and thermal Energies= -1251.013358
Sum of electronic and thermal Enthalpies= -1251.012414
Sum of electronic and thermal (Free) Energies= -1251.099257

ccTS

C -1.1890890000 -1.4571430000 -0.8942710000
C -0.0339160000 -0.9944110000 -0.3819910000
C -2.5114560000 -1.4673250000 -0.2745410000
H -1.1462470000 -1.8274880000 -1.9202720000
C 1.3135840000 -1.1672130000 -0.2550770000

C -3.6598770000 -1.4720960000 -1.0920860000
C -2.6809640000 -1.5445310000 1.1232670000
C 2.0212340000 0.0807530000 0.0060930000
C 2.0353090000 -2.5239660000 -0.2976820000
C -4.9338680000 -1.5158210000 -0.5308620000
H -3.5442340000 -1.4280720000 -2.1717080000
C -3.9566180000 -1.5965860000 1.6821440000
H -1.8080340000 -1.6090150000 1.7659960000
C 1.1293640000 1.1604870000 0.2021880000
O 3.3041920000 0.1485540000 -0.0298040000
C 1.0523270000 -3.6998280000 -0.4496240000
C 2.8450220000 -2.7229610000 1.0069340000
C 2.9935010000 -2.5193330000 -1.5191530000
C -5.0868180000 -1.5753090000 0.8585810000
H -5.8079330000 -1.5085580000 -1.1750210000
H -4.0700050000 -1.6701390000 2.7597570000
C -0.2137030000 0.8443610000 0.4865490000
H 1.4541760000 2.1760850000 0.0063990000
B 4.0834490000 1.4550220000 0.3477160000
H 0.4903870000 -3.6492710000 -1.3873080000
H 0.3357400000 -3.7456550000 0.3766250000
H 1.6173250000 -4.6373470000 -0.4550720000
H 3.3657140000 -3.6858290000 0.9655580000
H 2.1829190000 -2.7383750000 1.8801580000
H 3.5904080000 -1.9387760000 1.1470740000
H 2.4373260000 -2.3933950000 -2.4548090000
H 3.5151890000 -3.4816890000 -1.5645650000
H 3.7384180000 -1.7261010000 -1.4446130000
H -6.0797550000 -1.6212710000 1.2956710000
H -0.4233740000 0.2461100000 1.3738290000
C -1.2963840000 1.7710350000 0.1065700000
F 5.4095260000 1.0972140000 0.3039340000
F 3.6478220000 1.8260870000 1.6187160000
F 3.7379930000 2.4160720000 -0.6056420000
C -1.2253560000 2.5008200000 -1.0950100000
C -2.4027450000 1.9633770000 0.9520760000
C -2.2278890000 3.4072800000 -1.4329090000
H -0.3838910000 2.3482260000 -1.7650800000
C -3.4031690000 2.8754910000 0.6168040000
H -2.4695140000 1.4068410000 1.8819440000
C -3.3182080000 3.5981570000 -0.5764770000
H -2.1610250000 3.9646250000 -2.3623420000
H -4.2458590000 3.0233670000 1.2853150000
H -4.0982720000 4.3063940000 -0.8398880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.388032 (Hartree/Particle)
Thermal correction to Energy= 0.413111
Thermal correction to Enthalpy= 0.414055
Thermal correction to Gibbs (Free) Energy= 0.331448
Sum of electronic and zero-point Energies= -1251.010386
Sum of electronic and thermal Energies= -1250.985307
Sum of electronic and thermal Enthalpies= -1250.984363
Sum of electronic and thermal (Free) Energies= -1251.066970

ccPT

C 1.3354290000 -1.5655700000 0.0123300000
C 0.2155230000 -0.7958790000 -0.2028560000
C -1.1451200000 -1.1820290000 0.0629920000
C -2.0044920000 -0.0418720000 -0.1959530000
C -1.2188390000 1.0133630000 -0.6454470000
C 0.2169180000 0.6472870000 -0.7165620000
C -1.7571990000 -2.5151790000 0.4750550000
O -3.2960040000 -0.0605390000 -0.0323870000
C -0.7900990000 -3.6947800000 0.6994490000
C -2.7456560000 -2.9428270000 -0.6531120000
C -2.5420940000 -2.2972630000 1.8036800000
H -1.6033900000 1.9933860000 -0.8960580000
C 2.7341040000 -1.3232850000 -0.2942170000
H 1.1821440000 -2.4937280000 0.5426960000
C 3.6890830000 -2.0567420000 0.4516610000
C 5.0530300000 -1.8948060000 0.2358040000
C 5.5011300000 -1.0172740000 -0.7576760000
C 4.5746140000 -0.3103900000 -1.5311130000
C 3.2091650000 -0.4572160000 -1.3046700000
H 3.3439670000 -2.7455410000 1.2180310000
H 5.7661480000 -2.4559700000 0.8316520000
H 6.5649680000 -0.8963060000 -0.9382890000
H 4.9186910000 0.3525150000 -2.3189480000
H 2.5119800000 0.0705130000 -1.9410330000
B -4.1601060000 1.1584960000 -0.4100780000
F -5.4610100000 0.7812510000 -0.1540780000
F -3.9268680000 1.4291270000 -1.7673830000
F -3.7377710000 2.2373210000 0.3783450000
H -1.8610150000 -2.0163300000 2.6146610000
H -3.0242440000 -3.2408980000 2.0800500000
H -3.3099740000 -1.5312640000 1.7022750000
H -3.2359190000 -3.8736250000 -0.3488680000
H -2.2069470000 -3.1342700000 -1.5875630000
H -3.5128580000 -2.1902590000 -0.8312220000
H -0.1282370000 -3.5417230000 1.5581750000
H -0.1912280000 -3.9273880000 -0.1865860000
H -1.3901200000 -4.5822870000 0.9228280000
H 0.5254820000 0.6537070000 -1.7731080000
C 1.0722590000 1.6664270000 0.0379270000
C 1.1029970000 1.6858780000 1.4392690000
C 1.7657670000 2.6579910000 -0.6672910000
C 1.8316190000 2.6626720000 2.1186730000
C 2.5287140000 3.6435850000 1.4065310000
C 2.4904120000 3.6415640000 0.0107840000
H 0.5529290000 0.9372920000 2.0026190000
H 1.8466970000 2.6635670000 3.2045360000
H 3.0908720000 4.4066190000 1.9364580000
H 1.7348730000 2.6685640000 -1.7544340000
H 3.0209820000 4.4040280000 -0.5518950000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.391467 (Hartree/Particle)
Thermal correction to Energy= 0.416308
Thermal correction to Enthalpy= 0.417252
Thermal correction to Gibbs (Free) Energy= 0.334575
Sum of electronic and zero-point Energies= -1251.037637
Sum of electronic and thermal Energies= -1251.012796
Sum of electronic and thermal Enthalpies= -1251.011852
Sum of electronic and thermal (Free) Energies= -1251.094529

RB3LYP/6-31G(d)/SCRF=(PCM, CH_3OH, ε = 32.613)

1a

cRT

C 3.5799610000 -0.1435420000 -0.1109010000
C 2.3631590000 0.2904170000 -0.2722530000
C 1.1494650000 0.8191920000 -0.4048900000
C -0.0382200000 0.0055950000 -0.1601360000
C -0.0310450000 -1.4577660000 -0.1290650000
C 0.7498530000 -2.2145720000 -0.9136500000
H -0.7682640000 -1.9105990000 0.5248280000
C 0.9447540000 2.2938260000 -0.7025760000
O -1.1140790000 0.6541910000 0.0462610000
H 1.9024150000 2.7746490000 -0.9097680000
H 0.4749040000 2.7953420000 0.1498590000
H 0.2854120000 2.4259250000 -1.5667830000
B -2.5617030000 0.0446240000 0.2504460000
F -3.3599290000 1.1543350000 0.3736230000
F -2.5191740000 -0.7174020000 1.4047600000
F -2.8375340000 -0.7050160000 -0.8725110000
C 4.3487100000 -0.1142220000 1.1896340000
H 4.0872800000 -0.5737750000 -0.9763640000
H 3.7638780000 0.3350780000 1.9952500000
H 5.2743210000 0.4584060000 1.0611250000
H 4.6301480000 -1.1325120000 1.4812440000
H 1.4369580000 -1.7923160000 -1.6384150000
H 0.6840130000 -3.2976630000 -0.8731190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170985 (Hartree/Particle)
Thermal correction to Energy= 0.185548
Thermal correction to Enthalpy= 0.186492
Thermal correction to Gibbs (Free) Energy= 0.128679
Sum of electronic and zero-point Energies= -710.438688
Sum of electronic and thermal Energies= -710.424125
Sum of electronic and thermal Enthalpies= -710.423181
Sum of electronic and thermal (Free) Energies= -710.480994

cTS

C 3.4816420000 -0.3955550000 -0.0737260000

C 2.2076000000 -0.1007830000 -0.2717630000
C 1.1114210000 0.7033840000 -0.3135260000
C -0.1439770000 0.0329290000 -0.0920530000
C -0.0082010000 -1.3840690000 -0.0568670000
C 1.1114130000 -1.9188110000 -0.6645630000
C 1.1556190000 2.1739560000 -0.6328890000
O -1.2179130000 0.7228340000 0.1119620000
H 0.7421240000 2.7376800000 0.2117340000
H 0.5359810000 2.4020610000 -1.5069690000
H 2.1760830000 2.5139270000 -0.8152870000
H -0.6691260000 -1.9748180000 0.5678530000
B -2.6031580000 0.0528900000 0.1766340000
F -2.7769240000 -0.6804310000 -0.9894870000
F -3.4998680000 1.0966500000 0.2824660000
F -2.6263690000 -0.7735070000 1.2982770000
H 3.9434660000 -1.1688470000 -0.6853090000
C 4.3380080000 0.2275360000 0.9966430000
H 3.8073560000 1.0091770000 1.5443310000
H 5.2380870000 0.6563660000 0.5395060000
H 4.6710330000 -0.5393550000 1.7066430000
H 1.4904950000 -2.8908240000 -0.3545180000
H 1.4308940000 -1.6084100000 -1.6556900000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170263 (Hartree/Particle)
Thermal correction to Energy= 0.183890
Thermal correction to Enthalpy= 0.184834
Thermal correction to Gibbs (Free) Energy= 0.129087
Sum of electronic and zero-point Energies= -710.419132
Sum of electronic and thermal Energies= -710.405505
Sum of electronic and thermal Enthalpies= -710.404561
Sum of electronic and thermal (Free) Energies= -710.460308

cPT

C 3.4496570000 -0.5202170000 0.0000000000
C 2.0861000000 -0.5472210000 0.0000000000
C 1.1360800000 0.5204090000 0.0000000000
C -0.1921200000 -0.0245920000 0.0000000000
C -0.0979030000 -1.4124930000 0.0000000000
C 1.3119780000 -1.8499600000 0.0000000000
C 1.3668140000 1.9889750000 0.0000000000
O -1.2554420000 0.7484460000 0.0000000000
H 1.9412670000 2.2957180000 0.8821940000
H 0.4120990000 2.5170090000 0.0000000000
H 1.9412670000 2.2957180000 -0.8821930000
H -0.9442860000 -2.0860870000 0.0000000000
B -2.6379560000 0.1427120000 0.0000000000
F -2.7882520000 -0.6459730000 -1.1453250000
F -3.5202490000 1.2127660000 0.0000000000
F -2.7882520000 -0.6459720000 1.1453250000
H 3.9363210000 -1.4957450000 0.0000000000
C 4.3898020000 0.6302400000 0.0000000000
H 3.9154680000 1.6089880000 0.0000000000
H 5.0499970000 0.5536360000 -0.8752260000
H 5.0499970000 0.5536360000 0.8752270000
H 1.5497590000 -2.4711160000 0.8771770000
H 1.5497600000 -2.4711160000 -0.8771770000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172598 (Hartree/Particle)
Thermal correction to Energy= 0.186094
Thermal correction to Enthalpy= 0.187038
Thermal correction to Gibbs (Free) Energy= 0.130334
Sum of electronic and zero-point Energies= -710.469556
Sum of electronic and thermal Energies= -710.456060
Sum of electronic and thermal Enthalpies= -710.455116
Sum of electronic and thermal (Free) Energies= -710.511821

ccRT

C -3.5039770000 0.1399970000 0.6817300000
C -2.3080570000 0.4923410000 0.3070490000
C -1.1041210000 0.9431660000 -0.0364850000
C 0.0591790000 0.0648030000 0.0440540000
C -0.0264230000 -1.3937460000 0.1352770000
C -0.9617900000 -2.1250380000 -0.4876790000
H 0.7776050000 -1.8707010000 0.6850870000
C -0.8669460000 2.3951630000 -0.4103980000
O 1.1896530000 0.6502420000 0.0497380000
H -1.8165140000 2.9291680000 -0.4763840000
H -0.3499930000 2.4671280000 -1.3729950000
H -0.2370920000 2.8856610000 0.3390890000
B 2.6134030000 -0.0438770000 0.0415050000
F 3.4840780000 1.0158850000 -0.0103500000
F 2.6576820000 -0.8425670000 -1.0807460000
F 2.7164700000 -0.7669590000 1.2168460000
C -4.5698660000 -0.4529020000 -0.2084340000
H -3.7568830000 0.2708910000 1.7360950000
H -4.8362900000 -1.4562480000 0.1437390000
H -4.2422380000 -0.5184180000 -1.2484930000
H -5.4758100000 0.1619260000 -0.1633630000
H -1.7264410000 -1.6836450000 -1.1171640000
H -0.9526370000 -3.2082460000 -0.4134730000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171022 (Hartree/Particle)
Thermal correction to Energy= 0.185551
Thermal correction to Enthalpy= 0.186495
Thermal correction to Gibbs (Free) Energy= 0.128904
Sum of electronic and zero-point Energies= -710.438696
Sum of electronic and thermal Energies= -710.424168
Sum of electronic and thermal Enthalpies= -710.423224
Sum of electronic and thermal (Free) Energies= -710.480815

ccTS

C 3.4493840000 0.2055170000 -0.5101640000
C 2.1817970000 0.3034620000 -0.1448910000
C 1.0051980000 0.9737020000 0.0093840000
C -0.1751790000 0.1539260000 -0.0477670000
C 0.1295540000 -1.2371870000 -0.0757610000
C 1.3640660000 -1.6161410000 0.4155080000
H -0.5176280000 -1.9219420000 -0.6129460000
C 0.9068480000 2.4509630000 0.2788520000
O -1.3426870000 0.7022190000 -0.1362970000
H 1.8912620000 2.9203880000 0.3005190000
H 0.3931590000 2.6424290000 1.2275030000
H 0.3081850000 2.9197600000 -0.5111760000
B -2.6314410000 -0.1334490000 -0.0275980000
F -3.6573830000 0.7894920000 -0.0400050000
F -2.5758160000 -0.8499270000 1.1606920000
F -2.6812280000 -0.9875060000 -1.1274150000
C 4.5234130000 -0.6511070000 0.0928320000
H 3.7356950000 0.7936280000 -1.3861040000
H 4.9096430000 -1.3580120000 -0.6511060000
H 4.1747120000 -1.2072980000 0.9653340000
H 5.3649970000 -0.0169260000 0.3968560000
H 1.7392620000 -1.2409010000 1.3634880000
H 1.8187710000 -2.5489860000 0.0886070000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170121 (Hartree/Particle)
Thermal correction to Energy= 0.183744
Thermal correction to Enthalpy= 0.184688
Thermal correction to Gibbs (Free) Energy= 0.128974
Sum of electronic and zero-point Energies= -710.418391
Sum of electronic and thermal Energies= -710.404768
Sum of electronic and thermal Enthalpies= -710.403824
Sum of electronic and thermal (Free) Energies= -710.459538

ccPT

C 3.4234670000 0.3354250000 0.0000010000
C 2.1133840000 -0.0337570000 0.0000000000
C 1.0046240000 0.8636140000 0.0000000000
C -0.2194000000 0.1160700000 -0.0000010000
C 0.1004010000 -1.2349770000 -0.0000010000
C 1.5689520000 -1.4449590000 -0.0000010000
C 1.0119300000 2.3444270000 0.0000000000
O -1.3883140000 0.7193140000 -0.0000020000
H 2.0119000000 2.7788290000 0.0000010000
H 0.4585020000 2.7092180000 0.8750840000
H 0.4585050000 2.7092190000 -0.8750860000
H -0.6230650000 -2.0392840000 -0.0000020000
B -2.6609430000 -0.0913030000 0.0000000000
F -3.6968210000 0.8313960000 0.0000000000
F -2.6890080000 -0.8938940000 1.1454230000
F -2.6890100000 -0.8938960000 -1.1454200000
C 4.5914920000 -0.5818580000 0.0000010000

H 3.6563060000 1.3984240000 0.0000010000
H 4.3142440000 -1.6377090000 0.0000010000
H 5.2217480000 -0.3760860000 0.8761500000
H 5.2217490000 -0.3760850000 -0.8761470000
H 1.8978940000 -2.0204500000 0.8777080000
H 1.8978940000 -2.0204500000 -0.8777100000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172643 (Hartree/Particle)
Thermal correction to Energy= 0.186144
Thermal correction to Enthalpy= 0.187088
Thermal correction to Gibbs (Free) Energy= 0.130149
Sum of electronic and zero-point Energies= -710.474481
Sum of electronic and thermal Energies= -710.460980
Sum of electronic and thermal Enthalpies= -710.460036
Sum of electronic and thermal (Free) Energies= -710.516974

RM06-2X/6-31G(d)

6d

cRT

C -1.8816520000 -1.3398030000 0.8416050000
C -1.2835520000 -0.1754320000 0.8773080000
C -0.7427370000 1.0259960000 0.8822090000
C 0.3862380000 1.2727730000 -0.0501760000
C 1.4064650000 0.2727940000 -0.3200470000
C 1.6860650000 -0.7235630000 0.5433520000
H 1.9790710000 0.4305950000 -1.2262370000
C -1.2829960000 2.1838330000 1.7418090000
H -1.5401470000 -2.1153050000 1.5276760000
C -2.9967560000 -1.6940650000 -0.0584110000
O 0.4180700000 2.3971410000 -0.5994720000
C -2.2278740000 1.6200070000 2.8072330000
C -2.0625290000 3.1815260000 0.8680210000
C -0.1052770000 2.8886880000 2.4325590000
C -3.5419050000 -2.9791660000 0.0050830000
C -3.5255850000 -0.7738170000 -0.9716560000
C -4.5769160000 -1.1365720000 -1.8019570000
H -3.1034550000 0.2263470000 -1.0278280000
C -5.1165800000 -2.4213450000 -1.7327530000
H -4.9778480000 -0.4156090000 -2.5073580000
C -4.5966020000 -3.3410900000 -0.8274640000
H -3.1349440000 -3.6974980000 0.7119990000
H -5.9387200000 -2.7019060000 -2.3833290000
H -5.0106690000 -4.3426920000 -0.7681320000
B 1.6737360000 2.9554900000 -1.4821610000
F 1.2978070000 4.2261910000 -1.7536850000
F 1.7378800000 2.1250100000 -2.5718750000
F 2.7377920000 2.8248000000 -0.6339090000
H 0.5906870000 3.3255050000 1.7113580000
H 0.4462580000 2.1904070000 3.0720820000
H -0.4854750000 3.6973140000 3.0653330000
H -2.8871070000 2.6768420000 0.3528500000
H -1.4231170000 3.6592850000 0.1250300000
H -2.4909700000 3.9591170000 1.5102200000
H -3.0951450000 1.1308370000 2.3522230000
H -2.5885480000 2.4361650000 3.4408360000
H -1.7193720000 0.8893690000 3.4453190000
C 2.7230580000 -1.7391110000 0.3781280000
H 1.1157590000 -0.7894210000 1.4675830000
C 3.5995210000 -1.7570720000 -0.7181540000
C 2.8412110000 -2.7368760000 1.3552050000
C 4.5595370000 -2.7518270000 -0.8300250000
C 3.8018190000 -3.7346810000 1.2413270000
C 4.6623750000 -3.7433040000 0.1470030000
H 2.1690790000 -2.7246750000 2.2095920000
H 3.5366370000 -0.9858080000 -1.4789090000
H 3.8807780000 -4.5015020000 2.0050650000
H 5.2343230000 -2.7546280000 -1.6797800000
H 5.4164020000 -4.5186880000 0.0550070000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395314 (Hartree/Particle)
Thermal correction to Energy= 0.421280
Thermal correction to Enthalpy= 0.422224
Thermal correction to Gibbs (Free) Energy= 0.334545
Sum of electronic and zero-point Energies= -1250.432217
Sum of electronic and thermal Energies= -1250.406251
Sum of electronic and thermal Enthalpies= -1250.405307
Sum of electronic and thermal (Free) Energies= -1250.492986

cTS

C 1.7617170000 -0.2615160000 0.7149780000
C 0.4354520000 -0.3518110000 0.7114690000
C 2.6678090000 -1.1091080000 -0.0695370000
H 2.2234780000 0.5419430000 1.2892280000
C -0.7417490000 -1.0287320000 0.5932830000
C 4.0382990000 -1.0837410000 0.2164210000
C 2.2023930000 -1.9385460000 -1.0995910000
C -1.7903800000 -0.2101350000 0.0192550000
C -0.9985010000 -2.4372150000 1.1164440000
C 4.9209400000 -1.8930380000 -0.4898250000
H 4.4066520000 -0.4319490000 1.0041130000
C 3.0861980000 -2.7436460000 -1.8051030000
H 1.1461340000 -1.9294630000 -1.3544300000
C -1.3950620000 1.1532680000 -0.0481540000
O -2.8866840000 -0.7055640000 -0.4029930000
C 0.2307850000 -2.9931940000 1.8398590000
C -1.3423770000 -3.3486580000 -0.0779380000
C -2.1871230000 -2.3972260000 2.0930350000
C 4.4472060000 -2.7270000000 -1.4995220000
H 5.9800010000 -1.8700060000 -0.2536600000
H 2.7149390000 -3.3788840000 -2.6029720000
C -0.3292710000 1.5274600000 0.7754090000
H -1.8365480000 1.8169050000 -0.7838840000
B -4.0128260000 0.2916200000 -0.8820080000
H 0.5049980000 -2.3718520000 2.6986130000
H 1.0968940000 -3.0620720000 1.1741140000
H 0.0045830000 -3.9992140000 2.2067270000
H -1.5850300000 -4.3474150000 0.3007360000
H -0.4876890000 -3.4458420000 -0.7553410000
H -2.2004370000 -2.9695050000 -0.6357900000
H -1.9661330000 -1.7480690000 2.9472090000
H -2.3727120000 -3.4065270000 2.4749980000
H -3.0961220000 -2.0403410000 1.6045330000
H 5.1364420000 -3.3556990000 -2.0540230000
H -0.3837420000 1.2839620000 1.8371230000
C 0.5463850000 2.6692120000 0.4685170000
F -4.1664430000 1.1883170000 0.1549660000
F -5.0960540000 -0.4936810000 -1.1154560000
F -3.5016130000 0.9071990000 -2.0103940000
C 0.7822970000 3.0596700000 -0.8556080000
C 1.1796990000 3.3578250000 1.5091290000
C 1.6150020000 4.1367880000 -1.1284560000
H 0.3183510000 2.5063930000 -1.6676930000
C 2.0158000000 4.4349120000 1.2352170000
H 1.0000720000 3.0544780000 2.5379660000
C 2.2312130000 4.8262130000 -0.0838920000
H 1.7912000000 4.4363430000 -2.1563740000
H 2.4950670000 4.9698970000 2.0486270000
H 2.8838180000 5.6661290000 -0.3002320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394686 (Hartree/Particle)
Thermal correction to Energy= 0.419346
Thermal correction to Enthalpy= 0.420290
Thermal correction to Gibbs (Free) Energy= 0.338654
Sum of electronic and zero-point Energies= -1250.408666
Sum of electronic and thermal Energies= -1250.384006
Sum of electronic and thermal Enthalpies= -1250.383062
Sum of electronic and thermal (Free) Energies= -1250.464698

cPT

C -1.6335100000 0.9427520000 -0.7090700000
C -0.4489050000 0.3080290000 -0.8757610000
C -0.0456990000 -1.0505790000 -0.6194450000
C 1.3681320000 -1.0509350000 -0.3474320000
C 1.8787000000 0.1579350000 -0.8019530000
C 0.8219390000 1.0992820000 -1.2288070000
C -0.7885130000 -2.3506240000 -0.8302210000
C -2.7833470000 0.4637490000 0.0510500000
O 2.0170400000 -2.0535690000 0.1546010000
C -2.2113730000 -2.2182280000 -1.3883600000
C -0.8064810000 -3.1830180000 0.4702780000
C 0.0514120000 -3.1193980000 -1.8907470000
C -4.0887710000 0.7421660000 -0.3779180000

C -2.5899900000 -0.2430490000 1.2466170000
C -3.6816610000 -0.7150020000 1.9668160000
H -1.5791890000 -0.3923030000 1.6163180000
C -4.9744110000 -0.4812070000 1.5030930000
H -3.5230320000 -1.2577290000 2.8933070000
C -5.1761100000 0.2532950000 0.3334090000
H -4.2420750000 1.3136990000 -1.2891490000
H -5.8269050000 -0.8528510000 2.0625800000
H -6.1839830000 0.4480710000 -0.0185990000
B 3.4250040000 -1.7156020000 0.7096370000
F 4.2229250000 -1.4005690000 -0.3805860000
F 3.8313560000 -2.8217830000 1.3904250000
F 3.2484900000 -0.5936670000 1.5192360000
H -1.6885870000 1.9723060000 -1.0654160000
H 2.9385650000 0.3848440000 -0.8251980000
H 0.8288340000 1.2023190000 -2.3254460000
C 0.9638460000 2.4684260000 -0.5987930000
C 1.4783410000 2.5841300000 0.6962120000
C 0.5722390000 3.6158520000 -1.2889040000
H 0.0675900000 -2.5741900000 -2.8402170000
H -0.4246860000 -4.0893480000 -2.0623030000
H 1.0741470000 -3.2866290000 -1.5513190000
H -1.2303670000 -4.1659000000 0.2389610000
H -1.4429270000 -2.7118260000 1.2244570000
H 0.1988560000 -3.3164320000 0.8724690000
H -2.2650500000 -1.4809600000 -2.1965140000
H -2.9426940000 -1.9535120000 -0.6240130000
H -2.5061940000 -3.1879060000 -1.8012030000
C 1.5877640000 3.8366540000 1.2912330000
C 1.1825480000 4.9790150000 0.6032860000
C 0.6762720000 4.8681650000 -0.6887750000
H 0.1925570000 3.5295270000 -2.3050210000
H 1.2701860000 5.9547780000 1.0705490000
H 0.3715630000 5.7560730000 -1.2339020000
H 1.8164800000 1.6937660000 1.2248270000
H 1.9960960000 3.9204690000 2.2932890000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397426 (Hartree/Particle)
Thermal correction to Energy= 0.421728
Thermal correction to Enthalpy= 0.422672
Thermal correction to Gibbs (Free) Energy= 0.342545
Sum of electronic and zero-point Energies= -1250.428834
Sum of electronic and thermal Energies= -1250.404532
Sum of electronic and thermal Enthalpies= -1250.403588
Sum of electronic and thermal (Free) Energies= -1250.483715

ccRT

C -0.8105930000 -1.9864470000 -1.4398500000
C 0.3255690000 -1.6786320000 -0.8672160000
C 1.4531000000 -1.3353680000 -0.2764820000
C 1.7853060000 0.1144820000 -0.2436230000
C 0.7627230000 1.1498660000 -0.2609110000
C -0.4862870000 0.9474210000 0.2005550000
H 1.0913610000 2.1149120000 -0.6298380000
C 2.4418270000 -2.3691340000 0.2911840000
H -0.8296180000 -2.1421220000 -2.5177710000
C -2.0957910000 -2.0588920000 -0.7136110000
O 3.0021420000 0.4075190000 -0.2276150000
C 1.7659410000 -3.7435800000 0.3365140000
C 2.8396920000 -1.9620190000 1.7184220000
C 3.6895180000 -2.4661800000 -0.6039040000
C -3.2924180000 -1.8720420000 -1.4126340000
C -2.1439380000 -2.2684870000 0.6708430000
C -3.3615930000 -2.2722750000 1.3418640000
H -1.2178480000 -2.4332000000 1.2166900000
C -4.5490240000 -2.0694820000 0.6390090000
H -3.3845970000 -2.4378190000 2.4143730000
C -4.5103690000 -1.8718280000 -0.7395240000
H -3.2634560000 -1.7103330000 -2.4866360000
H -5.4995510000 -2.0741210000 1.1628070000
H -5.4307620000 -1.7171870000 -1.2937120000
B 3.5771770000 1.9290370000 -0.0601990000
F 4.9108620000 1.7247850000 0.0393200000
F 2.9668330000 2.3875820000 1.0732560000
F 3.1715090000 2.5772210000 -1.1982980000
H 4.2520840000 -1.5323010000 -0.6206370000
H 3.4072470000 -2.7272380000 -1.6292240000
H 4.3420960000 -3.2580460000 -0.2198650000
H 1.9571280000 -1.8929300000 2.3644730000
H 3.3651300000 -1.0045780000 1.7383300000
H 3.5065870000 -2.7220780000 2.1385870000
H 0.8666660000 -3.7307650000 0.9622660000
H 2.4616980000 -4.4752200000 0.7585320000
H 1.4790380000 -4.0827820000 -0.6636720000
C -1.5692790000 1.9279900000 0.2060650000
H -0.7505880000 -0.0239800000 0.6112630000
C -1.3549500000 3.2965180000 -0.0159540000
C -2.8752560000 1.4657800000 0.4211310000
C -2.4282070000 4.1759660000 -0.0341160000
C -3.9487100000 2.3479790000 0.3915490000
C -3.7266730000 3.7037680000 0.1639580000
H -3.0437040000 0.4058780000 0.5985510000
H -0.3452980000 3.6725900000 -0.1500940000
H -4.9563420000 1.9765010000 0.5494480000
H -2.2540770000 5.2345180000 -0.1977790000
H -4.5625930000 4.3962650000 0.1477220000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395712 (Hartree/Particle)
Thermal correction to Energy= 0.421340
Thermal correction to Enthalpy= 0.422284
Thermal correction to Gibbs (Free) Energy= 0.337928
Sum of electronic and zero-point Energies= -1250.436454
Sum of electronic and thermal Energies= -1250.410826
Sum of electronic and thermal Enthalpies= -1250.409882
Sum of electronic and thermal (Free) Energies= -1250.494238

ccTS

C 1.0305820000 1.5194700000 -0.9472530000
C -0.1026980000 1.0543570000 -0.4160890000
C 2.3462180000 1.4635610000 -0.3004680000
H 0.9868520000 1.9017250000 -1.9679960000
C -1.4568320000 1.1292250000 -0.2727430000
C 3.4828770000 1.1281040000 -1.0469320000
C 2.4800600000 1.7270970000 1.0688310000
C -2.0602290000 -0.1625850000 -0.0197280000
C -2.2646500000 2.4196730000 -0.2907740000
C 4.7209030000 1.0198200000 -0.4269950000
H 3.3818370000 0.9212200000 -2.1087940000
C 3.7242450000 1.6334350000 1.6843230000
H 1.6057800000 2.0337870000 1.6380900000
C -1.0633120000 -1.1550160000 0.1696190000
O -3.3212340000 -0.3455360000 -0.0525360000
C -1.3597410000 3.6465150000 -0.4330400000
C -3.0721410000 2.5362630000 1.0129310000
C -3.2219150000 2.3575290000 -1.4977600000
C 4.8437570000 1.2698920000 0.9398240000
H 5.5928420000 0.7386190000 -1.0088920000
H 3.8204760000 1.8499090000 2.7437620000
C 0.2183740000 -0.6935670000 0.4952970000
H -1.2714440000 -2.1933980000 -0.0657850000
B -3.8724240000 -1.7674900000 0.3580050000
H -0.7998200000 3.6300020000 -1.3735500000
H -0.6412610000 3.7171410000 0.3904520000
H -1.9777030000 4.5496420000 -0.4249760000
H -3.6638320000 3.4574060000 0.9892860000
H -2.4039180000 2.5855560000 1.8794950000
H -3.7526160000 1.6921340000 1.1397090000
H -2.6611620000 2.2822440000 -2.4353970000
H -3.8142590000 3.2783310000 -1.5280560000
H -3.9014800000 1.5069840000 -1.4225180000
H 5.8140760000 1.1938000000 1.4204040000
H 0.3422110000 -0.0646880000 1.3801210000
C 1.4165470000 -1.4680820000 0.1234430000
F -5.2219390000 -1.6177160000 0.3966720000
F -3.2899590000 -2.0416690000 1.5780540000
F -3.4230710000 -2.6320400000 -0.6229900000
C 1.4905720000 -2.0752480000 -1.1353670000
C 2.5019370000 -1.5674050000 0.9989270000
C 2.6315560000 -2.7746700000 -1.5091680000
H 0.6544060000 -1.9757290000 -1.8234600000
C 3.6418850000 -2.2700690000 0.6266420000
H 2.4505390000 -1.0871700000 1.9719070000
C 3.7085290000 -2.8710420000 -0.6286090000
H 2.6846060000 -3.2405380000 -2.4879390000
H 4.4797980000 -2.3425650000 1.3126100000
H 4.6016220000 -3.4133870000 -0.9233080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394348 (Hartree/Particle)
Thermal correction to Energy= 0.418871
Thermal correction to Enthalpy= 0.419815
Thermal correction to Gibbs (Free) Energy= 0.339541
Sum of electronic and zero-point Energies= -1250.408429
Sum of electronic and thermal Energies= -1250.383906
Sum of electronic and thermal Enthalpies= -1250.382962
Sum of electronic and thermal (Free) Energies= -1250.463236

ccPT

C -1.2238190000 1.6351930000 -0.0019700000
C -0.1360180000 0.8565930000 -0.2672820000
C 1.2373420000 1.1755700000 0.0167380000
C 2.0408360000 -0.0061160000 -0.1652700000
C 1.2110580000 -1.0255060000 -0.6167250000
C -0.1926720000 -0.5832070000 -0.7687640000
C 1.8969400000 2.4858540000 0.3806620000
O 3.3177830000 -0.0549420000 0.0508400000
C 0.9804920000 3.7082900000 0.5047010000
C 2.9284810000 2.7934920000 -0.7342980000
C 2.6299820000 2.2982820000 1.7300490000
H 1.5473980000 -2.0350390000 -0.8185800000
C -2.6264730000 1.3561990000 -0.2731730000
H -1.0621180000 2.5540030000 0.5461820000
C -3.5806850000 1.9252740000 0.5891280000
C -4.9348710000 1.6860030000 0.4096030000
C -5.3641530000 0.8998290000 -0.6591350000
C -4.4343690000 0.3623560000 -1.5467810000
C -3.0774070000 0.5863370000 -1.3575030000
H -3.2434160000 2.5432160000 1.4170940000
H -5.6569320000 2.1175550000 1.0948590000
H -6.4239110000 0.7194210000 -0.8087730000
H -4.7683990000 -0.2283180000 -2.3935660000
H -2.3660350000 0.1997270000 -2.0777850000
B 4.0362670000 -1.3798630000 -0.3069710000
F 5.3556570000 -1.1637560000 -0.0429160000
F 3.7622540000 -1.6140380000 -1.6480650000
F 3.4586820000 -2.3642420000 0.4819230000
H 1.9140180000 2.0771740000 2.5287450000
H 3.1372880000 3.2362850000 1.9785990000
H 3.3688560000 1.4990900000 1.6782430000
H 3.4688190000 3.7046580000 -0.4577720000
H 2.4204000000 2.9743260000 -1.6871490000
H 3.6468680000 1.9831700000 -0.8557330000
H 0.3282790000 3.6544580000 1.3821240000
H 0.3743970000 3.8705600000 -0.3920030000
H 1.6143290000 4.5902360000 0.6372670000
H -0.4462470000 -0.5931100000 -1.8393230000
C -1.1353910000 -1.5154610000 -0.0264550000
C -1.1166710000 -1.5517890000 1.3694120000
C -1.9765940000 -2.3831860000 -0.7205860000
C -1.9461640000 -2.4271930000 2.0597050000
C -2.7940160000 -3.2848590000 1.3602760000
C -2.8049090000 -3.2648210000 -0.0307320000
H -0.4461040000 -0.8898980000 1.9130940000
H -1.9256030000 -2.4468140000 3.1446830000
H -3.4393010000 -3.9707560000 1.8998140000
H -1.9843190000 -2.3700550000 -1.8083360000
H -3.4567100000 -3.9355030000 -0.5816250000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397698 (Hartree/Particle)
Thermal correction to Energy= 0.422110
Thermal correction to Enthalpy= 0.423054
Thermal correction to Gibbs (Free) Energy= 0.341495
Sum of electronic and zero-point Energies= -1250.433584
Sum of electronic and thermal Energies= -1250.409172
Sum of electronic and thermal Enthalpies= -1250.408228
Sum of electronic and thermal (Free) Energies= -1250.489787

RM06-2X/6-31G(d)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)

6d

cRT

C -1.8401210000 -1.2974450000 0.8625290000
C -1.2553650000 -0.1270770000 0.8739900000
C -0.7259520000 1.0825010000 0.8617570000
C 0.4201330000 1.3044860000 -0.0429860000
C 1.4106290000 0.2853730000 -0.3094670000
C 1.6630480000 -0.7167080000 0.5629760000
H 1.9918460000 0.4170220000 -1.2144300000
C -1.3057600000 2.2498010000 1.6832210000
H -1.4952250000 -2.0470500000 1.5752240000
C -2.9384250000 -1.6905540000 -0.0426430000
O 0.4884810000 2.4432670000 -0.5879860000
C -2.2854330000 1.6931130000 2.7211930000
C -2.0626600000 3.2297620000 0.7708160000
C -0.1619840000 2.9728780000 2.4105620000
C -3.4339740000 -2.9964880000 0.0194750000
C -3.4989920000 -0.7892250000 -0.9568320000
C -4.5333100000 -1.1914230000 -1.7917970000
H -3.1182110000 0.2276590000 -1.0094230000
C -5.0232460000 -2.4969410000 -1.7253360000
H -4.9607840000 -0.4853390000 -2.4966530000
C -4.4713910000 -3.3975110000 -0.8181370000
H -3.0020450000 -3.6986490000 0.7273530000
H -5.8322180000 -2.8080800000 -2.3785020000
H -4.8473130000 -4.4140890000 -0.7606850000
B 1.6999720000 2.9619970000 -1.4459650000
F 1.3655670000 4.2578550000 -1.7246260000
F 1.7653630000 2.1660300000 -2.5701960000
F 2.8106000000 2.8380800000 -0.6459300000
H 0.5550150000 3.4095360000 1.7100710000
H 0.3722920000 2.2858420000 3.0756620000
H -0.5742900000 3.7838420000 3.0196560000
H -2.8594100000 2.7113890000 0.2267170000
H -1.4002230000 3.7106610000 0.0501560000
H -2.5245060000 4.0071610000 1.3893430000
H -3.1342280000 1.1964600000 2.2400790000
H -2.6704240000 2.5155970000 3.3316960000
H -1.7963020000 0.9713970000 3.3837090000
C 2.6515180000 -1.7747110000 0.3967590000
H 1.1123130000 -0.7429350000 1.5004440000
C 3.4254420000 -1.9174670000 -0.7672120000
C 2.8227020000 -2.6916860000 1.4448830000
C 4.3453460000 -2.9501010000 -0.8718220000
C 3.7454400000 -3.7257430000 1.3385010000
C 4.5077250000 -3.8553030000 0.1797710000
H 2.2250620000 -2.5860540000 2.3463600000
H 3.3070630000 -1.2223510000 -1.5920450000
H 3.8695080000 -4.4280990000 2.1559620000
H 4.9389810000 -3.0536200000 -1.7739930000
H 5.2293920000 -4.6612860000 0.0925700000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395118 (Hartree/Particle)
Thermal correction to Energy= 0.420927
Thermal correction to Enthalpy= 0.421871
Thermal correction to Gibbs (Free) Energy= 0.335452
Sum of electronic and zero-point Energies= -1250.448497
Sum of electronic and thermal Energies= -1250.422688
Sum of electronic and thermal Enthalpies= -1250.421744
Sum of electronic and thermal (Free) Energies= -1250.508164

cTS

C 1.7608630000 -0.3263540000 0.7234250000
C 0.4360040000 -0.3983270000 0.7031780000
C 2.6629680000 -1.1716920000 -0.0679680000
H 2.2261370000 0.4513450000 1.3293520000
C -0.7690600000 -1.0164020000 0.5810120000
C 4.0332990000 -1.1510230000 0.2220870000
C 2.1935190000 -1.9958400000 -1.1011770000
C -1.7770530000 -0.1544090000 0.0047900000
C -1.0769870000 -2.4149920000 1.1095640000
C 4.9136130000 -1.9613340000 -0.4871280000
H 4.4025060000 -0.5040860000 1.0129160000
C 3.0754880000 -2.8014080000 -1.8091450000
H 1.1377310000 -1.9834570000 -1.3581670000
C -1.3593450000 1.1919570000 -0.0515490000
O -2.8959690000 -0.6257200000 -0.4337220000
C 0.1344200000 -3.0063630000 1.8358380000
C -1.4431690000 -3.3230560000 -0.0800010000
C -2.2608040000 -2.3338550000 2.0882310000
C 4.4369320000 -2.7895600000 -1.5012200000

H 5.9723680000 -1.9433880000 -0.2499310000
H 2.7034830000 -3.4332100000 -2.6091500000
C -0.2800340000 1.5468970000 0.7654980000
H -1.7920000000 1.8762500000 -0.7729380000
B -4.0039160000 0.3379560000 -0.8624630000
H 0.4263090000 -2.3910090000 2.6926500000
H 0.9971950000 -3.1016850000 1.1687190000
H -0.1228650000 -4.0046610000 2.2027680000
H -1.7032380000 -4.3154810000 0.3032250000
H -0.5944390000 -3.4367990000 -0.7619000000
H -2.2956790000 -2.9305540000 -0.6368470000
H -2.0176590000 -1.6863790000 2.9371420000
H -2.4768910000 -3.3352010000 2.4746720000
H -3.1599880000 -1.9519170000 1.6000340000
H 5.1245040000 -3.4184150000 -2.0575250000
H -0.3179230000 1.2737800000 1.8209180000
C 0.6173460000 2.6662860000 0.4626430000
F -4.2204330000 1.2176750000 0.1854610000
F -5.0964450000 -0.4536970000 -1.1239630000
F -3.5614940000 1.0151410000 -1.9921900000
C 0.8310740000 3.0861850000 -0.8579190000
C 1.2926360000 3.3095890000 1.5081180000
C 1.6849960000 4.1488530000 -1.1216460000
H 0.3374530000 2.5668900000 -1.6746890000
C 2.1490740000 4.3724580000 1.2418170000
H 1.1322700000 2.9800350000 2.5315720000
C 2.3427140000 4.7936230000 -0.0724420000
H 1.8468520000 4.4713830000 -2.1447990000
H 2.6630920000 4.8715650000 2.0564750000
H 3.0124920000 5.6214990000 -0.2822070000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394439 (Hartree/Particle)
Thermal correction to Energy= 0.419098
Thermal correction to Enthalpy= 0.420043
Thermal correction to Gibbs (Free) Energy= 0.338447
Sum of electronic and zero-point Energies= -1250.430105
Sum of electronic and thermal Energies= -1250.405445
Sum of electronic and thermal Enthalpies= -1250.404501
Sum of electronic and thermal (Free) Energies= -1250.486097

cPT

C -1.8104350000 0.4168680000 -0.7582550000
C -0.4691520000 0.1885720000 -0.7655370000
C 0.3037470000 -0.9707840000 -0.4500050000
C 1.6293950000 -0.5305640000 -0.0728790000
C 1.7517110000 0.8063450000 -0.3933300000
C 0.5119300000 1.3504780000 -0.9929340000
C 0.0164480000 -2.4297520000 -0.7307080000
C -2.8129430000 -0.3632830000 -0.0567130000
O 2.5354670000 -1.3392110000 0.4217460000
C -1.3450400000 -2.7326180000 -1.3702310000
C 0.1851100000 -3.2777580000 0.5472380000
C 1.0987420000 -2.8517110000 -1.7669230000
C -4.1177030000 -0.4590320000 -0.5677460000
C -2.4984640000 -0.9940700000 1.1588110000
C -3.4535120000 -1.7599240000 1.8162980000
H -1.5146540000 -0.8471470000 1.5959810000
C -4.7284890000 -1.8989210000 1.2692190000
H -3.2077000000 -2.2393190000 2.7581590000
C -5.0606590000 -1.2438620000 0.0806130000
H -4.3700690000 0.0541950000 -1.4911090000
H -5.4736660000 -2.4998760000 1.7802930000
H -6.0591070000 -1.3415030000 -0.3322750000
B 3.9426730000 -0.8206880000 0.5716430000
F 4.3949630000 -0.4266620000 -0.6850800000
F 4.6842190000 -1.8645460000 1.0844000000
F 3.9254340000 0.2733110000 1.4355220000
H -2.1512410000 1.3469180000 -1.2150170000
H 2.6485610000 1.3946480000 -0.2444290000
H 0.6461440000 1.4189220000 -2.0843130000
C 0.0999520000 2.7035020000 -0.4586600000
C 0.0266430000 2.9108020000 0.9225200000
C -0.2167530000 3.7482710000 -1.3253660000
H 0.9702070000 -2.2964910000 -2.7015320000
H 0.9643910000 -3.9162820000 -1.9796420000
H 2.1096310000 -2.6949610000 -1.3908180000
H 0.0815810000 -4.3323830000 0.2723140000
H -0.5962730000 -3.0399300000 1.2750470000
H 1.1634780000 -3.1265970000 1.0044270000
H -1.5805550000 -2.0330620000 -2.1787420000
H -2.1628320000 -2.7258850000 -0.6489900000
H -1.2968140000 -3.7375530000 -1.8003840000
C -0.3557660000 4.1480120000 1.4273830000
C -0.6704300000 5.1912680000 0.5552220000
C -0.6013940000 4.9899520000 -0.8200770000
H -0.1582820000 3.5926870000 -2.3996380000
H -0.9678680000 6.1577600000 0.9495100000
H -0.8431380000 5.7982460000 -1.5029170000
H 0.2702040000 2.0943830000 1.5999930000
H -0.4082720000 4.3006770000 2.5006870000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.396750 (Hartree/Particle)
Thermal correction to Energy= 0.421240
Thermal correction to Enthalpy= 0.422184
Thermal correction to Gibbs (Free) Energy= 0.340713
Sum of electronic and zero-point Energies= -1250.453333
Sum of electronic and thermal Energies= -1250.428843
Sum of electronic and thermal Enthalpies= -1250.427899
Sum of electronic and thermal (Free) Energies= -1250.509370

ccRT

C -0.8009360000 -1.9297620000 -1.4504410000
C 0.3352730000 -1.6285770000 -0.8773340000
C 1.4709300000 -1.2944030000 -0.2902010000
C 1.7860610000 0.1490950000 -0.2255020000
C 0.7635080000 1.1746420000 -0.2275440000
C -0.4910170000 0.9476730000 0.2195680000
H 1.0796480000 2.1501110000 -0.5793680000
C 2.4677680000 -2.3418320000 0.2393620000
H -0.8223790000 -2.0623710000 -2.5315740000
C -2.0810980000 -2.0247060000 -0.7157890000
O 3.0128810000 0.4530890000 -0.2019640000
C 1.7954100000 -3.7190000000 0.2471050000
C 2.8719790000 -1.9805060000 1.6768520000
C 3.7095040000 -2.4121110000 -0.6660230000
C -3.2810850000 -1.8022920000 -1.3994780000
C -2.1176420000 -2.2901060000 0.6596940000
C -3.3310700000 -2.3152670000 1.3395610000
H -1.1896550000 -2.4818780000 1.1932640000
C -4.5224330000 -2.0753270000 0.6542280000
H -3.3469570000 -2.5248620000 2.4043270000
C -4.4936880000 -1.8209720000 -0.7159930000
H -3.2592070000 -1.5998840000 -2.4665200000
H -5.4688500000 -2.0943780000 1.1849350000
H -5.4174110000 -1.6372180000 -1.2553160000
B 3.5758670000 1.9096010000 -0.0105150000
F 4.9270340000 1.7221890000 0.0790000000
F 3.0087310000 2.3937610000 1.1436660000
F 3.2000430000 2.6276760000 -1.1261920000
H 4.2750540000 -1.4796580000 -0.6553800000
H 3.4204010000 -2.6382610000 -1.6975820000
H 4.3625250000 -3.2170220000 -0.3114850000
H 1.9916600000 -1.9331920000 2.3271720000
H 3.3960090000 -1.0229510000 1.7251310000
H 3.5424330000 -2.7525350000 2.0683730000
H 0.9001420000 -3.7258000000 0.8781150000
H 2.4964850000 -4.4593990000 0.6440400000
H 1.5055260000 -4.0283350000 -0.7618110000
C -1.6017540000 1.8919010000 0.2076690000
H -0.7310380000 -0.0263010000 0.6390040000
C -1.4555280000 3.2437770000 -0.1437580000
C -2.8765730000 1.4029420000 0.5318130000
C -2.5623400000 4.0799500000 -0.1718160000
C -3.9850550000 2.2408130000 0.4924840000
C -3.8286920000 3.5800930000 0.1421080000
H -2.9928070000 0.3562330000 0.8035060000
H -0.4751530000 3.6439410000 -0.3822870000
H -4.9672300000 1.8486250000 0.7360000000
H -2.4418690000 5.1249560000 -0.4375960000
H -4.6911150000 4.2386630000 0.1156870000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395130 (Hartree/Particle)
Thermal correction to Energy= 0.420756
Thermal correction to Enthalpy= 0.421700
Thermal correction to Gibbs (Free) Energy= 0.337309

Sum of electronic and zero-point Energies= -1250.452274
Sum of electronic and thermal Energies= -1250.426648
Sum of electronic and thermal Enthalpies= -1250.425704
Sum of electronic and thermal (Free) Energies= -1250.510094

ccTS

C 1.0481890000 1.5071490000 -0.9744950000
C -0.0937380000 1.0654840000 -0.4474860000
C 2.3567830000 1.4694300000 -0.3165030000
H 1.0137510000 1.8544010000 -2.0084080000
C -1.4427440000 1.1240260000 -0.2847650000
C 3.5027960000 1.1705590000 -1.0655220000
C 2.4771070000 1.7207090000 1.0571240000
C -2.0317740000 -0.1728300000 -0.0343000000
C -2.2495530000 2.4181170000 -0.2840760000
C 4.7409210000 1.0826810000 -0.4413320000
H 3.4109280000 0.9827880000 -2.1316640000
C 3.7214570000 1.6486890000 1.6752230000
H 1.5955480000 2.0001960000 1.6289410000
C -1.0544180000 -1.1655910000 0.1697510000
O -3.3097990000 -0.3534820000 -0.0776980000
C -1.3374370000 3.6410870000 -0.4179730000
C -3.0453360000 2.5273500000 1.0266660000
C -3.2112160000 2.3798510000 -1.4877520000
C 4.8516460000 1.3184740000 0.9296290000
H 5.6220030000 0.8316340000 -1.0230210000
H 3.8088920000 1.8529310000 2.7375490000
C 0.2372730000 -0.7190440000 0.4837700000
H -1.2692680000 -2.2078890000 -0.0383390000
B -3.8937070000 -1.7016720000 0.3450330000
H -0.7812750000 3.6278560000 -1.3605040000
H -0.6176020000 3.6982460000 0.4050550000
H -1.9515290000 4.5466020000 -0.3998930000
H -3.6286590000 3.4539060000 1.0175680000
H -2.3690020000 2.5593380000 1.8872820000
H -3.7332450000 1.6884690000 1.1498710000
H -2.6538470000 2.3076790000 -2.4272760000
H -3.7924710000 3.3078460000 -1.5053070000
H -3.9017790000 1.5374780000 -1.4210110000
H 5.8213450000 1.2575210000 1.4133710000
H 0.3681220000 -0.0558220000 1.3424280000
C 1.4268140000 -1.5026180000 0.1247060000
F -5.2572810000 -1.5270950000 0.3430450000
F -3.3960200000 -1.9988650000 1.6034010000
F -3.4841090000 -2.6503970000 -0.5839110000
C 1.4850580000 -2.1683890000 -1.1067720000
C 2.5230760000 -1.5606170000 0.9931840000
C 2.6212080000 -2.8862350000 -1.4592610000
H 0.6443340000 -2.0972750000 -1.7923710000
C 3.6575490000 -2.2829700000 0.6415710000
H 2.4818750000 -1.0371890000 1.9438050000
C 3.7078090000 -2.9432420000 -0.5851170000
H 2.6656400000 -3.3943360000 -2.4169910000
H 4.5037130000 -2.3243680000 1.3197210000
H 4.5973260000 -3.4990070000 -0.8648260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394149 (Hartree/Particle)
Thermal correction to Energy= 0.418637
Thermal correction to Enthalpy= 0.419582
Thermal correction to Gibbs (Free) Energy= 0.339444
Sum of electronic and zero-point Energies= -1250.430113
Sum of electronic and thermal Energies= -1250.405625
Sum of electronic and thermal Enthalpies= -1250.404680
Sum of electronic and thermal (Free) Energies= -1250.484818

ccPT

C -1.2458680000 1.6177650000 -0.0063490000
C -0.1504090000 0.8413640000 -0.2793180000
C 1.2116080000 1.1753240000 0.0041210000
C 2.0220180000 -0.0069700000 -0.1925480000
C 1.2121180000 -1.0251120000 -0.6440320000
C -0.1988240000 -0.5953250000 -0.7823470000
C 1.8552070000 2.4926330000 0.3716240000
O 3.3169940000 -0.0418580000 0.0283170000
C 0.9250860000 3.7044140000 0.5000430000
C 2.8777370000 2.8189560000 -0.7460670000
C 2.5894980000 2.3138660000 1.7213560000
H 1.5481140000 -2.0303090000 -0.8642010000
C -2.6425670000 1.3429230000 -0.2756130000
H -1.0842110000 2.5291710000 0.5530450000
C -3.5911860000 1.9654760000 0.5599950000
C -4.9472450000 1.7303220000 0.3914190000
C -5.3822430000 0.8982050000 -0.6409220000
C -4.4586890000 0.3098020000 -1.5052750000
C -3.0998550000 0.5262060000 -1.3264790000
H -3.2473490000 2.6196250000 1.3562920000
H -5.6658360000 2.2002910000 1.0541670000
H -6.4436240000 0.7214260000 -0.7826820000
H -4.8002750000 -0.3137790000 -2.3246050000
H -2.3966260000 0.1007560000 -2.0319100000
B 4.0584640000 -1.3143220000 -0.2817500000
F 5.3828240000 -1.0693760000 0.0191120000
F 3.8799790000 -1.6126230000 -1.6313750000
F 3.5318890000 -2.3399300000 0.5017240000
H 1.8751460000 2.0816210000 2.5175030000
H 3.0818040000 3.2595380000 1.9697290000
H 3.3411190000 1.5267600000 1.6725500000
H 3.4027370000 3.7383650000 -0.4686010000
H 2.3627410000 2.9926210000 -1.6960720000
H 3.6100050000 2.0224850000 -0.8732600000
H 0.2772060000 3.6423310000 1.3792120000
H 0.3163320000 3.8608170000 -0.3955830000
H 1.5514720000 4.5915990000 0.6315510000
H -0.4575760000 -0.6036010000 -1.8509670000
C -1.1268030000 -1.5389160000 -0.0339150000
C -1.1341560000 -1.5469940000 1.3631110000
C -1.9317490000 -2.4423290000 -0.7272210000
C -1.9529940000 -2.4321270000 2.0556830000
C -2.7639480000 -3.3269380000 1.3575600000
C -2.7491570000 -3.3331660000 -0.0344490000
H -0.4995940000 -0.8514800000 1.9080180000
H -1.9563060000 -2.4264770000 3.1410700000
H -3.4030480000 -4.0175050000 1.8985250000
H -1.9233060000 -2.4477340000 -1.8146510000
H -3.3749070000 -4.0289550000 -0.5843260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397635 (Hartree/Particle)
Thermal correction to Energy= 0.422037
Thermal correction to Enthalpy= 0.422981
Thermal correction to Gibbs (Free) Energy= 0.341621
Sum of electronic and zero-point Energies= -1250.460024
Sum of electronic and thermal Energies= -1250.435622
Sum of electronic and thermal Enthalpies= -1250.434678
Sum of electronic and thermal (Free) Energies= -1250.516038

RM06-2X/6-31+G(d,p)

1a

cRT

C 3.5521650000 -0.1708740000 -0.0696610000
C 2.3537890000 0.3005080000 -0.2708140000
C 1.1568880000 0.8395960000 -0.4376290000
C -0.0526350000 0.0347450000 -0.1983280000
C -0.0597640000 -1.4359020000 -0.1973800000
C 0.7222950000 -2.1546490000 -1.0071870000
H -0.8128660000 -1.9018610000 0.4296640000
C 0.9520890000 2.3056440000 -0.7449170000
O -1.0983210000 0.6874370000 0.0135950000
H 1.9117370000 2.7909410000 -0.9213960000
H 0.4439090000 2.7946340000 0.0897780000
H 0.3170370000 2.4232470000 -1.6268070000
B -2.5579800000 0.0311990000 0.2859470000
F -3.3767580000 1.1113950000 0.3528920000
F -2.4086730000 -0.6540630000 1.4710130000
F -2.7729060000 -0.7948740000 -0.7900100000
C 4.2548510000 -0.1657490000 1.2647830000
H 4.0774580000 -0.6064750000 -0.9198810000
H 3.6358540000 0.2979380000 2.0336710000
H 5.1974030000 0.3835810000 1.1903190000
H 4.4882630000 -1.1894540000 1.5702810000
H 1.4194650000 -1.6934310000 -1.6985120000
H 0.6451770000 -3.2366500000 -1.0238570000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.172112 (Hartree/Particle)
Thermal correction to Energy= 0.186629
Thermal correction to Enthalpy= 0.187574
Thermal correction to Gibbs (Free) Energy= 0.130012
Sum of electronic and zero-point Energies= -710.185558
Sum of electronic and thermal Energies= -710.171041
Sum of electronic and thermal Enthalpies= -710.170097
Sum of electronic and thermal (Free) Energies= -710.227659

cTS

C 3.4295800000 -0.4575510000 -0.0404910000
C 2.1697090000 -0.1425500000 -0.2886950000
C 1.1121180000 0.7124010000 -0.3335180000
C -0.1651030000 0.0858050000 -0.1210040000
C -0.0448590000 -1.3412430000 -0.0835760000
C 1.0668980000 -1.8707710000 -0.7028630000
C 1.1991090000 2.1744640000 -0.6525700000
O -1.2107080000 0.7843470000 0.0619250000
H 0.7694690000 2.7379130000 0.1820050000
H 0.5989810000 2.4106390000 -1.5357020000
H 2.2306310000 2.4897210000 -0.8099510000
H -0.7186740000 -1.9253000000 0.5357620000
B -2.5904310000 0.0495870000 0.1933360000
F -2.6662430000 -0.7984060000 -0.9024480000
F -3.5289370000 1.0370170000 0.2030740000
F -2.5155140000 -0.6735670000 1.3765840000
H 3.8962290000 -1.2611080000 -0.6065560000
C 4.2444390000 0.2108840000 1.0339930000
H 3.6862360000 1.0188460000 1.5094450000
H 5.1643560000 0.6178590000 0.6032160000
H 4.5327690000 -0.5141780000 1.8012470000
H 1.4319810000 -2.8517200000 -0.4048930000
H 1.3707370000 -1.5594100000 -1.6991950000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171252 (Hartree/Particle)
Thermal correction to Energy= 0.184756
Thermal correction to Enthalpy= 0.185700
Thermal correction to Gibbs (Free) Energy= 0.130677
Sum of electronic and zero-point Energies= -710.158149
Sum of electronic and thermal Energies= -710.144645
Sum of electronic and thermal Enthalpies= -710.143701
Sum of electronic and thermal (Free) Energies= -710.198724

cPT

C 3.4059410000 -0.5582510000 0.0000000000
C 2.0528030000 -0.5589300000 0.0000000000
C 1.1214330000 0.5352020000 0.0000000000
C -0.2127720000 0.0368610000 0.0000000000
C -0.1506310000 -1.3600190000 0.0000000000
C 1.2446180000 -1.8373000000 0.0000000000
C 1.3766400000 1.9972890000 0.0000000000
O -1.2460700000 0.8173780000 0.0000000000
H 1.9522820000 2.2905910000 0.8844270000
H 0.4226020000 2.5260290000 0.0000000000
H 1.9522830000 2.2905910000 -0.8844270000
H -1.0279530000 -1.9970680000 0.0000000000
B -2.6214510000 0.1449290000 0.0000000000
F -2.6734460000 -0.6622280000 -1.1415280000
F -3.5499910000 1.1482070000 0.0000000000
F -2.6734460000 -0.6622280000 1.1415280000
H 3.8775400000 -1.5422310000 0.0000000000
C 4.3556890000 0.5896870000 0.0000000000
H 3.8728990000 1.5632280000 0.0000010000
H 5.0096750000 0.5208930000 -0.8766760000
H 5.0096760000 0.5208920000 0.8766770000
H 1.4582120000 -2.4587900000 0.8809530000
H 1.4582120000 -2.4587900000 -0.8809530000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173637 (Hartree/Particle)
Thermal correction to Energy= 0.186971
Thermal correction to Enthalpy= 0.187915
Thermal correction to Gibbs (Free) Energy= 0.132256
Sum of electronic and zero-point Energies= -710.203617
Sum of electronic and thermal Energies= -710.190284
Sum of electronic and thermal Enthalpies= -710.189339
Sum of electronic and thermal (Free) Energies= -710.244998

ccRT

C -3.4600510000 0.1185920000 0.7223010000
C -2.2877740000 0.5251600000 0.3244950000
C -1.1049980000 0.9808700000 -0.0549290000
C 0.0724800000 0.1001570000 0.0145630000
C -0.0170810000 -1.3666200000 0.0852480000
C -0.9741350000 -2.0592150000 -0.5380830000
H 0.8025120000 -1.8618530000 0.5956350000
C -0.8617600000 2.4199370000 -0.4474360000
O 1.1797690000 0.6817020000 0.0153660000
H -1.8049240000 2.9644920000 -0.4857790000
H -0.3719390000 2.4696680000 -1.4233250000
H -0.1951970000 2.8960130000 0.2759360000
B 2.6181810000 -0.0700460000 0.0621150000
F 3.5060410000 0.9494050000 -0.0562040000
F 2.5875040000 -0.9406030000 -0.9998520000
F 2.6317170000 -0.7077780000 1.2823520000
C -4.4956080000 -0.5122110000 -0.1731470000
H -3.6955990000 0.2241600000 1.7812370000
H -4.6805970000 -1.5451580000 0.1373560000
H -4.1743100000 -0.5091020000 -1.2161540000
H -5.4412960000 0.0312650000 -0.0995710000
H -1.7514380000 -1.5783490000 -1.1227370000
H -0.9700560000 -3.1437570000 -0.5108400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172103 (Hartree/Particle)
Thermal correction to Energy= 0.186595
Thermal correction to Enthalpy= 0.187539
Thermal correction to Gibbs (Free) Energy= 0.130114
Sum of electronic and zero-point Energies= -710.186071
Sum of electronic and thermal Energies= -710.171579
Sum of electronic and thermal Enthalpies= -710.170635
Sum of electronic and thermal (Free) Energies= -710.228060

ccTS

C -3.3968420000 0.1726690000 0.5275140000
C -2.1444340000 0.3064560000 0.1242240000
C -0.9900530000 1.0170940000 -0.0225910000
C 0.2038660000 0.2188500000 0.0199610000
C -0.1095700000 -1.1783140000 0.0396300000
C -1.3451060000 -1.5256990000 -0.4665170000
H 0.5379890000 -1.8724760000 0.5667110000
C -0.9083320000 2.4909790000 -0.2789960000
O 1.3513770000 0.7610680000 0.0947950000
H -1.8967860000 2.9483510000 -0.3109850000
H -0.3749970000 2.6886220000 -1.2130380000
H -0.3204330000 2.9495820000 0.5228370000
B 2.6163670000 -0.1630470000 0.0419210000
F 3.6827050000 0.6804920000 -0.0425630000
F 2.4396580000 -0.9716260000 -1.0728470000
F 2.5783500000 -0.9147510000 1.2092530000
C -4.4422040000 -0.7362660000 -0.0481150000
H -3.6775690000 0.7639630000 1.4010940000
H -4.7710350000 -1.4648450000 0.6993400000
H -4.0792290000 -1.2710580000 -0.9271950000
H -5.3204830000 -0.1532860000 -0.3408660000
H -1.6917460000 -1.1433740000 -1.4232630000
H -1.8089330000 -2.4604420000 -0.1578430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171185 (Hartree/Particle)
Thermal correction to Energy= 0.184642
Thermal correction to Enthalpy= 0.185586
Thermal correction to Gibbs (Free) Energy= 0.130740
Sum of electronic and zero-point Energies= -710.157706
Sum of electronic and thermal Energies= -710.144249
Sum of electronic and thermal Enthalpies= -710.143304
Sum of electronic and thermal (Free) Energies= -710.19815

ccPT

C 3.3916200000 0.3219900000 0.0000010000
C 2.0862770000 -0.0245560000 0.0000000000
C 0.9824100000 0.8905360000 0.0000000000
C -0.2481810000 0.1759570000 0.0000000000
C 0.0539190000 -1.1850370000 0.0000000000

C 1.5173950000 -1.4234230000 0.0000000000
C 0.9983430000 2.3662250000 0.0000000000
O -1.3930800000 0.7838780000 0.0000000000
H 1.9976940000 2.7995280000 0.0000000000
H 0.4331040000 2.7199890000 0.8704900000
H 0.4331050000 2.7199890000 -0.8704890000
H -0.6991770000 -1.9649350000 0.0000000000
B -2.6398490000 -0.1036990000 0.0000000000
F -3.7210010000 0.7338940000 -0.0000010000
F -2.5599660000 -0.9085270000 1.1416420000
F -2.5599650000 -0.9085270000 -1.1416430000
C 4.5349120000 -0.6326500000 0.0000010000
H 3.6429000000 1.3815680000 0.0000010000
H 4.2095470000 -1.6739660000 0.0000010000
H 5.1676360000 -0.4604860000 0.8776860000
H 5.1676360000 -0.4604860000 -0.8776840000
H 1.8298230000 -1.9997710000 0.8813830000
H 1.8298230000 -1.9997710000 -0.8813830000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173358 (Hartree/Particle)
Thermal correction to Energy= 0.186779
Thermal correction to Enthalpy= 0.187723
Thermal correction to Gibbs (Free) Energy= 0.132553
Sum of electronic and zero-point Energies= -710.208713
Sum of electronic and thermal Energies= -710.195292
Sum of electronic and thermal Enthalpies= -710.194348
Sum of electronic and thermal (Free) Energies= -710.249518

6d

cRT

C -1.8283460000 -1.3974200000 0.8580210000
C -1.2647280000 -0.2158540000 0.9082590000
C -0.7605530000 1.0024170000 0.9250730000
C 0.3585430000 1.2846250000 -0.0081650000
C 1.4090430000 0.3225000000 -0.2881120000
C 1.7192760000 -0.6781160000 0.5628920000
H 1.9842470000 0.5119220000 -1.1867920000
C -1.3489760000 2.1385240000 1.7841420000
H -1.4724690000 -2.1654990000 1.5452550000
C -2.9214100000 -1.7773320000 -0.0603920000
O 0.3498780000 2.4150240000 -0.5556480000
C -2.2426560000 1.5335130000 2.8719960000
C -2.1979360000 3.0791100000 0.9107480000
C -0.2027220000 2.9172270000 2.4490130000
C -3.4562490000 -3.0671910000 0.0154780000
C -3.4377560000 -0.8787340000 -1.0035030000
C -4.4694580000 -1.2668840000 -1.8493300000
H -3.0232190000 0.1236740000 -1.0732910000
C -5.0003490000 -2.5559920000 -1.7670510000
H -4.8601070000 -0.5635250000 -2.5776650000
C -4.4910630000 -3.4546850000 -0.8330710000
H -3.0586740000 -3.7692460000 0.7435950000
H -5.8055140000 -2.8561580000 -2.4297520000
H -4.8972510000 -4.4587370000 -0.7639180000
B 1.5037580000 2.9864650000 -1.5146180000
F 1.1047170000 4.2641590000 -1.7579460000
F 1.5005680000 2.1660080000 -2.6228090000
F 2.6620740000 2.8778830000 -0.7773950000
H 0.4350730000 3.4140210000 1.7140100000
H 0.4175540000 2.2533910000 3.0616000000
H -0.6208350000 3.6873030000 3.1049130000
H -3.0121840000 2.5250390000 0.4318380000
H -1.6012760000 3.5667050000 0.1388440000
H -2.6423830000 3.8522000000 1.5469390000
H -3.0891110000 0.9911880000 2.4392740000
H -2.6377470000 2.3359960000 3.5020780000
H -1.6822190000 0.8416770000 3.5098980000
C 2.7903640000 -1.6556840000 0.3851710000
H 1.1495960000 -0.7760540000 1.4847330000
C 3.6719760000 -1.6286540000 -0.7083650000
C 2.9358320000 -2.6645190000 1.3489800000
C 4.6641190000 -2.5920180000 -0.8302310000
C 3.9287130000 -3.6309490000 1.2245420000
C 4.7940990000 -3.5957170000 0.1330800000
H 2.2611720000 -2.6862050000 2.2010400000
H 3.5890970000 -0.8491660000 -1.4586590000
H 4.0288310000 -4.4064380000 1.9767350000
H 5.3423400000 -2.5606860000 -1.6765010000
H 5.5724610000 -4.3453830000 0.0323990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392968 (Hartree/Particle)
Thermal correction to Energy= 0.418987
Thermal correction to Enthalpy= 0.419931
Thermal correction to Gibbs (Free) Energy= 0.332626
Sum of electronic and zero-point Energies= -1250.506866
Sum of electronic and thermal Energies= -1250.480847
Sum of electronic and thermal Enthalpies= -1250.479903
Sum of electronic and thermal (Free) Energies= -1250.567208

cTS

C 1.7610810000 -0.3075180000 0.7240340000
C 0.4333390000 -0.3667000000 0.7298830000
C 2.6382180000 -1.1739020000 -0.0747820000
H 2.2468880000 0.4791360000 1.3017200000
C -0.7658150000 -1.0031510000 0.6159370000
C 4.0107350000 -1.1928110000 0.2072110000
C 2.1432990000 -1.9786900000 -1.1115560000
C -1.7862360000 -0.1519300000 0.0387900000
C -1.0670310000 -2.4008510000 1.1472210000
C 4.8666150000 -2.0232350000 -0.5102360000
H 4.4020670000 -0.5600880000 0.9992440000
C 3.0007610000 -2.8034420000 -1.8294370000
H 1.0867940000 -1.9387370000 -1.3618010000
C -1.3606890000 1.2001770000 -0.0288470000
O -2.8959390000 -0.6246870000 -0.3858270000
C 0.1481990000 -2.9908540000 1.8692090000
C -1.4431590000 -3.3092200000 -0.0409510000
C -2.2503300000 -2.3159650000 2.1285190000
C 4.3637090000 -2.8325900000 -1.5277030000
H 5.9264020000 -2.0359200000 -0.2771760000
H 2.6079050000 -3.4186100000 -2.6325480000
C -0.2823460000 1.5509100000 0.7895740000
H -1.7971720000 1.8812860000 -0.7527890000
B -3.9932500000 0.3490870000 -0.9048900000
H 0.4442640000 -2.3751160000 2.7245750000
H 1.0095890000 -3.0899210000 1.2012340000
H -0.1076980000 -3.9877350000 2.2404180000
H -1.7039890000 -4.2996000000 0.3465900000
H -0.5977050000 -3.4293090000 -0.7257190000
H -2.2981110000 -2.9150340000 -0.5925950000
H -2.0074520000 -1.6639230000 2.9744240000
H -2.4619360000 -3.3152020000 2.5223740000
H -3.1517990000 -1.9403430000 1.6404060000
H 5.0312410000 -3.4766530000 -2.0908230000
H -0.3303810000 1.2984930000 1.8494810000
C 0.6215090000 2.6674900000 0.4756440000
F -4.1772070000 1.2935450000 0.0967860000
F -5.0899650000 -0.4317160000 -1.1371640000
F -3.4747290000 0.9403640000 -2.0524780000
C 0.8696410000 3.0409640000 -0.8522820000
C 1.2711300000 3.3478390000 1.5131500000
C 1.7330080000 4.0935830000 -1.1324190000
H 0.3934210000 2.4939370000 -1.6616240000
C 2.1365060000 4.4013440000 1.2320120000
H 1.0825300000 3.0576840000 2.5440830000
C 2.3657310000 4.7756140000 -0.0911860000
H 1.9198260000 4.3792500000 -2.1622760000
H 2.6278850000 4.9305770000 2.0418020000
H 3.0410650000 5.5957760000 -0.3129270000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392395 (Hartree/Particle)
Thermal correction to Energy= 0.417154
Thermal correction to Enthalpy= 0.418098
Thermal correction to Gibbs (Free) Energy= 0.336257
Sum of electronic and zero-point Energies= -1250.484526
Sum of electronic and thermal Energies= -1250.459768
Sum of electronic and thermal Enthalpies= -1250.458824
Sum of electronic and thermal (Free) Energies= -1250.540665

cPT

C -1.7915920000 0.5139060000 -0.6869830000
C -0.4718370000 0.2146750000 -0.7681260000
C 0.2602740000 -0.9926590000 -0.4973760000

C 1.6022000000 -0.6252040000 -0.1213860000
C 1.7861140000 0.7150840000 -0.4401500000
C 0.5668030000 1.3258890000 -1.0157310000
C -0.0927460000 -2.4311550000 -0.8005390000
C -2.8185270000 -0.2538770000 0.0090880000
O 2.4658890000 -1.4702990000 0.3528550000
C -1.4759260000 -2.6553410000 -1.4260030000
C 0.0580180000 -3.3097840000 0.4610560000
C 0.9638270000 -2.8822790000 -1.8526550000
C -4.1323970000 -0.2911460000 -0.4827150000
C -2.5138000000 -0.9231580000 1.2042590000
C -3.4894460000 -1.6657360000 1.8616500000
H -1.5154560000 -0.8340670000 1.6238250000
C -4.7781620000 -1.7429650000 1.3351290000
H -3.2461020000 -2.1773830000 2.7872840000
C -5.0993550000 -1.0500030000 0.1651550000
H -4.3794170000 0.2498560000 -1.3919790000
H -5.5384070000 -2.3257240000 1.8450640000
H -6.1066220000 -1.0982080000 -0.2353990000
B 3.8862920000 -0.9656460000 0.6163810000
F 4.3793550000 -0.4932750000 -0.6032900000
F 4.5883690000 -2.0357700000 1.1045620000
F 3.7830720000 0.0893380000 1.5265990000
H -2.0946220000 1.4926330000 -1.0616240000
H 2.7234280000 1.2447330000 -0.3078250000
H 0.6860830000 1.3851600000 -2.1097430000
C 0.2361070000 2.7001420000 -0.4826550000
C 0.3451360000 2.9620580000 0.8869900000
C -0.1990050000 3.7114910000 -1.3399090000
H 0.8613330000 -2.3004340000 -2.7745700000
H 0.7734310000 -3.9328320000 -2.0904810000
H 1.9825190000 -2.7881830000 -1.4763740000
H -0.1023950000 -4.3522310000 0.1678600000
H -0.6987670000 -3.0505270000 1.2070330000
H 1.0514150000 -3.2147820000 0.9007810000
H -1.6883850000 -1.9322790000 -2.2203190000
H -2.2829980000 -2.6190070000 -0.6936690000
H -1.4859940000 -3.6535200000 -1.8734560000
C 0.0185480000 4.2176420000 1.3895780000
C -0.4211760000 5.2238610000 0.5280150000
C -0.5287190000 4.9702090000 -0.8371450000
H -0.2732690000 3.5170710000 -2.4074760000
H -0.6725980000 6.2038240000 0.9206360000
H -0.8614160000 5.7516520000 -1.5128680000
H 0.6944400000 2.1789540000 1.5575700000
H 0.1120110000 4.4133900000 2.4528630000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394694 (Hartree/Particle)
Thermal correction to Energy= 0.419283
Thermal correction to Enthalpy= 0.420227
Thermal correction to Gibbs (Free) Energy= 0.338547
Sum of electronic and zero-point Energies= -1250.505809
Sum of electronic and thermal Energies= -1250.481220
Sum of electronic and thermal Enthalpies= -1250.480276
Sum of electronic and thermal (Free) Energies= -1250.561957

ccRT

C -0.8069660000 -1.9931460000 -1.4380100000
C 0.3190020000 -1.6875670000 -0.8427000000
C 1.4412010000 -1.3418410000 -0.2416720000
C 1.7768710000 0.1069250000 -0.2269290000
C 0.7666420000 1.1506250000 -0.2271340000
C -0.4918620000 0.9528490000 0.2174400000
H 1.1071600000 2.1224360000 -0.5669590000
C 2.4204310000 -2.3708040000 0.3535420000
H -0.7991410000 -2.1552680000 -2.5151390000
C -2.1091260000 -2.0587760000 -0.7399680000
O 3.0005000000 0.3895520000 -0.2374380000
C 1.7224600000 -3.7319200000 0.4542880000
C 2.8385940000 -1.9199730000 1.7625580000
C 3.6566960000 -2.5182450000 -0.5512030000
C -3.2887260000 -1.8604300000 -1.4665160000
C -2.1910210000 -2.2768440000 0.6423810000
C -3.4254130000 -2.2781840000 1.2850210000
H -1.2809140000 -2.4544850000 1.2102130000
C -4.5958300000 -2.0631600000 0.5554800000
H -3.4746110000 -2.4511760000 2.3553640000
C -4.5234370000 -1.8566520000 -0.8215350000
H -3.2344750000 -1.6916970000 -2.5383840000
H -5.5583060000 -2.0655220000 1.0567880000
H -5.4294210000 -1.6923290000 -1.3960730000
B 3.6082440000 1.8721800000 -0.1317020000
F 4.9488970000 1.6539770000 -0.0468350000
F 3.0429400000 2.4096480000 1.0031250000
F 3.2056660000 2.5154980000 -1.2824630000
H 4.2262070000 -1.5908120000 -0.6165960000
H 3.3597680000 -2.8224960000 -1.5601750000
H 4.3076820000 -3.2967970000 -0.1391300000
H 1.9623830000 -1.7957410000 2.4089320000
H 3.3972220000 -0.9818670000 1.7434050000
H 3.4811110000 -2.6851950000 2.2095370000
H 0.8328120000 -3.6820370000 1.0913330000
H 2.4120160000 -4.4590130000 0.8932260000
H 1.4177930000 -4.1019800000 -0.5293430000
C -1.5614490000 1.9479460000 0.2345050000
H -0.7730770000 -0.0232210000 0.6051670000
C -1.3301430000 3.3178470000 0.0295050000
C -2.8741680000 1.4987940000 0.4454270000
C -2.3935490000 4.2110930000 0.0258040000
C -3.9381050000 2.3951210000 0.4299080000
C -3.6988570000 3.7521170000 0.2205300000
H -3.0561900000 0.4383400000 0.6068240000
H -0.3176370000 3.6856390000 -0.1048050000
H -4.9500920000 2.0346340000 0.5842270000
H -2.2066500000 5.2693170000 -0.1243030000
H -4.5258410000 4.4552150000 0.2151210000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.393242 (Hartree/Particle)
Thermal correction to Energy= 0.419007
Thermal correction to Enthalpy= 0.419951
Thermal correction to Gibbs (Free) Energy= 0.335252
Sum of electronic and zero-point Energies= -1250.510900
Sum of electronic and thermal Energies= -1250.485135
Sum of electronic and thermal Enthalpies= -1250.484191
Sum of electronic and thermal (Free) Energies= -1250.568889

ccTS

C 1.0411680000 1.5051710000 -0.9595800000
C -0.0920530000 1.0543130000 -0.4164230000
C 2.3613290000 1.4602670000 -0.3197260000
H 0.9910370000 1.8713530000 -1.9860450000
C -1.4453210000 1.1300730000 -0.2654630000
C 3.4952930000 1.1277390000 -1.0738200000
C 2.5055570000 1.7415720000 1.0458690000
C -2.0472850000 -0.1614570000 -0.0070830000
C -2.2518960000 2.4226780000 -0.2775830000
C 4.7412740000 1.0379870000 -0.4639430000
H 3.3876600000 0.9101830000 -2.1329630000
C 3.7574380000 1.6668060000 1.6510500000
H 1.6353100000 2.0480210000 1.6213850000
C -1.0597600000 -1.1571520000 0.1945550000
O -3.3135150000 -0.3352710000 -0.0437280000
C -1.3433570000 3.6479890000 -0.4180630000
C -3.0546210000 2.5367880000 1.0302650000
C -3.2126720000 2.3679370000 -1.4833090000
C 4.8744930000 1.3047100000 0.8999740000
H 5.6102130000 0.7582470000 -1.0508000000
H 3.8614580000 1.8969270000 2.7067480000
C 0.2277870000 -0.7014060000 0.5098530000
H -1.2761250000 -2.2009340000 -0.0117850000
B -3.9045410000 -1.7251880000 0.3327980000
H -0.7864270000 3.6342830000 -1.3601280000
H -0.6231380000 3.7146050000 0.4041070000
H -1.9595230000 4.5518410000 -0.4050830000
H -3.6370340000 3.4636060000 1.0143250000
H -2.3832670000 2.5740600000 1.8949680000
H -3.7436310000 1.6994740000 1.1540340000
H -2.6548510000 2.2883940000 -2.4222390000
H -3.7957350000 3.2943760000 -1.5109120000
H -3.9008860000 1.5247340000 -1.4076940000
H 5.8497040000 1.2429210000 1.3723550000
H 0.3577330000 -0.0563490000 1.3818790000
C 1.4187120000 -1.4879890000 0.1425910000
F -5.2592400000 -1.5478010000 0.3549860000
F -3.3604170000 -2.0537600000 1.5677170000
F -3.4728840000 -2.6095750000 -0.6497520000

C 1.4812400000 -2.1199100000 -1.1058550000
C 2.5071350000 -1.5824990000 1.0167950000
C 2.6143810000 -2.8391020000 -1.4707500000
H 0.6440710000 -2.0253480000 -1.7935200000
C 3.6383000000 -2.3067440000 0.6544650000
H 2.4643510000 -1.0852400000 1.9817500000
C 3.6940920000 -2.9319520000 -0.5908350000
H 2.6587920000 -3.3237260000 -2.4406520000
H 4.4770750000 -2.3775160000 1.3394120000
H 4.5795210000 -3.4905240000 -0.8777730000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392023 (Hartree/Particle)
Thermal correction to Energy= 0.416655
Thermal correction to Enthalpy= 0.417599
Thermal correction to Gibbs (Free) Energy= 0.337100
Sum of electronic and zero-point Energies= -1250.484343
Sum of electronic and thermal Energies= -1250.459710
Sum of electronic and thermal Enthalpies= -1250.458766
Sum of electronic and thermal (Free) Energies= -1250.539265

ccPT

C -1.2073720000 1.6474590000 -0.0292200000
C -0.1264300000 0.8538190000 -0.2844720000
C 1.2495250000 1.1709700000 -0.0048430000
C 2.0391430000 -0.0245830000 -0.1549830000
C 1.2087960000 -1.0448980000 -0.5949470000
C -0.1908950000 -0.5909780000 -0.7676130000
C 1.9203150000 2.4844480000 0.3254050000
O 3.3179190000 -0.0773560000 0.0748730000
C 1.0133550000 3.7183450000 0.4099350000
C 2.9589000000 2.7507850000 -0.7955010000
C 2.6459850000 2.3288030000 1.6841810000
H 1.5419180000 -2.0589860000 -0.7861330000
C -2.6156030000 1.3729160000 -0.2756080000
H -1.0317290000 2.5754720000 0.4984550000
C -3.5518580000 1.9771930000 0.5845590000
C -4.9115410000 1.7376130000 0.4390150000
C -5.3639060000 0.9157770000 -0.5941780000
C -4.4519980000 0.3441090000 -1.4813890000
C -3.0897990000 0.5680050000 -1.3255120000
H -3.1973590000 2.6219230000 1.3843970000
H -5.6188360000 2.1951180000 1.1226470000
H -6.4266550000 0.7332090000 -0.7167660000
H -4.8042440000 -0.2754810000 -2.2994890000
H -2.3951160000 0.1477920000 -2.0430180000
B 4.0494590000 -1.3845310000 -0.2293840000
F 5.3719480000 -1.1544890000 0.0492840000
F 3.8147110000 -1.6769640000 -1.5769920000
F 3.4808600000 -2.3748080000 0.5739480000
H 1.9255540000 2.1266100000 2.4837320000
H 3.1500050000 3.2734980000 1.9117270000
H 3.3869400000 1.5304710000 1.6579990000
H 3.5001250000 3.6686510000 -0.5455800000
H 2.4556740000 2.9024710000 -1.7558960000
H 3.6768880000 1.9365050000 -0.8880810000
H 0.3602170000 3.6984160000 1.2876510000
H 0.4120460000 3.8606450000 -0.4931800000
H 1.6558470000 4.5969680000 0.5172970000
H -0.4227980000 -0.6037790000 -1.8435210000
C -1.1576930000 -1.5137370000 -0.0445640000
C -1.2637870000 -1.4733620000 1.3476430000
C -1.9040400000 -2.4512670000 -0.7587740000
C -2.1247120000 -2.3413320000 2.0122450000
C -2.8789180000 -3.2678290000 1.2915750000
C -2.7625020000 -3.3259210000 -0.0951000000
H -0.6705810000 -0.7569400000 1.9116950000
H -2.2021640000 -2.2998740000 3.0939010000
H -3.5487850000 -3.9455670000 1.8107560000
H -1.8160910000 -2.4971010000 -1.8422120000
H -3.3389660000 -4.0501850000 -0.6617280000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395356 (Hartree/Particle)
Thermal correction to Energy= 0.419897
Thermal correction to Enthalpy= 0.420841
Thermal correction to Gibbs (Free) Energy= 0.338889
Sum of electronic and zero-point Energies= -1250.510827
Sum of electronic and thermal Energies= -1250.486285
Sum of electronic and thermal Enthalpies= -1250.485341
Sum of electronic and thermal (Free) Energies= -1250.567294

RM06-2X/6-31+G(d,p)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)

6d

cRT

C -1.7979760000 -1.3498310000 0.8721290000
C -1.2434680000 -0.1644010000 0.8948160000
C -0.7450710000 1.0594490000 0.8927500000
C 0.3940440000 1.3117270000 -0.0111890000
C 1.4159370000 0.3295050000 -0.2788180000
C 1.6894940000 -0.6821430000 0.5803930000
H 2.0099980000 0.4931080000 -1.1703580000
C -1.3621920000 2.2072260000 1.7167570000
H -1.4382150000 -2.0928370000 1.5845760000
C -2.8790270000 -1.7657320000 -0.0454210000
O 0.4240780000 2.4565120000 -0.5603820000
C -2.2947790000 1.6145250000 2.7789200000
C -2.1812580000 3.1401430000 0.8078360000
C -0.2406870000 2.9906680000 2.4170130000
C -3.3539300000 -3.0803170000 0.0196060000
C -3.4423680000 -0.8792910000 -0.9740970000
C -4.4608060000 -1.3045260000 -1.8197010000
H -3.0788760000 0.1435710000 -1.0311520000
C -4.9309880000 -2.6186700000 -1.7502610000
H -4.8902700000 -0.6105200000 -2.5351140000
C -4.3752720000 -3.5045600000 -0.8290570000
H -2.9201810000 -3.7711960000 0.7372610000
H -5.7262820000 -2.9473840000 -2.4114170000
H -4.7350530000 -4.5267360000 -0.7692540000
B 1.5563010000 2.9993480000 -1.4647170000
F 1.1988350000 4.3045680000 -1.7193260000
F 1.5836450000 2.2252360000 -2.6155500000
F 2.7400900000 2.9010360000 -0.7516320000
H 0.4249210000 3.4787960000 1.7007210000
H 0.3543790000 2.3311330000 3.0578030000
H -0.6829240000 3.7680330000 3.0478550000
H -2.9728430000 2.5815950000 0.2977530000
H -1.5572800000 3.6290440000 0.0586160000
H -2.6526620000 3.9129860000 1.4242830000
H -3.1295770000 1.0749180000 2.3207310000
H -2.7049660000 2.4247320000 3.3888820000
H -1.7590880000 0.9238250000 3.4384160000
C 2.7096710000 -1.7069850000 0.4020820000
H 1.1329630000 -0.7401190000 1.5130740000
C 3.4918100000 -1.8101340000 -0.7623720000
C 2.9039970000 -2.6340440000 1.4391980000
C 4.4434370000 -2.8140710000 -0.8772760000
C 3.8587590000 -3.6393710000 1.3219650000
C 4.6294660000 -3.7294130000 0.1635830000
H 2.3005690000 -2.5596830000 2.3397880000
H 3.3561700000 -1.1094000000 -1.5795700000
H 4.0010470000 -4.3491810000 2.1297890000
H 5.0428530000 -2.8876060000 -1.7784270000
H 5.3752930000 -4.5120060000 0.0678190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392601 (Hartree/Particle)
Thermal correction to Energy= 0.418490
Thermal correction to Enthalpy= 0.419434
Thermal correction to Gibbs (Free) Energy= 0.332912
Sum of electronic and zero-point Energies= -1250.525670
Sum of electronic and thermal Energies= -1250.499781
Sum of electronic and thermal Enthalpies= -1250.498837
Sum of electronic and thermal (Free) Energies= -1250.585358

cTS

C 1.7581860000 -0.3771360000 0.7332300000
C 0.4325690000 -0.4193020000 0.7195890000
C 2.6342370000 -1.2382340000 -0.0723570000
H 2.2444900000 0.3821260000 1.3461300000
C -0.7942270000 -0.9914860000 0.6023010000
C 4.0066590000 -1.2564280000 0.2131120000
C 2.1380200000 -2.0404310000 -1.1113340000
C -1.7697200000 -0.0958650000 0.0219990000
C -1.1499990000 -2.3764690000 1.1401370000

C 4.8631790000 -2.0845470000 -0.5076220000
H 4.3966560000 -0.6266380000 1.0077570000
C 2.9964880000 -2.8626440000 -1.8316110000
H 1.0817230000 -2.0020250000 -1.3631080000
C -1.3199620000 1.2375100000 -0.0376270000
O -2.9037320000 -0.5422490000 -0.4186570000
C 0.0441620000 -3.0026740000 1.8676770000
C -1.5482060000 -3.2812080000 -0.0426560000
C -2.3279050000 -2.2473590000 2.1218520000
C 4.3601920000 -2.8907140000 -1.5286270000
H 5.9227760000 -2.0976250000 -0.2742680000
H 2.6047950000 -3.4767700000 -2.6359120000
C -0.2301910000 1.5694820000 0.7761380000
H -1.7428130000 1.9380470000 -0.7503860000
B -3.9872090000 0.3981190000 -0.8843010000
H 0.3580730000 -2.3923990000 2.7201120000
H 0.9019020000 -3.1316710000 1.1997940000
H -0.2454630000 -3.9893280000 2.2408340000
H -1.8274550000 -4.2644190000 0.3497130000
H -0.7087920000 -3.4184030000 -0.7312420000
H -2.3966620000 -2.8729510000 -0.5938920000
H -2.0626390000 -1.5965220000 2.9613330000
H -2.5712760000 -3.2367960000 2.5215550000
H -3.2178380000 -1.8465160000 1.6321250000
H 5.0283560000 -3.5324810000 -2.0936480000
H -0.2634660000 1.2849800000 1.8286410000
C 0.6960490000 2.6618200000 0.4682630000
F -4.2380690000 1.3272210000 0.1268810000
F -5.0949950000 -0.3924780000 -1.1405570000
F -3.5469950000 1.0517000000 -2.0393460000
C 0.9275860000 3.0645920000 -0.8559200000
C 1.3833480000 3.2955840000 1.5133090000
C 1.8129450000 4.1018460000 -1.1240960000
H 0.4258100000 2.5518810000 -1.6719510000
C 2.2694860000 4.3343230000 1.2426640000
H 1.2101730000 2.9781060000 2.5383750000
C 2.4822030000 4.7385970000 -0.0754700000
H 1.9900750000 4.4102640000 -2.1489680000
H 2.7922100000 4.8268160000 2.0556960000
H 3.1752110000 5.5462010000 -0.2884440000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.391975 (Hartree/Particle)
Thermal correction to Energy= 0.416771
Thermal correction to Enthalpy= 0.417715
Thermal correction to Gibbs (Free) Energy= 0.335632
Sum of electronic and zero-point Energies= -1250.508805
Sum of electronic and thermal Energies= -1250.484009
Sum of electronic and thermal Enthalpies= -1250.483065
Sum of electronic and thermal (Free) Energies= -1250.565148

cPT

C -1.8256480000 0.3384710000 -0.7682250000
C -0.4736660000 0.1670080000 -0.7793660000
C 0.3504840000 -0.9585070000 -0.4741920000
C 1.6596000000 -0.4566670000 -0.1134340000
C 1.7209460000 0.8851970000 -0.4190710000
C 0.4515710000 1.3742660000 -1.0056980000
C 0.1228170000 -2.4288340000 -0.7507360000
C -2.7947620000 -0.4718980000 -0.0553770000
O 2.6068100000 -1.2326170000 0.3710380000
C -1.2326950000 -2.7861050000 -1.3754850000
C 0.3382980000 -3.2688340000 0.5269560000
C 1.2112140000 -2.8081540000 -1.7981550000
C -4.1015470000 -0.6077050000 -0.5562250000
C -2.4526530000 -1.0863960000 1.1621500000
C -3.3812830000 -1.8755590000 1.8318720000
H -1.4703050000 -0.9103590000 1.5917740000
C -4.6565280000 -2.0555350000 1.2946980000
H -3.1146360000 -2.3426230000 2.7741470000
C -5.0168450000 -1.4173730000 0.1033550000
H -4.3764770000 -0.1062290000 -1.4795560000
H -5.3797520000 -2.6752760000 1.8146650000
H -6.0149160000 -1.5467610000 -0.3014050000
B 3.9708810000 -0.6823100000 0.5920080000
F 4.4788240000 -0.1953530000 -0.6226800000
F 4.7490490000 -1.7284180000 1.0742890000
F 3.9100810000 0.3671590000 1.5221020000
H -2.2064530000 1.2506570000 -1.2298680000
H 2.5916290000 1.5139840000 -0.2735460000
H 0.5777700000 1.4525430000 -2.0974280000
C -0.0202260000 2.7053260000 -0.4647470000
C -0.1137380000 2.9013290000 0.9179590000
C -0.3750360000 3.7413790000 -1.3287160000
H 1.0623870000 -2.2469640000 -2.7260230000
H 1.1047040000 -3.8732790000 -2.0215290000
H 2.2194060000 -2.6292880000 -1.4253680000
H 0.2621320000 -4.3256030000 0.2528790000
H -0.4371310000 -3.0544540000 1.2676720000
H 1.3188510000 -3.0887980000 0.9682070000
H -1.5005790000 -2.1046430000 -2.1890970000
H -2.0437050000 -2.8019490000 -0.6472390000
H -1.1518900000 -3.7927370000 -1.7952920000
C -0.5575510000 4.1178490000 1.4271990000
C -0.9118730000 5.1523730000 0.5575930000
C -0.8201010000 4.9629880000 -0.8193820000
H -0.3017310000 3.5955060000 -2.4033850000
H -1.2566070000 6.1017160000 0.9547870000
H -1.0915590000 5.7638040000 -1.4997370000
H 0.1598460000 2.0938970000 1.5949590000
H -0.6261310000 4.2611150000 2.5007990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394236 (Hartree/Particle)
Thermal correction to Energy= 0.418855
Thermal correction to Enthalpy= 0.419800
Thermal correction to Gibbs (Free) Energy= 0.338125
Sum of electronic and zero-point Energies= -1250.533532
Sum of electronic and thermal Energies= -1250.508913
Sum of electronic and thermal Enthalpies= -1250.507968
Sum of electronic and thermal (Free) Energies= -1250.589643

ccRT

C -0.8015540000 -1.9372370000 -1.4458270000
C 0.3247370000 -1.6380270000 -0.8510850000
C 1.4570200000 -1.3039300000 -0.2552720000
C 1.7774290000 0.1379140000 -0.2082950000
C 0.7689690000 1.1719690000 -0.1965390000
C -0.4953300000 0.9530830000 0.2360520000
H 1.0970990000 2.1532000000 -0.5208420000
C 2.4436420000 -2.3505350000 0.2977960000
H -0.7961500000 -2.0779920000 -2.5262110000
C -2.0990140000 -2.0242280000 -0.7393010000
O 3.0128480000 0.4316020000 -0.2090480000
C 1.7462720000 -3.7144240000 0.3636730000
C 2.8752340000 -1.9472450000 1.7168860000
C 3.6692180000 -2.4734800000 -0.6245060000
C -3.2823230000 -1.7960580000 -1.4520450000
C -2.1693980000 -2.2912580000 0.6353260000
C -3.3999970000 -2.3122590000 1.2865660000
H -1.2572320000 -2.4905370000 1.1924330000
C -4.5747420000 -2.0660590000 0.5731040000
H -3.4419420000 -2.5227340000 2.3503770000
C -4.5122300000 -1.8102210000 -0.7968850000
H -3.2352560000 -1.5923990000 -2.5180340000
H -5.5334310000 -2.0808280000 1.0813360000
H -5.4219010000 -1.6213380000 -1.3577650000
B 3.6078500000 1.8536660000 -0.0763440000
F 4.9674080000 1.6516550000 0.0101420000
F 3.0801440000 2.4213880000 1.0717820000
F 3.2506750000 2.5649820000 -1.2125780000
H 4.2412110000 -1.5459330000 -0.6675540000
H 3.3600480000 -2.7449950000 -1.6389850000
H 4.3222540000 -3.2656770000 -0.2433370000
H 2.0043000000 -1.8445900000 2.3732840000
H 3.4335660000 -1.0084560000 1.7236540000
H 3.5221980000 -2.7269350000 2.1309790000
H 0.8628570000 -3.6824830000 1.0097850000
H 2.4409940000 -4.4524240000 0.7750950000
H 1.4345970000 -4.0542090000 -0.6285330000
C -1.5909740000 1.9141050000 0.2334480000
H -0.7521730000 -0.0238930000 0.6381670000
C -1.4248010000 3.2688230000 -0.1042780000
C -2.8735150000 1.4405750000 0.5567810000
C -2.5197990000 4.1224740000 -0.1184090000
C -3.9703570000 2.2964580000 0.5314290000
C -3.7938780000 3.6381930000 0.1955230000
H -3.0057080000 0.3920510000 0.8145930000

H -0.4408570000 3.6588210000 -0.3439720000
H -4.9577670000 1.9176130000 0.7742520000
H -2.3845100000 5.1682460000 -0.3732870000
H -4.6459290000 4.3103200000 0.1797240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392740 (Hartree/Particle)
Thermal correction to Energy= 0.418428
Thermal correction to Enthalpy= 0.419372
Thermal correction to Gibbs (Free) Energy= 0.335154
Sum of electronic and zero-point Energies= -1250.528838
Sum of electronic and thermal Energies= -1250.503150
Sum of electronic and thermal Enthalpies= -1250.502206
Sum of electronic and thermal (Free) Energies= -1250.586424

ccTS

C 1.0552160000 1.4912360000 -0.9863660000
C -0.0856050000 1.0690770000 -0.4429540000
C 2.3719120000 1.4608580000 -0.3422550000
H 1.0101120000 1.8205950000 -2.0258970000
C -1.4329970000 1.1261960000 -0.2686950000
C 3.5086730000 1.1550010000 -1.1047240000
C 2.5119030000 1.7336440000 1.0261500000
C -2.0185500000 -0.1719650000 -0.0168750000
C -2.2393470000 2.4219940000 -0.2570750000
C 4.7576210000 1.0803300000 -0.4974370000
H 3.4026830000 0.9529610000 -2.1670280000
C 3.7669900000 1.6761850000 1.6266820000
H 1.6392910000 2.0177310000 1.6092680000
C -1.0508600000 -1.1680730000 0.1973730000
O -3.3026940000 -0.3446140000 -0.0682810000
C -1.3235360000 3.6438560000 -0.3847800000
C -3.0294520000 2.5230300000 1.0587250000
C -3.2049990000 2.3961570000 -1.4589260000
C 4.8883150000 1.3384090000 0.8690200000
H 5.6306010000 0.8230720000 -1.0884790000
H 3.8693460000 1.8966100000 2.6843540000
C 0.2454510000 -0.7282800000 0.5075770000
H -1.2715760000 -2.2142950000 0.0125910000
B -3.9293390000 -1.6634680000 0.3047560000
H -0.7713250000 3.6372740000 -1.3294040000
H -0.6011770000 3.6928070000 0.4363310000
H -1.9356650000 4.5499780000 -0.3570310000
H -3.6034350000 3.4550260000 1.0616400000
H -2.3494380000 2.5392720000 1.9167460000
H -3.7255960000 1.6902950000 1.1756950000
H -2.6509190000 2.3244990000 -2.4002560000
H -3.7773610000 3.3293950000 -1.4690130000
H -3.9034090000 1.5604100000 -1.3948870000
H 5.8652320000 1.2878300000 1.3391060000
H 0.3782470000 -0.0482180000 1.3524260000
C 1.4306430000 -1.5188200000 0.1550800000
F -5.2991550000 -1.4582450000 0.2750160000
F -3.4896480000 -2.0261530000 1.5792240000
F -3.5377370000 -2.6269860000 -0.6303530000
C 1.4852800000 -2.2024600000 -1.0681580000
C 2.5279500000 -1.5688290000 1.0248390000
C 2.6197270000 -2.9298630000 -1.4114400000
H 0.6457750000 -2.1373460000 -1.7558960000
C 3.6594490000 -2.3031610000 0.6838110000
H 2.4893670000 -1.0326600000 1.9685860000
C 3.7070390000 -2.9801950000 -0.5353150000
H 2.6623330000 -3.4504960000 -2.3623820000
H 4.5051460000 -2.3402160000 1.3627140000
H 4.5939440000 -3.5437840000 -0.8072580000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.391635 (Hartree/Particle)
Thermal correction to Energy= 0.416286
Thermal correction to Enthalpy= 0.417230
Thermal correction to Gibbs (Free) Energy= 0.336632
Sum of electronic and zero-point Energies= -1250.508998
Sum of electronic and thermal Energies= -1250.484347
Sum of electronic and thermal Enthalpies= -1250.483403
Sum of electronic and thermal (Free) Energies= -1250.564001

ccPT

C -1.2332260000 1.6294090000 -0.0323450000
C -0.1434310000 0.8380460000 -0.2931000000
C 1.2200810000 1.1692500000 -0.0121110000
C 2.0173740000 -0.0267880000 -0.1837310000
C 1.2066320000 -1.0452090000 -0.6245430000
C -0.2006310000 -0.6030920000 -0.7791020000
C 1.8741530000 2.4885770000 0.3283390000
O 3.3157200000 -0.0656550000 0.0485690000
C 0.9518230000 3.7098620000 0.4284120000
C 2.9002030000 2.7820110000 -0.7969750000
C 2.6049410000 2.3347240000 1.6843460000
H 1.5367610000 -2.0556260000 -0.8344340000
C -2.6337640000 1.3573120000 -0.2833140000
H -1.0608830000 2.5495210000 0.5090940000
C -3.5687050000 2.0047010000 0.5510140000
C -4.9289990000 1.7669580000 0.4104210000
C -5.3815330000 0.9083110000 -0.5936700000
C -4.4715620000 0.2966570000 -1.4589120000
C -3.1086840000 0.5142480000 -1.3068390000
H -3.2119080000 2.6789610000 1.3244670000
H -5.6363340000 2.2544070000 1.0725120000
H -6.4450670000 0.7283890000 -0.7132460000
H -4.8272610000 -0.3474730000 -2.2559870000
H -2.4186070000 0.0645470000 -2.0100390000
B 4.0760720000 -1.3130090000 -0.2186290000
F 5.4040650000 -1.0471860000 0.0982710000
F 3.9445500000 -1.6624090000 -1.5729440000
F 3.5715110000 -2.3552150000 0.5757550000
H 1.8881060000 2.1177820000 2.4823360000
H 3.0948210000 3.2857300000 1.9147690000
H 3.3581720000 1.5484870000 1.6545280000
H 3.4249850000 3.7077130000 -0.5425160000
H 2.3871700000 2.9310580000 -1.7520720000
H 3.6331590000 1.9830960000 -0.9020230000
H 0.3026100000 3.6722370000 1.3075320000
H 0.3478210000 3.8537900000 -0.4722410000
H 1.5856030000 4.5936430000 0.5428160000
H -0.4416140000 -0.6141800000 -1.8522290000
C -1.1504000000 -1.5366850000 -0.0451060000
C -1.2788470000 -1.4685970000 1.3449240000
C -1.8632420000 -2.5073380000 -0.7510180000
C -2.1269980000 -2.3456500000 2.0163290000
C -2.8466090000 -3.3072540000 1.3046850000
C -2.7089980000 -3.3900170000 -0.0798230000
H -0.7206410000 -0.7202320000 1.9032850000
H -2.2254020000 -2.2794630000 3.0951390000
H -3.5091980000 -3.9889130000 1.8281990000
H -1.7644530000 -2.5696810000 -1.8322990000
H -3.2625740000 -4.1368250000 -0.6400150000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395080 (Hartree/Particle)
Thermal correction to Energy= 0.419663
Thermal correction to Enthalpy= 0.420607
Thermal correction to Gibbs (Free) Energy= 0.338565
Sum of electronic and zero-point Energies= -1250.540533
Sum of electronic and thermal Energies= -1250.515950
Sum of electronic and thermal Enthalpies= -1250.515006
Sum of electronic and thermal (Free) Energies= -1250.597049

RMP2/6-31+G(d,p)

1a

cRT

C 3.5637830000 -0.1877080000 -0.0336200000
C 2.3615170000 0.2831310000 -0.2723880000
C 1.1637890000 0.8329420000 -0.4578060000
C -0.0408750000 0.0331020000 -0.2077090000
C -0.0373640000 -1.4323310000 -0.2174040000
C 0.7401720000 -2.1358300000 -1.0631760000
H -0.7572220000 -1.9226760000 0.4228540000
C 0.9726840000 2.2920190000 -0.7999520000
O -1.0931180000 0.6952750000 0.0232370000
H 1.9357750000 2.7571720000 -0.9965670000
H 0.4812180000 2.8074010000 0.0246680000
H 0.3351010000 2.3917790000 -1.6783070000
B -2.5790150000 0.0251580000 0.3012350000
F -3.3830700000 1.1272170000 0.3971670000
F -2.4167720000 -0.6859720000 1.4800600000

F -2.8057710000 -0.7761730000 -0.8023120000
C 4.2270670000 -0.1463250000 1.3187410000
H 4.1075960000 -0.6510370000 -0.8524930000
H 3.5931070000 0.3536840000 2.0479110000
H 5.1770970000 0.3849710000 1.2554890000
H 4.4321810000 -1.1585200000 1.6687680000
H 1.4029890000 -1.6553810000 -1.7684810000
H 0.6780710000 -3.2150330000 -1.0902620000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173003 (Hartree/Particle)
Thermal correction to Energy= 0.187755
Thermal correction to Enthalpy= 0.188699
Thermal correction to Gibbs (Free) Energy= 0.130485
Sum of electronic and zero-point Energies= -708.501495
Sum of electronic and thermal Energies= -708.486744
Sum of electronic and thermal Enthalpies= -708.485800
Sum of electronic and thermal (Free) Energies= -708.544014

cTS

C 3.4610270000 -0.4281440000 -0.0425570000
C 2.1934890000 -0.1169150000 -0.3027060000
C 1.1210130000 0.7237450000 -0.3469880000
C -0.1512470000 0.0811980000 -0.1220850000
C -0.0257270000 -1.3485710000 -0.0912320000
C 1.0632350000 -1.8814720000 -0.7580500000
C 1.1857840000 2.1842340000 -0.6819770000
O -1.2032920000 0.7835680000 0.0790270000
H 2.2143890000 2.5242100000 -0.7743970000
H 0.6839210000 2.7422310000 0.1101060000
H 0.6468280000 2.3859890000 -1.6084540000
H -0.6630910000 -1.9399110000 0.5534720000
B -2.6045230000 0.0401870000 0.2043190000
F -2.6806630000 -0.8008390000 -0.9096010000
F -3.5351060000 1.0503290000 0.2167260000
F -2.5345920000 -0.6921060000 1.3937350000
H 3.9485360000 -1.1992120000 -0.6304900000
C 4.2338250000 0.1857940000 1.0936650000
H 3.6568990000 0.9679050000 1.5832490000
H 5.1660140000 0.6120700000 0.7199340000
H 4.4899560000 -0.5733530000 1.8346070000
H 1.4151920000 -2.8751390000 -0.4985150000
H 1.3551580000 -1.5299470000 -1.7394800000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172401 (Hartree/Particle)
Thermal correction to Energy= 0.186121
Thermal correction to Enthalpy= 0.187065
Thermal correction to Gibbs (Free) Energy= 0.131342
Sum of electronic and zero-point Energies= -708.481327
Sum of electronic and thermal Energies= -708.467608
Sum of electronic and thermal Enthalpies= -708.466663
Sum of electronic and thermal (Free) Energies= -708.522386

cPT

C 3.4224220000 -0.5612540000 0.0124470000
C 2.0568570000 -0.5673380000 -0.0365020000
C 1.1361970000 0.5215480000 -0.0367630000
C -0.2044630000 0.0222970000 0.0033800000
C -0.1398520000 -1.3894980000 -0.0045870000
C 1.2602070000 -1.8506570000 -0.0546340000
C 1.4012990000 1.9814540000 -0.0948950000
O -1.2334380000 0.8087950000 0.0304270000
H 1.6852920000 2.3547640000 0.8938530000
H 0.4886630000 2.4953580000 -0.3924070000
H 2.2063030000 2.2163300000 -0.7890920000
H -1.0073740000 -2.0331210000 0.0222600000
B -2.6377680000 0.1472370000 0.0187520000
F -2.6938220000 -0.6478810000 -1.1430220000
F -3.5452240000 1.1840130000 0.0234340000
F -2.7069430000 -0.6696090000 1.1638100000
H 3.9030820000 -1.5359760000 -0.0254740000
C 4.3318490000 0.6206560000 0.1062150000
H 3.8922300000 1.4383870000 0.6707790000
H 4.5806780000 0.9935860000 -0.8918070000
H 5.2668230000 0.3325020000 0.5836810000
H 1.5070870000 -2.5029120000 0.7914610000
H 1.4603550000 -2.4274180000 -0.9663910000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.174435 (Hartree/Particle)
Thermal correction to Energy= 0.188001
Thermal correction to Enthalpy= 0.188945
Thermal correction to Gibbs (Free) Energy= 0.133449
Sum of electronic and zero-point Energies= -708.523244
Sum of electronic and thermal Energies= -708.509678
Sum of electronic and thermal Enthalpies= -708.508733
Sum of electronic and thermal (Free) Energies= -708.564230

ccRT

C -3.4685630000 0.1195080000 0.7462570000
C -2.2915800000 0.5140120000 0.3189760000
C -1.1075540000 0.9775360000 -0.0740470000
C 0.0655550000 0.1005040000 0.0057430000
C -0.0379670000 -1.3604860000 0.0675060000
C -0.9901290000 -2.0383820000 -0.6023340000
H 0.7439250000 -1.8775670000 0.6060190000
C -0.8792300000 2.4136410000 -0.4825320000
O 1.1840270000 0.6900900000 0.0259860000
H -1.8292390000 2.9396980000 -0.5398940000
H -0.3812430000 2.4551710000 -1.4511000000
H -0.2331770000 2.9084880000 0.2420400000
B 2.6469310000 -0.0792940000 0.0771700000
F 3.5281830000 0.9620900000 -0.0177300000
F 2.6231010000 -0.9326510000 -1.0104900000
F 2.6444750000 -0.7356030000 1.2980050000
C -4.5196770000 -0.5164580000 -0.1241170000
H -3.6874900000 0.2406720000 1.8040020000
H -4.7040570000 -1.5431210000 0.1959660000
H -4.2132120000 -0.5232630000 -1.1683620000
H -5.4587170000 0.0313700000 -0.0432900000
H -1.7265840000 -1.5400060000 -1.2162600000
H -1.0040260000 -3.1194730000 -0.5836390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172982 (Hartree/Particle)
Thermal correction to Energy= 0.187722
Thermal correction to Enthalpy= 0.188666
Thermal correction to Gibbs (Free) Energy= 0.130534
Sum of electronic and zero-point Energies= -708.501787
Sum of electronic and thermal Energies= -708.487047
Sum of electronic and thermal Enthalpies= -708.486103
Sum of electronic and thermal (Free) Energies= -708.544236

ccTS

C -3.4195810000 0.1709210000 0.5552880000
C -2.1637180000 0.3043390000 0.1332690000
C -1.0040950000 1.0086000000 -0.0219810000
C 0.1929570000 0.2061870000 0.0269620000
C -0.1128350000 -1.1959130000 0.0482630000
C -1.3310540000 -1.5630050000 -0.4982930000
H 0.5102460000 -1.8844420000 0.6046070000
C -0.9195430000 2.4793980000 -0.2987460000
O 1.3440870000 0.7624620000 0.1098140000
H -1.8978250000 2.9499000000 -0.2426270000
H -0.4801040000 2.6576810000 -1.2810050000
H -0.2515700000 2.9293340000 0.4375680000
B 2.6384610000 -0.1590700000 0.0440200000
F 3.6899160000 0.7201320000 -0.0438620000
F 2.4643500000 -0.9648650000 -1.0855980000
F 2.6191250000 -0.9174710000 1.2190260000
C -4.4748190000 -0.7061010000 -0.0494480000
H -3.6782640000 0.7145460000 1.4628190000
H -4.7743690000 -1.4870840000 0.6515230000
H -4.1300060000 -1.1721510000 -0.9700310000
H -5.3624420000 -0.1142650000 -0.2771010000
H -1.6701870000 -1.1501040000 -1.4395910000
H -1.7748620000 -2.5144730000 -0.2227540000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.172302 (Hartree/Particle)
Thermal correction to Energy= 0.185999
Thermal correction to Enthalpy= 0.186944
Thermal correction to Gibbs (Free) Energy= 0.131335
Sum of electronic and zero-point Energies= -708.480760
Sum of electronic and thermal Energies= -708.467063

Sum of electronic and thermal Enthalpies= -708.466119
Sum of electronic and thermal (Free) Energies= -708.521727

ccPT

C 3.4074080000 0.3253460000 0.0000390000
C 2.0886180000 -0.0191920000 0.0000060000
C 0.9906590000 0.8917410000 -0.0000150000
C -0.2424710000 0.1731060000 -0.0000230000
C 0.0671790000 -1.2028180000 -0.0000480000
C 1.5323270000 -1.4214580000 -0.0000090000
C 1.0043060000 2.3710140000 0.0000160000
O -1.3891990000 0.7800640000 -0.0000250000
H 2.0055420000 2.7934620000 -0.0005270000
H 0.4509460000 2.7284120000 0.8717850000
H 0.4499450000 2.7284450000 -0.8710950000
H -0.6741500000 -1.9889650000 -0.0000870000
B -2.6593890000 -0.1087540000 -0.0000180000
F -3.7311900000 0.7578760000 -0.0000130000
F -2.5857510000 -0.9151170000 1.1533770000
F -2.5857660000 -0.9151200000 -1.1534110000
C 4.5464280000 -0.6345460000 0.0000850000
H 3.6608640000 1.3813800000 0.0000400000
H 4.2157080000 -1.6706220000 0.0000810000
H 5.1763090000 -0.4674490000 0.8765480000
H 5.1763700000 -0.4674610000 -0.8763380000
H 1.8532960000 -1.9909190000 0.8798750000
H 1.8533450000 -1.9909240000 -0.8798710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173811 (Hartree/Particle)
Thermal correction to Energy= 0.187775
Thermal correction to Enthalpy= 0.188719
Thermal correction to Gibbs (Free) Energy= 0.130399
Sum of electronic and zero-point Energies= -708.528268
Sum of electronic and thermal Energies= -708.514304
Sum of electronic and thermal Enthalpies= -708.513360
Sum of electronic and thermal (Free) Energies= -708.571680

RωB97X-D/6-31G(d)

6d

cRT

C -1.8605940000 -1.4345720000 0.8155190000
C -1.2680310000 -0.2706080000 0.8888670000
C -0.7373460000 0.9326240000 0.9132400000
C 0.3413380000 1.2191460000 -0.0652500000
C 1.4043370000 0.2741300000 -0.3476590000
C 1.7434440000 -0.7138180000 0.5038720000
H 1.9566290000 0.4665410000 -1.2594160000
C -1.2348570000 2.0574730000 1.8423040000
H -1.4948380000 -2.2401070000 1.4518560000
C -2.9999990000 -1.7501760000 -0.0683380000
O 0.2881700000 2.3311670000 -0.6384900000
C -2.0924590000 1.4490030000 2.9590290000
C -2.0884980000 3.0643660000 1.0488020000
C -0.0193450000 2.7650480000 2.4675720000
C -3.5598110000 -3.0299680000 -0.0303470000
C -3.5375660000 -0.7999400000 -0.9447500000
C -4.6112390000 -1.1266830000 -1.7611930000
H -3.1066540000 0.1969460000 -0.9863160000
C -5.1651210000 -2.4055100000 -1.7161590000
H -5.0175850000 -0.3810560000 -2.4377440000
C -4.6364490000 -3.3559360000 -0.8488930000
H -3.1485630000 -3.7751320000 0.6460060000
H -6.0047360000 -2.6583260000 -2.3562930000
H -5.0610770000 -4.3544110000 -0.8083290000
B 1.4922120000 3.0430040000 -1.5049660000
F 0.9296640000 4.2262850000 -1.8525650000
F 1.7460130000 2.1959460000 -2.5581390000
F 2.5158720000 3.1209560000 -0.5988840000
H 0.6242670000 3.2252130000 1.7125270000
H 0.5836170000 2.0620710000 3.0543880000
H -0.3625290000 3.5568470000 3.1420350000
H -2.9449480000 2.5615840000 0.5854880000
H -1.5095130000 3.5587630000 0.2671500000
H -2.4746910000 3.8294600000 1.7321660000
H -2.9828730000 0.9537970000 2.5580430000
H -2.4223600000 2.2415530000 3.6387260000
H -1.5273790000 0.7139840000 3.5431770000
C 2.8211650000 -1.6826060000 0.3239420000
H 1.1861940000 -0.8109010000 1.4329540000
C 3.6787260000 -1.6712430000 -0.7868160000
C 3.0001400000 -2.6682870000 1.3040360000
C 4.6795660000 -2.6235360000 -0.9091430000
C 4.0014290000 -3.6231760000 1.1798140000
C 4.8427630000 -3.6018810000 0.0714550000
H 2.3442000000 -2.6828680000 2.1709460000
H 3.5695960000 -0.9119100000 -1.5542350000
H 4.1266040000 -4.3807730000 1.9469450000
H 5.3383850000 -2.6028950000 -1.7714120000
H 5.6283570000 -4.3445200000 -0.0290460000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395505 (Hartree/Particle)
Thermal correction to Energy= 0.421495
Thermal correction to Enthalpy= 0.422439
Thermal correction to Gibbs (Free) Energy= 0.334518
Sum of electronic and zero-point Energies= -1250.550890
Sum of electronic and thermal Energies= -1250.524899
Sum of electronic and thermal Enthalpies= -1250.523955
Sum of electronic and thermal (Free) Energies= -1250.611876

cTS

C 1.7591670000 -0.3075310000 0.7213770000
C 0.4344620000 -0.3649390000 0.7264250000
C 2.6383860000 -1.1743040000 -0.0740070000
H 2.2446870000 0.4786890000 1.2980450000
C -0.7609560000 -1.0021540000 0.6101200000
C 4.0087180000 -1.1958270000 0.2107790000
C 2.1483260000 -1.9789690000 -1.1108640000
C -1.7758360000 -0.1607490000 0.0088160000
C -1.0602000000 -2.3972020000 1.1536550000
C 4.8652570000 -2.0246800000 -0.5040600000
H 4.4004750000 -0.5650270000 1.0044580000
C 3.0059070000 -2.8046130000 -1.8249380000
H 1.0934300000 -1.9395360000 -1.3658660000
C -1.3456890000 1.1899600000 -0.0708380000
O -2.8733740000 -0.6323030000 -0.4321370000
C 0.1478830000 -2.9769230000 1.8993620000
C -1.4138440000 -3.3192430000 -0.0320280000
C -2.2571710000 -2.3110740000 2.1202480000
C 4.3659440000 -2.8335450000 -1.5212400000
H 5.9248390000 -2.0369350000 -0.2679990000
H 2.6133860000 -3.4211510000 -2.6276110000
C -0.2967090000 1.5626800000 0.7669290000
H -1.7516340000 1.8437730000 -0.8341300000
B -4.0190640000 0.3587500000 -0.9045760000
H 0.4376520000 -2.3483740000 2.7481600000
H 1.0168440000 -3.0904940000 1.2436930000
H -0.1120050000 -3.9675190000 2.2866680000
H -1.6784970000 -4.3097900000 0.3542720000
H -0.5576700000 -3.4404750000 -0.7042520000
H -2.2610520000 -2.9317280000 -0.6011910000
H -2.0281660000 -1.6539810000 2.9669210000
H -2.4758900000 -3.3081030000 2.5176890000
H -3.1535930000 -1.9380080000 1.6201670000
H 5.0351600000 -3.4785040000 -2.0821760000
H -0.3661690000 1.3201190000 1.8268060000
C 0.6126640000 2.6778230000 0.4647870000
F -4.1995810000 1.2352320000 0.1480890000
F -5.0837740000 -0.4523390000 -1.1540770000
F -3.5194520000 1.0005350000 -2.0277220000
C 0.9002430000 3.0363060000 -0.8577700000
C 1.2354800000 3.3684190000 1.5100980000
C 1.7723610000 4.0824480000 -1.1255760000
H 0.4474560000 2.4821100000 -1.6751180000
C 2.1100120000 4.4151820000 1.2417060000
H 1.0199790000 3.0915080000 2.5394070000
C 2.3769560000 4.7740030000 -0.0767270000
H 1.9884300000 4.3554090000 -2.1535640000
H 2.5806630000 4.9515270000 2.0596300000
H 3.0610820000 5.5899040000 -0.2888090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395139 (Hartree/Particle)
Thermal correction to Energy= 0.419814

Thermal correction to Enthalpy= 0.420758
Thermal correction to Gibbs (Free) Energy= 0.338775
Sum of electronic and zero-point Energies= -1250.527838
Sum of electronic and thermal Energies= -1250.503163
Sum of electronic and thermal Enthalpies= -1250.502219
Sum of electronic and thermal (Free) Energies= -1250.584202

cPT

C -1.6583380000 0.8744220000 -0.7025820000
C -0.4582450000 0.2810640000 -0.8940880000
C 0.0043780000 -1.0613240000 -0.6541680000
C 1.4148660000 -1.0018340000 -0.3796380000
C 1.8715680000 0.2215770000 -0.8434510000
C 0.7770610000 1.1228730000 -1.2552940000
C -0.6887150000 -2.3893780000 -0.8702510000
C -2.7934830000 0.3685690000 0.0643730000
O 2.1021990000 -1.9736990000 0.1260610000
C -2.1105490000 -2.3002000000 -1.4413320000
C -0.6958310000 -3.2085590000 0.4405830000
C 0.1843990000 -3.1392600000 -1.9178020000
C -4.1051890000 0.6109350000 -0.3642140000
C -2.5831350000 -0.3152490000 1.2688760000
C -3.6621570000 -0.7981980000 1.9998380000
H -1.5700580000 -0.4412770000 1.6389910000
C -4.9603720000 -0.5979490000 1.5387940000
H -3.4881990000 -1.3244540000 2.9331180000
C -5.1800830000 0.1124990000 0.3587770000
H -4.2756270000 1.1643600000 -1.2835920000
H -5.8033060000 -0.9784410000 2.1071950000
H -6.1928300000 0.2816830000 0.0066840000
B 3.4751260000 -1.6005360000 0.7548010000
F 4.3169800000 -1.2240100000 -0.2865770000
F 3.8864050000 -2.7204760000 1.4172640000
F 3.2223600000 -0.5147740000 1.5979840000
H -1.7441060000 1.9064080000 -1.0429470000
H 2.9203350000 0.4886040000 -0.8818950000
H 0.7714550000 1.2298190000 -2.3509290000
C 0.8718420000 2.4942120000 -0.6199770000
C 1.3718310000 2.6236560000 0.6789040000
C 0.4470010000 3.6304180000 -1.3080410000
H 0.2024940000 -2.5968410000 -2.8693880000
H -0.2608210000 -4.1229740000 -2.0965160000
H 1.2069410000 -3.2808100000 -1.5652870000
H -1.0818250000 -4.2095580000 0.2198390000
H -1.3556000000 -2.7511960000 1.1831600000
H 0.3084940000 -3.3026850000 0.8572210000
H -2.1699980000 -1.5978360000 -2.2796860000
H -2.8481500000 -2.0113260000 -0.6927100000
H -2.3950580000 -3.2890570000 -1.8147990000
C 1.4344240000 3.8761360000 1.2789980000
C 0.9961970000 5.0065870000 0.5925870000
C 0.5040120000 4.8830340000 -0.7031180000
H 0.0756020000 3.5371760000 -2.3265380000
H 1.0468990000 5.9832520000 1.0641660000
H 0.1726430000 5.7620070000 -1.2477860000
H 1.7348710000 1.7454140000 1.2096890000
H 1.8320090000 3.9691710000 2.2848320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397914 (Hartree/Particle)
Thermal correction to Energy= 0.422236
Thermal correction to Enthalpy= 0.423180
Thermal correction to Gibbs (Free) Energy= 0.342795
Sum of electronic and zero-point Energies= -1250.551616
Sum of electronic and thermal Energies= -1250.527294
Sum of electronic and thermal Enthalpies= -1250.526350
Sum of electronic and thermal (Free) Energies= -1250.606735

ccRT

C -0.8123570000 -2.0179790000 -1.4550450000
C 0.3112020000 -1.7033030000 -0.8646690000
C 1.4270880000 -1.3506900000 -0.2616730000
C 1.7712230000 0.0953840000 -0.2792560000
C 0.7589910000 1.1362940000 -0.2729510000
C -0.4817630000 0.9562540000 0.2187950000
H 1.0918680000 2.0950100000 -0.6530850000
C 2.3887230000 -2.3694390000 0.3795370000
H -0.8045130000 -2.2072600000 -2.5275790000
C -2.1163580000 -2.0604790000 -0.7604790000
O 2.9902240000 0.3784530000 -0.3242140000
C 1.6880670000 -3.7298720000 0.4950820000
C 2.7699760000 -1.8846420000 1.7897050000
C 3.6506250000 -2.5361940000 -0.4879590000
C -3.2905960000 -1.8330700000 -1.4843950000
C -2.2045410000 -2.2822810000 0.6191310000
C -3.4373310000 -2.2587180000 1.2611650000
H -1.2994390000 -2.4804830000 1.1870510000
C -4.6009170000 -2.0161210000 0.5335940000
H -3.4899240000 -2.4347120000 2.3312340000
C -4.5232570000 -1.8056970000 -0.8408100000
H -3.2341780000 -1.6598440000 -2.5555890000
H -5.5637640000 -1.9992260000 1.0347780000
H -5.4253670000 -1.6184900000 -1.4151150000
B 3.6490920000 1.8756920000 -0.1325040000
F 4.9765810000 1.6073430000 -0.1968470000
F 3.1883520000 2.2744430000 1.0927260000
F 3.1606470000 2.6228690000 -1.1781310000
H 4.2205870000 -1.6086800000 -0.5557210000
H 3.3831480000 -2.8578230000 -1.5005420000
H 4.2931630000 -3.3065700000 -0.0463660000
H 1.8790860000 -1.7685080000 2.4181580000
H 3.3044850000 -0.9317720000 1.7656750000
H 3.4232220000 -2.6237300000 2.2659340000
H 0.7863780000 -3.6702380000 1.1151510000
H 2.3677910000 -4.4506720000 0.9610700000
H 1.4002870000 -4.1218660000 -0.4858230000
C -1.5521900000 1.9498900000 0.2451390000
H -0.7491580000 -0.0097440000 0.6382690000
C -1.3287340000 3.3154180000 0.0157090000
C -2.8589280000 1.5054720000 0.4893810000
C -2.3913940000 4.2075570000 0.0195720000
C -3.9219110000 2.3996570000 0.4819810000
C -3.6898120000 3.7519290000 0.2473300000
H -3.0401210000 0.4495500000 0.6710450000
H -0.3200000000 3.6833100000 -0.1444670000
H -4.9301010000 2.0396970000 0.6623680000
H -2.2077060000 5.2636580000 -0.1511390000
H -4.5180480000 4.4542020000 0.2478870000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395977 (Hartree/Particle)
Thermal correction to Energy= 0.421704
Thermal correction to Enthalpy= 0.422648
Thermal correction to Gibbs (Free) Energy= 0.337432
Sum of electronic and zero-point Energies= -1250.555432
Sum of electronic and thermal Energies= -1250.529705
Sum of electronic and thermal Enthalpies= -1250.528761
Sum of electronic and thermal (Free) Energies= -1250.613977

ccTS

C 1.0350090000 1.5169840000 -0.9679490000
C -0.0940510000 1.0552650000 -0.4338620000
C 2.3552830000 1.4722510000 -0.3285230000
H 0.9840440000 1.8974100000 -1.9884860000
C -1.4440050000 1.1290330000 -0.2800270000
C 3.4885050000 1.1367480000 -1.0779340000
C 2.4982760000 1.7502410000 1.0360780000
C -2.0487130000 -0.1658410000 -0.0487290000
C -2.2448600000 2.4273930000 -0.2634990000
C 4.7313970000 1.0428330000 -0.4663850000
H 3.3839130000 0.9176950000 -2.1368050000
C 3.7462970000 1.6695120000 1.6438420000
H 1.6276640000 2.0534610000 1.6118450000
C -1.0588130000 -1.1631340000 0.1386650000
O -3.3080390000 -0.3467030000 -0.0976100000
C -1.3326100000 3.6557510000 -0.3685740000
C -3.0524820000 2.5131680000 1.0452920000
C -3.2019230000 2.4064900000 -1.4742340000
C 4.8627310000 1.3066120000 0.8958510000
H 5.6006830000 0.7613280000 -1.0523480000
H 3.8475560000 1.8950440000 2.7011280000
C 0.2187730000 -0.7238720000 0.4896110000
H -1.2715780000 -2.1945790000 -0.1175950000
B -3.9157920000 -1.7468210000 0.3376080000
H -0.7706730000 3.6687130000 -1.3081980000
H -0.6148320000 3.7013910000 0.4576210000
H -1.9458580000 4.5620550000 -0.3339830000

H -3.6360590000 3.4402030000 1.0530580000
H -2.3849420000 2.5277190000 1.9144160000
H -3.7425310000 1.6732070000 1.1479780000
H -2.6418060000 2.3539230000 -2.4145360000
H -3.7914990000 3.3299600000 -1.4816210000
H -3.8868630000 1.5578550000 -1.4251630000
H 5.8369110000 1.2400660000 1.3705110000
H 0.3338890000 -0.0847860000 1.3663530000
C 1.4174060000 -1.5057820000 0.1410970000
F -5.2620250000 -1.5415090000 0.3410490000
F -3.3731590000 -2.0090950000 1.5811900000
F -3.4822970000 -2.6554670000 -0.6147320000
C 1.5070610000 -2.1343260000 -1.1056900000
C 2.4925630000 -1.5926790000 1.0296100000
C 2.6505080000 -2.8416300000 -1.4535090000
H 0.6822090000 -2.0467010000 -1.8080990000
C 3.6351250000 -2.3024560000 0.6836540000
H 2.4342130000 -1.0946470000 1.9926340000
C 3.7160420000 -2.9252260000 -0.5591640000
H 2.7142970000 -3.3235770000 -2.4241030000
H 4.4647710000 -2.3635290000 1.3806910000
H 4.6119650000 -3.4738620000 -0.8337560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394801 (Hartree/Particle)
Thermal correction to Energy= 0.419360
Thermal correction to Enthalpy= 0.420304
Thermal correction to Gibbs (Free) Energy= 0.339659
Sum of electronic and zero-point Energies= -1250.527617
Sum of electronic and thermal Energies= -1250.503058
Sum of electronic and thermal Enthalpies= -1250.502114
Sum of electronic and thermal (Free) Energies= -1250.582758

ccPT

C -1.2103100000 1.6479280000 0.0251950000
C -0.1318200000 0.8617550000 -0.2366290000
C 1.2468910000 1.1546970000 0.0491170000
C 2.0284240000 -0.0371510000 -0.1508400000
C 1.1810840000 -1.0340920000 -0.6130320000
C -0.2142460000 -0.5727080000 -0.7492940000
C 1.9251730000 2.4530240000 0.4310020000
O 3.3023580000 -0.1084400000 0.0624920000
C 1.0227710000 3.6865260000 0.5716750000
C 2.9639680000 2.7622920000 -0.6786340000
C 2.6502440000 2.2335140000 1.7818720000
H 1.4976720000 -2.0466230000 -0.8253990000
C -2.6108920000 1.3725760000 -0.2772890000
H -1.0510840000 2.5582810000 0.5874060000
C -3.5783420000 1.7841920000 0.6532240000
C -4.9240730000 1.5259430000 0.4380170000
C -5.3304710000 0.8864120000 -0.7315910000
C -4.3863080000 0.5120230000 -1.6833810000
C -3.0368250000 0.7489680000 -1.4582630000
H -3.2622500000 2.2886660000 1.5624330000
H -5.6582930000 1.8303130000 1.1770030000
H -6.3843030000 0.6938330000 -0.9070980000
H -4.7019430000 0.0363490000 -2.6064970000
H -2.3128730000 0.4860500000 -2.2213570000
B 4.0554600000 -1.4002600000 -0.3602780000
F 5.3702490000 -1.1536020000 -0.0807760000
F 3.7932240000 -1.5746370000 -1.7157270000
F 3.5111000000 -2.4430740000 0.3821670000
H 1.9289240000 2.0107980000 2.5761580000
H 3.1751130000 3.1566800000 2.0498330000
H 3.3758830000 1.4222710000 1.7202390000
H 3.5156610000 3.6650270000 -0.3956970000
H 2.4626410000 2.9554780000 -1.6332740000
H 3.6752760000 1.9460480000 -0.8056040000
H 0.3595210000 3.6238400000 1.4408430000
H 0.4291950000 3.8784320000 -0.3280050000
H 1.6640340000 4.5591580000 0.7308500000
H -0.4799470000 -0.5685390000 -1.8160190000
C -1.1718130000 -1.4896920000 -0.0054630000
C -1.1074350000 -1.5777710000 1.3863730000
C -2.0877360000 -2.2798430000 -0.6956290000
C -1.9624860000 -2.4271010000 2.0767990000
C -2.8845350000 -3.2068480000 1.3812970000
C -2.9429810000 -3.1347410000 -0.0061730000
H -0.3825370000 -0.9768520000 1.9301500000
H -1.9044950000 -2.4868140000 3.1592570000
H -3.5511030000 -3.8725340000 1.9209540000
H -2.1376780000 -2.2250100000 -1.7802620000
H -3.6544360000 -3.7436400000 -0.5555470000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397911 (Hartree/Particle)
Thermal correction to Energy= 0.422433
Thermal correction to Enthalpy= 0.423377
Thermal correction to Gibbs (Free) Energy= 0.340581
Sum of electronic and zero-point Energies= -1250.556336
Sum of electronic and thermal Energies= -1250.531814
Sum of electronic and thermal Enthalpies= -1250.530870
Sum of electronic and thermal (Free) Energies= -1250.613666

RωB97X-D/6-31G(d)/ SCRF=(PCM, CH_2Cl_2, ε = 8.93)

6d

cRT

C -1.7945900000 -1.3811660000 0.8582890000
C -1.2357420000 -0.2003990000 0.8938520000
C -0.7387510000 1.0211710000 0.8887560000
C 0.3725840000 1.2807070000 -0.0467490000
C 1.3985410000 0.3045780000 -0.3210390000
C 1.7116790000 -0.6811120000 0.5501570000
H 1.9547790000 0.4549660000 -1.2380990000
C -1.3236980000 2.1607780000 1.7475710000
H -1.4235420000 -2.1418730000 1.5444380000
C -2.8950440000 -1.7714770000 -0.0452980000
O 0.3724300000 2.4121370000 -0.6129780000
C -2.2395180000 1.5628370000 2.8237620000
C -2.1505110000 3.1215890000 0.8730150000
C -0.1738940000 2.9176850000 2.4350220000
C -3.3782670000 -3.0827500000 -0.0014570000
C -3.4698890000 -0.8635070000 -0.9436140000
C -4.5053700000 -1.2628300000 -1.7783410000
H -3.1014690000 0.1580840000 -0.9869530000
C -4.9826950000 -2.5728350000 -1.7287800000
H -4.9427570000 -0.5499070000 -2.4705320000
C -4.4165860000 -3.4809800000 -0.8386690000
H -2.9374800000 -3.7939200000 0.6920250000
H -5.7927680000 -2.8821280000 -2.3820040000
H -4.7821380000 -4.5023020000 -0.7942610000
B 1.5349710000 3.0417270000 -1.4710760000
F 1.0471210000 4.2792740000 -1.8035980000
F 1.7292950000 2.2280980000 -2.5729710000
F 2.6347950000 3.0876770000 -0.6425050000
H 0.5001390000 3.3852240000 1.7118540000
H 0.4119820000 2.2442840000 3.0708180000
H -0.5851490000 3.7097950000 3.0697820000
H -2.9564230000 2.5822930000 0.3629250000
H -1.5339400000 3.6186880000 0.1223630000
H -2.6057240000 3.8884620000 1.5100310000
H -3.0925590000 1.0394640000 2.3796090000
H -2.6273640000 2.3670730000 3.4573610000
H -1.6985120000 0.8559680000 3.4623460000
C 2.7361090000 -1.7018480000 0.3732960000
H 1.1799740000 -0.7224000000 1.4975670000
C 3.4933380000 -1.8279560000 -0.8031130000
C 2.9622420000 -2.6022770000 1.4253040000
C 4.4493670000 -2.8262220000 -0.9163070000
C 3.9206380000 -3.6017360000 1.3101960000
C 4.6653550000 -3.7141440000 0.1389270000
H 2.3802170000 -2.5137380000 2.3387180000
H 3.3354290000 -1.1475360000 -1.6334580000
H 4.0861070000 -4.2910990000 2.1317090000
H 5.0292270000 -2.9155190000 -1.8291690000
H 5.4149860000 -4.4936840000 0.0451140000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395226 (Hartree/Particle)
Thermal correction to Energy= 0.421058
Thermal correction to Enthalpy= 0.422002
Thermal correction to Gibbs (Free) Energy= 0.335149
Sum of electronic and zero-point Energies= -1250.567482
Sum of electronic and thermal Energies= -1250.541651
Sum of electronic and thermal Enthalpies= -1250.540707
Sum of electronic and thermal (Free) Energies= -1250.627560

cTS

C 1.7540890000 -0.3750090000 0.7280540000
C 0.4306580000 -0.4058570000 0.7167810000
C 2.6246780000 -1.2458880000 -0.0716880000
H 2.2462210000 0.3857270000 1.3323680000
C -0.7929330000 -0.9804110000 0.5969980000
C 3.9953300000 -1.2755870000 0.2139540000
C 2.1258760000 -2.0472400000 -1.1077580000
C -1.7632440000 -0.0930930000 -0.0043560000
C -1.1480650000 -2.3622620000 1.1465410000
C 4.8451580000 -2.1107030000 -0.5028150000
H 4.3917830000 -0.6478810000 1.0072420000
C 2.9772540000 -2.8786840000 -1.8232030000
H 1.0712750000 -2.0014600000 -1.3631390000
C -1.3041230000 1.2377270000 -0.0737790000
O -2.8853550000 -0.5363210000 -0.4588460000
C 0.0395370000 -2.9819430000 1.8938070000
C -1.5316370000 -3.2799140000 -0.0325370000
C -2.3365750000 -2.2280770000 2.1170480000
C 4.3381680000 -2.9158090000 -1.5202330000
H 5.9047840000 -2.1303420000 -0.2683600000
H 2.5802280000 -3.4931770000 -2.6249850000
C -0.2366710000 1.5831550000 0.7563570000
H -1.6999280000 1.9164240000 -0.8199480000
B -4.0099180000 0.4158280000 -0.8828990000
H 0.3514300000 -2.3606220000 2.7396310000
H 0.9023220000 -3.1272410000 1.2359450000
H -0.2552840000 -3.9618870000 2.2827470000
H -1.8169640000 -4.2620120000 0.3600840000
H -0.6843280000 -3.4224750000 -0.7113480000
H -2.3728570000 -2.8760140000 -0.5989760000
H -2.0802420000 -1.5733370000 2.9571470000
H -2.5893320000 -3.2144310000 2.5204650000
H -3.2215030000 -1.8263410000 1.6181070000
H 5.0023480000 -3.5649080000 -2.0822430000
H -0.2921990000 1.3146800000 1.8109080000
C 0.7004520000 2.6692410000 0.4571150000
F -4.2697880000 1.2667120000 0.1829110000
F -5.0783200000 -0.4039700000 -1.1776480000
F -3.5743560000 1.1295870000 -1.9978620000
C 0.9675060000 3.0549660000 -0.8636960000
C 1.3697700000 3.3091080000 1.5080640000
C 1.8671990000 4.0796600000 -1.1232550000
H 0.4810690000 2.5385540000 -1.6862050000
C 2.2710980000 4.3345820000 1.2463660000
H 1.1721820000 3.0071170000 2.5333180000
C 2.5179830000 4.7213260000 -0.0689790000
H 2.0701630000 4.3740440000 -2.1478180000
H 2.7801810000 4.8307960000 2.0662010000
H 3.2242240000 5.5195310000 -0.2751990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394736 (Hartree/Particle)
Thermal correction to Energy= 0.419441
Thermal correction to Enthalpy= 0.420385
Thermal correction to Gibbs (Free) Energy= 0.338186
Sum of electronic and zero-point Energies= -1250.549682
Sum of electronic and thermal Energies= -1250.524977
Sum of electronic and thermal Enthalpies= -1250.524033
Sum of electronic and thermal (Free) Energies= -1250.606232

cPT

C -1.8456170000 0.1240700000 -0.7389280000
C -0.4876860000 0.1461040000 -0.7067430000
C 0.4817070000 -0.8455640000 -0.3670380000
C 1.6789080000 -0.1635550000 0.0726970000
C 1.5636920000 1.1671470000 -0.2596300000
C 0.2683330000 1.4699220000 -0.9074300000
C 0.4982400000 -2.3263250000 -0.6848410000
C -2.7235740000 -0.8271030000 -0.0818270000
O 2.6821180000 -0.7921850000 0.6337900000
C -0.7592200000 -2.8731230000 -1.3748660000
C 0.7869020000 -3.1591890000 0.5828060000
C 1.6714250000 -2.4949100000 -1.6972460000
C -3.9730390000 -1.1306400000 -0.6445140000
C -2.3582180000 -1.4142690000 1.1398280000
C -3.1994540000 -2.3333160000 1.7539810000
H -1.4285240000 -1.1203830000 1.6175880000
C -4.4128800000 -2.6706150000 1.1579280000
H -2.9124010000 -2.7794360000 2.7005460000
C -4.8005290000 -2.0648110000 -0.0385340000
H -4.2725420000 -0.6548890000 -1.5737480000
H -5.0688900000 -3.3912230000 1.6358510000
H -5.7532700000 -2.3177780000 -0.4920670000
B 4.0952330000 -0.2912540000 0.5069850000
F 4.4617370000 -0.3739200000 -0.8387430000
F 4.8636940000 -1.1274100000 1.2998640000
F 4.1736570000 1.0355810000 0.9491870000
H -2.3338410000 0.9833820000 -1.1980420000
H 2.3333550000 1.9082100000 -0.0903030000
H 0.4297210000 1.5575460000 -1.9929930000
C -0.4075950000 2.7259520000 -0.4044720000
C -0.5732970000 2.9276340000 0.9690120000
C -0.8846040000 3.6845460000 -1.2968630000
H 1.4371800000 -1.9858510000 -2.6382420000
H 1.7884490000 -3.5625520000 -1.9079710000
H 2.6166860000 -2.1099540000 -1.3143200000
H 0.8728440000 -4.2112200000 0.2915340000
H -0.0363190000 -3.0743840000 1.2987720000
H 1.7148830000 -2.8504970000 1.0646910000
H -1.0906760000 -2.2275050000 -2.1943420000
H -1.5901660000 -3.0170950000 -0.6840510000
H -0.5143610000 -3.8516320000 -1.7997480000
C -1.2043370000 4.0723590000 1.4404930000
C -1.6786650000 5.0287450000 0.5425800000
C -1.5184600000 4.8331490000 -0.8255590000
H -0.7584320000 3.5360890000 -2.3663150000
H -2.1713230000 5.9233340000 0.9109370000
H -1.8840700000 5.5742450000 -1.5296800000
H -0.2083120000 2.1799550000 1.6698590000
H -1.3271000000 4.2198750000 2.5090420000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397649 (Hartree/Particle)
Thermal correction to Energy= 0.421974
Thermal correction to Enthalpy= 0.422918
Thermal correction to Gibbs (Free) Energy= 0.342083
Sum of electronic and zero-point Energies= -1250.576402
Sum of electronic and thermal Energies= -1250.552077
Sum of electronic and thermal Enthalpies= -1250.551132
Sum of electronic and thermal (Free) Energies= -1250.631967

ccRT

C -0.7986510000 -1.9511300000 -1.4590190000
C 0.3257140000 -1.6412390000 -0.8708060000
C 1.4537450000 -1.3016890000 -0.2753940000
C 1.7761350000 0.1395830000 -0.2488470000
C 0.7581990000 1.1650450000 -0.2404640000
C -0.4871960000 0.9569470000 0.2399270000
H 1.0715310000 2.1331910000 -0.6126350000
C 2.4303530000 -2.3439390000 0.3050270000
H -0.7952640000 -2.1093050000 -2.5366120000
C -2.0956460000 -2.0263160000 -0.7527240000
O 3.0050580000 0.4393250000 -0.2674170000
C 1.7358400000 -3.7111770000 0.3700420000
C 2.8323660000 -1.9263260000 1.7304590000
C 3.6774260000 -2.4699020000 -0.5900040000
C -3.2765480000 -1.7762870000 -1.4591120000
C -2.1679420000 -2.2991970000 0.6189330000
C -3.3955820000 -2.3040610000 1.2726970000
H -1.2583890000 -2.5138070000 1.1735310000
C -4.5665280000 -2.0371250000 0.5647210000
H -3.4375460000 -2.5192100000 2.3358570000
C -4.5030890000 -1.7756060000 -0.8022770000
H -3.2308400000 -1.5659840000 -2.5239440000
H -5.5243780000 -2.0397180000 1.0753850000
H -5.4111780000 -1.5694670000 -1.3601620000
B 3.6317400000 1.8718590000 -0.0638480000
F 4.9813490000 1.6313150000 -0.0953740000
F 3.1817410000 2.3207660000 1.1581440000
F 3.2017750000 2.6623320000 -1.1145610000
H 4.2469600000 -1.5398890000 -0.6243020000
H 3.3929700000 -2.7445420000 -1.6116250000
H 4.3273400000 -3.2586390000 -0.1944860000
H 1.9499140000 -1.8362230000 2.3739910000
H 3.3702910000 -0.9749410000 1.7425120000

H 3.4896130000 -2.6887920000 2.1620780000
H 0.8424140000 -3.6808250000 1.0033440000
H 2.4252710000 -4.4470660000 0.7962560000
H 1.4385060000 -4.0609040000 -0.6238190000
C -1.5918250000 1.9078630000 0.2414890000
H -0.7231830000 -0.0085000000 0.6789430000
C -1.4490800000 3.2519960000 -0.1386950000
C -2.8603950000 1.4357370000 0.6107000000
C -2.5506710000 4.0951200000 -0.1513450000
C -3.9636480000 2.2798780000 0.5875340000
C -3.8098480000 3.6107360000 0.2076380000
H -2.9800850000 0.3963530000 0.9038790000
H -0.4754530000 3.6443270000 -0.4144010000
H -4.9407700000 1.8985430000 0.8663470000
H -2.4305020000 5.1340060000 -0.4411610000
H -4.6689350000 4.2743220000 0.1928400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395497 (Hartree/Particle)
Thermal correction to Energy= 0.421128
Thermal correction to Enthalpy= 0.422072
Thermal correction to Gibbs (Free) Energy= 0.337477
Sum of electronic and zero-point Energies= -1250.571427
Sum of electronic and thermal Energies= -1250.545796
Sum of electronic and thermal Enthalpies= -1250.544852
Sum of electronic and thermal (Free) Energies= -1250.629447

ccTS

C 1.0486730000 1.5047080000 -0.9882250000
C -0.0857760000 1.0640970000 -0.4532920000
C 2.3664890000 1.4734630000 -0.3472560000
H 1.0003800000 1.8540030000 -2.0201120000
C -1.4313090000 1.1212020000 -0.2807230000
C 3.5022610000 1.1695540000 -1.1075880000
C 2.5067260000 1.7382700000 1.0208870000
C -2.0207570000 -0.1789900000 -0.0536310000
C -2.2318090000 2.4220750000 -0.2453510000
C 4.7490260000 1.0905480000 -0.5005520000
H 3.3985190000 0.9696710000 -2.1702560000
C 3.7588990000 1.6745610000 1.6222280000
H 1.6340790000 2.0167840000 1.6055940000
C -1.0489760000 -1.1755520000 0.1491720000
O -3.2965880000 -0.3574610000 -0.1178780000
C -1.3129990000 3.6465720000 -0.3443150000
C -3.0253380000 2.5003070000 1.0717990000
C -3.1954310000 2.4241580000 -1.4503420000
C 4.8791350000 1.3405430000 0.8650460000
H 5.6220220000 0.8350130000 -1.0926920000
H 3.8596730000 1.8872140000 2.6818910000
C 0.2375060000 -0.7472090000 0.4910910000
H -1.2666040000 -2.2118900000 -0.0801050000
B -3.9418560000 -1.6796720000 0.3089050000
H -0.7580530000 3.6635430000 -1.2877870000
H -0.5911860000 3.6784000000 0.4786510000
H -1.9223190000 4.5548730000 -0.2972820000
H -3.6004660000 3.4321730000 1.0951470000
H -2.3480470000 2.4979140000 1.9329730000
H -3.7226190000 1.6657670000 1.1727870000
H -2.6402660000 2.3731870000 -2.3932410000
H -3.7728820000 3.3551030000 -1.4448890000
H -3.8918220000 1.5845110000 -1.4072880000
H 5.8557290000 1.2852950000 1.3358720000
H 0.3572660000 -0.0779010000 1.3445440000
C 1.4297120000 -1.5335720000 0.1534450000
F -5.3002380000 -1.4537420000 0.2343090000
F -3.5208040000 -1.9636640000 1.6013590000
F -3.5271620000 -2.6699380000 -0.5798780000
C 1.5091170000 -2.2063900000 -1.0725020000
C 2.5125970000 -1.5865300000 1.0378940000
C 2.6508500000 -2.9245420000 -1.4031220000
H 0.6817190000 -2.1415030000 -1.7739900000
C 3.6523920000 -2.3091870000 0.7087760000
H 2.4600910000 -1.0568520000 1.9838450000
C 3.7230880000 -2.9758570000 -0.5125470000
H 2.7104030000 -3.4374440000 -2.3577190000
H 4.4879110000 -2.3451680000 1.4002540000
H 4.6178330000 -3.5319270000 -0.7751670000
C 3.6270893000 1.4144898000 0.2587942000
H 3.9837438000 0.4056798000 0.2587942000
H 3.9837622000 1.9188880000 1.1324457000
H 3.9837622000 1.9188880000 -0.6148573000
H 2.5570893000 1.4145030000 0.2587942000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394305 (Hartree/Particle)
Thermal correction to Energy= 0.418963
Thermal correction to Enthalpy= 0.419907
Thermal correction to Gibbs (Free) Energy= 0.338413
Sum of electronic and zero-point Energies= -1250.549892
Sum of electronic and thermal Energies= -1250.525234
Sum of electronic and thermal Enthalpies= -1250.524290
Sum of electronic and thermal (Free) Energies= -1250.605784

ccPT

C -1.2366170000 1.6244330000 -0.0007680000
C -0.1500300000 0.8441520000 -0.2827330000
C 1.2161890000 1.1653440000 -0.0063650000
C 2.0119320000 -0.0258970000 -0.2005310000
C 1.1923840000 -1.0302820000 -0.6586230000
C -0.2127760000 -0.5892210000 -0.7914380000
C 1.8718020000 2.4819040000 0.3550990000
O 3.3024870000 -0.0722450000 0.0283250000
C 0.9517660000 3.7060420000 0.4654210000
C 2.9084170000 2.7891810000 -0.7570390000
C 2.5892910000 2.3032200000 1.7156890000
H 1.5138430000 -2.0370960000 -0.8872070000
C -2.6378610000 1.3567790000 -0.2624630000
H -1.0655430000 2.5312950000 0.5619800000
C -3.5773830000 1.9102450000 0.6274090000
C -4.9329670000 1.6666160000 0.4667420000
C -5.3765710000 0.8997100000 -0.6103470000
C -4.4618910000 0.3836950000 -1.5264920000
C -3.1030330000 0.6053060000 -1.3547250000
H -3.2306560000 2.5150160000 1.4606340000
H -5.6452980000 2.0810570000 1.1723530000
H -6.4381580000 0.7175730000 -0.7446420000
H -4.8089180000 -0.1906130000 -2.3790390000
H -2.4066230000 0.2330790000 -2.0958790000
B 4.0839680000 -1.3286550000 -0.2553780000
F 5.3951940000 -1.0361590000 0.0805150000
F 3.9569970000 -1.6431140000 -1.6112960000
F 3.5727410000 -2.3688250000 0.5260360000
H 1.8643910000 2.0840980000 2.5067810000
H 3.0941020000 3.2418670000 1.9668220000
H 3.3305880000 1.5049540000 1.6799740000
H 3.4399120000 3.7079930000 -0.4891130000
H 2.4058500000 2.9535600000 -1.7159250000
H 3.6372280000 1.9864830000 -0.8675370000
H 0.2971600000 3.6613370000 1.3411940000
H 0.3504830000 3.8620540000 -0.4357320000
H 1.5834760000 4.5904430000 0.5934080000
H -0.4717890000 -0.5858320000 -1.8595110000
C -1.1517070000 -1.5292820000 -0.0521150000
C -1.1615700000 -1.5542920000 1.3441390000
C -1.9734420000 -2.4084380000 -0.7554080000
C -1.9981270000 -2.4305920000 2.0254190000
C -2.8256640000 -3.3006880000 1.3169280000
C -2.8087350000 -3.2906840000 -0.0744890000
H -0.5172860000 -0.8778140000 1.9002630000
H -2.0027270000 -2.4365330000 3.1110660000
H -3.4796530000 -3.9844100000 1.8493580000
H -1.9667820000 -2.4011420000 -1.8424180000
H -3.4481680000 -3.9667580000 -0.6336890000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.398270 (Hartree/Particle)
Thermal correction to Energy= 0.422629
Thermal correction to Enthalpy= 0.423573
Thermal correction to Gibbs (Free) Energy= 0.342058
Sum of electronic and zero-point Energies= -1250.582774
Sum of electronic and thermal Energies= -1250.558415
Sum of electronic and thermal Enthalpies= -1250.557471
Sum of electronic and thermal (Free) Energies= -1250.638986

RωB97X-D/6-31+G(d,p)

1a

cRT

C 3.5627400000 -0.1604070000 -0.0589770000
C 2.3628500000 0.2994790000 -0.2707680000
C 1.1630560000 0.8288270000 -0.4440090000
C -0.0378570000 0.0165100000 -0.1978210000
C -0.0297640000 -1.4525990000 -0.1889810000
C 0.7358910000 -2.1783850000 -1.0076030000
H -0.7648260000 -1.9204110000 0.4572550000
C 0.9565400000 2.2904160000 -0.7710060000
O -1.0902150000 0.6604580000 0.0146420000
H 1.9159500000 2.7772250000 -0.9494760000
H 0.4443110000 2.7933400000 0.0531750000
H 0.3274480000 2.3983530000 -1.6587610000
B -2.5758150000 0.0377190000 0.2866730000
F -3.3554720000 1.1488350000 0.3845840000
F -2.4459240000 -0.6776890000 1.4605110000
F -2.8318400000 -0.7554010000 -0.8084500000
C 4.2626040000 -0.1374420000 1.2754000000
H 4.0940430000 -0.6032030000 -0.9010960000
H 3.6430240000 0.3307160000 2.0421090000
H 5.2035360000 0.4153520000 1.1972220000
H 4.5015440000 -1.1570300000 1.5924190000
H 1.4167600000 -1.7260000000 -1.7206940000
H 0.6617650000 -3.2607080000 -1.0098720000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171808 (Hartree/Particle)
Thermal correction to Energy= 0.186442
Thermal correction to Enthalpy= 0.187386
Thermal correction to Gibbs (Free) Energy= 0.129356
Sum of electronic and zero-point Energies= -710.249572
Sum of electronic and thermal Energies= -710.234938
Sum of electronic and thermal Enthalpies= -710.233994
Sum of electronic and thermal (Free) Energies= -710.292025

cTS

C 3.4467260000 -0.4352330000 -0.0370250000
C 2.1850870000 -0.1382170000 -0.2902340000
C 1.1177240000 0.7021190000 -0.3382220000
C -0.1518840000 0.0633910000 -0.1161280000
C -0.0184050000 -1.3604070000 -0.0750320000
C 1.0842070000 -1.8904470000 -0.7052260000
C 1.1961150000 2.1615860000 -0.6703890000
O -1.2014640000 0.7538350000 0.0735770000
H 0.7561110000 2.7331310000 0.1530960000
H 0.6039360000 2.3867970000 -1.5620170000
H 2.2265860000 2.4843070000 -0.8224880000
H -0.6769610000 -1.9477780000 0.5559420000
B -2.6058950000 0.0538730000 0.1931740000
F -2.7106500000 -0.7800630000 -0.9157210000
F -3.5125470000 1.0764840000 0.2085030000
F -2.5653170000 -0.6819150000 1.3748290000
H 3.9262640000 -1.2301700000 -0.6036010000
C 4.2512980000 0.2319490000 1.0444500000
H 3.6897510000 1.0356310000 1.5241690000
H 5.1724120000 0.6455170000 0.6214630000
H 4.5399920000 -0.4959900000 1.8095850000
H 1.4519280000 -2.8709790000 -0.4096020000
H 1.3825890000 -1.5795110000 -1.7026840000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171031 (Hartree/Particle)
Thermal correction to Energy= 0.184649
Thermal correction to Enthalpy= 0.185594
Thermal correction to Gibbs (Free) Energy= 0.130017
Sum of electronic and zero-point Energies= -710.222489
Sum of electronic and thermal Energies= -710.208871
Sum of electronic and thermal Enthalpies= -710.207927
Sum of electronic and thermal (Free) Energies= -710.263503

cPT

C 3.4221340000 -0.5434440000 -0.0045500000
C 2.0704500000 -0.5694070000 0.0153710000
C 1.1289480000 0.5136590000 0.0159030000
C -0.2001910000 0.0037380000 -0.0110930000
C -0.1223320000 -1.3892760000 -0.0008650000
C 1.2754600000 -1.8549390000 0.0325450000
C 1.3842470000 1.9726860000 0.0597830000
O -1.2348130000 0.7800060000 -0.0299860000
H 2.1488610000 2.2277660000 0.7976500000
H 0.4533720000 2.4964040000 0.2844620000
H 1.7362450000 2.3196640000 -0.9202680000
H -0.9880040000 -2.0399850000 -0.0125790000
B -2.6342940000 0.1520220000 -0.0093710000
F -2.7356190000 -0.6651940000 -1.1450970000
F -3.5245570000 1.1960390000 -0.0129430000
F -2.7117920000 -0.6369110000 1.1486920000
H 3.9137640000 -1.5155540000 0.0323580000
C 4.3367190000 0.6350260000 -0.0630300000
H 3.8968550000 1.4949700000 -0.5676120000
H 5.2636810000 0.3667220000 -0.5750340000
H 4.6124870000 0.9446910000 0.9534980000
H 1.4787760000 -2.4453300000 0.9369330000
H 1.5090340000 -2.5031680000 -0.8229290000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173558 (Hartree/Particle)
Thermal correction to Energy= 0.186950
Thermal correction to Enthalpy= 0.187894
Thermal correction to Gibbs (Free) Energy= 0.132235
Sum of electronic and zero-point Energies= -710.272196
Sum of electronic and thermal Energies= -710.258805
Sum of electronic and thermal Enthalpies= -710.257861
Sum of electronic and thermal (Free) Energies= -710.313520

ccRT

C -3.4741330000 -0.1320930000 -0.7185890000
C -2.2976620000 -0.5243540000 -0.3220040000
C -1.1105170000 -0.9714050000 0.0524640000
C 0.0590630000 -0.0836670000 -0.0230190000
C -0.0431540000 1.3806090000 -0.0967990000
C -0.9841540000 2.0789180000 0.5435730000
H 0.7615930000 1.8774080000 -0.6284110000
C -0.8668620000 -2.4082360000 0.4534730000
O 1.1723200000 -0.6562290000 -0.0266010000
H -1.8097840000 -2.9545380000 0.4953090000
H -0.3789830000 -2.4553470000 1.4307920000
H -0.2011910000 -2.8927690000 -0.2654230000
B 2.6382260000 0.0644490000 -0.0604720000
F 3.4949660000 -0.9896540000 0.0205640000
F 2.6437230000 0.9013610000 1.0321490000
F 2.6698680000 0.7389300000 -1.2647640000
C -4.5169680000 0.4947660000 0.1688750000
H -3.7109640000 -0.2488330000 -1.7758560000
H -4.1946210000 0.5195000000 1.2118430000
H -5.4530690000 -0.0679290000 0.1094140000
H -4.7243760000 1.5181260000 -0.1599640000
H -1.7487630000 1.6058590000 1.1507120000
H -0.9802250000 3.1631510000 0.5073590000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171777 (Hartree/Particle)
Thermal correction to Energy= 0.186381
Thermal correction to Enthalpy= 0.187325
Thermal correction to Gibbs (Free) Energy= 0.129475
Sum of electronic and zero-point Energies= -710.250015
Sum of electronic and thermal Energies= -710.235410
Sum of electronic and thermal Enthalpies= -710.234466
Sum of electronic and thermal (Free) Energies= -710.292316

ccTS

C -3.4084870000 0.1830640000 0.5306680000
C -2.1576300000 0.3013350000 0.1232030000
C -0.9984310000 1.0013460000 -0.0239640000
C 0.1904290000 0.1960450000 0.0266390000
C -0.1294110000 -1.1979050000 0.0435720000
C -1.3541830000 -1.5494390000 -0.4786590000
H 0.5060140000 -1.8936480000 0.5814400000
C -0.9159640000 2.4736450000 -0.2889400000
O 1.3392320000 0.7333890000 0.1113070000
H -1.9043260000 2.9326890000 -0.3203460000
H -0.3879800000 2.6681100000 -1.2269610000
H -0.3258370000 2.9402830000 0.5065390000
B 2.6355220000 -0.1541770000 0.0426310000
F 3.6730430000 0.7328650000 -0.0237490000

F 2.4936760000 -0.9465530000 -1.0931910000
F 2.6288880000 -0.9295130000 1.1997230000
C -4.4715370000 -0.7065650000 -0.0399910000
H -3.6770350000 0.7735370000 1.4080880000
H -4.8064060000 -1.4331760000 0.7072960000
H -4.1271810000 -1.2455220000 -0.9245670000
H -5.3435970000 -0.1086300000 -0.3227150000
H -1.6976640000 -1.1629450000 -1.4340680000
H -1.8166290000 -2.4872610000 -0.1785330000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170986 (Hartree/Particle)
Thermal correction to Energy= 0.184555
Thermal correction to Enthalpy= 0.185499
Thermal correction to Gibbs (Free) Energy= 0.130137
Sum of electronic and zero-point Energies= -710.221966
Sum of electronic and thermal Energies= -710.208397
Sum of electronic and thermal Enthalpies= -710.207453
Sum of electronic and thermal (Free) Energies= -710.262815

ccPT

C 3.4026500000 0.3296580000 0.0000010000
C 2.1006730000 -0.0255140000 0.0000000000
C 0.9883560000 0.8791070000 0.0000000000
C -0.2353140000 0.1521680000 0.0000000000
C 0.0813250000 -1.2031610000 0.0000000000
C 1.5441470000 -1.4283220000 0.0000000000
C 0.9964110000 2.3548430000 0.0000000000
O -1.3833830000 0.7510050000 0.0000000000
H 1.9936240000 2.7945850000 0.0000000000
H 0.4318580000 2.7089170000 0.8704140000
H 0.4318590000 2.7089170000 -0.8704140000
H -0.6585470000 -1.9940670000 0.0000000000
B -2.6585980000 -0.1001110000 0.0000000000
F -3.7107680000 0.7812660000 -0.0000010000
F -2.6145490000 -0.9072960000 1.1471620000
F -2.6145490000 -0.9072960000 -1.1471630000
C 4.5583110000 -0.6090340000 0.0000010000
H 3.6470670000 1.3903620000 0.0000010000
H 4.2528450000 -1.6567370000 0.0000010000
H 5.1885600000 -0.4267030000 0.8777270000
H 5.1885600000 -0.4267030000 -0.8777250000
H 1.8618320000 -2.0022930000 0.8806970000
H 1.8618320000 -2.0022930000 -0.8806970000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173301 (Hartree/Particle)
Thermal correction to Energy= 0.186805
Thermal correction to Enthalpy= 0.187749
Thermal correction to Gibbs (Free) Energy= 0.132070
Sum of electronic and zero-point Energies= -710.277126
Sum of electronic and thermal Energies= -710.263622
Sum of electronic and thermal Enthalpies= -710.262678
Sum of electronic and thermal (Free) Energies= -710.318357

1b

cRT

C -1.0461910000 -1.0858340000 -0.5650740000
C 0.1090140000 -0.2582520000 -0.1736370000
C 0.0239080000 1.1769040000 0.0728910000
C -0.8210610000 1.9840730000 -0.5854330000
H 0.7680860000 1.5833110000 0.7504950000
C -2.2713940000 -0.6849560000 -0.2734170000
H -1.4950220000 1.5627960000 -1.3281990000
C -0.8703920000 3.4640350000 -0.4083130000
C -3.4909930000 -0.3560120000 0.0464250000
H -4.0743800000 0.2083910000 -0.6808610000
C -4.1491120000 -0.6916860000 1.3599470000
O 1.1922360000 -0.8806880000 -0.0538150000
B 2.6368820000 -0.2393160000 0.3068930000
C -0.7552870000 -2.4371510000 -1.1775030000
H -0.1937260000 -3.0568250000 -0.4738840000
H -0.1403830000 -2.3260260000 -2.0748750000
H -1.6855950000 -2.9421730000 -1.4400860000
H -0.1701190000 3.8067210000 0.3559780000
H -1.8829260000 3.7770940000 -0.1296810000
H -0.6325120000 3.9650370000 -1.3529810000
H -3.4782930000 -1.2592860000 2.0071090000
H -5.0545440000 -1.2815800000 1.1881820000
H -4.4439930000 0.2249460000 1.8797620000
F 2.8550120000 0.7212290000 -0.6579560000
F 2.4906460000 0.2916390000 1.5751180000
F 3.4754710000 -1.3114290000 0.2405920000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199899 (Hartree/Particle)
Thermal correction to Energy= 0.216167
Thermal correction to Enthalpy= 0.217111
Thermal correction to Gibbs (Free) Energy= 0.155225
Sum of electronic and zero-point Energies= -749.536347
Sum of electronic and thermal Energies= -749.520080
Sum of electronic and thermal Enthalpies= -749.519135
Sum of electronic and thermal (Free) Energies= -749.581021

cTS

C -0.8935410000 -1.0327360000 -0.3674150000
C 0.3063930000 -0.2872450000 -0.1106600000
C 0.0338310000 1.1060220000 0.0030020000
C -1.1286540000 1.5686560000 -0.5920930000
H 0.6497670000 1.7309310000 0.6423840000
C -2.0319080000 -0.2926630000 -0.2599410000
H -1.3564460000 1.2565310000 -1.6101350000
C -1.7810090000 2.8523100000 -0.1727020000
C -3.3128790000 -0.1577500000 0.0311150000
H -3.8844130000 0.6307270000 -0.4548670000
C -4.0251420000 -0.9932170000 1.0588190000
O 1.4243110000 -0.8801540000 0.0406960000
B 2.7436310000 -0.0520280000 0.1943240000
C -0.8392290000 -2.4676140000 -0.7927970000
H -0.3363190000 -3.0459740000 -0.0109130000
H -0.2391670000 -2.5794830000 -1.7005940000
H -1.8366420000 -2.8763500000 -0.9583550000
H -1.6079940000 3.0719130000 0.8824280000
H -2.8587280000 2.8203990000 -0.3544440000
H -1.3807750000 3.6760210000 -0.7739180000
H -3.3757140000 -1.7730930000 1.4607040000
H -4.9080160000 -1.4618870000 0.6122000000
H -4.3711090000 -0.3673120000 1.8880190000
F 2.7676920000 0.8399240000 -0.8761670000
F 2.6368720000 0.6281760000 1.4073790000
F 3.7538510000 -0.9742810000 0.1683800000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198879 (Hartree/Particle)
Thermal correction to Energy= 0.214217
Thermal correction to Enthalpy= 0.215161
Thermal correction to Gibbs (Free) Energy= 0.155603
Sum of electronic and zero-point Energies= -749.509188
Sum of electronic and thermal Energies= -749.493850
Sum of electronic and thermal Enthalpies= -749.492906
Sum of electronic and thermal (Free) Energies= -749.552465

cPT

C 0.9397100000 -0.8265850000 0.0074270000
C -0.3428730000 -0.2114380000 0.0382530000
C -0.1523050000 1.1476600000 0.2773560000
C 1.2776720000 1.4992770000 0.4123870000
H -0.9624140000 1.8635360000 0.3547370000
C 1.9642220000 0.1629320000 0.1878840000
H 1.4599210000 1.8204940000 1.4509380000
C 1.7146460000 2.6342720000 -0.5276300000
C 3.3076020000 0.0155970000 0.1746790000
H 3.8861410000 0.9176270000 0.3722140000
C 4.1141830000 -1.2166470000 -0.0742910000
O -1.4352680000 -0.8869860000 -0.1216990000
B -2.7778170000 -0.1537060000 -0.0238100000
C 1.0755780000 -2.2929860000 -0.1560650000
H 1.4048420000 -2.5241120000 -1.1775070000
H 0.1030500000 -2.7655120000 -0.0063820000
H 1.8117380000 -2.7122650000 0.5338290000
H 1.5832820000 2.3403680000 -1.5724230000
H 2.7634230000 2.8957590000 -0.3662650000
H 1.1142500000 3.5282460000 -0.3420930000
H 3.6181250000 -1.9255230000 -0.7373200000
H 4.3184010000 -1.7300350000 0.8743850000

H 5.0815570000 -0.9529460000 -0.5076790000
F -2.8245480000 0.4496720000 1.2428390000
F -2.7803670000 0.8364810000 -1.0180680000
F -3.7508280000 -1.1043430000 -0.2051910000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.202371 (Hartree/Particle)
Thermal correction to Energy= 0.217147
Thermal correction to Enthalpy= 0.218092
Thermal correction to Gibbs (Free) Energy= 0.159612
Sum of electronic and zero-point Energies= -749.551356
Sum of electronic and thermal Energies= -749.536579
Sum of electronic and thermal Enthalpies= -749.535635
Sum of electronic and thermal (Free) Energies= -749.594114

ccRT

C 3.3256190000 -0.7659050000 0.7656870000
C 2.1313390000 -1.0182770000 0.3106280000
C 0.9203740000 -1.3209640000 -0.1234710000
C -0.1732670000 -0.3446110000 0.0265260000
C 0.0459840000 1.0890900000 0.1876500000
C 1.0689720000 1.7446970000 -0.3800730000
H -0.7356830000 1.6277950000 0.7138670000
H 1.7898620000 1.1953270000 -0.9818050000
C 1.2683330000 3.2201000000 -0.2903600000
C 0.5635190000 -2.6859550000 -0.6657200000
H 3.5261630000 -1.0049660000 1.8097640000
C 4.4395560000 -0.1469130000 -0.0371820000
O -1.3289400000 -0.8335270000 0.0155700000
B -2.7244080000 -0.0107500000 0.0938200000
H 1.4573480000 -3.3049560000 -0.7517670000
H 0.0910620000 -2.5962460000 -1.6477180000
H -0.1538410000 -3.1780540000 -0.0040890000
H 4.1438690000 0.0152160000 -1.0758830000
H 5.3208530000 -0.7949130000 -0.0267350000
H 4.7314370000 0.8135270000 0.3999200000
H 2.2593460000 3.4427810000 0.1207900000
H 0.5103120000 3.6964270000 0.3345170000
H 1.2315770000 3.6672940000 -1.2896920000
F -3.6656970000 -0.9878480000 -0.0332220000
F -2.6753700000 0.8798310000 -0.9577290000
F -2.7101910000 0.6097020000 1.3290680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.200176 (Hartree/Particle)
Thermal correction to Energy= 0.216335
Thermal correction to Enthalpy= 0.217279
Thermal correction to Gibbs (Free) Energy= 0.155782
Sum of electronic and zero-point Energies= -749.536482
Sum of electronic and thermal Energies= -749.520323
Sum of electronic and thermal Enthalpies= -749.519379
Sum of electronic and thermal (Free) Energies= -749.580875

ccTS

C 3.2061610000 0.7345550000 -0.5151180000
C 1.9415250000 0.6689210000 -0.1281410000
C 0.7289050000 1.2765130000 0.0093590000
C -0.3868260000 0.3745720000 -0.0327430000
C 0.0483050000 -0.9774150000 -0.0512320000
C 1.3230390000 -1.2404170000 0.4314970000
H -0.5468740000 -1.7324310000 -0.5560010000
H 1.6072320000 -0.8398580000 1.4035880000
C 2.0540210000 -2.4845040000 0.0123320000
C 0.5261650000 2.7370190000 0.2688450000
H 3.4057570000 1.3617840000 -1.3854000000
C 4.3810760000 0.0246230000 0.0849340000
O -1.5808870000 0.8147960000 -0.1106860000
B -2.7908500000 -0.1732510000 -0.0309260000
H 1.4678760000 3.2859710000 0.2472900000
H 0.0309420000 2.8929090000 1.2319590000
H -0.1469590000 3.1369980000 -0.4964020000
H 4.1262430000 -0.4836500000 1.0165980000
H 5.1688370000 0.7524610000 0.3033110000
H 4.8036920000 -0.7032460000 -0.6165330000
H 1.8596010000 -2.7311510000 -1.0331980000
H 1.7175030000 -3.3218350000 0.6342010000
H 3.1311220000 -2.3888950000 0.1571970000
F -3.9037630000 0.6209110000 0.0224680000
F -2.5905470000 -0.9396070000 1.1160770000
F -2.7232290000 -0.9662330000 -1.1768660000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199105 (Hartree/Particle)
Thermal correction to Energy= 0.214337
Thermal correction to Enthalpy= 0.215282
Thermal correction to Gibbs (Free) Energy= 0.155766
Sum of electronic and zero-point Energies= -749.507480
Sum of electronic and thermal Energies= -749.492247
Sum of electronic and thermal Enthalpies= -749.491303
Sum of electronic and thermal (Free) Energies= -749.550818

cPT

C 3.1994100000 0.7584230000 0.1044870000
C 1.9336060000 0.2896760000 0.0843980000
C 0.7656970000 1.1010140000 -0.1074070000
C -0.4089300000 0.3105380000 0.0304730000
C -0.0037830000 -0.9934310000 0.2890920000
C 1.4739590000 -1.1381550000 0.3018560000
H -0.6900640000 -1.8201910000 0.4306660000
H 1.8026880000 -1.5015110000 1.2865120000
C 1.9479270000 -2.1299900000 -0.7800240000
C 0.6768990000 2.5487310000 -0.3803610000
H 3.3540650000 1.8180150000 -0.0910260000
C 4.4307440000 -0.0328090000 0.3816410000
O -1.5935600000 0.8227080000 -0.0831310000
B -2.8086230000 -0.1009090000 0.0501740000
H 1.6410780000 3.0365240000 -0.5219750000
H 0.1345850000 3.0288740000 0.4429740000
H 0.0462740000 2.6994850000 -1.2638350000
H 4.2191320000 -1.0450700000 0.7275980000
H 5.0358860000 0.4743070000 1.1401710000
H 5.0494460000 -0.0915740000 -0.5223270000
H 3.0334010000 -2.2495170000 -0.7630900000
H 1.6523570000 -1.7773090000 -1.7718050000
H 1.4944790000 -3.1105250000 -0.6158710000
F -3.9169160000 0.6914130000 -0.1184840000
F -2.7414080000 -0.6918590000 1.3214770000
F -2.6833330000 -1.0909560000 -0.9372980000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201951 (Hartree/Particle)
Thermal correction to Energy= 0.216889
Thermal correction to Enthalpy= 0.217833
Thermal correction to Gibbs (Free) Energy= 0.159086
Sum of electronic and zero-point Energies= -749.555783
Sum of electronic and thermal Energies= -749.540845
Sum of electronic and thermal Enthalpies= -749.539901
Sum of electronic and thermal (Free) Energies= -749.598648

1c

c/s RT

C -2.6468970000 -2.1445520000 -0.0136050000
C -1.4063370000 -1.9294170000 -0.3486260000
H -3.4254310000 -1.7672890000 -0.6765180000
C -3.0828290000 -2.8634960000 1.2368220000
C -0.1327200000 -1.7678570000 -0.6635460000
H -2.2251030000 -3.1967430000 1.8235530000
H -3.6924780000 -3.7347210000 0.9789540000
H -3.6953390000 -2.2020080000 1.8572040000
C 0.6025880000 -0.5979910000 -0.1511260000
C 0.6557330000 -2.8011580000 -1.4352180000
C -0.0535140000 0.6277680000 0.2888160000
O 1.8501160000 -0.7299450000 -0.1048960000
H 1.4446180000 -3.2207680000 -0.8058820000
H 1.1407720000 -2.3432330000 -2.3016690000
H -0.0006850000 -3.6036510000 -1.7737760000
C -1.1741330000 1.0984460000 -0.2767400000
H 0.4773210000 1.2052480000 1.0392920000
B 2.9148410000 0.4013300000 0.3528630000
H -1.6378180000 0.5501840000 -1.0969090000
C -1.8402890000 2.3854580000 0.1001240000
F 2.6682740000 1.4827160000 -0.4672940000
F 4.1183220000 -0.2040620000 0.1456150000
F 2.6263440000 0.6545460000 1.6813240000

C -3.2914710000 2.1096480000 0.5202720000
C -1.7782480000 3.3712990000 -1.0757760000
H -1.3022310000 2.8200570000 0.9504310000
H -3.3362700000 1.4220740000 1.3700570000
H -3.7869750000 3.0419590000 0.8071800000
H -3.8598400000 1.6696070000 -0.3076830000
H -0.7436750000 3.5829140000 -1.3585100000
H -2.2979820000 2.9671060000 -1.9521480000
H -2.2617640000 4.3144660000 -0.8039000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257353 (Hartree/Particle)
Thermal correction to Energy= 0.276244
Thermal correction to Enthalpy= 0.277188
Thermal correction to Gibbs (Free) Energy= 0.208614
Sum of electronic and zero-point Energies= -828.093410
Sum of electronic and thermal Energies= -828.074519
Sum of electronic and thermal Enthalpies= -828.073575
Sum of electronic and thermal (Free) Energies= -828.142150

c/s TS

C -2.7803990000 -1.4910830000 0.0394120000
C -1.5219570000 -1.1661810000 -0.2098310000
H -3.5772350000 -0.8774140000 -0.3696420000
C -3.1772970000 -2.6441440000 0.9182140000
C -0.2335530000 -1.5764820000 -0.3921960000
H -2.3091080000 -3.2224530000 1.2397910000
H -3.8651820000 -3.3033680000 0.3786030000
H -3.7031960000 -2.2842370000 1.8089450000
C 0.7448620000 -0.5808050000 -0.0750380000
C 0.1672530000 -2.9001480000 -0.9666060000
C 0.1328490000 0.6739860000 0.1826300000
O 1.9860300000 -0.8730040000 -0.0098250000
H 0.8426140000 -3.3968610000 -0.2623770000
H 0.7290890000 -2.7641040000 -1.8954570000
H -0.6970310000 -3.5392110000 -1.1509250000
C -1.1452040000 0.8837340000 -0.3184160000
H 0.6116710000 1.3831450000 0.8512350000
B 3.0460820000 0.2548100000 0.1896440000
H -1.3503140000 0.6482330000 -1.3644990000
C -1.9866810000 2.0158950000 0.2336300000
F 2.7783620000 1.2186330000 -0.7835320000
F 4.2615470000 -0.3562030000 0.0395830000
F 2.8346820000 0.7725180000 1.4685080000
C -3.4936310000 1.8121260000 0.0586470000
C -1.5350430000 3.3081610000 -0.4729880000
H -1.7707270000 2.1135830000 1.3034990000
H -3.8744690000 1.0215840000 0.7092050000
H -4.0249300000 2.7333530000 0.3137200000
H -3.7433880000 1.5657350000 -0.9805750000
H -0.4634660000 3.4839810000 -0.3472510000
H -1.7457800000 3.2569460000 -1.5470800000
H -2.0757100000 4.1661690000 -0.0626050000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256655 (Hartree/Particle)
Thermal correction to Energy= 0.274416
Thermal correction to Enthalpy= 0.275361
Thermal correction to Gibbs (Free) Energy= 0.210244
Sum of electronic and zero-point Energies= -828.063278
Sum of electronic and thermal Energies= -828.045517
Sum of electronic and thermal Enthalpies= -828.044572
Sum of electronic and thermal (Free) Energies= -828.109689

c/s PT

C 2.9169350000 -1.1010140000 0.4177590000
C 1.6620690000 -0.6315920000 0.2400540000
H 3.6547540000 -0.3774570000 0.7585500000
C 3.4297180000 -2.4938610000 0.2412950000
C 0.4853510000 -1.3563050000 -0.1576560000
H 2.6650890000 -3.2569810000 0.3858350000
H 4.2445940000 -2.6835710000 0.9439740000
H 3.8446930000 -2.6174220000 -0.7673950000
C -0.6723990000 -0.5744460000 0.0990840000
C 0.3704190000 -2.7095600000 -0.7477150000
C -0.2476480000 0.6388160000 0.6329760000
O -1.8706020000 -1.0066760000 -0.1392280000
H 1.2125710000 -2.9550900000 -1.3964250000
H -0.5724980000 -2.7806810000 -1.2952200000
H 0.3247390000 -3.4574640000 0.0555600000
C 1.2239950000 0.7803390000 0.5995750000
H -0.9297320000 1.3993840000 0.9914360000
B -3.0355670000 -0.0233980000 0.0034320000
H 1.6090430000 1.0844300000 1.5843780000
C 1.6566670000 1.8745290000 -0.4361830000
F -3.0970710000 0.3626070000 1.3505580000
F -4.1594920000 -0.6863760000 -0.4207900000
F -2.7228360000 1.0952990000 -0.7908310000
C 3.1725670000 2.0860570000 -0.4500420000
C 0.9353030000 3.1983100000 -0.1608790000
H 1.3446800000 1.5084180000 -1.4227050000
H 3.7110500000 1.2041080000 -0.8051610000
H 3.4252750000 2.9125780000 -1.1204610000
H 3.5451190000 2.3461440000 0.5481510000
H -0.1433890000 3.1217080000 -0.3176710000
H 1.1129250000 3.5361230000 0.8672000000
H 1.3104560000 3.9747750000 -0.8334220000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.259556 (Hartree/Particle)
Thermal correction to Energy= 0.276981
Thermal correction to Enthalpy= 0.277925
Thermal correction to Gibbs (Free) Energy= 0.213289
Sum of electronic and zero-point Energies= -828.106502
Sum of electronic and thermal Energies= -828.089077
Sum of electronic and thermal Enthalpies= -828.088133
Sum of electronic and thermal (Free) Energies= -828.152769

cc/s RT

C 2.4451300000 2.2763050000 -0.6913200000
C 1.2480200000 2.0822910000 -0.2157820000
C 3.7236020000 1.9488000000 0.0340410000
H 2.5251040000 2.6874010000 -1.6973710000
C 0.0176520000 1.9203130000 0.2395260000
H 4.3573640000 2.8372480000 0.1095800000
H 4.2838410000 1.1875150000 -0.5185830000
H 3.5290760000 1.5766060000 1.0421590000
C -0.6946270000 0.6610490000 -0.0383460000
C -0.7509720000 3.0167490000 0.9397610000
C -0.0088690000 -0.5824770000 -0.3723090000
O -1.9465540000 0.7275220000 0.0226710000
H -1.6117480000 3.3168380000 0.3367330000
H -0.1092580000 3.8826240000 1.1070100000
H -1.1351910000 2.6618110000 1.8999610000
C 1.1797630000 -0.9212250000 0.1467550000
H -0.5668450000 -1.2801520000 -0.9890570000
B -2.9782740000 -0.5074830000 -0.1634460000
H 1.6772420000 -0.2471070000 0.8442480000
C 1.8829070000 -2.2178010000 -0.1114360000
F -4.1916080000 0.0628690000 0.0815300000
F -2.5878320000 -1.4469040000 0.7684640000
F -2.8023090000 -0.9346440000 -1.4665640000
C 3.2941340000 -1.9419600000 -0.6501600000
C 1.9329520000 -3.0501990000 1.1784750000
H 1.3177190000 -2.7760930000 -0.8665510000
H 3.8896010000 -1.3907770000 0.0873270000
H 3.8110200000 -2.8828520000 -0.8610230000
H 3.2610050000 -1.3548570000 -1.5729300000
H 2.4805400000 -2.5184790000 1.9652380000
H 0.9267730000 -3.2657610000 1.5473630000
H 2.4451460000 -3.9996930000 0.9956570000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257469 (Hartree/Particle)
Thermal correction to Energy= 0.276280
Thermal correction to Enthalpy= 0.277224
Thermal correction to Gibbs (Free) Energy= 0.209232
Sum of electronic and zero-point Energies= -828.094229
Sum of electronic and thermal Energies= -828.075419
Sum of electronic and thermal Enthalpies= -828.074474
Sum of electronic and thermal (Free) Energies= -828.142466

cc/s TS

C 2.5986690000 1.8608610000 -0.4011040000
C 1.3967290000 1.3577800000 -0.1391630000
C 3.9018360000 1.5439440000 0.2601430000

H 2.6242090000 2.6334220000 -1.1723720000
C 0.0843880000 1.7169360000 0.0062860000
H 4.2837220000 2.4640900000 0.7167620000
H 4.6557440000 1.2078920000 -0.4578580000
H 3.7961340000 0.7950140000 1.0448210000
C -0.8438440000 0.6331220000 -0.0748590000
C -0.3845200000 3.0977850000 0.3452810000
C -0.1662460000 -0.6037900000 -0.1853770000
O -2.1044780000 0.8397680000 -0.0965300000
H -0.7754420000 3.1320570000 1.3672240000
H -1.2184230000 3.3544450000 -0.3152700000
H 0.4108340000 3.8359940000 0.2382380000
C 1.1637810000 -0.6701170000 0.2232170000
H -0.6415770000 -1.4301710000 -0.7055910000
B -3.0926030000 -0.3648830000 -0.0366960000
H 1.4275870000 -0.3373510000 1.2291890000
C 1.9768840000 -1.8452590000 -0.2979730000
F -4.3355340000 0.1881340000 0.1144380000
F -2.6908950000 -1.1466600000 1.0482070000
F -2.9344340000 -1.0656820000 -1.2336540000
C 3.4830780000 -1.6169780000 -0.3979420000
C 1.6783620000 -3.0509550000 0.6122540000
H 1.6077640000 -2.0745960000 -1.3041080000
H 3.9227770000 -1.3961560000 0.5801980000
H 3.9624560000 -2.5254810000 -0.7736750000
H 3.7232790000 -0.8036950000 -1.0857340000
H 2.0310140000 -2.8628050000 1.6327210000
H 0.6081630000 -3.2687770000 0.6597680000
H 2.1936670000 -3.9397220000 0.2359060000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257095 (Hartree/Particle)
Thermal correction to Energy= 0.274533
Thermal correction to Enthalpy= 0.275477
Thermal correction to Gibbs (Free) Energy= 0.210985
Sum of electronic and zero-point Energies= -828.057549
Sum of electronic and thermal Energies= -828.040111
Sum of electronic and thermal Enthalpies= -828.039167
Sum of electronic and thermal (Free) Energies= -828.103659

cc/s PT

C -2.6804220000 -1.6479290000 0.2281280000
C -1.5510410000 -0.9195950000 0.0981230000
C -3.9732250000 -1.2195670000 0.8320620000
H -2.6405600000 -2.6892750000 -0.0872630000
C -0.2919090000 -1.4925320000 -0.2990590000
H -4.2368770000 -1.9050320000 1.6451410000
H -4.7808320000 -1.2879050000 0.0938250000
H -3.9457950000 -0.2043940000 1.2266480000
C 0.7701960000 -0.6127230000 0.0399700000
C -0.0251610000 -2.8091190000 -0.9108010000
C 0.2020280000 0.5108240000 0.6262780000
O 2.0134560000 -0.9141590000 -0.1749740000
H 0.6146240000 -2.6595180000 -1.7878330000
H -0.9228150000 -3.3578140000 -1.1950510000
H 0.5767850000 -3.4082470000 -0.2169740000
C -1.2803260000 0.5124520000 0.5242750000
H 0.7853420000 1.3168730000 1.0528960000
B 3.0702380000 0.1604400000 0.0875750000
H -1.7471120000 0.7600610000 1.4872400000
C -1.7290190000 1.5829450000 -0.5325630000
F 4.2722620000 -0.3676060000 -0.3127150000
F 3.0301750000 0.4647930000 1.4568560000
F 2.6927830000 1.2945400000 -0.6553010000
C -3.2469180000 1.6524380000 -0.6962260000
C -1.1652770000 2.9642610000 -0.1829040000
H -1.2937370000 1.2648050000 -1.4887190000
H -3.7353770000 1.9417270000 0.2417340000
H -3.5005250000 2.4095710000 -1.4439100000
H -3.6700840000 0.7032820000 -1.0336690000
H -1.4589120000 3.2630260000 0.8305590000
H -0.0750960000 2.9959100000 -0.2504160000
H -1.5583940000 3.7137350000 -0.8755420000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.259539 (Hartree/Particle)
Thermal correction to Energy= 0.276833
Thermal correction to Enthalpy= 0.277777
Thermal correction to Gibbs (Free) Energy= 0.213944
Sum of electronic and zero-point Energies= -828.109479
Sum of electronic and thermal Energies= -828.092185
Sum of electronic and thermal Enthalpies= -828.091241
Sum of electronic and thermal (Free) Energies= -828.155073

c/d RT

C -3.3236200000 -1.3269620000 0.0938750000
C -2.0814070000 -1.4818660000 -0.2675010000
H -3.9828120000 -0.7720290000 -0.5734800000
C -3.9108960000 -1.8505460000 1.3791700000
C -0.8237840000 -1.7046410000 -0.6076950000
H -3.1657050000 -2.3906260000 1.9656920000
H -4.7460840000 -2.5244270000 1.1656030000
H -4.2978210000 -1.0232070000 1.9818410000
C 0.2297790000 -0.7779580000 -0.1577330000
C -0.3860370000 -2.9497160000 -1.3448490000
C -0.0249810000 0.6036430000 0.2298130000
O 1.3868570000 -1.2648480000 -0.1197300000
H 0.2654870000 -3.5547600000 -0.7093330000
H 0.1868570000 -2.6840080000 -2.2375530000
H -1.2541080000 -3.5412160000 -1.6382970000
C -0.9656370000 1.3609680000 -0.3540210000
H 0.6778430000 1.0228210000 0.9410830000
B 2.7436320000 -0.4741240000 0.2705760000
H -1.5876200000 0.9253410000 -1.1345690000
C -1.2050990000 2.8183880000 -0.0887700000
F 2.8011000000 0.5984910000 -0.5958020000
F 3.7151870000 -1.4104340000 0.0769380000
F 2.5768080000 -0.0921470000 1.5894150000
C -1.0079790000 3.6067350000 -1.3958420000
C -0.3621040000 3.3978990000 1.0454830000
H -2.2677450000 2.9021080000 0.1867880000
H -1.6383760000 3.2179450000 -2.2019090000
H -1.2628390000 4.6595790000 -1.2445420000
H 0.0356560000 3.5499280000 -1.7209050000
H -0.5154060000 2.8551110000 1.9830100000
H 0.7047240000 3.3639550000 0.8006450000
H -0.6323240000 4.4440390000 1.2143560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257483 (Hartree/Particle)
Thermal correction to Energy= 0.276220
Thermal correction to Enthalpy= 0.277164
Thermal correction to Gibbs (Free) Energy= 0.209153
Sum of electronic and zero-point Energies= -828.092992
Sum of electronic and thermal Energies= -828.074254
Sum of electronic and thermal Enthalpies= -828.073310
Sum of electronic and thermal (Free) Energies= -828.141321

c/d TS

C -2.8604910000 -1.3932920000 -0.0619180000
C -1.5811940000 -1.2194650000 -0.3371630000
H -3.5972050000 -0.7697810000 -0.5649910000
C -3.3651070000 -2.3619050000 0.9721020000
C -0.2913010000 -1.6431380000 -0.4228550000
H -2.5523870000 -2.9553070000 1.3949820000
H -4.1015900000 -3.0370910000 0.5246090000
H -3.8650080000 -1.8263550000 1.7860850000
C 0.6750090000 -0.6183070000 -0.1381100000
C 0.1354520000 -3.0140320000 -0.8499330000
C 0.0592670000 0.6597920000 -0.0276920000
O 1.9028560000 -0.9113720000 0.0404450000
H 0.7527970000 -3.4514560000 -0.0586110000
H 0.7622500000 -2.9628020000 -1.7449860000
H -0.7217010000 -3.6615960000 -1.0378160000
C -1.1668480000 0.8223290000 -0.6503980000
H 0.4906600000 1.4079410000 0.6294700000
B 2.9638560000 0.2220940000 0.2294860000
H -1.2809190000 0.4661990000 -1.6739570000
C -2.1504920000 1.8956430000 -0.2566670000
F 2.7926280000 1.0978130000 -0.8411510000
F 4.1755690000 -0.4134670000 0.2351210000
F 2.6551390000 0.8482600000 1.4379650000
C -1.7921630000 3.2022580000 -0.9869360000
C -2.2434490000 2.0949980000 1.2566410000
H -3.1331330000 1.5736580000 -0.6259110000
H -1.7546290000 3.0616020000 -2.0712180000
H -2.5393610000 3.9705500000 -0.7680370000

H -0.8151650000 3.5711900000 -0.6598940000
H -2.4475500000 1.1484320000 1.7670680000
H -1.3145360000 2.5057860000 1.6642730000
H -3.0467700000 2.7967930000 1.4980860000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256362 (Hartree/Particle)
Thermal correction to Energy= 0.274255
Thermal correction to Enthalpy= 0.275200
Thermal correction to Gibbs (Free) Energy= 0.209725
Sum of electronic and zero-point Energies= -828.066924
Sum of electronic and thermal Energies= -828.049031
Sum of electronic and thermal Enthalpies= -828.048087
Sum of electronic and thermal (Free) Energies= -828.113561

c/d PT

C -3.0972720000 -0.8051820000 -0.3837360000
C -1.7817870000 -0.5000110000 -0.3500860000
H -3.7668940000 0.0137360000 -0.6466270000
C -3.7666490000 -2.1114540000 -0.1075950000
C -0.6626520000 -1.3279250000 0.0022610000
H -3.1310060000 -2.9724890000 -0.3130430000
H -4.6768060000 -2.2010010000 -0.7054200000
H -4.0725190000 -2.1601060000 0.9457410000
C 0.5488500000 -0.6150700000 -0.2083980000
C -0.6510870000 -2.7115970000 0.5322410000
C 0.2179120000 0.6478670000 -0.6942210000
O 1.7115720000 -1.1307600000 0.0394930000
H -1.4303510000 -2.8672020000 1.2817930000
H 0.3318430000 -2.9271050000 0.9557240000
H -0.8238970000 -3.4246720000 -0.2844260000
C -1.2415340000 0.8637320000 -0.7400780000
H 0.9580280000 1.3869830000 -0.9761920000
B 2.9341470000 -0.2110820000 -0.0019380000
H -1.5469660000 1.1120060000 -1.7684230000
C -1.7190710000 2.0339240000 0.1757330000
F 3.0704490000 0.2515310000 -1.3189290000
F 4.0020100000 -0.9619150000 0.4205530000
F 2.6529670000 0.8744250000 0.8493840000
C -1.2228400000 3.3774460000 -0.3625780000
C -1.2985690000 1.8305210000 1.6322240000
H -2.8155770000 2.0354920000 0.1241050000
H -1.5105900000 3.5263060000 -1.4084980000
H -1.6482110000 4.1977500000 0.2227830000
H -0.1330920000 3.4563830000 -0.2921950000
H -1.6383090000 0.8668130000 2.0251740000
H -0.2096380000 1.8729240000 1.7399860000
H -1.7299660000 2.6158000000 2.2595860000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.259569 (Hartree/Particle)
Thermal correction to Energy= 0.276976
Thermal correction to Enthalpy= 0.277920
Thermal correction to Gibbs (Free) Energy= 0.213467
Sum of electronic and zero-point Energies= -828.110302
Sum of electronic and thermal Energies= -828.092896
Sum of electronic and thermal Enthalpies= -828.091952
Sum of electronic and thermal (Free) Energies= -828.156405

cc/d RT

C 2.6465630000 -2.0277320000 0.7872460000
C 1.4258150000 -1.9720220000 0.3358920000
C 3.8828300000 -1.7721190000 -0.0335700000
H 2.7802360000 -2.2607600000 1.8433850000
C 0.1734300000 -1.9528040000 -0.0862760000
H 4.5471570000 -2.6407680000 -0.0016240000
H 4.4340010000 -0.9182710000 0.3735250000
H 3.6360520000 -1.5647460000 -1.0770620000
C -0.6043640000 -0.7056100000 0.0142260000
C -0.5519500000 -3.1908550000 -0.5603440000
C 0.0095010000 0.6143020000 0.1015280000
O -1.8511740000 -0.8521110000 0.0315350000
H -1.3707390000 -3.4316590000 0.1224500000
H 0.1347420000 -4.0366480000 -0.6114150000
H -0.9911240000 -3.0229820000 -1.5475510000
C 1.1526620000 0.9263520000 -0.5264940000
H -0.5764350000 1.3655620000 0.6188960000
B -2.9511340000 0.3353610000 0.0753210000
H 1.6599780000 0.1623010000 -1.1136410000
C 1.8160400000 2.2721560000 -0.5292910000
F -4.1349170000 -0.3352840000 -0.0050180000
F -2.6682300000 1.1317990000 -1.0151710000
F -2.7426710000 0.9799090000 1.2811130000
C 1.0758690000 3.3399510000 0.2732240000
C 3.2701580000 2.1087160000 -0.0518740000
H 1.8529160000 2.5904650000 -1.5816750000
H 1.0203930000 3.0686700000 1.3332080000
H 1.6035550000 4.2950180000 0.2005670000
H 0.0572220000 3.4892840000 -0.0956430000
H 3.2964060000 1.7736100000 0.9907070000
H 3.8130300000 1.3782980000 -0.6605920000
H 3.8007170000 3.0628930000 -0.1163350000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257685 (Hartree/Particle)
Thermal correction to Energy= 0.276299
Thermal correction to Enthalpy= 0.277243
Thermal correction to Gibbs (Free) Energy= 0.210065
Sum of electronic and zero-point Energies= -828.093891
Sum of electronic and thermal Energies= -828.075277
Sum of electronic and thermal Enthalpies= -828.074333
Sum of electronic and thermal (Free) Energies= -828.141511

cc/d TS

C -2.5323900000 1.7347340000 0.4631540000
C -1.3224800000 1.3269860000 0.1057100000
C -3.8410080000 1.3865420000 -0.1720160000
H -2.5701780000 2.3965270000 1.3303110000
C -0.0036930000 1.6677970000 0.0044990000
H -4.3963350000 2.3078900000 -0.3745110000
H -4.4631060000 0.7788410000 0.4945430000
H -3.7070480000 0.8557350000 -1.1150420000
C 0.8958440000 0.5546660000 0.0198540000
C 0.5036710000 3.0606090000 -0.2036950000
C 0.1891700000 -0.6731900000 -0.0118490000
O 2.1575720000 0.7306910000 0.1072860000
H -0.2953380000 3.7987370000 -0.1299900000
H 0.9968020000 3.1502020000 -1.1765580000
H 1.2674740000 3.2691890000 0.5522980000
C -1.1224900000 -0.6611840000 -0.4793660000
H 0.6291040000 -1.5594870000 0.4348840000
B 3.1317990000 -0.4831800000 -0.0052580000
H -1.3316510000 -0.1939680000 -1.4422040000
C -2.0400430000 -1.8029270000 -0.0714650000
F 4.3879520000 0.0597350000 -0.0335710000
F 2.7841660000 -1.1559300000 -1.1766600000
F 2.8947030000 -1.2834730000 1.1139990000
C -2.4937660000 -1.6923820000 1.3907510000
C -3.2117570000 -2.0350120000 -1.0265390000
H -1.3965440000 -2.6918030000 -0.1341200000
H -3.1861910000 -0.8571980000 1.5284940000
H -3.0058730000 -2.6093940000 1.6957080000
H -1.6416760000 -1.5394300000 2.0592170000
H -3.9720270000 -1.2549030000 -0.9384770000
H -2.8770810000 -2.0758730000 -2.0678800000
H -3.6976400000 -2.9875190000 -0.7968230000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256501 (Hartree/Particle)
Thermal correction to Energy= 0.274180
Thermal correction to Enthalpy= 0.275124
Thermal correction to Gibbs (Free) Energy= 0.210769
Sum of electronic and zero-point Energies= -828.061423
Sum of electronic and thermal Energies= -828.043745
Sum of electronic and thermal Enthalpies= -828.042800
Sum of electronic and thermal (Free) Energies= -828.107155

cc/d PT

C -2.7195040000 1.5115560000 -0.1592570000
C -1.5630640000 0.8146400000 -0.1512120000
C -4.0156960000 1.1216930000 -0.7807200000
H -2.7053620000 2.5016880000 0.2935410000
C -0.3162470000 1.3782280000 0.2948640000
H -4.3453580000 1.9165630000 -1.4586000000
H -4.7928870000 1.0253880000 -0.0134080000
H -3.9585860000 0.1878260000 -1.3382400000

C 0.7670720000 0.5664880000 -0.1340290000
C -0.0792760000 2.6235970000 1.0512000000
C 0.2264740000 -0.5144280000 -0.8175840000
O 2.0019910000 0.8711000000 0.1245500000
H 0.5813300000 2.3935640000 1.8947380000
H -0.9878150000 3.1063230000 1.4106860000
H 0.4902770000 3.3193320000 0.4233930000
C -1.2552810000 -0.5454970000 -0.7507380000
H 0.8239070000 -1.2972820000 -1.2706860000
B 3.0731150000 -0.1851720000 -0.1464820000
H -1.6935330000 -0.6570240000 -1.7512830000
C -1.6936600000 -1.7877890000 0.1064960000
F 4.2591590000 0.3328320000 0.3107400000
F 3.0790140000 -0.4419950000 -1.5256960000
F 2.6782770000 -1.3469480000 0.5451540000
C -1.1299770000 -1.7414890000 1.5287640000
C -3.2074030000 -1.9937700000 0.1237110000
H -1.2489510000 -2.6504030000 -0.4051460000
H -1.4834360000 -0.8531020000 2.0657740000
H -1.4689530000 -2.6180270000 2.0881330000
H -0.0369090000 -1.7381710000 1.5432990000
H -3.7111960000 -1.2003520000 0.6852770000
H -3.6289640000 -2.0308740000 -0.8860780000
H -3.4437510000 -2.9427670000 0.6138520000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.260101 (Hartree/Particle)
Thermal correction to Energy= 0.277211
Thermal correction to Enthalpy= 0.278155
Thermal correction to Gibbs (Free) Energy= 0.214863
Sum of electronic and zero-point Energies= -828.110500
Sum of electronic and thermal Energies= -828.093391
Sum of electronic and thermal Enthalpies= -828.092447
Sum of electronic and thermal (Free) Energies= -828.155739

c/u RT

C -2.8359490000 -1.9213450000 0.0713610000
C -1.5711770000 -1.8608360000 -0.2356160000
H -3.5584700000 -1.6187750000 -0.6864520000
C -3.3711670000 -2.3628760000 1.4089120000
C -0.2782750000 -1.8508680000 -0.5104220000
H -2.5637630000 -2.6444550000 2.0870090000
H -4.0407780000 -3.2192210000 1.2845040000
H -3.9482390000 -1.5546120000 1.8686510000
C 0.5279720000 -0.6621730000 -0.1796590000
C 0.4536180000 -3.0618580000 -1.0420280000
C -0.0412070000 0.6681840000 -0.0024960000
O 1.7580180000 -0.8737540000 -0.0425720000
H 1.1825250000 -3.4143070000 -0.3079120000
H 1.0055860000 -2.8065170000 -1.9507890000
H -0.2515590000 -3.8637790000 -1.2637980000
C -1.0999060000 1.1026960000 -0.7018150000
H 0.5121960000 1.3266390000 0.6573930000
B 2.8905540000 0.2402500000 0.2698770000
H -1.5687600000 0.4339270000 -1.4218590000
C -1.7171070000 2.4668320000 -0.6073850000
F 2.7702420000 1.1739190000 -0.7384740000
F 4.0484340000 -0.4783590000 0.2411610000
F 2.5666680000 0.7477290000 1.5151840000
C -1.0039190000 3.4161690000 0.3529150000
C -3.2054650000 2.3087770000 -0.2468660000
H -1.6698140000 2.8940570000 -1.6198080000
H 0.0450980000 3.5566400000 0.0774670000
H -1.4903360000 4.3955480000 0.3401450000
H -1.0406960000 3.0391810000 1.3809070000
H -3.7257460000 1.6556800000 -0.9552150000
H -3.3130430000 1.8806050000 0.7554610000
H -3.7037190000 3.2823550000 -0.2567650000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257284 (Hartree/Particle)
Thermal correction to Energy= 0.276089
Thermal correction to Enthalpy= 0.277033
Thermal correction to Gibbs (Free) Energy= 0.208830
Sum of electronic and zero-point Energies= -828.093404
Sum of electronic and thermal Energies= -828.074599
Sum of electronic and thermal Enthalpies= -828.073655
Sum of electronic and thermal (Free) Energies= -828.141858

c/u TS

C 2.7036350000 1.3962490000 0.0185120000
C 1.4396970000 1.1442590000 -0.2753390000
H 3.4862840000 0.8306820000 -0.4796100000
C 3.1271420000 2.3827190000 1.0709900000
C 0.1412680000 1.5410910000 -0.3732680000
H 2.2729350000 2.9279170000 1.4766490000
H 3.8387690000 3.0988760000 0.6476920000
H 3.6332240000 1.8683750000 1.8951430000
C -0.8087480000 0.4922300000 -0.1327900000
C -0.3056430000 2.9115860000 -0.7798050000
C -0.1717190000 -0.7743560000 -0.0433810000
O -2.0473150000 0.7573140000 0.0199660000
H 0.5401370000 3.5843490000 -0.9260380000
H -0.9580250000 3.3131040000 0.0023920000
H -0.9039790000 2.8675750000 -1.6945890000
C 1.0851430000 -0.8989340000 -0.6179460000
H -0.6142710000 -1.5617120000 0.5590090000
B -3.0914480000 -0.3968740000 0.1584570000
H 1.2377300000 -0.5220050000 -1.6293830000
C 2.0314580000 -2.0008420000 -0.1878790000
F -2.8809620000 -1.2457150000 -0.9270440000
F -4.3142950000 0.2176130000 0.1496190000
F -2.8009340000 -1.0455150000 1.3598740000
C 2.4205610000 -1.8940250000 1.2924600000
C 3.2570610000 -2.1094760000 -1.0977120000
H 1.4491060000 -2.9263700000 -0.3075380000
H 1.5388270000 -1.8283000000 1.9356230000
H 2.9961630000 -2.7727070000 1.5967900000
H 3.0361440000 -1.0064760000 1.4697920000
H 2.9686190000 -2.2039030000 -2.1491560000
H 3.9096220000 -1.2354360000 -1.0004780000
H 3.8510630000 -2.9885740000 -0.8334020000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256074 (Hartree/Particle)
Thermal correction to Energy= 0.274050
Thermal correction to Enthalpy= 0.274994
Thermal correction to Gibbs (Free) Energy= 0.209402
Sum of electronic and zero-point Energies= -828.065261
Sum of electronic and thermal Energies= -828.047285
Sum of electronic and thermal Enthalpies= -828.046341
Sum of electronic and thermal (Free) Energies= -828.111933

c/u PT

C 2.9167300000 0.9844060000 -0.4405810000
C 1.6417860000 0.5442350000 -0.3500790000
H 3.6412750000 0.2724320000 -0.8301790000
C 3.4681580000 2.3298030000 -0.0930640000
C 0.4770440000 1.2605860000 0.0946370000
H 2.7500250000 3.1376980000 -0.2360110000
H 4.3522450000 2.5416080000 -0.6984050000
H 3.7880500000 2.3470620000 0.9568980000
C -0.6941130000 0.5144530000 -0.2057440000
C 0.3866740000 2.5705490000 0.7796000000
C -0.2913530000 -0.6679570000 -0.8201260000
O -1.8832840000 0.9405180000 0.0858350000
H 0.4146850000 3.3785780000 0.0361970000
H 1.2071620000 2.7282700000 1.4818610000
H -0.5761920000 2.6405510000 1.2907200000
C 1.1776090000 -0.8154930000 -0.8431580000
H -0.9823100000 -1.4219710000 -1.1797530000
B -3.0503090000 -0.0418350000 -0.0317670000
H 1.5303360000 -0.9996070000 -1.8683700000
C 1.6105610000 -2.0466160000 0.0246930000
F -3.1686930000 -0.4004350000 -1.3823750000
F -4.1575890000 0.6066800000 0.4543170000
F -2.6999860000 -1.1758840000 0.7260080000
C 1.1467430000 -1.9251430000 1.4774570000
C 3.1140730000 -2.3184430000 -0.0563260000
H 1.0939410000 -2.9026490000 -0.4270330000
H 0.0580640000 -1.8649500000 1.5600140000
H 1.4800980000 -2.7969290000 2.0477800000
H 1.5753270000 -1.0360990000 1.9551240000
H 3.4775150000 -2.3166010000 -1.0897970000
H 3.6832160000 -1.5779820000 0.5157200000
H 3.3373150000 -3.2999090000 0.3719820000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.259780 (Hartree/Particle)
Thermal correction to Energy= 0.277027
Thermal correction to Enthalpy= 0.277972
Thermal correction to Gibbs (Free) Energy= 0.214273
Sum of electronic and zero-point Energies= -828.108418
Sum of electronic and thermal Energies= -828.091170
Sum of electronic and thermal Enthalpies= -828.090226
Sum of electronic and thermal (Free) Energies= -828.153924

cc/u RT

C -2.8271080000 -2.0271570000 -0.8207490000
C -1.6236620000 -1.9839010000 -0.3240620000
C -4.0734560000 -1.6000840000 -0.0907340000
H -2.9359890000 -2.3797950000 -1.8460240000
C -0.3928970000 -1.9794220000 0.1573420000
H -4.8003100000 -2.4173220000 -0.0681550000
H -4.5418510000 -0.7557080000 -0.6068950000
H -3.8547300000 -1.3049660000 0.9376970000
C 0.4615550000 -0.7964340000 -0.0453530000
C 0.2337020000 -3.1861020000 0.8170710000
C -0.0620390000 0.5326320000 -0.3373670000
O 1.6961700000 -1.0077360000 0.0438530000
H 1.0699100000 -3.5519750000 0.2158440000
H -0.5035740000 -3.9817690000 0.9304820000
H 0.6323530000 -2.9209660000 1.8001190000
C -1.2203230000 0.9871760000 0.1634400000
H 0.6043190000 1.1800580000 -0.8962700000
B 2.8664020000 0.1060120000 -0.0589730000
H -1.8141420000 0.3351170000 0.8022600000
C -1.7646690000 2.3752750000 -0.0069830000
F 3.9989420000 -0.6101620000 0.1904780000
F 2.5586980000 1.0450160000 0.9044850000
F 2.7814990000 0.6070380000 -1.3451540000
C -1.9375330000 3.0220050000 1.3786750000
C -0.9427990000 3.2628070000 -0.9395710000
H -2.7701780000 2.2514490000 -0.4380980000
H -0.9634340000 3.1611950000 1.8580790000
H -2.4149280000 4.0013550000 1.2824030000
H -2.5576490000 2.4061920000 2.0380110000
H 0.0597700000 3.4371920000 -0.5350310000
H -0.8380030000 2.8188300000 -1.9340070000
H -1.4298060000 4.2351430000 -1.0549090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257548 (Hartree/Particle)
Thermal correction to Energy= 0.276246
Thermal correction to Enthalpy= 0.277190
Thermal correction to Gibbs (Free) Energy= 0.209425
Sum of electronic and zero-point Energies= -828.093453
Sum of electronic and thermal Energies= -828.074755
Sum of electronic and thermal Enthalpies= -828.073810
Sum of electronic and thermal (Free) Energies= -828.141575

cc/u TS

C -2.6747800000 1.7496260000 0.4293970000
C -1.4455280000 1.4428730000 0.0464770000
C -3.9622410000 1.2861740000 -0.1807750000
H -2.7518090000 2.3864590000 1.3122230000
C -0.1303940000 1.7832500000 -0.0607760000
H -4.6259260000 2.1438470000 -0.3258540000
H -4.4815240000 0.5855250000 0.4833960000
H -3.8103440000 0.8080100000 -1.1498990000
C 0.7696750000 0.6666490000 -0.0014270000
C 0.3794820000 3.1708890000 -0.2982390000
C 0.0629280000 -0.5643220000 -0.0126370000
O 2.0273060000 0.8460570000 0.1154530000
H 1.0902770000 3.4221500000 0.4957560000
H -0.4291930000 3.9021200000 -0.3057990000
H 0.9328120000 3.2231810000 -1.2406050000
C -1.2221860000 -0.5557130000 -0.5369160000
H 0.4804540000 -1.4268320000 0.4969240000
B 3.0031450000 -0.3731720000 0.0642540000
H -1.3815610000 -0.0897610000 -1.5089980000
C -2.2231300000 -1.6287680000 -0.1723620000
F 4.2599570000 0.1678940000 0.0504200000
F 2.6827430000 -1.0808700000 -1.0936730000
F 2.7359510000 -1.1370470000 1.2017450000
C -1.8659680000 -2.9244940000 -0.9233420000
C -2.3194820000 -1.8568810000 1.3377990000
H -3.2028210000 -1.3017310000 -0.5354850000
H -0.8962390000 -3.3107210000 -0.5947950000
H -2.6226990000 -3.6896240000 -0.7270020000
H -1.8154170000 -2.7629280000 -2.0040670000
H -1.3831980000 -2.2524200000 1.7437250000
H -2.5469020000 -0.9245060000 1.8640820000
H -3.1082150000 -2.5808430000 1.5618790000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256607 (Hartree/Particle)
Thermal correction to Energy= 0.274313
Thermal correction to Enthalpy= 0.275257
Thermal correction to Gibbs (Free) Energy= 0.210567
Sum of electronic and zero-point Energies= -828.065429
Sum of electronic and thermal Energies= -828.047723
Sum of electronic and thermal Enthalpies= -828.046778
Sum of electronic and thermal (Free) Energies= -828.111468

cc/u PT

C 2.8492320000 -1.5197880000 -0.1700110000
C 1.6484940000 -0.9051560000 -0.2096930000
C 4.1599720000 -0.9287210000 -0.5613310000
H 2.8815390000 -2.5537310000 0.1690310000
C 0.3993390000 -1.5332210000 0.1164260000
H 4.6893670000 -1.6084030000 -1.2369190000
H 4.7963090000 -0.8107710000 0.3245260000
H 4.0616840000 0.0412170000 -1.0502980000
C -0.6763470000 -0.6467780000 -0.1589220000
C 0.1524020000 -2.8889990000 0.6454620000
C -0.1303670000 0.5260060000 -0.6667690000
O -1.9125840000 -0.9750700000 0.0561180000
H -0.4369370000 -2.8007590000 1.5655280000
H 1.0579100000 -3.4638410000 0.8386850000
H -0.4918170000 -3.4316210000 -0.0561410000
C 1.3518390000 0.5137840000 -0.6500850000
H -0.7305680000 1.3668010000 -0.9925630000
B -2.9810980000 0.1097700000 -0.0881150000
H 1.7430650000 0.6949970000 -1.6617970000
C 1.9367360000 1.6189590000 0.2888360000
F -4.1709240000 -0.4601280000 0.2902990000
F -2.9738140000 0.5352940000 -1.4250470000
F -2.5926280000 1.1760480000 0.7450470000
C 1.6826350000 3.0108090000 -0.2938420000
C 1.3947560000 1.5071040000 1.7153070000
H 3.0210010000 1.4596240000 0.3200590000
H 0.6147920000 3.2518180000 -0.3017720000
H 2.1837510000 3.7701700000 0.3134230000
H 2.0608160000 3.0963650000 -1.3180000000
H 0.3201230000 1.7140810000 1.7515330000
H 1.5603900000 0.5108100000 2.1383040000
H 1.8988980000 2.2300240000 2.3630780000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.259271 (Hartree/Particle)
Thermal correction to Energy= 0.276779
Thermal correction to Enthalpy= 0.277723
Thermal correction to Gibbs (Free) Energy= 0.213165
Sum of electronic and zero-point Energies= -828.114576
Sum of electronic and thermal Energies= -828.097068
Sum of electronic and thermal Enthalpies= -828.096124
Sum of electronic and thermal (Free) Energies= -828.160682

1d

cRT

C -0.2286590000 3.5606920000 0.2602610000
C -0.9795810000 2.5818340000 -0.1595040000
C -1.7927140000 1.6162560000 -0.5500580000
C -1.4946450000 0.2178180000 -0.1873820000
C -0.1579750000 -0.2712520000 0.1005990000
C 0.9487120000 0.2529950000 -0.4603920000
H -0.1173830000 -1.1541110000 0.7276140000
C -3.1081400000 1.8872890000 -1.2440880000
O -2.4970020000 -0.5393300000 -0.1269370000
H -3.2019750000 2.9488650000 -1.4761080000
H -3.9409140000 1.5817800000 -0.6057380000

H -3.1785630000 1.3090950000 -2.1696070000
B -2.4792330000 -2.1213850000 0.1908250000
F -3.7888020000 -2.4804090000 0.0710890000
F -1.9757030000 -2.2320020000 1.4763720000
F -1.6432510000 -2.6752220000 -0.7573590000
C -0.3731240000 4.2341750000 1.6004860000
H 0.5680080000 3.9106770000 -0.3961830000
H -1.2002030000 3.8089820000 2.1715750000
H -0.5512290000 5.3056240000 1.4678850000
H 0.5477660000 4.1195090000 2.1803030000
H 0.8404170000 1.0912480000 -1.1443020000
C 2.3204310000 -0.2164440000 -0.2670380000
C 3.3634190000 0.5155640000 -0.8521850000
C 2.6357220000 -1.3619010000 0.4808490000
C 4.6883460000 0.1266600000 -0.6866440000
C 4.9875760000 -1.0080410000 0.0631180000
C 3.9582380000 -1.7513870000 0.6428450000
H 3.1300410000 1.3983210000 -1.4418220000
H 5.4842550000 0.7048250000 -1.1445330000
H 6.0196050000 -1.3183390000 0.1917040000
H 4.1888790000 -2.6415500000 1.2187310000
H 1.8476390000 -1.9601960000 0.9257460000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.254299 (Hartree/Particle)
Thermal correction to Energy= 0.273493
Thermal correction to Enthalpy= 0.274437
Thermal correction to Gibbs (Free) Energy= 0.203634
Sum of electronic and zero-point Energies= -941.164675
Sum of electronic and thermal Energies= -941.145481
Sum of electronic and thermal Enthalpies= -941.144537
Sum of electronic and thermal (Free) Energies= -941.215340

cTS

C 1.3890780000 2.5436940000 0.1023010000
C 0.2823410000 1.8984440000 -0.2149550000
C -1.0714090000 1.7708080000 -0.2897320000
C -1.5371560000 0.4223780000 -0.1193510000
C -0.4627740000 -0.5064550000 -0.1327960000
C 0.7252020000 -0.0774870000 -0.7207580000
C -2.0231830000 2.8828470000 -0.6059070000
O -2.7777610000 0.1823880000 0.0628010000
H -1.5048730000 3.8350820000 -0.7238300000
H -2.7493790000 2.9636300000 0.2095530000
H -2.5938850000 2.6573000000 -1.5115930000
H -0.5513020000 -1.4560040000 0.3838590000
B -3.2984620000 -1.2877480000 0.1312940000
F -4.6623410000 -1.1868860000 0.1946430000
F -2.7278870000 -1.8526990000 1.2740010000
F -2.8347550000 -1.9214990000 -1.0199360000
H 2.3115550000 2.2855540000 -0.4157050000
C 1.4786690000 3.5516670000 1.2133610000
H 0.5004420000 3.7539980000 1.6534020000
H 1.8989230000 4.4889930000 0.8347360000
H 2.1476750000 3.1880390000 2.0004510000
H 0.6809420000 0.3832610000 -1.7069260000
C 2.0412850000 -0.6311620000 -0.3707760000
C 3.0764700000 -0.6076610000 -1.3130290000
C 2.2915200000 -1.1501740000 0.9063700000
C 4.3323800000 -1.1150660000 -0.9953300000
H 2.8906570000 -0.2028420000 -2.3046570000
C 3.5451490000 -1.6587020000 1.2229550000
H 1.5036360000 -1.1441540000 1.6541160000
C 4.5665420000 -1.6430990000 0.2725710000
H 5.1253150000 -1.1017890000 -1.7358640000
H 3.7293260000 -2.0627710000 2.2129100000
H 5.5455300000 -2.0391030000 0.5227680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.253193 (Hartree/Particle)
Thermal correction to Energy= 0.271374
Thermal correction to Enthalpy= 0.272318
Thermal correction to Gibbs (Free) Energy= 0.205259
Sum of electronic and zero-point Energies= -941.140009
Sum of electronic and thermal Energies= -941.121828
Sum of electronic and thermal Enthalpies= -941.120884
Sum of electronic and thermal (Free) Energies= -941.187943

cPT

C -1.6292260000 2.4497610000 0.2077390000
C -0.6055480000 1.5765290000 0.3330990000
C 0.7652780000 1.6933250000 -0.0674230000
C 1.4409110000 0.4548610000 0.1335540000
C 0.5449850000 -0.4251480000 0.7341070000
C -0.7847240000 0.1894560000 0.9430490000
C 1.4920010000 2.8721560000 -0.5955050000
O 2.6801470000 0.2883940000 -0.2001330000
H 1.2235540000 3.0306360000 -1.6479570000
H 2.5663420000 2.6838990000 -0.5534050000
H 1.2440390000 3.7823570000 -0.0444870000
H 0.7891470000 -1.4422030000 1.0163630000
B 3.3138000000 -1.0956950000 -0.0159630000
F 3.2352600000 -1.4097860000 1.3486210000
F 4.6035440000 -0.9929860000 -0.4736030000
F 2.5355010000 -1.9997710000 -0.7563510000
H -2.5888240000 2.1042680000 0.5933310000
C -1.6534070000 3.8039620000 -0.4129630000
H -0.7715900000 4.0344220000 -1.0073680000
H -1.7528980000 4.5659740000 0.3703790000
H -2.5388470000 3.8974940000 -1.0493740000
C -1.9448430000 -0.6161900000 0.3865490000
H -0.9409720000 0.3137970000 2.0267330000
C -1.8472300000 -1.2175610000 -0.8716360000
C -2.9241740000 -1.9244360000 -1.3961320000
C -4.1094940000 -2.0379910000 -0.6702560000
C -4.2103240000 -1.4464990000 0.5857240000
C -3.1294360000 -0.7411030000 1.1125770000
H -0.9224630000 -1.1421740000 -1.4383980000
H -2.8346670000 -2.3942220000 -2.3702540000
H -4.9471000000 -2.5935370000 -1.0794580000
H -5.1255470000 -1.5401090000 1.1615700000
H -3.2077060000 -0.2931340000 2.1003250000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255460 (Hartree/Particle)
Thermal correction to Energy= 0.273549
Thermal correction to Enthalpy= 0.274493
Thermal correction to Gibbs (Free) Energy= 0.206290
Sum of electronic and zero-point Energies= -941.178076
Sum of electronic and thermal Energies= -941.159988
Sum of electronic and thermal Enthalpies= -941.159043
Sum of electronic and thermal (Free) Energies= -941.227246

ccRT

C -0.1683880000 3.4423040000 0.9142700000
C 0.7341270000 2.6635410000 0.3885350000
C -1.3860600000 3.9558400000 0.1914360000
H -0.0460610000 3.7209320000 1.9605050000
C 1.6745600000 1.8845890000 -0.1159760000
H -2.2939640000 3.5587850000 0.6575850000
H -1.3772510000 3.6691590000 -0.8626480000
H -1.4334790000 5.0470540000 0.2505010000
C 1.5514200000 0.4206600000 0.0159140000
C 2.9513270000 2.4230930000 -0.7190300000
C 0.2833680000 -0.2638330000 0.2034990000
O 2.6372960000 -0.2114490000 -0.0306270000
H 3.8086550000 2.1295410000 -0.1080390000
H 2.9104790000 3.5111030000 -0.7833060000
H 3.1073370000 2.0084050000 -1.7187280000
C -0.8806200000 0.2035320000 -0.2865530000
H 0.3509240000 -1.2290100000 0.6917840000
B 2.8080350000 -1.8163750000 0.0203130000
H -0.8779450000 1.1413400000 -0.8363800000
C -2.1868110000 -0.4466060000 -0.1814630000
F 4.1503120000 -1.9941560000 -0.1357330000
F 2.0402900000 -2.2974490000 -1.0207110000
F 2.3248370000 -2.1978690000 1.2607440000
C -3.3167080000 0.2557400000 -0.6241390000
C -2.3562750000 -1.7357490000 0.3469750000
C -4.5864390000 -0.3033940000 -0.5291210000
H -3.1949760000 1.2510060000 -1.0440340000
C -3.6238420000 -2.2948710000 0.4379040000
H -1.4963590000 -2.3116420000 0.6725390000
C -4.7416330000 -1.5805280000 0.0042420000
H -5.4514750000 0.2538390000 -0.8736060000
H -3.7416380000 -3.2944710000 0.8430580000
H -5.7299070000 -2.0232250000 0.0765590000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.254221 (Hartree/Particle)
Thermal correction to Energy= 0.273357
Thermal correction to Enthalpy= 0.274301
Thermal correction to Gibbs (Free) Energy= 0.204235
Sum of electronic and zero-point Energies= -941.165509
Sum of electronic and thermal Energies= -941.146373
Sum of electronic and thermal Enthalpies= -941.145429
Sum of electronic and thermal (Free) Energies= -941.215495

ccTS

C 1.3066920000 2.6207360000 -0.6012140000
C 0.2382320000 1.9754680000 -0.1616760000
C 2.6819730000 2.6159270000 -0.0081300000
H 1.1753880000 3.1708850000 -1.5344600000
C -1.1180120000 1.8706020000 -0.0647980000
H 3.3581580000 1.9936520000 -0.6057220000
H 2.6890280000 2.2403150000 1.0156060000
H 3.0836380000 3.6332860000 -0.0069800000
C -1.5994560000 0.5182320000 -0.0191040000
C -2.0616150000 3.0256220000 0.0612820000
C -0.5306820000 -0.4046540000 0.1089350000
O -2.8447670000 0.2669430000 -0.1448970000
H -2.6164770000 2.9698070000 1.0026760000
H -2.8032790000 2.9578930000 -0.7414010000
H -1.5411970000 3.9814170000 -0.0036700000
C 0.6718300000 0.0945450000 0.6123690000
H -0.6253990000 -1.4161480000 -0.2714660000
B -3.3752880000 -1.1924290000 0.0190160000
H 0.6514590000 0.6567580000 1.5452070000
C 1.9599240000 -0.5478240000 0.3002730000
F -4.7395130000 -1.0905830000 -0.0347820000
F -2.8938890000 -1.6477940000 1.2450910000
F -2.8291200000 -1.9283920000 -1.0343230000
C 2.9586310000 -0.6422390000 1.2760600000
C 2.2050310000 -1.0545820000 -0.9812560000
C 4.1740800000 -1.2503180000 0.9832900000
H 2.7758260000 -0.2471880000 2.2721080000
C 3.4231320000 -1.6567300000 -1.2768320000
H 1.4417590000 -0.9600320000 -1.7487660000
C 4.4078770000 -1.7565250000 -0.2947570000
H 4.9382700000 -1.3303230000 1.7493970000
H 3.6059150000 -2.0457400000 -2.2730660000
H 5.3583670000 -2.2266130000 -0.5258990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.253470 (Hartree/Particle)
Thermal correction to Energy= 0.271434
Thermal correction to Enthalpy= 0.272378
Thermal correction to Gibbs (Free) Energy= 0.206192
Sum of electronic and zero-point Energies= -941.138875
Sum of electronic and thermal Energies= -941.120911
Sum of electronic and thermal Enthalpies= -941.119967
Sum of electronic and thermal (Free) Energies= -941.186153

ccPT

C -1.4623410000 2.6915190000 -0.0188390000
C -0.5532530000 1.7063440000 -0.1818670000
C 0.8009300000 1.7529610000 0.2818010000
C 1.4755700000 0.5406460000 -0.0380940000
C 0.5774370000 -0.2683820000 -0.7237620000
C -0.7587500000 0.3683470000 -0.8716230000
C 1.5040850000 2.8484220000 0.9773900000
O 2.7126650000 0.3442270000 0.2912080000
H 0.8763740000 3.7106630000 1.2009880000
H 2.3585000000 3.1601970000 0.3649330000
H 1.9440190000 2.4524770000 1.8997280000
H 0.8094540000 -1.2600810000 -1.0928920000
B 3.3677440000 -0.9937680000 -0.0715500000
F 4.6575940000 -0.9295880000 0.3950130000
F 3.2919420000 -1.1249080000 -1.4664740000
F 2.6087910000 -2.0015010000 0.5415920000
C -2.8718450000 2.6780630000 -0.4939290000
H -1.1528540000 3.5832830000 0.5235530000
H -3.1267920000 1.7761530000 -1.0499960000
H -3.0602730000 3.5543840000 -1.1242620000
H -3.5496320000 2.7590860000 0.3641910000
H -0.9623910000 0.5369570000 -1.9393250000
C -1.8720670000 -0.5020150000 -0.3021770000
C -1.9001560000 -0.8022490000 1.0617920000
C -2.8562550000 -1.0299360000 -1.1367210000
C -3.8661780000 -1.8370980000 -0.6154100000
C -3.8953640000 -2.1237500000 0.7461880000
C -2.9082360000 -1.6053110000 1.5838840000
H -1.1249280000 -0.4141400000 1.7175530000
H -2.9176840000 -1.8353410000 2.6443420000
H -4.6788520000 -2.7543180000 1.1536620000
H -2.8354260000 -0.8126070000 -2.2018420000
H -4.6259710000 -2.2430860000 -1.2755140000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.255531 (Hartree/Particle)
Thermal correction to Energy= 0.273643
Thermal correction to Enthalpy= 0.274587
Thermal correction to Gibbs (Free) Energy= 0.206931
Sum of electronic and zero-point Energies= -941.182434
Sum of electronic and thermal Energies= -941.164323
Sum of electronic and thermal Enthalpies= -941.163378
Sum of electronic and thermal (Free) Energies= -941.231034

2a

cRT

C -3.0453510000 -1.5144060000 -0.1273480000
C -2.0358290000 -0.7134400000 0.0628110000
C -1.0269080000 0.1333980000 0.1827570000
C 0.3286430000 -0.4454490000 0.1724710000
C 0.6162810000 -1.7806750000 0.7143920000
C -0.0526830000 -2.3007890000 1.7470140000
H 1.4794230000 -2.2832150000 0.2914260000
C -1.2302340000 1.6628350000 0.2140130000
O 1.2438130000 0.2526370000 -0.3196870000
C -2.7028310000 1.9738510000 0.5150890000
C -0.8632060000 2.2720650000 -1.1525320000
C -0.3590690000 2.2776200000 1.3244600000
B 2.8306610000 -0.1025720000 -0.3813170000
F 3.3657460000 1.0234310000 -0.9316390000
F 2.9174520000 -1.2266040000 -1.1774460000
F 3.1922300000 -0.3319190000 0.9273640000
H -1.4767950000 1.8346110000 -1.9471960000
H 0.1882550000 2.1152320000 -1.3966470000
H -1.0543670000 3.3503160000 -1.1314620000
H -3.0174230000 1.5437050000 1.4719970000
H -3.3661680000 1.5905340000 -0.2662180000
H -2.8390160000 3.0580730000 0.5701540000
H -0.5981830000 1.8388850000 2.2995060000
H -0.5537500000 3.3530270000 1.3844770000
H 0.7073710000 2.1438360000 1.1325000000
H -3.5510060000 -1.9166420000 0.7498680000
C -3.5584280000 -1.9266270000 -1.4827780000
H -2.9793290000 -1.4639790000 -2.2840500000
H -4.6072120000 -1.6344090000 -1.5934660000
H -3.5032170000 -3.0137320000 -1.5940020000
H -0.8697470000 -1.7767680000 2.2320500000
H 0.2361970000 -3.2621750000 2.1585430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257230 (Hartree/Particle)
Thermal correction to Energy= 0.275655
Thermal correction to Enthalpy= 0.276599
Thermal correction to Gibbs (Free) Energy= 0.210430
Sum of electronic and zero-point Energies= -828.084281
Sum of electronic and thermal Energies= -828.065855
Sum of electronic and thermal Enthalpies= -828.064911
Sum of electronic and thermal (Free) Energies= -828.131081

cTS

C 2.9351880000 -1.5765510000 -0.0134820000
C 1.7870100000 -0.9630260000 -0.2376020000
C 0.8996990000 0.0644730000 -0.1352370000
C -0.4715710000 -0.3832910000 -0.0516720000
C -0.5875570000 -1.7773630000 -0.3415300000
C 0.4415970000 -2.3457230000 -1.0565090000
C 1.2836790000 1.5430150000 -0.1882610000
O -1.4132240000 0.3942220000 0.3074100000

C 2.7750890000 1.7199630000 -0.5017110000
C 0.9802910000 2.1589580000 1.1939930000
C 0.4578560000 2.2548460000 -1.2767340000
H -1.3740440000 -2.3610080000 0.1249670000
B -2.9134330000 -0.0568720000 0.2294220000
F -3.0961820000 -0.5628990000 -1.0539810000
F -3.6332320000 1.0790190000 0.4849300000
F -3.0715240000 -1.0508100000 1.1914840000
H 3.2789260000 -2.3264040000 -0.7221970000
C 3.7826950000 -1.3371370000 1.2050620000
H 3.9230080000 -2.2693330000 1.7614080000
H 3.3289850000 -0.6000220000 1.8701780000
H 4.7741340000 -0.9805570000 0.9056270000
H 0.6560720000 1.8210040000 -2.2626600000
H 0.7399440000 3.3119190000 -1.3114870000
H -0.6133550000 2.1956390000 -1.0771840000
H 3.0430060000 1.2692950000 -1.4625850000
H 3.4118370000 1.2822010000 0.2729370000
H 3.0047380000 2.7882800000 -0.5544460000
H -0.0785850000 2.0753460000 1.4451700000
H 1.2497820000 3.2200900000 1.1794700000
H 1.5680670000 1.6703120000 1.9784330000
H 0.6195330000 -3.4166810000 -0.9795380000
H 0.8455020000 -1.8862820000 -1.9542850000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256917 (Hartree/Particle)
Thermal correction to Energy= 0.274085
Thermal correction to Enthalpy= 0.275029
Thermal correction to Gibbs (Free) Energy= 0.212399
Sum of electronic and zero-point Energies= -828.058394
Sum of electronic and thermal Energies= -828.041226
Sum of electronic and thermal Enthalpies= -828.040282
Sum of electronic and thermal (Free) Energies= -828.102912

cPT

C -2.9101740000 -1.5821760000 -0.1357780000
C -1.6524860000 -1.2444830000 0.2258960000
C -0.8723210000 -0.0348750000 0.0958100000
C 0.5106270000 -0.4071290000 0.0007440000
C 0.6236720000 -1.7398580000 0.3831180000
C -0.6887390000 -2.3399380000 0.6582570000
C -1.2941920000 1.4137610000 0.1835170000
O 1.4498030000 0.4183420000 -0.3383760000
C -2.7385280000 1.6261960000 0.6647130000
C -1.0867880000 2.0646700000 -1.2046360000
C -0.3710440000 2.1109540000 1.2205330000
H 1.5704630000 -2.2587120000 0.4693490000
B 2.9180330000 -0.0012820000 -0.2042090000
F 3.1140620000 -0.3719260000 1.1347960000
F 3.6566900000 1.0973510000 -0.5720030000
F 3.1196450000 -1.1070640000 -1.0400130000
H -3.1949400000 -2.6044060000 0.1141000000
C -3.9220810000 -0.8482390000 -0.9495940000
H -4.3659190000 -1.5443320000 -1.6678830000
H -3.4961330000 -0.0126970000 -1.5035310000
H -4.7406640000 -0.4804770000 -0.3197830000
H -0.5132300000 1.6767620000 2.2154440000
H -0.6520860000 3.1669800000 1.2695480000
H 0.6815980000 2.0446580000 0.9514920000
H -2.9781380000 0.9924160000 1.5245130000
H -3.4787840000 1.4547940000 -0.1145220000
H -2.8498380000 2.6669290000 0.9807070000
H -0.0434080000 1.9965660000 -1.5183820000
H -1.3664370000 3.1209120000 -1.1395800000
H -1.7179960000 1.5928970000 -1.9650040000
H -0.8269770000 -3.2956420000 0.1386690000
H -0.8173450000 -2.5355120000 1.7324260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.259597 (Hartree/Particle)
Thermal correction to Energy= 0.276594
Thermal correction to Enthalpy= 0.277539
Thermal correction to Gibbs (Free) Energy= 0.214672
Sum of electronic and zero-point Energies= -828.093684
Sum of electronic and thermal Energies= -828.076686
Sum of electronic and thermal Enthalpies= -828.075742
Sum of electronic and thermal (Free) Energies= -828.138609

ccRT

C 3.0255260000 -1.1795270000 -0.9679030000
C 2.0100820000 -0.4946400000 -0.5255340000
C 0.9846980000 0.2353400000 -0.1189580000
C -0.3212620000 -0.4437820000 -0.0534720000
C -0.4458870000 -1.8790950000 0.2400330000
C 0.3930990000 -2.5290390000 1.0510410000
C 1.1065260000 1.7456020000 0.1701140000
O -1.3400110000 0.2537810000 -0.2590750000
C 2.5894110000 2.1167010000 0.3114670000
C 0.3877750000 2.0774470000 1.4905630000
C 0.4982110000 2.5582820000 -0.9884640000
H -1.3292040000 -2.3643480000 -0.1610480000
B -2.8952970000 -0.2170060000 -0.1622030000
F -3.5709810000 0.9442330000 -0.3898120000
F -3.0317260000 -0.7226910000 1.1112670000
F -3.0455900000 -1.1706770000 -1.1481660000
H 1.0009170000 2.3216950000 -1.9320730000
H 0.6333470000 3.6270950000 -0.7910650000
H -0.5689530000 2.3633150000 -1.1025870000
H 3.1425250000 1.9368810000 -0.6152320000
H 3.0715490000 1.5474000000 1.1137840000
H 2.6744090000 3.1803290000 0.5534340000
H -0.6869300000 1.8946940000 1.4317620000
H 0.5325250000 3.1366430000 1.7254770000
H 0.7989230000 1.4911290000 2.3198040000
C 3.9995490000 -1.9290700000 -0.0983790000
H 3.1710370000 -1.2217880000 -2.0469080000
H 3.7904850000 -1.7751210000 0.9622750000
H 5.0219200000 -1.5961860000 -0.3002150000
H 3.9513740000 -3.0013010000 -0.3140420000
H 1.2376840000 -2.0397920000 1.5249840000
H 0.2232750000 -3.5729670000 1.2926150000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.257092 (Hartree/Particle)
Thermal correction to Energy= 0.275544
Thermal correction to Enthalpy= 0.276488
Thermal correction to Gibbs (Free) Energy= 0.210302
Sum of electronic and zero-point Energies= -828.084837
Sum of electronic and thermal Energies= -828.066385
Sum of electronic and thermal Enthalpies= -828.065441
Sum of electronic and thermal (Free) Energies= -828.131627

ccTS

C 3.0747690000 -1.0363280000 -0.6141300000
C 1.8855420000 -0.6395460000 -0.1979640000
C 0.8762820000 0.2725520000 -0.0938160000
C -0.4324470000 -0.3349890000 -0.0859900000
C -0.3478100000 -1.7558450000 0.0397630000
C 0.8095530000 -2.2569130000 0.5905460000
C 1.0873240000 1.7764770000 0.0805160000
O -1.4972150000 0.3456150000 -0.2422610000
C 2.5762430000 2.1208350000 0.2152400000
C 0.3456130000 2.2577250000 1.3420690000
C 0.5197060000 2.4824420000 -1.1696580000
H -1.1024430000 -2.3844030000 -0.4212550000
B -2.9092390000 -0.3091960000 -0.0554150000
F -3.7884720000 0.7392810000 -0.0847800000
F -2.8653820000 -0.9735800000 1.1673130000
F -3.0667190000 -1.2048630000 -1.1098870000
H 1.0384360000 2.1519130000 -2.0756820000
H 0.6694650000 3.5622530000 -1.0676400000
H -0.5483120000 2.2917880000 -1.2869230000
H 3.1414360000 1.8461670000 -0.6807780000
H 3.0324300000 1.6206920000 1.0755190000
H 2.6817020000 3.2004330000 0.3572470000
H -0.7274960000 2.0692290000 1.2776540000
H 0.4951260000 3.3355070000 1.4616630000
H 0.7366120000 1.7621770000 2.2371810000
C 3.9693310000 -2.0610980000 0.0156220000
H 3.4255680000 -0.5827920000 -1.5419630000
H 3.5656100000 -2.4411120000 0.9558700000
H 4.9498770000 -1.6196830000 0.2200510000
H 4.1298840000 -2.9035970000 -0.6649180000
H 1.2346130000 -1.8430970000 1.5004020000
H 1.1019230000 -3.2838310000 0.3817370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256559 (Hartree/Particle)
Thermal correction to Energy= 0.273824
Thermal correction to Enthalpy= 0.274768
Thermal correction to Gibbs (Free) Energy= 0.211706
Sum of electronic and zero-point Energies= -828.057419
Sum of electronic and thermal Energies= -828.040154
Sum of electronic and thermal Enthalpies= -828.039210
Sum of electronic and thermal (Free) Energies= -828.102272

ccPT

C -3.1781610000 -0.7961060000 0.0000010000
C -1.8261430000 -0.8528380000 0.0000010000
C -0.8646760000 0.2272070000 0.0000000000
C 0.4558370000 -0.3426520000 0.0000000000
C 0.3402990000 -1.7253500000 0.0000000000
C -1.0646410000 -2.1567430000 0.0000000000
C -1.0539820000 1.7260160000 0.0000010000
O 1.5418060000 0.3688560000 -0.0000010000
C -2.5039020000 2.2264250000 0.0000010000
C -0.3589870000 2.2846780000 -1.2693520000
C -0.3589860000 2.2846780000 1.2693530000
H 1.1904180000 -2.3958810000 -0.0000010000
B 2.9078620000 -0.3181670000 -0.0000010000
F 3.8370480000 0.6952450000 -0.0000010000
F 2.9726540000 -1.1219960000 -1.1477540000
F 2.9726550000 -1.1219960000 1.1477520000
H -0.8443560000 1.9057810000 2.1746560000
H -0.4558490000 3.3747530000 1.2628200000
H 0.7001310000 2.0296400000 1.2971370000
H -3.0520500000 1.9175720000 0.8955530000
H -3.0520500000 1.9175720000 -0.8955500000
H -2.4849330000 3.3199580000 0.0000010000
H 0.7001300000 2.0296400000 -1.2971380000
H -0.4558500000 3.3747530000 -1.2628190000
H -0.8443580000 1.9057820000 -2.1746550000
C -4.0870350000 -1.9774630000 0.0000010000
H -3.6744940000 0.1645420000 0.0000010000
H -3.5616730000 -2.9331160000 0.0000010000
H -4.7432980000 -1.9385630000 -0.8769770000
H -4.7432980000 -1.9385630000 0.8769810000
H -1.2955850000 -2.7711410000 -0.8807020000
H -1.2955840000 -2.7711410000 0.8807030000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.259830 (Hartree/Particle)
Thermal correction to Energy= 0.276815
Thermal correction to Enthalpy= 0.277759
Thermal correction to Gibbs (Free) Energy= 0.214914
Sum of electronic and zero-point Energies= -828.104947
Sum of electronic and thermal Energies= -828.087962
Sum of electronic and thermal Enthalpies= -828.087018
Sum of electronic and thermal (Free) Energies= -828.149863

2b

cRT

C -3.0114770000 1.2767860000 0.6495490000
C -2.0347740000 0.5201100000 0.2342760000
C -1.0573620000 -0.2927560000 -0.1250750000
C 0.3218000000 0.2121200000 0.0391670000
C 0.6745640000 1.6095490000 -0.1808050000
C 0.0079340000 2.4050070000 -1.0316030000
H 1.5811720000 1.9520840000 0.3074150000
C -1.3104710000 -1.7423030000 -0.5885500000
O 1.1892750000 -0.6271360000 0.3827630000
C -2.7841810000 -1.8979340000 -0.9881370000
C -0.9980580000 -2.7256130000 0.5553720000
C -0.4303110000 -2.0517950000 -1.8129920000
B 2.7800570000 -0.3834140000 0.5225210000
F 3.2519050000 -1.6274730000 0.8253840000
F 2.9270170000 0.5434070000 1.5368050000
F 3.1796300000 0.0943760000 -0.7085180000
H -1.6178150000 -2.5067740000 1.4313490000
H 0.0510760000 -2.6819360000 0.8507860000
H -1.2222360000 -3.7464290000 0.2274110000
H -3.0584130000 -1.2042190000 -1.7902210000
H -3.4541420000 -1.7222360000 -0.1410050000
H -2.9560400000 -2.9169500000 -1.3478380000
H -0.6306040000 -1.3482200000 -2.6287800000
H -0.6549750000 -3.0592790000 -2.1770590000
H 0.6345150000 -2.0150980000 -1.5734340000
H -3.4982890000 1.9284220000 -0.0755790000
C -3.5136400000 1.3121990000 2.0697890000
H -2.9548510000 0.6223160000 2.7048820000
H -4.5731680000 1.0399430000 2.1029630000
H -3.4177080000 2.3214820000 2.4816150000
H -0.8504690000 2.0092460000 -1.5706030000
C 0.3930430000 3.8129370000 -1.3346230000
H 1.2598890000 4.1335310000 -0.7535500000
H -0.4457270000 4.4861210000 -1.1241140000
H 0.6239260000 3.9195240000 -2.4001800000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.285109 (Hartree/Particle)
Thermal correction to Energy= 0.305249
Thermal correction to Enthalpy= 0.306193
Thermal correction to Gibbs (Free) Energy= 0.235788
Sum of electronic and zero-point Energies= -867.371491
Sum of electronic and thermal Energies= -867.351351
Sum of electronic and thermal Enthalpies= -867.350407
Sum of electronic and thermal (Free) Energies= -867.420812

cTS

C -2.9681780000 1.0964300000 0.2388750000
C -1.7813130000 0.6147660000 -0.0837110000
C -0.8296390000 -0.3632820000 -0.0992100000
C 0.5038710000 0.1720660000 0.0238630000
C 0.5128940000 1.5845570000 -0.1357160000
C -0.5714180000 2.1523480000 -0.7864050000
H 1.2749600000 2.1814710000 0.3559840000
C -1.1103430000 -1.8483410000 -0.3128930000
O 1.5071940000 -0.5665750000 0.3044490000
C -2.5869090000 -2.0956440000 -0.6477850000
C -0.7551910000 -2.5863830000 0.9955910000
C -0.2407350000 -2.3786740000 -1.4690190000
B 2.9595830000 0.0014060000 0.2626810000
F 3.7722080000 -1.0900400000 0.4227700000
F 3.0547860000 0.9257350000 1.3026540000
F 3.0994060000 0.6268310000 -0.9751070000
H -1.3721400000 -2.2294370000 1.8272140000
H 0.2964380000 -2.4526240000 1.2558240000
H -0.9469850000 -3.6565880000 0.8658200000
H -2.8915330000 -1.5596000000 -1.5522610000
H -3.2492250000 -1.7946040000 0.1691800000
H -2.7399280000 -3.1649270000 -0.8213930000
H -0.4745020000 -1.8572590000 -2.4034530000
H -0.4457460000 -3.4436310000 -1.6176310000
H 0.8241560000 -2.2625240000 -1.2605070000
H -3.3854970000 1.9087750000 -0.3526250000
C -3.7655100000 0.6366440000 1.4274990000
H -3.2415090000 -0.1428020000 1.9838060000
H -4.7349800000 0.2458870000 1.0997530000
H -3.9615330000 1.4751820000 2.1035310000
H -0.9081500000 1.7168090000 -1.7254460000
C -0.9348920000 3.5960160000 -0.6023330000
H -0.7175020000 3.9453480000 0.4087560000
H -1.9926290000 3.7676870000 -0.8179210000
H -0.3625960000 4.2026630000 -1.3130190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284786 (Hartree/Particle)
Thermal correction to Energy= 0.303695
Thermal correction to Enthalpy= 0.304639
Thermal correction to Gibbs (Free) Energy= 0.237931
Sum of electronic and zero-point Energies= -867.345144
Sum of electronic and thermal Energies= -867.326235
Sum of electronic and thermal Enthalpies= -867.325290
Sum of electronic and thermal (Free) Energies= -867.391998

cPT

C -2.9396250000 1.1121320000 0.1990660000
C -1.6739780000 0.8898340000 -0.2119240000
C -0.8056300000 -0.2613720000 -0.0919660000
C 0.5434880000 0.2087980000 0.0155400000
C 0.5560630000 1.5343360000 -0.3991520000

C -0.7947420000 2.0498650000 -0.6973300000
H 1.4630980000 2.1180530000 -0.5070880000
C -1.1208640000 -1.7341920000 -0.2164490000
O 1.5383880000 -0.5430470000 0.3682110000
C -2.5391880000 -2.0348180000 -0.7267230000
C -0.8828790000 -2.4009970000 1.1593530000
C -0.1350920000 -2.3403550000 -1.2530410000
B 2.9713610000 -0.0198080000 0.2241270000
F 3.7893740000 -1.0536700000 0.6115040000
F 3.0921230000 1.1141040000 1.0376750000
F 3.1396990000 0.3381610000 -1.1225480000
H -1.5562350000 -1.9986140000 1.9231380000
H 0.1487180000 -2.2613560000 1.4885480000
H -1.0802540000 -3.4734980000 1.0651540000
H -2.7951600000 -1.4190090000 -1.5946900000
H -3.3072070000 -1.9029510000 0.0329130000
H -2.5807850000 -3.0815930000 -1.0399060000
H -0.2875400000 -1.8900120000 -2.2391850000
H -0.3435710000 -3.4110630000 -1.3349340000
H 0.9058430000 -2.2109940000 -0.9617120000
H -3.3336580000 2.1016730000 -0.0259540000
C -3.8387260000 0.2846620000 1.0558910000
H -3.3232640000 -0.5409420000 1.5446950000
H -4.6805950000 -0.1101470000 0.4752560000
H -4.2672810000 0.9259260000 1.8328510000
H -0.9124920000 2.0922240000 -1.7920480000
C -1.0499610000 3.4444050000 -0.1213710000
H -1.0125320000 3.4284380000 0.9714290000
H -2.0200510000 3.8387310000 -0.4345420000
H -0.2848840000 4.1374170000 -0.4812880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.288018 (Hartree/Particle)
Thermal correction to Energy= 0.306538
Thermal correction to Enthalpy= 0.307482
Thermal correction to Gibbs (Free) Energy= 0.241450
Sum of electronic and zero-point Energies= -867.373512
Sum of electronic and thermal Energies= -867.354992
Sum of electronic and thermal Enthalpies= -867.354048
Sum of electronic and thermal (Free) Energies= -867.420081

ccRT

C -3.0245540000 0.6214070000 -1.2332350000
C -1.9904030000 0.0549280000 -0.6786720000
C -4.0491760000 1.4440760000 -0.4978660000
H -3.1509300000 0.4977240000 -2.3083290000
C -0.9414630000 -0.5531130000 -0.1538650000
H -3.8454730000 1.4721130000 0.5747860000
H -5.0495980000 1.0267950000 -0.6466010000
H -4.0591260000 2.4696110000 -0.8810910000
C 0.3323460000 0.1950180000 -0.1689870000
C -0.9942580000 -2.0066200000 0.3586880000
C 0.3890070000 1.6448450000 -0.0161580000
O 1.3792510000 -0.4789350000 -0.3245670000
C -0.3476080000 -2.9558290000 -0.6676730000
C -2.4587470000 -2.4187430000 0.5634160000
C -0.2610820000 -2.1018290000 1.7090110000
C -0.5184590000 2.3421840000 0.6842090000
H 1.2742420000 2.1283210000 -0.4166530000
B 2.9022700000 0.0579630000 -0.2631720000
H 0.7086170000 -2.7285460000 -0.8182880000
H -0.8612490000 -2.8885380000 -1.6324060000
H -0.4309390000 -3.9877420000 -0.3098430000
H -2.9659450000 -1.7580430000 1.2751560000
H -2.4963110000 -3.4373800000 0.9612020000
H -3.0189960000 -2.4030750000 -0.3762340000
H 0.8038260000 -1.8793680000 1.6154230000
H -0.3551670000 -3.1188770000 2.1024960000
H -0.6992380000 -1.4165890000 2.4432900000
H -1.3517170000 1.8180470000 1.1477090000
C -0.4430130000 3.8122810000 0.9213480000
F 3.6324510000 -1.0872690000 -0.3936580000
F 3.0171400000 0.6710050000 0.9674650000
F 3.0294800000 0.9380420000 -1.3205780000
H 0.4145350000 4.2635820000 0.4185790000
H -1.3593160000 4.2983790000 0.5679050000
H -0.3697460000 4.0176160000 1.9949420000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284882 (Hartree/Particle)
Thermal correction to Energy= 0.305082
Thermal correction to Enthalpy= 0.306027
Thermal correction to Gibbs (Free) Energy= 0.235471
Sum of electronic and zero-point Energies= -867.372132
Sum of electronic and thermal Energies= -867.351932
Sum of electronic and thermal Enthalpies= -867.350987
Sum of electronic and thermal (Free) Energies= -867.421543

ccTS

C 3.0773340000 -0.3786960000 -0.6395450000
C 1.8335610000 -0.2008340000 -0.2211620000
C 4.1433020000 -1.2215440000 -0.0089170000
H 3.3498690000 0.1419650000 -1.5581990000
C 0.7267630000 0.5896110000 -0.1029030000
H 3.8516980000 -1.5886340000 0.9766150000
H 5.0505130000 -0.6210880000 0.1110510000
H 4.4044510000 -2.0742500000 -0.6453540000
C -0.5001530000 -0.1686490000 -0.0982020000
C 0.7583030000 2.1036630000 0.0978720000
C -0.2473510000 -1.5611640000 -0.0062020000
O -1.6423930000 0.3874220000 -0.2315350000
C 0.0945020000 2.7566630000 -1.1340870000
C 2.1940730000 2.6284310000 0.2266090000
C -0.0233330000 2.4687060000 1.3745720000
C 0.9868990000 -1.9548160000 0.4914810000
H -0.9456660000 -2.2677530000 -0.4444910000
B -2.9595970000 -0.4288460000 -0.0567920000
H -0.9430260000 2.4375100000 -1.2453860000
H 0.6402040000 2.5084430000 -2.0505690000
H 0.1117970000 3.8447600000 -1.0129670000
H 2.7190110000 2.1723820000 1.0720710000
H 2.1652890000 3.7097470000 0.3905320000
H 2.7788780000 2.4453010000 -0.6800250000
H -1.0659620000 2.1517650000 1.3150280000
H -0.0042840000 3.5544000000 1.5135730000
H 0.4344400000 2.0081060000 2.2566560000
H 1.3355780000 -1.5239820000 1.4285330000
C 1.5348070000 -3.3143790000 0.1565330000
F -3.9613460000 0.5059770000 -0.0746640000
F -2.8449820000 -1.1028920000 1.1579960000
F -3.0157290000 -1.3270200000 -1.1224230000
H 1.4680320000 -3.5176230000 -0.9144550000
H 2.5705520000 -3.4316370000 0.4761510000
H 0.9420150000 -4.0710820000 0.6830070000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284685 (Hartree/Particle)
Thermal correction to Energy= 0.303593
Thermal correction to Enthalpy= 0.304538
Thermal correction to Gibbs (Free) Energy= 0.237470
Sum of electronic and zero-point Energies= -867.342701
Sum of electronic and thermal Energies= -867.323793
Sum of electronic and thermal Enthalpies= -867.322849
Sum of electronic and thermal (Free) Energies= -867.389916

ccPT

C -3.1203060000 -0.2954690000 -0.3228900000
C -1.7922450000 -0.5038280000 -0.1705020000
C -0.7401050000 0.4837610000 -0.0558870000
C 0.5245250000 -0.1945340000 -0.1358160000
C 0.2843060000 -1.5563360000 -0.2209160000
C -1.1542940000 -1.8789500000 -0.1818770000
C -0.7969690000 1.9821250000 0.1295820000
O 1.6700860000 0.4179110000 -0.1126630000
C -2.1953690000 2.6029700000 0.2434630000
C -0.0747040000 2.6423830000 -1.0725300000
C -0.0341420000 2.3033540000 1.4432850000
H 1.0711740000 -2.2999230000 -0.2653660000
B 2.9664730000 -0.3904410000 -0.0944010000
F 3.9843290000 0.5326960000 -0.0405050000
F 2.9958040000 -1.1716250000 -1.2590260000
F 2.9220010000 -1.2228920000 1.0349630000
H -0.5460980000 1.8627800000 2.3049960000
H -0.0206480000 3.3896110000 1.5750810000
H 0.9943290000 1.9444870000 1.4145470000
H -2.7786110000 2.1729450000 1.0636630000
H -2.7613850000 2.5320960000 -0.6903880000

H -2.0757510000 3.6687510000 0.4579920000
H 0.9605590000 2.3118990000 -1.1533490000
H -0.0862400000 3.7271900000 -0.9278940000
H -0.5975480000 2.4187810000 -2.0081850000
C -4.1515890000 -1.3506710000 -0.5397410000
H -3.5033680000 0.7154510000 -0.3072420000
H -3.7362510000 -2.3441890000 -0.7076170000
H -4.7727130000 -1.0851650000 -1.4016430000
H -4.8253620000 -1.3928700000 0.3251820000
H -1.4371910000 -2.4361520000 -1.0863060000
C -1.4953600000 -2.7324410000 1.0593360000
H -1.2380200000 -2.1877240000 1.9717810000
H -0.9238620000 -3.6636840000 1.0437410000
H -2.5577630000 -2.9831690000 1.0924020000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.288260 (Hartree/Particle)
Thermal correction to Energy= 0.306758
Thermal correction to Enthalpy= 0.307702
Thermal correction to Gibbs (Free) Energy= 0.241417
Sum of electronic and zero-point Energies= -867.383407
Sum of electronic and thermal Energies= -867.364910
Sum of electronic and thermal Enthalpies= -867.363965
Sum of electronic and thermal (Free) Energies= -867.430250

2c

c/s RT

C -0.9279680000 2.9426630000 -0.8935200000
C -0.1580520000 2.0307030000 -0.3700630000
C 0.6702960000 1.1217330000 0.1135180000
C 0.3639410000 -0.2887430000 -0.2022100000
C -1.0039110000 -0.7779660000 -0.3218850000
C -2.0288610000 -0.2439460000 0.3590250000
H -1.1386000000 -1.6735930000 -0.9198640000
H -1.8523780000 0.6028750000 1.0228000000
C -3.4352320000 -0.7548560000 0.3183670000
C 1.9540970000 1.4937410000 0.8831010000
O 1.3437950000 -1.0557050000 -0.3679000000
C 1.8639900000 2.9542860000 1.3462600000
C 3.1837430000 1.3367060000 -0.0313540000
C 2.0915730000 0.5898620000 2.1216450000
C -4.3750860000 0.3663660000 -0.1491510000
C -3.8410490000 -1.2807620000 1.7030570000
H -3.4858810000 -1.5814020000 -0.3996330000
H -4.3484090000 1.2128660000 0.5471690000
H -5.4059310000 0.0024930000 -0.1933110000
H -4.0973360000 0.7306920000 -1.1425770000
H -3.7928880000 -0.4830560000 2.4532760000
H -3.1844270000 -2.0936010000 2.0244090000
H -4.8683060000 -1.6566750000 1.6777670000
B 1.2955440000 -2.6516700000 -0.6019250000
F 2.6157520000 -2.9978110000 -0.6118160000
F 0.6513700000 -2.8319900000 -1.8112130000
F 0.5833950000 -3.1522750000 0.4691700000
H 3.0897880000 1.9749070000 -0.9163490000
H 3.3152530000 0.3043750000 -0.3580700000
H 4.0827970000 1.6431960000 0.5142040000
H 0.9924690000 3.1191140000 1.9889300000
H 1.7988030000 3.6442770000 0.4994300000
H 2.7607720000 3.2082390000 1.9195000000
H 1.2136060000 0.6776520000 2.7712980000
H 2.9684660000 0.8969690000 2.7003210000
H 2.2229620000 -0.4600080000 1.8517150000
H -1.7678600000 3.3033580000 -0.3001910000
C -0.7390060000 3.5294280000 -2.2682990000
H 0.1275700000 3.0941330000 -2.7693720000
H -0.5983320000 4.6127140000 -2.2014030000
H -1.6257210000 3.3478770000 -2.8834280000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342175 (Hartree/Particle)
Thermal correction to Energy= 0.365057
Thermal correction to Enthalpy= 0.366001
Thermal correction to Gibbs (Free) Energy= 0.288442
Sum of electronic and zero-point Energies= -945.928964
Sum of electronic and thermal Energies= -945.906082
Sum of electronic and thermal Enthalpies= -945.905138
Sum of electronic and thermal (Free) Energies= -945.982696

c/s TS

C -2.6915060000 1.1730210000 -0.4573750000
C -1.4756430000 0.7924730000 -0.0958970000
C -0.1477610000 1.0844150000 0.0560110000
C 0.6874930000 -0.0705650000 -0.1389760000
C -0.0822370000 -1.2577760000 -0.1775680000
C -1.3701960000 -1.2098530000 0.3465990000
C -2.3520810000 -2.3055330000 -0.0229590000
C 0.4093580000 2.4369510000 0.4940990000
O 1.9539970000 0.0191180000 -0.3000090000
C -0.7071870000 3.4168950000 0.8767780000
C 1.2138410000 3.0180320000 -0.6884060000
C 1.3325280000 2.2424940000 1.7132600000
C -3.8232740000 -1.9342740000 0.1817660000
C -1.9933870000 -3.5356850000 0.8339940000
H -2.1993310000 -2.5629210000 -1.0770500000
H -3.9897050000 -1.4961970000 1.1733590000
H -4.4448640000 -2.8313580000 0.1119150000
H -4.1779390000 -1.2334300000 -0.5769840000
H -2.1481050000 -3.3245480000 1.8980050000
H -0.9514780000 -3.8366610000 0.6981330000
H -2.6339130000 -4.3790830000 0.5597790000
H -1.5210310000 -0.8030930000 1.3481410000
H 0.2890320000 -2.1265090000 -0.7127200000
B 2.8467700000 -1.2541480000 -0.3101010000
F 2.5034920000 -1.9859190000 0.8281120000
F 4.1359010000 -0.7885880000 -0.2934850000
F 2.5253090000 -1.9626090000 -1.4687890000
H -3.5494970000 0.7031500000 0.0120740000
C -2.9713710000 2.1774190000 -1.5389720000
H -3.5701470000 1.7213440000 -2.3344390000
H -2.0501170000 2.5643980000 -1.9782580000
H -3.5513620000 3.0137430000 -1.1335190000
H 0.7776390000 1.8201230000 2.5579040000
H 1.7302160000 3.2138670000 2.0239650000
H 2.1740040000 1.5868010000 1.4847970000
H -1.3321140000 3.0227140000 1.6843420000
H -1.3528910000 3.6589140000 0.0284460000
H -0.2564880000 4.3511200000 1.2247620000
H 2.0365360000 2.3590520000 -0.9721520000
H 1.6309150000 3.9871370000 -0.3953660000
H 0.5710430000 3.1752070000 -1.5612080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342665 (Hartree/Particle)
Thermal correction to Energy= 0.363967
Thermal correction to Enthalpy= 0.364911
Thermal correction to Gibbs (Free) Energy= 0.292708
Sum of electronic and zero-point Energies= -945.898465
Sum of electronic and thermal Energies= -945.877162
Sum of electronic and thermal Enthalpies= -945.876218
Sum of electronic and thermal (Free) Energies= -945.948422

c/s PT

C -2.7481210000 -0.8018360000 0.4796740000
C -1.5851320000 -0.3682710000 -0.0460930000
C -0.2720390000 -0.9840770000 -0.0528310000
C 0.7051160000 0.0524080000 0.0565750000
C 0.0746220000 1.2435010000 -0.2769620000
C -1.3801620000 1.0891610000 -0.4969830000
C -2.2845840000 2.1969940000 0.1045840000
C 0.1231250000 -2.4195520000 -0.3143710000
O 1.9578440000 -0.1591140000 0.3169620000
C -1.0289370000 -3.3105450000 -0.8053240000
C 0.7583500000 -3.0005530000 0.9709090000
C 1.1909750000 -2.4065160000 -1.4433370000
C -3.5734020000 2.3492370000 -0.7135930000
C -1.5737950000 3.5521980000 0.1942330000
H -2.5418790000 1.8922840000 1.1263730000
H -3.3445320000 2.7724910000 -1.6987900000
H -4.2709520000 3.0278090000 -0.2142630000
H -4.0917590000 1.4006170000 -0.8826280000
H -1.2103960000 3.8776480000 -0.7874190000
H -0.7256850000 3.5308180000 0.8838340000
H -2.2734670000 4.3120990000 0.5542320000
H -1.5347370000 1.0918190000 -1.5899000000
H 0.6161100000 2.1696350000 -0.4210120000

B 2.9558260000 0.9964200000 0.2088010000
F 2.8904810000 1.4723250000 -1.1103250000
F 4.1828570000 0.4672330000 0.5280970000
F 2.5400960000 1.9991720000 1.0967220000
H -3.5924230000 -0.1238030000 0.3850840000
C -3.0327230000 -1.9961780000 1.3292160000
H -3.5880160000 -1.6671200000 2.2139010000
H -2.1337330000 -2.5087500000 1.6681460000
H -3.6776290000 -2.7090390000 0.8025110000
H 0.7681540000 -2.0055430000 -2.3701470000
H 1.5000900000 -3.4387380000 -1.6318940000
H 2.0707700000 -1.8242100000 -1.1738800000
H -1.5953800000 -2.8292860000 -1.6087240000
H -1.7211880000 -3.5964740000 -0.0156400000
H -0.6055360000 -4.2356010000 -1.2063590000
H 1.6282000000 -2.4153570000 1.2755720000
H 1.0782390000 -4.0273870000 0.7675160000
H 0.0432050000 -3.0274970000 1.7991530000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345356 (Hartree/Particle)
Thermal correction to Energy= 0.366455
Thermal correction to Enthalpy= 0.367400
Thermal correction to Gibbs (Free) Energy= 0.295781
Sum of electronic and zero-point Energies= -945.926024
Sum of electronic and thermal Energies= -945.904924
Sum of electronic and thermal Enthalpies= -945.903980
Sum of electronic and thermal (Free) Energies= -945.975598

cc/s RT

C 1.7111170000 2.3610850000 -1.3673710000
C 0.6953250000 1.8236700000 -0.7532360000
C 3.0557160000 2.6154840000 -0.7392930000
H 1.5797580000 2.6374060000 -2.4130810000
C -0.3631130000 1.2990800000 -0.1609600000
H 3.0635290000 2.3346490000 0.3161700000
H 3.3169620000 3.6751940000 -0.8158960000
H 3.8316680000 2.0437320000 -1.2586250000
C -0.5356120000 -0.1618220000 -0.2914700000
C -1.4269410000 2.1575910000 0.5520460000
C 0.5992660000 -1.0751010000 -0.3633610000
O -1.7145310000 -0.5896610000 -0.3422510000
C -0.8559930000 3.5581770000 0.8142600000
C -1.7872190000 1.5105660000 1.9017780000
C -2.6832040000 2.2879460000 -0.3296110000
C 1.7726690000 -0.8281490000 0.2373560000
H 0.4111790000 -2.0284720000 -0.8468440000
B -2.1844510000 -2.1338790000 -0.3594490000
H -0.6158900000 4.0786000000 -0.1177580000
H 0.0526630000 3.5135190000 1.4247470000
H -1.5968920000 4.1564450000 1.3531700000
H -2.2550250000 0.5319210000 1.7766210000
H -2.4955580000 2.1525380000 2.4349410000
H -0.8982220000 1.3962290000 2.5320940000
H -2.4323230000 2.7418450000 -1.2940530000
H -3.4118100000 2.9348970000 0.1708260000
H -3.1510180000 1.3193500000 -0.5109840000
H 1.9082670000 0.0993300000 0.7941220000
C 2.9365060000 -1.7694840000 0.2505450000
F -3.5448630000 -2.0384120000 -0.3074960000
F -1.6098150000 -2.6977440000 0.7617280000
F -1.6956900000 -2.6597850000 -1.5401080000
C 4.1664350000 -1.0774300000 -0.3555740000
C 3.2134050000 -2.2374820000 1.6868600000
H 2.6852340000 -2.6435580000 -0.3610310000
H 5.0203260000 -1.7613300000 -0.3638180000
H 3.9751830000 -0.7552480000 -1.3835290000
H 4.4472800000 -0.1968760000 0.2340320000
H 3.4592400000 -1.3874130000 2.3337990000
H 2.3448870000 -2.7496800000 2.1092320000
H 4.0622360000 -2.9277240000 1.7021800000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342519 (Hartree/Particle)
Thermal correction to Energy= 0.365204
Thermal correction to Enthalpy= 0.366148
Thermal correction to Gibbs (Free) Energy= 0.289790
Sum of electronic and zero-point Energies= -945.929616
Sum of electronic and thermal Energies= -945.906931
Sum of electronic and thermal Enthalpies= -945.905987
Sum of electronic and thermal (Free) Energies= -945.982344

cc/s TS

C 2.4686410000 1.6097260000 -0.5626070000
C 1.3332680000 0.9784220000 -0.2743020000
C 3.7710600000 1.5425660000 0.1681990000
H 2.4249380000 2.3109470000 -1.3963290000
C -0.0211950000 1.1456290000 -0.1489010000
H 3.9724030000 2.5400330000 0.5766410000
H 4.6067680000 1.2934190000 -0.4915370000
H 3.7459860000 0.8388830000 1.0002180000
C -0.7455910000 -0.0961540000 -0.1789540000
C -0.7190150000 2.4766480000 0.1371680000
C 0.1350130000 -1.1980670000 -0.1826300000
O -2.0229660000 -0.1482980000 -0.2485590000
C 1.4548750000 -0.9963970000 0.2186500000
H -0.1852620000 -2.1351640000 -0.6281010000
B -2.7752340000 -1.4966960000 -0.0707720000
H 1.6507330000 -0.5693740000 1.2045920000
C 2.4505260000 -2.0584560000 -0.2331880000
F -4.1013590000 -1.1591710000 0.0134400000
F -2.2735190000 -2.0789550000 1.0948380000
F -2.4701240000 -2.2797430000 -1.1851720000
C 3.8998150000 -1.6107710000 -0.4052390000
C 2.3680830000 -3.2170020000 0.7778890000
H 2.1045480000 -2.4270230000 -1.2055230000
H 4.3301330000 -1.2559930000 0.5363870000
H 4.5000900000 -2.4629870000 -0.7367640000
H 3.9938940000 -0.8247830000 -1.1573410000
H 2.7066160000 -2.8915650000 1.7682360000
H 1.3482280000 -3.5977830000 0.8777490000
H 3.0120630000 -4.0407020000 0.4555650000
C -1.6663680000 2.7747240000 -1.0461710000
H -2.4227320000 1.9969140000 -1.1598720000
H -2.1739200000 3.7277150000 -0.8642070000
H -1.1062060000 2.8620280000 -1.9832220000
C -1.5272900000 2.3563490000 1.4446290000
H -2.0370290000 3.3045390000 1.6437920000
H -2.2821300000 1.5709160000 1.3841500000
H -0.8659880000 2.1445390000 2.2917810000
C 0.2687380000 3.6417770000 0.2793360000
H 0.9912960000 3.4700730000 1.0834690000
H 0.8171950000 3.8309130000 -0.6482290000
H -0.2900680000 4.5511820000 0.5196510000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342852 (Hartree/Particle)
Thermal correction to Energy= 0.363897
Thermal correction to Enthalpy= 0.364841
Thermal correction to Gibbs (Free) Energy= 0.293072
Sum of electronic and zero-point Energies= -945.891509
Sum of electronic and thermal Energies= -945.870464
Sum of electronic and thermal Enthalpies= -945.869520
Sum of electronic and thermal (Free) Energies= -945.941289

cc/s PT

C -2.7347840000 0.9206070000 -0.8147000000
C -1.5853220000 0.3175520000 -0.4406730000
C -0.3378860000 0.9861350000 -0.1247230000
C 0.7320010000 0.0629870000 -0.3643620000
C 0.1763050000 -1.1648130000 -0.6851510000
C -1.2933270000 -1.1696670000 -0.5369430000
C -0.0736940000 2.3716330000 0.4108680000
O 1.9925470000 0.3707670000 -0.2649220000
C -1.3146190000 3.2303500000 0.6944160000
C 0.8357260000 3.1285390000 -0.5871690000
C 0.6771230000 2.1729700000 1.7569850000
C -1.6888750000 -1.9499450000 0.7687340000
H 0.7712930000 -2.0329980000 -0.9389160000
C -3.2011270000 -2.0127950000 0.9802710000
H -3.6502910000 -1.0190280000 1.0532230000
H -3.4191930000 -2.5432430000 1.9118440000
H -3.6932240000 -2.5612650000 0.1685550000
C -1.0862270000 -3.3580930000 0.7681470000
H -1.2458760000 -1.3853500000 1.5997370000
H -1.3848500000 -3.9123760000 -0.1297850000
H -1.4445400000 -3.9182150000 1.6365550000

H 0.0054180000 -3.3386320000 0.8159290000
H -1.7814850000 -1.6551040000 -1.3916150000
B 3.0248320000 -0.7516140000 -0.2120620000
F 4.2293580000 -0.1495520000 0.0646850000
F 3.0122750000 -1.4124560000 -1.4483320000
F 2.6132800000 -1.6391310000 0.8009020000
H 0.0354380000 1.6693880000 2.4873770000
H 0.9349540000 3.1595290000 2.1541310000
H 1.5953040000 1.5994870000 1.6300330000
H -2.0574820000 2.7040880000 1.3015580000
H -1.7882480000 3.5973270000 -0.2208300000
H -0.9969650000 4.1136860000 1.2557350000
H 1.7797030000 2.6069890000 -0.7460250000
H 1.0460640000 4.1219960000 -0.1787260000
H 0.3311340000 3.2569600000 -1.5504020000
C -3.9609770000 0.2624150000 -1.3506320000
H -2.7773560000 2.0021960000 -0.7929450000
H -3.8822180000 -0.8217850000 -1.4175310000
H -4.1767180000 0.6589630000 -2.3492850000
H -4.8255150000 0.5123280000 -0.7246350000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345882 (Hartree/Particle)
Thermal correction to Energy= 0.366779
Thermal correction to Enthalpy= 0.367723
Thermal correction to Gibbs (Free) Energy= 0.296631
Sum of electronic and zero-point Energies= -945.937889
Sum of electronic and thermal Energies= -945.916993
Sum of electronic and thermal Enthalpies= -945.916048
Sum of electronic and thermal (Free) Energies= -945.987140

c/d RT

C -1.4430070000 -2.8742590000 -0.9482180000
C -1.3605880000 -1.6916620000 -0.4066430000
C -1.3268580000 -0.4692200000 0.0934830000
C -0.1171540000 0.3299070000 -0.1904890000
C 1.2092560000 -0.2652150000 -0.2834550000
C 1.5624500000 -1.3590430000 0.4094590000
H 1.9342760000 0.2979530000 -0.8597440000
H 0.8221300000 -1.8432530000 1.0450030000
C 2.9350630000 -1.9619920000 0.4554030000
C -2.5195810000 0.1520900000 0.8487350000
O -0.2823590000 1.5644600000 -0.3510160000
C -3.4816130000 -0.9617760000 1.2842310000
C -3.2753990000 1.1316260000 -0.0689430000
C -2.0089980000 0.8830100000 2.1036720000
C 3.4341250000 -1.9651940000 1.9114690000
C 3.9451320000 -1.3011920000 -0.4806260000
H 2.8100580000 -3.0126220000 0.1506700000
H 3.5687660000 -0.9398390000 2.2701360000
H 4.3962130000 -2.4808590000 1.9800460000
H 2.7298890000 -2.4711810000 2.5795160000
H 4.1230170000 -0.2588630000 -0.1958580000
H 3.6058840000 -1.3182830000 -1.5206190000
H 4.9016210000 -1.8289060000 -0.4300050000
B 0.8688350000 2.6758990000 -0.5501250000
F 0.1644960000 3.8449530000 -0.5672140000
F 1.4856380000 2.3665180000 -1.7478620000
F 1.7050170000 2.5312920000 0.5391300000
H -3.6370810000 0.6179460000 -0.9659700000
H -2.6444610000 1.9667880000 -0.3758180000
H -4.1432650000 1.5329770000 0.4655040000
H -2.9830670000 -1.6944370000 1.9279890000
H -3.9017810000 -1.4928880000 0.4247000000
H -4.3109290000 -0.5238780000 1.8479840000
H -1.4515710000 0.2012780000 2.7557040000
H -2.8613180000 1.2682400000 2.6722440000
H -1.3669270000 1.7299210000 1.8530750000
H -1.1117260000 -3.7299010000 -0.3603520000
C -1.9648080000 -3.1390010000 -2.3367340000
H -2.2649760000 -2.2129340000 -2.8305160000
H -2.8283720000 -3.8100510000 -2.2946620000
H -1.1961670000 -3.6257100000 -2.9448300000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.343082 (Hartree/Particle)
Thermal correction to Energy= 0.365647
Thermal correction to Enthalpy= 0.366591
Thermal correction to Gibbs (Free) Energy= 0.290330
Sum of electronic and zero-point Energies= -945.927738
Sum of electronic and thermal Energies= -945.905173
Sum of electronic and thermal Enthalpies= -945.904229
Sum of electronic and thermal (Free) Energies= -945.980490

c/d TS

C -2.6698990000 1.3363940000 -0.2667190000
C -1.4435090000 0.9760380000 0.0641580000
C -0.0920300000 1.1462120000 0.1141720000
C 0.6226060000 -0.0964920000 -0.0518200000
C -0.2485180000 -1.2151240000 0.0367140000
C -1.4619520000 -1.0224550000 0.6767810000
C -2.6565980000 -1.9129530000 0.4418480000
C 0.6054110000 2.4731940000 0.4025890000
O 1.8733720000 -0.1285190000 -0.3099830000
C -0.4075630000 3.5696210000 0.7566740000
C 1.3762400000 2.8858520000 -0.8694330000
C 1.5847180000 2.2988010000 1.5790370000
C -2.5425250000 -3.1547050000 1.3443440000
C -2.8403080000 -2.2917750000 -1.0282990000
H -3.5409440000 -1.3514430000 0.7704670000
H -1.6719020000 -3.7560140000 1.0650670000
H -3.4362640000 -3.7765460000 1.2393110000
H -2.4396090000 -2.8798750000 2.3982440000
H -2.0284690000 -2.9358020000 -1.3801510000
H -2.8657300000 -1.4014170000 -1.6645450000
H -3.7770660000 -2.8395260000 -1.1645830000
H -1.4683110000 -0.5130240000 1.6397450000
H -0.0038480000 -2.1275020000 -0.4973340000
B 2.6558890000 -1.4768390000 -0.3202600000
F 2.3540360000 -2.1156350000 0.8815120000
F 3.9741730000 -1.1220940000 -0.4384810000
F 2.1758750000 -2.2082900000 -1.4071760000
H -3.5076450000 0.9309840000 0.2971700000
C -2.9954960000 2.2284110000 -1.4323340000
H -3.6513350000 1.7095500000 -2.1391290000
H -2.0930770000 2.5411690000 -1.9610270000
H -3.5283780000 3.1201820000 -1.0849710000
H 1.0527590000 1.9952880000 2.4871060000
H 2.0806050000 3.2532550000 1.7826610000
H 2.3534810000 1.5560330000 1.3593260000
H -1.0002020000 3.3032420000 1.6376170000
H -1.0947140000 3.7750810000 -0.0695870000
H 0.1305130000 4.4959320000 0.9789470000
H 2.1239040000 2.1388800000 -1.1423820000
H 1.8867780000 3.8369740000 -0.6857800000
H 0.6928020000 3.0249940000 -1.7139700000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342069 (Hartree/Particle)
Thermal correction to Energy= 0.363607
Thermal correction to Enthalpy= 0.364551
Thermal correction to Gibbs (Free) Energy= 0.291795
Sum of electronic and zero-point Energies= -945.903240
Sum of electronic and thermal Energies= -945.881702
Sum of electronic and thermal Enthalpies= -945.880758
Sum of electronic and thermal (Free) Energies= -945.953514

c/d PT

C -2.9582890000 0.2616070000 0.1332900000
C -1.6719360000 0.2110750000 -0.2707220000
C -0.6616980000 -0.8175760000 -0.1455750000
C 0.6166020000 -0.1773380000 -0.0717480000
C 0.4559030000 1.1194210000 -0.5389880000
C -0.9572880000 1.4710850000 -0.7790310000
C -1.3542940000 2.8439640000 -0.1875670000
C -0.7851060000 -2.3221300000 -0.2357980000
O 1.7052410000 -0.7796910000 0.2930230000
C -2.1495760000 -2.8137610000 -0.7454760000
C -0.4735740000 -2.9164640000 1.1584600000
C 0.2764700000 -2.8266480000 -1.2508340000
C -0.6650220000 3.9813490000 -0.9483350000
C -1.0601300000 2.9248920000 1.3129720000
H -2.4337230000 2.9651900000 -0.3427580000
H 0.4201820000 3.9629910000 -0.8054330000
H -1.0237010000 4.9485630000 -0.5848920000
H -0.8678980000 3.9297810000 -2.0230760000
H 0.0165730000 2.8705250000 1.5060010000

H -1.5409890000 2.1117620000 1.8659830000
H -1.4244400000 3.8714360000 1.7225130000
H -1.1318410000 1.5061860000 -1.8669110000
H 1.2891790000 1.7908240000 -0.7067740000
B 3.0348160000 -0.0224130000 0.2481340000
F 3.2425710000 0.3717160000 -1.0823980000
F 3.9866820000 -0.9026130000 0.7027230000
F 2.8986750000 1.1114230000 1.0636230000
H -3.4803410000 1.1874570000 -0.1022230000
C -3.7439400000 -0.6648960000 0.9998870000
H -4.2506770000 -0.0730200000 1.7692450000
H -3.1283930000 -1.4117730000 1.4990360000
H -4.5294690000 -1.1704540000 0.4262920000
H 0.0757610000 -2.4250710000 -2.2493990000
H 0.2055240000 -3.9168670000 -1.3049840000
H 1.2904950000 -2.5590150000 -0.9587850000
H -2.4756880000 -2.2537120000 -1.6276020000
H -2.9342010000 -2.7661530000 0.0067820000
H -2.0540290000 -3.8634110000 -1.0364510000
H 0.5299740000 -2.6377420000 1.4863490000
H -0.5321840000 -4.0075530000 1.0934900000
H -1.1962050000 -2.5825690000 1.9099940000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345354 (Hartree/Particle)
Thermal correction to Energy= 0.366524
Thermal correction to Enthalpy= 0.367469
Thermal correction to Gibbs (Free) Energy= 0.295470
Sum of electronic and zero-point Energies= -945.931157
Sum of electronic and thermal Energies= -945.909986
Sum of electronic and thermal Enthalpies= -945.909042
Sum of electronic and thermal (Free) Energies= -945.981040

cc/d RT

C 1.4864350000 2.5522970000 -1.2814310000
C 0.5089900000 1.9103490000 -0.7066320000
C 2.7178570000 3.0525210000 -0.5743300000
H 1.4091980000 2.7329480000 -2.3531550000
C -0.5134390000 1.2760410000 -0.1605220000
H 2.6738960000 2.8479550000 0.4976800000
H 2.8245710000 4.1323380000 -0.7149320000
H 3.6126970000 2.5740440000 -0.9853760000
C -0.4668480000 -0.1996790000 -0.1918810000
C -1.7486660000 2.0140710000 0.3935110000
C 0.7827030000 -0.9447510000 -0.0956460000
O -1.5649920000 -0.7961260000 -0.3129900000
C -1.4040960000 3.4957360000 0.5993420000
C -2.1433690000 1.4055050000 1.7514340000
C -2.9210970000 1.9076620000 -0.5997510000
C 1.8460280000 -0.4944350000 0.5875550000
H 0.7638000000 -1.9415580000 -0.5209960000
B -1.8118210000 -2.3897610000 -0.2618270000
H -1.1508360000 3.9875910000 -0.3446130000
H -0.5600740000 3.6197080000 1.2868030000
H -2.2682400000 4.0126870000 1.0274910000
H -2.4587200000 0.3642240000 1.6588220000
H -2.9803440000 1.9707320000 2.1734620000
H -1.3110590000 1.4579640000 2.4622150000
H -2.6443740000 2.3328380000 -1.5701830000
H -3.7764080000 2.4722920000 -0.2130980000
H -3.2313160000 0.8724200000 -0.7480610000
H 1.7888700000 0.4805170000 1.0695620000
C 3.1404920000 -1.2270730000 0.7816520000
F -3.1708830000 -2.4898240000 -0.3364280000
F -1.2757530000 -2.8011100000 0.9419070000
F -1.1427350000 -2.9071280000 -1.3550890000
C 3.1817200000 -2.6133230000 0.1421630000
C 4.2938590000 -0.3379800000 0.2825720000
H 3.2644310000 -1.3404670000 1.8688490000
H 4.1402020000 -3.0947390000 0.3553720000
H 2.3871450000 -3.2594850000 0.5256960000
H 3.0753810000 -2.5489750000 -0.9462710000
H 4.2131730000 -0.1770430000 -0.7979190000
H 4.2918320000 0.6395210000 0.7753700000
H 5.2561480000 -0.8167870000 0.4846260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342932 (Hartree/Particle)
Thermal correction to Energy= 0.365389
Thermal correction to Enthalpy= 0.366333
Thermal correction to Gibbs (Free) Energy= 0.290892
Sum of electronic and zero-point Energies= -945.929078
Sum of electronic and thermal Energies= -945.906620
Sum of electronic and thermal Enthalpies= -945.905676
Sum of electronic and thermal (Free) Energies= -945.981117

cc/d TS

C 2.4611090000 1.4475150000 -0.5888820000
C 1.3054230000 0.9242980000 -0.2005540000
C 3.7965450000 1.3127260000 0.0698060000
H 2.4263960000 2.0576710000 -1.4920340000
C -0.0486190000 1.0975270000 -0.1042240000
H 3.7255970000 0.8199900000 1.0397710000
H 4.2135720000 2.3129960000 0.2264940000
H 4.5077250000 0.7661390000 -0.5592230000
C -0.7689420000 -0.1473730000 -0.0862180000
C -0.7450070000 2.4455420000 0.0789720000
C 0.1106990000 -1.2483580000 0.0262140000
O -2.0410630000 -0.2036100000 -0.2129740000
C 0.2560580000 3.6015890000 0.2008670000
C -1.6114500000 2.4041490000 1.3530480000
C -1.6359480000 2.6858010000 -1.1597010000
C 1.4040150000 -1.0133000000 0.4880220000
H -0.1910840000 -2.2168430000 -0.3605370000
B -2.8092170000 -1.5409090000 -0.0104480000
H 0.8505180000 3.7272980000 -0.7090540000
H 0.9400320000 3.4610570000 1.0438560000
H -0.2949960000 4.5322880000 0.3655270000
H -2.3716850000 1.6231420000 1.3002970000
H -2.1184440000 3.3663540000 1.4778240000
H -0.9914270000 2.2324080000 2.2395530000
H -1.0345600000 2.7167700000 -2.0744930000
H -2.1410220000 3.6514130000 -1.0527970000
H -2.3944840000 1.9084840000 -1.2638120000
H 1.5368880000 -0.4777670000 1.4286100000
C 2.4729050000 -2.0391940000 0.1393540000
F -4.1362840000 -1.1981670000 -0.0369640000
F -2.3900990000 -2.0553220000 1.2166140000
F -2.4318680000 -2.3842310000 -1.0570320000
C 2.9034950000 -1.9613100000 -1.3317570000
C 3.6668620000 -2.0633490000 1.0952690000
H 1.9529540000 -2.9999290000 0.2613420000
H 3.5302990000 -2.8209060000 -1.5855360000
H 2.0362240000 -1.9637020000 -1.9982020000
H 3.4798770000 -1.0534340000 -1.5296690000
H 4.3359090000 -1.2136200000 0.9411950000
H 3.3426100000 -2.0637680000 2.1408040000
H 4.2550870000 -2.9707140000 0.9312460000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342345 (Hartree/Particle)
Thermal correction to Energy= 0.363664
Thermal correction to Enthalpy= 0.364608
Thermal correction to Gibbs (Free) Energy= 0.292691
Sum of electronic and zero-point Energies= -945.895976
Sum of electronic and thermal Energies= -945.874658
Sum of electronic and thermal Enthalpies= -945.873714
Sum of electronic and thermal (Free) Energies= -945.945631

cc/d PT

C -2.7647610000 0.7595480000 -0.8475950000
C -1.5893820000 0.1782010000 -0.5230520000
C -0.3549620000 0.8762490000 -0.2178040000
C 0.7362720000 -0.0115220000 -0.4933770000
C 0.2110430000 -1.2553510000 -0.7992220000
C -1.2576060000 -1.2956930000 -0.6640660000
C -0.1178360000 2.2529290000 0.3523020000
O 1.9895410000 0.3318120000 -0.4056180000
C -1.3748610000 3.0701040000 0.6827580000
C 0.7535160000 3.0613920000 -0.6390980000
C 0.6612490000 2.0381830000 1.6804810000
C -1.6367340000 -2.1746460000 0.5869400000
H 0.8250730000 -2.1231440000 -1.0119780000
C -1.0567340000 -1.6213880000 1.8901440000
H 0.0347800000 -1.5666610000 1.8717740000
H -1.3461630000 -2.2680120000 2.7233510000
H -1.4489600000 -0.6193870000 2.1030550000

C -3.1438200000 -2.3953800000 0.7096520000
H -1.1715800000 -3.1496880000 0.3966860000
H -3.6651110000 -1.4608100000 0.9424660000
H -3.3486220000 -3.0982110000 1.5225820000
H -3.5730770000 -2.8164190000 -0.2051970000
H -1.7240170000 -1.7525540000 -1.5455770000
B 3.0398380000 -0.7593530000 -0.2335240000
F 4.2257470000 -0.1124730000 0.0225840000
F 3.0754080000 -1.5273390000 -1.4051820000
F 2.6146170000 -1.5617620000 0.8448740000
H 0.0432490000 1.5048030000 2.4096350000
H 0.9060550000 3.0209270000 2.0949470000
H 1.5883600000 1.4866580000 1.5257640000
H -2.0899550000 2.5088220000 1.2921050000
H -1.8778180000 3.4471620000 -0.2126030000
H -1.0688170000 3.9471100000 1.2601960000
H 1.7076100000 2.5690960000 -0.8281730000
H 0.9455140000 4.0482240000 -0.2062710000
H 0.2286900000 3.2034850000 -1.5895640000
C -3.9862140000 0.0878330000 -1.3766740000
H -2.8375040000 1.8378150000 -0.7838160000
H -3.8665360000 -0.9843320000 -1.5231790000
H -4.2627230000 0.5431250000 -2.3342140000
H -4.8309250000 0.2556820000 -0.6982500000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.346112 (Hartree/Particle)
Thermal correction to Energy= 0.366843
Thermal correction to Enthalpy= 0.367787
Thermal correction to Gibbs (Free) Energy= 0.297463
Sum of electronic and zero-point Energies= -945.939474
Sum of electronic and thermal Energies= -945.918742
Sum of electronic and thermal Enthalpies= -945.917798
Sum of electronic and thermal (Free) Energies= -945.988123

c/u RT

C -0.1543190000 -3.1068650000 0.7939950000
C 0.3916460000 -2.0215340000 0.3223230000
C 0.9878180000 -0.9209020000 -0.1010320000
C 0.2535930000 0.3465330000 0.0937050000
C -1.1988240000 0.4272130000 0.0080690000
C -1.9238000000 -0.3907160000 -0.7705410000
H -1.6525670000 1.2588780000 0.5346170000
H -1.4126900000 -1.1611330000 -1.3461390000
C -3.4123400000 -0.3467950000 -0.9476860000
C 2.4192170000 -0.9203220000 -0.6753200000
O 0.9440130000 1.3646360000 0.3455640000
C 2.8092890000 -2.3516300000 -1.0692550000
C 3.4138690000 -0.4071370000 0.3830150000
C 2.4699560000 -0.0308070000 -1.9306950000
C -4.1049590000 0.7842010000 -0.1905560000
C -3.9924160000 -1.7216470000 -0.5682840000
H -3.5869260000 -0.2049970000 -2.0244220000
H -3.9732940000 0.6736860000 0.8913620000
H -5.1785310000 0.7702790000 -0.3983050000
H -3.7169310000 1.7637510000 -0.4837110000
H -3.8403630000 -1.9202440000 0.4979370000
H -3.5218060000 -2.5300150000 -1.1375030000
H -5.0670050000 -1.7481140000 -0.7699580000
B 0.4130230000 2.8805680000 0.4930010000
F 1.5657250000 3.5925120000 0.6583000000
F -0.4176800000 2.8792640000 1.5979200000
F -0.2569480000 3.1469910000 -0.6841120000
H 3.3787630000 -1.0336300000 1.2805730000
H 3.2033720000 0.6241250000 0.6690470000
H 4.4303780000 -0.4520140000 -0.0226740000
H 2.1181470000 -2.7667500000 -1.8106990000
H 2.8227540000 -3.0204820000 -0.2032990000
H 3.8123760000 -2.3462560000 -1.5064120000
H 1.7533630000 -0.3747850000 -2.6848580000
H 3.4704580000 -0.0812510000 -2.3717950000
H 2.2604060000 1.0159950000 -1.7012610000
H -0.7657530000 -3.7055790000 0.1193040000
C -0.0024670000 -3.5884110000 2.2135240000
H 0.6251140000 -2.9119150000 2.7966280000
H 0.4479140000 -4.5857530000 2.2289130000
H -0.9818440000 -3.6597180000 2.6965980000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342757 (Hartree/Particle)
Thermal correction to Energy= 0.365372
Thermal correction to Enthalpy= 0.366316
Thermal correction to Gibbs (Free) Energy= 0.289855
Sum of electronic and zero-point Energies= -945.928246
Sum of electronic and thermal Energies= -945.905631
Sum of electronic and thermal Enthalpies= -945.904687
Sum of electronic and thermal (Free) Energies= -945.981148

c/u TS

C -2.6589960000 1.0629760000 -0.3453250000
C -1.4245990000 0.7604110000 0.0199340000
C -0.0898570000 1.0349930000 0.0820750000
C 0.7199890000 -0.1527250000 -0.0296230000
C -0.0615640000 -1.3290240000 0.0929060000
C -1.3153600000 -1.2081330000 0.6779530000
C -2.3859000000 -2.2507200000 0.4243980000
C 0.5029870000 2.4180240000 0.3408720000
O 1.9755420000 -0.0955340000 -0.2641420000
C -0.5892400000 3.4488570000 0.6537840000
C 1.2593550000 2.8498970000 -0.9336680000
C 1.4767140000 2.3483690000 1.5331600000
C -2.7851930000 -2.3411390000 -1.0542600000
C -3.6002090000 -2.0869230000 1.3412430000
H -1.9020600000 -3.2026030000 0.6892920000
H -3.3174670000 -1.4389660000 -1.3711950000
H -3.4453490000 -3.1979660000 -1.2155080000
H -1.9106630000 -2.4622930000 -1.6992000000
H -4.1634090000 -1.1767860000 1.1100310000
H -3.3042390000 -2.0452370000 2.3940340000
H -4.2848240000 -2.9307710000 1.2195490000
H -1.4044940000 -0.6722760000 1.6228170000
H 0.2744100000 -2.2518610000 -0.3698340000
B 2.8627390000 -1.3744270000 -0.2133370000
F 2.5987650000 -1.9892110000 1.0098710000
F 4.1502250000 -0.9196750000 -0.3329310000
F 2.4577880000 -2.1845210000 -1.2752450000
H -3.4914190000 0.6421430000 0.2112850000
C -2.9939360000 1.9040370000 -1.5447170000
H -3.6003250000 1.3309740000 -2.2542480000
H -2.0938640000 2.2481390000 -2.0575230000
H -3.5839470000 2.7750400000 -1.2395910000
H 0.9555210000 2.0335250000 2.4436110000
H 1.8994840000 3.3417930000 1.7138430000
H 2.2995280000 1.6570020000 1.3442010000
H -1.1757560000 3.1624640000 1.5325020000
H -1.2754070000 3.5890070000 -0.1864500000
H -0.1193590000 4.4147300000 0.8618100000
H 2.0622620000 2.1513410000 -1.1762530000
H 1.6978020000 3.8400150000 -0.7712010000
H 0.5793850000 2.9162600000 -1.7898000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342086 (Hartree/Particle)
Thermal correction to Energy= 0.363558
Thermal correction to Enthalpy= 0.364502
Thermal correction to Gibbs (Free) Energy= 0.292244
Sum of electronic and zero-point Energies= -945.901015
Sum of electronic and thermal Energies= -945.879544
Sum of electronic and thermal Enthalpies= -945.878600
Sum of electronic and thermal (Free) Energies= -945.950857

c/u PT

C 2.7921920000 0.6075300000 0.1558070000
C 1.5579030000 0.2510200000 -0.2578490000
C 0.2798130000 0.9154230000 -0.1192510000
C -0.7439210000 -0.0844870000 -0.0831260000
C -0.1907130000 -1.2481020000 -0.5956050000
C 1.2669520000 -1.1516280000 -0.8146510000
C 1.9889280000 -2.4097410000 -0.2616310000
C -0.0658420000 2.3873230000 -0.1822100000
O -1.9663860000 0.1466920000 0.2805370000
C 1.0860000000 3.2922770000 -0.6489960000
C -0.5753430000 2.8254700000 1.2115660000
C -1.2112360000 2.5586110000 -1.2176990000
C 1.9394030000 -2.4922640000 1.2664900000
C 3.4092490000 -2.6165890000 -0.7992830000
H 1.3915790000 -3.2454700000 -0.6503940000

H 2.5583820000 -1.7161980000 1.7289510000
H 2.3172690000 -3.4614690000 1.6044800000
H 0.9174080000 -2.3840610000 1.6427690000
H 4.1420150000 -1.9634010000 -0.3151950000
H 3.4635720000 -2.4502100000 -1.8801310000
H 3.7306980000 -3.6440370000 -0.6044390000
H 1.4568940000 -1.0993460000 -1.8989260000
H -0.7708070000 -2.1393700000 -0.8066260000
B -3.0063340000 -0.9726210000 0.1790740000
F -3.0644900000 -1.3616870000 -1.1678520000
F -4.1858080000 -0.4340390000 0.6338060000
F -2.5494010000 -2.0407680000 0.9645010000
H 3.5902420000 -0.0750130000 -0.1209060000
C 3.2236930000 1.6951080000 1.0813590000
H 3.8709380000 1.2558190000 1.8481940000
H 2.3927980000 2.1875580000 1.5841060000
H 3.8267460000 2.4449960000 0.5566080000
H -0.8740680000 2.2635530000 -2.2166750000
H -1.4840350000 3.6173250000 -1.2524220000
H -2.0967310000 1.9811650000 -0.9573660000
H 1.5942390000 2.8795260000 -1.5261260000
H 1.8262520000 3.4833790000 0.1252570000
H 0.6703980000 4.2626600000 -0.9338950000
H -1.4485710000 2.2418070000 1.5097030000
H -0.8578150000 3.8818740000 1.1630990000
H 0.2001750000 2.7172170000 1.9766460000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344866 (Hartree/Particle)
Thermal correction to Energy= 0.366197
Thermal correction to Enthalpy= 0.367141
Thermal correction to Gibbs (Free) Energy= 0.294331
Sum of electronic and zero-point Energies= -945.928175
Sum of electronic and thermal Energies= -945.906845
Sum of electronic and thermal Enthalpies= -945.905900
Sum of electronic and thermal (Free) Energies= -945.978710

cc/u RT

C 0.6609100000 -2.9481400000 -1.4448770000
C 0.9354280000 -1.8466310000 -0.8053490000
C -0.0396100000 -4.1365580000 -0.8411340000
H 0.9491940000 -3.0084550000 -2.4938220000
C 1.2439970000 -0.7205540000 -0.1869620000
H -0.2491060000 -3.9811640000 0.2194510000
H 0.5776810000 -5.0342880000 -0.9418590000
H -0.9841630000 -4.3247800000 -1.3618360000
C 0.2602260000 0.3764970000 -0.2867330000
C 2.5943370000 -0.5065490000 0.5255830000
C -1.1758010000 0.1345850000 -0.3526190000
O 0.7181160000 1.5453530000 -0.3140920000
C 3.2677830000 -1.8667870000 0.7549250000
C 2.3534660000 0.1617740000 1.8913810000
C 3.5196190000 0.3684050000 -0.3409340000
C -1.7624650000 -0.9171610000 0.2393040000
H -1.7601240000 0.9222710000 -0.8144250000
B -0.1310540000 2.9167260000 -0.2959240000
H 3.4940680000 -2.3709400000 -0.1894140000
H 2.6360660000 -2.5314420000 1.3544970000
H 4.2094570000 -1.7189680000 1.2922200000
H 1.9294910000 1.1628650000 1.7898350000
H 3.3056820000 0.2556240000 2.4229830000
H 1.6814920000 -0.4423960000 2.5111640000
H 3.6900340000 -0.0988790000 -1.3164780000
H 4.4888290000 0.4759890000 0.1579850000
H 3.1021940000 1.3637190000 -0.4990600000
H -1.1415010000 -1.6374030000 0.7701920000
C -3.2385940000 -1.1745630000 0.3099430000
F 0.8384480000 3.8746840000 -0.2250270000
F -0.9311480000 2.8327370000 0.8263140000
F -0.8540870000 2.9252740000 -1.4738560000
C -3.6681210000 -1.2362210000 1.7865560000
C -4.0891420000 -0.1814490000 -0.4794950000
H -3.3871450000 -2.1790300000 -0.1158030000
H -4.7240670000 -1.5109610000 1.8621450000
H -3.0849880000 -1.9739460000 2.3470360000
H -3.5330390000 -0.2603380000 2.2635200000
H -3.9936730000 0.8302830000 -0.0714880000
H -3.8035430000 -0.1525510000 -1.5352180000
H -5.1436160000 -0.4658150000 -0.4236700000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342533 (Hartree/Particle)
Thermal correction to Energy= 0.365216
Thermal correction to Enthalpy= 0.366161
Thermal correction to Gibbs (Free) Energy= 0.289502
Sum of electronic and zero-point Energies= -945.928873
Sum of electronic and thermal Energies= -945.906189
Sum of electronic and thermal Enthalpies= -945.905245
Sum of electronic and thermal (Free) Energies= -945.981903

cc/u TS

C 2.4467230000 1.6718810000 -0.5795870000
C 1.3033150000 1.1438090000 -0.1706520000
C 3.7973520000 1.5358960000 0.0536220000
H 2.3970940000 2.2600130000 -1.4967800000
C -0.0568680000 1.2054770000 -0.0713360000
H 3.7430420000 1.1018290000 1.0533090000
H 4.2555540000 2.5259050000 0.1397920000
H 4.4653580000 0.9247160000 -0.5643610000
C -0.6742620000 -0.0972460000 -0.0875580000
C -0.8550400000 2.4925130000 0.1287590000
C 0.2918140000 -1.1290650000 0.0119080000
O -1.9335970000 -0.2518320000 -0.2438340000
C 0.0641040000 3.7106330000 0.2863250000
C -1.7316190000 2.3624850000 1.3892210000
C -1.7451020000 2.6938870000 -1.1169060000
C 1.5340810000 -0.7972100000 0.5345240000
H 0.0863390000 -2.0964350000 -0.4352580000
B -2.5909420000 -1.6558910000 -0.0962490000
H 0.6703330000 3.8836950000 -0.6081070000
H 0.7380630000 3.6028870000 1.1421870000
H -0.5493860000 4.6017090000 0.4494990000
H -2.4352310000 1.5321030000 1.3090290000
H -2.3060000000 3.2839950000 1.5283980000
H -1.1124170000 2.2136300000 2.2804260000
H -1.1359140000 2.7902260000 -2.0218990000
H -2.3227210000 3.6163330000 -0.9968030000
H -2.4417350000 1.8644370000 -1.2490540000
H 1.5721810000 -0.2528550000 1.4776770000
C 2.7506390000 -1.6453400000 0.2369080000
F -3.9410130000 -1.4239040000 -0.1347680000
F -2.1470930000 -2.1732790000 1.1203700000
F -2.1279810000 -2.4283280000 -1.1626700000
C 2.6698530000 -2.9413660000 1.0644060000
C 2.9164970000 -1.9361090000 -1.2563860000
H 3.6313980000 -1.0950200000 0.5819770000
H 3.5770990000 -3.5343330000 0.9162280000
H 2.5695020000 -2.7312650000 2.1332650000
H 1.8118050000 -3.5475380000 0.7582830000
H 2.0952420000 -2.5504060000 -1.6384190000
H 2.9421680000 -1.0096400000 -1.8386210000
H 3.8475870000 -2.4817470000 -1.4347250000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342197 (Hartree/Particle)
Thermal correction to Energy= 0.363592
Thermal correction to Enthalpy= 0.364537
Thermal correction to Gibbs (Free) Energy= 0.292349
Sum of electronic and zero-point Energies= -945.900757
Sum of electronic and thermal Energies= -945.879362
Sum of electronic and thermal Enthalpies= -945.878418
Sum of electronic and thermal (Free) Energies= -945.950605

cc/u PT

C -2.9570140000 0.6441440000 -0.5942110000
C -1.6906800000 0.1927100000 -0.4537420000
C -0.4898890000 0.9634310000 -0.2079980000
C 0.6404970000 0.1104060000 -0.4372380000
C 0.1761050000 -1.1567840000 -0.7499630000
C -1.2888120000 -1.2557290000 -0.6465520000
C -0.3017720000 2.3849230000 0.2650250000
O 1.8777000000 0.5005490000 -0.3314130000
C -1.5828990000 3.1927220000 0.5092970000
C 0.5559340000 3.1415060000 -0.7793200000
C 0.4646760000 2.2993660000 1.6134470000
C -1.7260640000 -2.1861720000 0.5381790000
H 0.8355580000 -1.9848240000 -0.9798790000

C -1.3618900000 -3.6411160000 0.2365930000
H -1.7655590000 -3.9683150000 -0.7275000000
H -1.7678970000 -4.2988270000 1.0106940000
H -0.2767560000 -3.7848390000 0.2211640000
C -1.1400690000 -1.7334520000 1.8766910000
H -2.8184240000 -2.1149790000 0.6001260000
H -0.0498360000 -1.8324730000 1.8916450000
H -1.5478820000 -2.3472100000 2.6850650000
H -1.3864390000 -0.6895530000 2.0983500000
H -1.7124740000 -1.6736780000 -1.5699500000
B 2.9736240000 -0.5511940000 -0.1939860000
F 4.1296570000 0.1365600000 0.0897470000
F 3.0435360000 -1.2709580000 -1.3946620000
F 2.5826050000 -1.4129990000 0.8501520000
H -0.1399770000 1.7892030000 2.3703090000
H 0.6588950000 3.3180810000 1.9630450000
H 1.4174780000 1.7808520000 1.5079030000
H -2.2563090000 2.7037040000 1.2199810000
H -2.1215960000 3.4109930000 -0.4179220000
H -1.2993680000 4.1562920000 0.9423390000
H 1.5239410000 2.6636080000 -0.9287600000
H 0.7202320000 4.1616240000 -0.4183870000
H 0.0328460000 3.2011390000 -1.7393900000
C -4.1528630000 -0.1853910000 -0.9216510000
H -3.1547280000 1.7026920000 -0.4919630000
H -3.9207710000 -1.2307400000 -1.1255790000
H -4.6639070000 0.2337030000 -1.7952470000
H -4.8704820000 -0.1416700000 -0.0933110000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345332 (Hartree/Particle)
Thermal correction to Energy= 0.366460
Thermal correction to Enthalpy= 0.367404
Thermal correction to Gibbs (Free) Energy= 0.295224
Sum of electronic and zero-point Energies= -945.943163
Sum of electronic and thermal Energies= -945.922035
Sum of electronic and thermal Enthalpies= -945.921091
Sum of electronic and thermal (Free) Energies= -945.993270

2d

cRT

C 0.5212520000 -3.0294930000 1.1849900000
C 1.0095330000 -2.0109340000 0.5341350000
C 1.5528560000 -0.9736120000 -0.0760950000
C 0.9142320000 0.3406540000 0.1540520000
C -0.5238740000 0.5029330000 0.2586000000
C -1.3962190000 -0.3504810000 -0.3139740000
H -0.8512300000 1.4092350000 0.7536640000
C 2.8511320000 -1.0767980000 -0.9020960000
O 1.6870630000 1.3267730000 0.2634460000
C 3.1018970000 -2.5452380000 -1.2713250000
C 4.0454830000 -0.5584460000 -0.0789550000
C 2.7013190000 -0.2582970000 -2.1970470000
B 1.2647150000 2.8725370000 0.3984440000
F 2.4652300000 3.5221330000 0.3977890000
F 0.5674090000 2.9712560000 1.5901800000
F 0.4753810000 3.1320970000 -0.7045210000
H 4.1542620000 -1.1343120000 0.8461580000
H 3.9313730000 0.4954180000 0.1783670000
H 4.9656660000 -0.6746090000 -0.6618490000
H 2.2688150000 -2.9622830000 -1.8473890000
H 3.2469670000 -3.1666670000 -0.3824160000
H 4.0062770000 -2.6157400000 -1.8833330000
H 1.8435050000 -0.6046470000 -2.7842710000
H 3.5990770000 -0.3806750000 -2.8111720000
H 2.5790970000 0.8084360000 -1.9971580000
H -0.2256400000 -3.6462160000 0.6854910000
C 0.9156600000 -3.4105090000 2.5882670000
H 1.6650930000 -2.7253560000 2.9888510000
H 1.3237850000 -4.4259170000 2.6046370000
H 0.0406810000 -3.3941320000 3.2452210000
H -1.0039930000 -1.2064660000 -0.8583480000
C -2.8531920000 -0.2334890000 -0.3055460000
C -3.6066340000 -1.2589680000 -0.8949570000
C -3.5275400000 0.8555250000 0.2696890000
C -4.9146090000 0.9058810000 0.2592550000
C -4.9963410000 -1.2090370000 -0.9025490000
C -5.6524790000 -0.1255700000 -0.3238680000
H -3.0945830000 -2.1024520000 -1.3506730000
H -5.5651640000 -2.0110160000 -1.3614830000
H -6.7368250000 -0.0799960000 -0.3303190000
H -2.9699920000 1.6718330000 0.7165250000
H -5.4242800000 1.7545940000 0.7032280000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.339450 (Hartree/Particle)
Thermal correction to Energy= 0.362558
Thermal correction to Enthalpy= 0.363502
Thermal correction to Gibbs (Free) Energy= 0.284326
Sum of electronic and zero-point Energies= -1059.000070
Sum of electronic and thermal Energies= -1058.976962
Sum of electronic and thermal Enthalpies= -1058.976018
Sum of electronic and thermal (Free) Energies= -1059.055194

cTS

C -1.1614360000 2.3656980000 -0.4296400000
C -0.2324680000 1.5150060000 -0.0344920000
C 1.0507520000 1.0595320000 0.0576120000
C 1.1280740000 -0.3792120000 -0.0210440000
C -0.1486640000 -0.9801770000 0.1171180000
C -1.1532210000 -0.1949340000 0.6806730000
C 2.2692400000 1.9425810000 0.3118470000
O 2.2339600000 -0.9833810000 -0.2412080000
C 1.8573450000 3.3943230000 0.5882070000
C 3.1534750000 1.8967940000 -0.9527990000
C 3.0550140000 1.4063230000 1.5237440000
H -0.3383930000 -1.9647550000 -0.2964240000
B 2.3355460000 -2.5343220000 -0.1640810000
F 1.8049290000 -2.9045700000 1.0703930000
F 3.6723580000 -2.8105960000 -0.2925680000
F 1.5613510000 -3.0384600000 -1.2109720000
H -2.1119790000 2.3837830000 0.1012320000
C -1.0321520000 3.2522540000 -1.6355200000
H -0.0704930000 3.1164470000 -2.1340090000
H -1.1328360000 4.3024760000 -1.3408490000
H -1.8313920000 3.0350560000 -2.3516720000
H 2.4364750000 1.4229580000 2.4275490000
H 3.9269930000 2.0439280000 1.7010390000
H 3.4063120000 0.3863390000 1.3591860000
H 1.2004910000 3.4688910000 1.4607040000
H 1.3443550000 3.8451000000 -0.2665310000
H 2.7537530000 3.9887280000 0.7885350000
H 3.4841500000 0.8796710000 -1.1708800000
H 4.0374100000 2.5231210000 -0.7934580000
H 2.6138220000 2.2861630000 -1.8227770000
C -2.5824230000 -0.4098680000 0.4106090000
H -0.9487100000 0.3207580000 1.6178070000
C -3.0145710000 -0.9624350000 -0.8022670000
C -3.5334630000 -0.0237140000 1.3625330000
C -4.8910300000 -0.2079310000 1.1197620000
C -5.3097090000 -0.7725450000 -0.0831800000
C -4.3700680000 -1.1481620000 -1.0438680000
H -2.2855670000 -1.2359900000 -1.5596620000
H -6.3680940000 -0.9168370000 -0.2751180000
H -4.6963910000 -1.5807000000 -1.9839010000
H -3.2051820000 0.4098120000 2.3038280000
H -5.6200410000 0.0851500000 1.8680250000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.338931 (Hartree/Particle)
Thermal correction to Energy= 0.360764
Thermal correction to Enthalpy= 0.361708
Thermal correction to Gibbs (Free) Energy= 0.287253
Sum of electronic and zero-point Energies= -1058.976284
Sum of electronic and thermal Energies= -1058.954452
Sum of electronic and thermal Enthalpies= -1058.953507
Sum of electronic and thermal (Free) Energies= -1059.027963

cPT

C 1.2284430000 2.3409330000 0.1985570000
C 0.4542930000 1.3433690000 -0.2757370000
C -0.9464280000 1.0322990000 -0.1206530000
C -1.0923690000 -0.3945220000 -0.1341610000
C 0.0691180000 -0.9262860000 -0.6780540000
C 1.1010800000 0.1027320000 -0.9228330000
C -2.1443550000 1.9525060000 -0.0963890000

O -2.1716830000 -1.0053360000 0.2396400000
C -1.8291070000 3.3928230000 -0.5297140000
C -2.7419730000 1.9243670000 1.3310630000
C -3.1962790000 1.4024010000 -1.0962970000
H 0.2032880000 -1.9769730000 -0.9061320000
B -2.2477850000 -2.5332340000 0.1417750000
F -2.0616950000 -2.8714850000 -1.2059620000
F -3.4900710000 -2.8780650000 0.6168840000
F -1.1988630000 -3.0500120000 0.9151570000
H 2.2813580000 2.2689540000 -0.0720610000
C 0.9219890000 3.4257550000 1.1749510000
H -0.0337220000 3.2945240000 1.6804160000
H 0.9387640000 4.4072750000 0.6866460000
H 1.7105900000 3.4408430000 1.9342960000
H -2.7974820000 1.4033180000 -2.1159340000
H -4.0668620000 2.0643380000 -1.0743050000
H -3.5197440000 0.3938650000 -0.8441550000
H -1.2624050000 3.4140450000 -1.4659330000
H -1.2810550000 3.9600300000 0.2199160000
H -2.7722450000 3.9191290000 -0.7007630000
H -3.0364180000 0.9107910000 1.6108360000
H -3.6287270000 2.5657470000 1.3492750000
H -2.0336040000 2.3044990000 2.0738660000
C 2.4834760000 -0.2857410000 -0.4503780000
H 1.1417460000 0.3114040000 -2.0031720000
C 2.6483570000 -0.9290300000 0.7801780000
C 3.6077070000 0.0094210000 -1.2219810000
C 4.8830840000 -0.3261850000 -0.7699940000
C 5.0403400000 -0.9643820000 0.4571450000
C 3.9197420000 -1.2676230000 1.2304780000
H 1.7764770000 -1.1722480000 1.3834450000
H 6.0318290000 -1.2315710000 0.8083730000
H 4.0359050000 -1.7738010000 2.1833030000
H 3.4873230000 0.4991660000 -2.1853080000
H 5.7503360000 -0.0954390000 -1.3803950000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341548 (Hartree/Particle)
Thermal correction to Energy= 0.363247
Thermal correction to Enthalpy= 0.364192
Thermal correction to Gibbs (Free) Energy= 0.289552
Sum of electronic and zero-point Energies= -1059.001076
Sum of electronic and thermal Energies= -1058.979377
Sum of electronic and thermal Enthalpies= -1058.978433
Sum of electronic and thermal (Free) Energies= -1059.053072

ccRT

C -0.2525870000 2.8877170000 -1.5385060000
C -0.8893050000 1.9827150000 -0.8500590000
C 0.8422560000 3.7648360000 -0.9904370000
H -0.5189740000 3.0061810000 -2.5881840000
C -1.5553480000 1.0595670000 -0.1806470000
H 0.9680060000 3.6213160000 0.0852360000
H 0.6129800000 4.8191930000 -1.1706480000
H 1.7917740000 3.5409490000 -1.4878090000
C -1.0221290000 -0.3181520000 -0.2477520000
C -2.8768260000 1.3537980000 0.5567220000
C 0.4009830000 -0.6040710000 -0.2947870000
O -1.8691890000 -1.2470580000 -0.2726100000
C -3.0130960000 2.8685460000 0.7648580000
C -2.8603140000 0.6645110000 1.9330650000
C -4.0723870000 0.8539640000 -0.2756970000
C 1.3302550000 0.2297860000 0.2120360000
H 0.6624370000 -1.5777010000 -0.6919220000
B -1.5682070000 -2.8267590000 -0.2226800000
H -3.0621810000 3.4050700000 -0.1874280000
H -2.1729330000 3.2711990000 1.3413630000
H -3.9340880000 3.0774930000 1.3175690000
H -2.8256180000 -0.4235690000 1.8471190000
H -3.7704240000 0.9263590000 2.4818750000
H -2.0023910000 0.9960490000 2.5286740000
H -4.0879080000 1.3383780000 -1.2576050000
H -5.0048450000 1.1043100000 0.2417640000
H -4.0386790000 -0.2266750000 -0.4207630000
H 1.0003600000 1.1634830000 0.6611640000
C 2.7738520000 0.0010560000 0.2451510000
F -2.8160480000 -3.3775000000 -0.1755300000
F -0.8168270000 -3.0175850000 0.9202300000
F -0.8644840000 -3.1139460000 -1.3792770000
C 3.6009710000 1.0380520000 0.7000260000
C 3.3644930000 -1.2049610000 -0.1638240000
C 4.9826700000 0.8854710000 0.7339930000
H 3.1529410000 1.9730690000 1.0263410000
C 4.7438110000 -1.3578270000 -0.1260590000
H 2.7470070000 -2.0316650000 -0.4988430000
C 5.5562560000 -0.3140030000 0.3192570000
H 5.6095490000 1.6980950000 1.0861650000
H 5.1885580000 -2.2963170000 -0.4401430000
H 6.6338920000 -0.4397100000 0.3475050000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.339425 (Hartree/Particle)
Thermal correction to Energy= 0.362540
Thermal correction to Enthalpy= 0.363484
Thermal correction to Gibbs (Free) Energy= 0.284501
Sum of electronic and zero-point Energies= -1059.000831
Sum of electronic and thermal Energies= -1058.977716
Sum of electronic and thermal Enthalpies= -1058.976772
Sum of electronic and thermal (Free) Energies= -1059.055755

ccTS

C 1.0764570000 2.4238460000 -0.6853990000
C 0.1935080000 1.5536140000 -0.2210050000
C 2.4112150000 2.7748340000 -0.1043270000
H 0.8123090000 2.9069040000 -1.6269810000
C -1.0979340000 1.1218650000 -0.1082230000
H 2.5128730000 2.4436170000 0.9295360000
H 2.5454160000 3.8600760000 -0.1342450000
H 3.2217220000 2.3250270000 -0.6894220000
C -1.2014640000 -0.3162640000 -0.0599980000
C -2.3098040000 2.0390530000 0.0403710000
C 0.0675880000 -0.9217160000 0.1043550000
O -2.3191750000 -0.9192440000 -0.2117940000
C -1.8945030000 3.5122540000 0.1429570000
C -3.0963790000 1.6514260000 1.3073240000
C -3.1961520000 1.8523420000 -1.2105490000
C 1.0933120000 -0.1149560000 0.5999220000
H 0.2446620000 -1.9333470000 -0.2448440000
B -2.4415600000 -2.4558460000 0.0059630000
H -1.3816390000 3.8563990000 -0.7603000000
H -1.2361480000 3.6896450000 0.9993500000
H -2.7901110000 4.1273120000 0.2717570000
H -3.4497660000 0.6197960000 1.2642660000
H -3.9674610000 2.3068350000 1.4076490000
H -2.4775700000 1.7741920000 2.2027690000
H -2.6519720000 2.1264610000 -2.1205700000
H -4.0703610000 2.5064640000 -1.1278880000
H -3.5420750000 0.8216750000 -1.3044690000
H 0.9213680000 0.4407000000 1.5207890000
C 2.5053830000 -0.4164690000 0.3075040000
F -3.7849150000 -2.7197530000 -0.0703940000
F -1.8907480000 -2.7219160000 1.2584280000
F -1.6975450000 -3.0639820000 -1.0062040000
C 3.4854920000 -0.2429630000 1.2910740000
C 2.8823560000 -0.8670300000 -0.9628420000
C 4.8172100000 -0.5329310000 1.0168780000
H 3.1992800000 0.1100660000 2.2785420000
C 4.2152590000 -1.1501710000 -1.2401270000
H 2.1273620000 -0.9787960000 -1.7362350000
C 5.1834100000 -0.9848310000 -0.2504650000
H 5.5691450000 -0.4072380000 1.7889540000
H 4.4997590000 -1.4972260000 -2.2279900000
H 6.2235600000 -1.2059610000 -0.4672880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.338985 (Hartree/Particle)
Thermal correction to Energy= 0.360662
Thermal correction to Enthalpy= 0.361606
Thermal correction to Gibbs (Free) Energy= 0.287770
Sum of electronic and zero-point Energies= -1058.974297
Sum of electronic and thermal Energies= -1058.952619
Sum of electronic and thermal Enthalpies= -1058.951675
Sum of electronic and thermal (Free) Energies= -1059.025512

ccPT

C -1.2249750000 2.5070980000 -0.5464200000
C -0.5096240000 1.3577390000 -0.5441640000

C 0.8506020000 1.1404360000 -0.1109590000
C 1.1544880000 -0.2593120000 -0.2489990000
C 0.0483730000 -0.8977810000 -0.7853680000
C -1.0817610000 0.0278680000 -1.0068180000
C 1.8997420000 2.1036850000 0.3942340000
O 2.2992220000 -0.7777300000 0.0778170000
C 1.4873960000 3.5785410000 0.4834270000
C 3.1173460000 2.0111310000 -0.5625560000
C 2.3097360000 1.6385670000 1.8164160000
H 0.0039290000 -1.9602590000 -0.9905920000
B 2.5444470000 -2.2756310000 -0.1092040000
F 3.8321770000 -2.4992160000 0.3197460000
F 2.3628540000 -2.5628840000 -1.4700330000
F 1.5861050000 -2.9557620000 0.6548280000
H 1.4599470000 1.7032860000 2.5040980000
H 3.0943810000 2.3072080000 2.1837390000
H 2.6933450000 0.6186420000 1.8147150000
H 0.6833280000 3.7445460000 1.2070280000
H 1.2028110000 3.9926570000 -0.4887130000
H 2.3514660000 4.1501470000 0.8340020000
H 3.5132860000 0.9975040000 -0.6193120000
H 3.9031320000 2.6721880000 -0.1842020000
H 2.8446090000 2.3484170000 -1.5678220000
C -2.6345180000 2.6456770000 -1.0092380000
H -0.7785280000 3.4092980000 -0.1528390000
H -2.9592860000 1.8385450000 -1.6648110000
H -2.7715940000 3.6026040000 -1.5205970000
H -3.3007160000 2.6497640000 -0.1357620000
H -1.3068560000 0.0814590000 -2.0819940000
C -2.3333730000 -0.4401620000 -0.2717560000
C -3.4472240000 -0.8876300000 -0.9804370000
C -4.5813200000 -1.3357610000 -0.3054430000
C -4.6070890000 -1.3412490000 1.0862380000
C -3.4922870000 -0.9030540000 1.8001190000
C -2.3603380000 -0.4596020000 1.1245010000
H -3.4318070000 -0.8875700000 -2.0676460000
H -5.4417890000 -1.6821190000 -0.8689340000
H -5.4882510000 -1.6916540000 1.6137860000
H -3.5001890000 -0.9167980000 2.8852120000
H -1.4885170000 -0.1342580000 1.6866000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341607 (Hartree/Particle)
Thermal correction to Energy= 0.363366
Thermal correction to Enthalpy= 0.364310
Thermal correction to Gibbs (Free) Energy= 0.288521
Sum of electronic and zero-point Energies= -1059.010369
Sum of electronic and thermal Energies= -1058.988611
Sum of electronic and thermal Enthalpies= -1058.987667
Sum of electronic and thermal (Free) Energies= -1059.063455

3a

cRT

C 2.5650970000 -0.0210010000 -0.8306570000
C 1.3419770000 0.4215190000 -0.8399330000
C 0.1191760000 0.9244280000 -0.7874090000
C -1.0061170000 0.0622920000 -0.4043030000
C -0.9580210000 -1.4053130000 -0.4677260000
C -0.3099660000 -2.0710620000 -1.4267920000
H -1.5702490000 -1.9243440000 0.2620890000
C -0.1640600000 2.3974820000 -0.9722960000
O -2.0295090000 0.6595210000 0.0023020000
H 0.7439110000 2.9213870000 -1.2733870000
H -0.5379720000 2.8298080000 -0.0404730000
H -0.9354390000 2.5480670000 -1.7323570000
B -3.4298350000 -0.0251060000 0.4798080000
F -4.2169890000 1.0515560000 0.7524270000
F -3.0914150000 -0.7817320000 1.5851780000
F -3.8392180000 -0.7843620000 -0.5930020000
C 3.4684480000 -0.0818820000 0.3951280000
H 2.9838760000 -0.3994310000 -1.7642520000
H 0.2404240000 -1.5676260000 -2.2143910000
H -0.3546920000 -3.1543150000 -1.4666480000
C 2.7655790000 0.4842770000 1.6326870000
H 2.4825570000 1.5317020000 1.4858660000
H 1.8606210000 -0.0833000000 1.8721310000
H 3.4340940000 0.4329390000 2.4974830000
C 4.7369100000 0.7321140000 0.0903010000
H 5.4322160000 0.6745170000 0.9342990000
H 5.2519940000 0.3486390000 -0.7970530000
H 4.4955380000 1.7854520000 -0.0827900000
C 3.8381020000 -1.5564800000 0.6306220000
H 4.3380220000 -1.9858870000 -0.2443490000
H 4.5199290000 -1.6417800000 1.4832290000
H 2.9462790000 -2.1538670000 0.8439820000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256926 (Hartree/Particle)
Thermal correction to Energy= 0.275393
Thermal correction to Enthalpy= 0.276337
Thermal correction to Gibbs (Free) Energy= 0.209214
Sum of electronic and zero-point Energies= -828.088548
Sum of electronic and thermal Energies= -828.070081
Sum of electronic and thermal Enthalpies= -828.069137
Sum of electronic and thermal (Free) Energies= -828.136261

cTS

C 2.4471450000 -0.5533630000 -0.6486420000
C 1.1766890000 -0.2036710000 -0.7341770000
H 2.8126470000 -1.3447040000 -1.3023510000
C 3.4588140000 -0.0052890000 0.3462440000
C 0.1286260000 0.6575430000 -0.6342190000
C 4.6408190000 0.5604210000 -0.4619230000
C 2.8624750000 1.0880330000 1.2371850000
C 3.9417230000 -1.1804250000 1.2163010000
C -1.1167410000 0.0351420000 -0.2719800000
C 0.1894910000 2.1232460000 -0.9400040000
H 1.9982760000 0.7213620000 1.7996360000
H 3.6134020000 1.4277570000 1.9567450000
H 2.5473180000 1.9564810000 0.6511030000
H 4.3230150000 1.3959890000 -1.0933210000
H 5.4183000000 0.9228030000 0.2185520000
H 5.0871190000 -0.2050110000 -1.1055960000
H 4.3700220000 -1.9806090000 0.6032410000
H 4.7155360000 -0.8386880000 1.9115020000
H 3.1176510000 -1.5993860000 1.8018520000
C -1.0088550000 -1.3888450000 -0.2880160000
O -2.1183320000 0.7408440000 0.0691630000
H 0.0327840000 2.6863020000 -0.0137080000
H -0.6149520000 2.4064910000 -1.6238800000
H 1.1540520000 2.4024820000 -1.3658730000
C 0.0098750000 -1.9107350000 -1.0554360000
H -1.6005290000 -1.9869000000 0.3967280000
B -3.5083510000 0.0647610000 0.3478060000
H 0.4010360000 -2.9002010000 -0.8261840000
H 0.1836780000 -1.5859960000 -2.0777220000
F -3.7790080000 -0.7274620000 -0.7639890000
F -4.3829100000 1.1022060000 0.5172500000
F -3.3326720000 -0.7148620000 1.4895100000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256492 (Hartree/Particle)
Thermal correction to Energy= 0.273846
Thermal correction to Enthalpy= 0.274790
Thermal correction to Gibbs (Free) Energy= 0.210536
Sum of electronic and zero-point Energies= -828.060930
Sum of electronic and thermal Energies= -828.043576
Sum of electronic and thermal Enthalpies= -828.042632
Sum of electronic and thermal (Free) Energies= -828.106886

cPT

C -2.3991950000 0.8711250000 0.0336420000
C -1.0492860000 0.7326310000 0.0534780000
C -0.1495170000 -0.3890610000 0.0558560000
C 1.1996990000 0.0717120000 0.0066050000
C 1.1878660000 1.4636510000 0.0110010000
C -0.1862400000 1.9815890000 0.0579440000
C -0.3749730000 -1.8501710000 0.1090580000
O 2.1944150000 -0.7556400000 -0.0220060000
H -1.3689060000 -2.1449970000 0.4297320000
H 0.3866400000 -2.2925100000 0.7592520000
H -0.1779800000 -2.2685150000 -0.8872380000
H 2.0807190000 2.0758820000 -0.0140900000
B 3.6245870000 -0.1999880000 -0.0256440000
F 3.7530410000 0.5998790000 -1.1704460000
F 4.4595030000 -1.2893300000 -0.0306410000

F 3.7585400000 0.5931780000 1.1241420000
H -2.7125330000 1.9169500000 0.0621940000
C -3.5640970000 -0.0953380000 -0.0288180000
H -0.3580880000 2.5807210000 0.9635250000
H -0.4038420000 2.6379130000 -0.7959870000
C -3.4420790000 -1.0534980000 -1.2291350000
H -3.3988920000 -0.4904430000 -2.1663610000
H -2.5591380000 -1.6893900000 -1.1811170000
H -4.3223300000 -1.7031110000 -1.2663680000
C -4.8489210000 0.7345750000 -0.2163950000
H -5.7218360000 0.0765730000 -0.2577870000
H -4.9952240000 1.4340320000 0.6136230000
H -4.8169590000 1.3087770000 -1.1483900000
C -3.6842370000 -0.8621910000 1.3054790000
H -3.8489040000 -0.1684860000 2.1355880000
H -4.5402070000 -1.5430890000 1.2591100000
H -2.7946560000 -1.4489340000 1.5387910000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.259284 (Hartree/Particle)
Thermal correction to Energy= 0.276415
Thermal correction to Enthalpy= 0.277360
Thermal correction to Gibbs (Free) Energy= 0.214048
Sum of electronic and zero-point Energies= -828.100156
Sum of electronic and thermal Energies= -828.083024
Sum of electronic and thermal Enthalpies= -828.082080
Sum of electronic and thermal (Free) Energies= -828.145391

ccRT

C 2.4579070000 0.3575260000 -0.8752440000
C 1.2645190000 0.6653970000 -0.4590270000
C 0.0615340000 1.0639370000 -0.0765740000
C -1.0692370000 0.1274090000 -0.0884620000
C -0.9221370000 -1.3321600000 -0.1884560000
C 0.0486320000 -2.0154300000 0.4208770000
H -1.7229120000 -1.8416950000 -0.7142650000
C -0.2402440000 2.5070630000 0.2587540000
O -2.2038210000 0.6559960000 -0.0365460000
H 0.6765290000 3.0976370000 0.2420620000
H -0.6981980000 2.5810940000 1.2488260000
H -0.9512810000 2.9238070000 -0.4592250000
B -3.6403260000 -0.1167500000 -0.0159210000
F -4.5308530000 0.9035550000 0.1223810000
F -3.5680350000 -0.9714590000 1.0606780000
F -3.7046010000 -0.7726640000 -1.2296870000
C 3.6305740000 -0.1039800000 -0.0190370000
H 2.6381610000 0.4219050000 -1.9498200000
H 0.8093300000 -1.5304330000 1.0217610000
H 0.0746120000 -3.0986080000 0.3660960000
C 3.8808730000 -1.5936670000 -0.3097160000
H 3.0162220000 -2.2021660000 -0.0272880000
H 4.0795530000 -1.7619730000 -1.3731780000
H 4.7485560000 -1.9475940000 0.2570440000
C 3.3557810000 0.1074390000 1.4736570000
H 4.2232890000 -0.2082620000 2.0612950000
H 3.1605050000 1.1617050000 1.6938110000
H 2.4950460000 -0.4732980000 1.8188690000
C 4.8623100000 0.7181320000 -0.4343720000
H 4.7042250000 1.7852440000 -0.2492370000
H 5.7390400000 0.3984290000 0.1382680000
H 5.0878570000 0.5851060000 -1.4977900000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256782 (Hartree/Particle)
Thermal correction to Energy= 0.275285
Thermal correction to Enthalpy= 0.276229
Thermal correction to Gibbs (Free) Energy= 0.209543
Sum of electronic and zero-point Energies= -828.088085
Sum of electronic and thermal Energies= -828.069583
Sum of electronic and thermal Enthalpies= -828.068638
Sum of electronic and thermal (Free) Energies= -828.135325

ccTS

C 2.3607600000 0.5087530000 -0.5607570000
C 1.1177810000 0.4874460000 -0.1106360000
C -0.0851450000 1.1197960000 0.0130300000
C -1.2284470000 0.2502750000 -0.0200300000
C -0.8306090000 -1.1205090000 -0.0105580000
C 0.4098340000 -1.3841540000 0.5300610000
H -1.4192370000 -1.8627520000 -0.5392250000
C -0.2531560000 2.5943970000 0.2136100000
O -2.4041910000 0.7237250000 -0.1278240000
H 0.7024760000 3.1176870000 0.1742670000
H -0.7464900000 2.8008780000 1.1681720000
H -0.9137240000 2.9808410000 -0.5693490000
B -3.6494740000 -0.2309470000 -0.0615170000
F -4.7357790000 0.5987590000 -0.0339620000
F -3.4877510000 -0.9902270000 1.0941760000
F -3.5805530000 -1.0306620000 -1.2006150000
C 3.6276120000 -0.1645740000 -0.0705200000
H 2.4883460000 1.0994110000 -1.4723480000
H 0.7068980000 -0.9659170000 1.4860740000
H 0.9293240000 -2.2998700000 0.2557250000
C 3.9858700000 -1.3030820000 -1.0438070000
H 3.2101910000 -2.0750330000 -1.0493430000
H 4.0999510000 -0.9305400000 -2.0668420000
H 4.9309080000 -1.7687700000 -0.7452440000
C 3.5185070000 -0.7108610000 1.3585110000
H 4.5100660000 -1.0113430000 1.7105120000
H 3.1331850000 0.0473170000 2.0481430000
H 2.8799940000 -1.5949570000 1.4162160000
C 4.7350440000 0.9071310000 -0.1102380000
H 4.5137920000 1.7282160000 0.5790530000
H 5.6932550000 0.4658950000 0.1816720000
H 4.8503890000 1.3253430000 -1.1156880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256205 (Hartree/Particle)
Thermal correction to Energy= 0.273667
Thermal correction to Enthalpy= 0.274612
Thermal correction to Gibbs (Free) Energy= 0.210349
Sum of electronic and zero-point Energies= -828.056721
Sum of electronic and thermal Energies= -828.039259
Sum of electronic and thermal Enthalpies= -828.038315
Sum of electronic and thermal (Free) Energies= -828.102578

ccPT

C -2.3331270000 0.5660860000 0.0000010000
C -1.0645780000 0.0969780000 0.0000000000
C 0.0872400000 0.9576750000 0.0000010000
C 1.2845750000 0.1888250000 0.0000000000
C 0.9203560000 -1.1515680000 -0.0000010000
C -0.5481710000 -1.3250690000 -0.0000010000
C 0.1511720000 2.4329230000 0.0000020000
O 2.4532320000 0.7492690000 0.0000000000
H -0.8195780000 2.9276020000 0.0000030000
H 0.7343290000 2.7564460000 -0.8699820000
H 0.7343300000 2.7564440000 0.8699860000
H 1.6297290000 -1.9699670000 -0.0000020000
B 3.6973620000 -0.1435960000 -0.0000010000
F 4.7796690000 0.7016480000 -0.0000010000
F 3.6279960000 -0.9494860000 -1.1472640000
F 3.6279970000 -0.9494870000 1.1472610000
C -3.6716690000 -0.1212290000 0.0000010000
H -2.4321290000 1.6520250000 0.0000020000
H -0.8783610000 -1.8918840000 -0.8787170000
H -0.8783600000 -1.8918850000 0.8787140000
C -4.4224400000 0.3683310000 1.2581190000
H -4.5027390000 1.4599670000 1.2791310000
H -5.4364850000 -0.0436180000 1.2646060000
H -3.9154340000 0.0434510000 2.1717690000
C -4.4224410000 0.3683340000 -1.2581160000
H -5.4364850000 -0.0436150000 -1.2646040000
H -4.5027400000 1.4599700000 -1.2791250000
H -3.9154360000 0.0434560000 -2.1717680000
C -3.6302320000 -1.6521720000 -0.0000010000
H -3.1323100000 -2.0473540000 -0.8895090000
H -3.1323100000 -2.0473560000 0.8895050000
H -4.6537690000 -2.0386050000 -0.0000010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.258742 (Hartree/Particle)
Thermal correction to Energy= 0.276116
Thermal correction to Enthalpy= 0.277060
Thermal correction to Gibbs (Free) Energy= 0.211651
Sum of electronic and zero-point Energies= -828.110253
Sum of electronic and thermal Energies= -828.092879

Sum of electronic and thermal Enthalpies= -828.091935
Sum of electronic and thermal (Free) Energies= -828.157344

3b

cRT

C -2.5805570000 0.0269050000 -0.7630230000
C -1.3628990000 -0.4094640000 -0.9060840000
C -0.1431880000 -0.9110460000 -1.0001400000
C 0.9863150000 -0.1959570000 -0.3842050000
C 0.9605860000 1.2271810000 -0.0615550000
C 0.2976140000 2.1349570000 -0.7927180000
H 1.6029220000 1.5342280000 0.7578480000
C 0.1342880000 -2.2735050000 -1.5921350000
O 1.9888840000 -0.9069830000 -0.1267840000
H -0.7747040000 -2.6870550000 -2.0308260000
H 0.5035910000 -2.9522670000 -0.8189910000
H 0.9078150000 -2.2075590000 -2.3621120000
B 3.3856050000 -0.4019060000 0.5162040000
F 4.1515980000 -1.5294850000 0.5188090000
F 3.0558750000 0.0640340000 1.7763710000
F 3.8341150000 0.5942360000 -0.3253900000
C -3.4756110000 -0.2440130000 0.4398530000
H -0.2655840000 1.8123290000 -1.6655590000
C 0.3144310000 3.6010060000 -0.5195120000
H 0.8973970000 3.8431250000 0.3713220000
H -0.7088280000 3.9705980000 -0.3868120000
H 0.7377350000 4.1401020000 -1.3739500000
C -2.7757480000 -1.1453090000 1.4615460000
C -4.7622190000 -0.9179730000 -0.0646100000
H -2.5138830000 -2.1140910000 1.0238750000
H -3.4371490000 -1.3269330000 2.3142490000
H -1.8579030000 -0.6829150000 1.8385780000
H -4.5428870000 -1.8849330000 -0.5278920000
H -5.2750660000 -0.2930360000 -0.8037740000
H -5.4511950000 -1.0866040000 0.7697090000
C -3.8142760000 1.1120200000 1.0829400000
H -2.9087470000 1.6096920000 1.4441790000
H -4.4886120000 0.9682080000 1.9336830000
H -4.3112420000 1.7776330000 0.3686560000
H -2.9994690000 0.6570090000 -1.5491940000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.285221 (Hartree/Particle)
Thermal correction to Energy= 0.305287
Thermal correction to Enthalpy= 0.306231
Thermal correction to Gibbs (Free) Energy= 0.235319
Sum of electronic and zero-point Energies= -867.375236
Sum of electronic and thermal Energies= -867.355171
Sum of electronic and thermal Enthalpies= -867.354227
Sum of electronic and thermal (Free) Energies= -867.425139

cTS

C -2.4129410000 0.3790300000 -0.5342510000
C -1.1339780000 0.0862540000 -0.6834020000
H -2.8043110000 1.2608050000 -1.0421100000
C -3.4027400000 -0.3353530000 0.3720170000
C -0.0782450000 -0.7751010000 -0.7135250000
C -2.7840200000 -1.5533950000 1.0631080000
C -4.5966750000 -0.7721200000 -0.4958870000
C -3.8752270000 0.6790490000 1.4299950000
C 1.1543110000 -0.1909670000 -0.2632930000
C -0.1200910000 -2.1782740000 -1.2340440000
H -2.4760570000 -2.3125820000 0.3381640000
H -3.5188620000 -2.0112610000 1.7321370000
H -1.9106030000 -1.2756040000 1.6611430000
H -4.2858430000 -1.4907250000 -1.2606350000
H -5.0590660000 0.0841290000 -0.9984910000
H -5.3596310000 -1.2471370000 0.1295410000
H -3.0415240000 1.0044500000 2.0599730000
H -4.6336900000 0.2237960000 2.0753280000
H -4.3191580000 1.5647570000 0.9626950000
C 1.0219130000 1.2128170000 -0.0855450000
O 2.1708600000 -0.9221910000 -0.0196290000
H -1.0813250000 -2.4043120000 -1.6974750000
H 0.0455140000 -2.8705620000 -0.4013950000
H 0.6880840000 -2.3465660000 -1.9508100000
C -0.0157670000 1.8301500000 -0.7703590000
H 1.6199590000 1.7292990000 0.6588680000
B 3.5395830000 -0.2674440000 0.3532610000
H -0.1366520000 1.6229710000 -1.8325820000
C -0.5843910000 3.1445680000 -0.3223300000
F 3.8070490000 0.6711980000 -0.6419330000
F 4.4368770000 -1.3002380000 0.3932690000
F 3.3505330000 0.3566790000 1.5873520000
H 0.0119360000 3.9590040000 -0.7482710000
H -0.5789530000 3.2400300000 0.7652010000
H -1.6076260000 3.2755600000 -0.6836610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284529 (Hartree/Particle)
Thermal correction to Energy= 0.303522
Thermal correction to Enthalpy= 0.304466
Thermal correction to Gibbs (Free) Energy= 0.236617
Sum of electronic and zero-point Energies= -867.347643
Sum of electronic and thermal Energies= -867.328650
Sum of electronic and thermal Enthalpies= -867.327706
Sum of electronic and thermal (Free) Energies= -867.395556

cPT

C -2.3784260000 0.6335170000 -0.1923180000
C -1.0278040000 0.5307870000 -0.1248170000
C -0.1196530000 -0.5601620000 0.1117340000
C 1.2249350000 -0.1145710000 -0.0477590000
C 1.1992070000 1.2426240000 -0.3441820000
C -0.1769260000 1.7708140000 -0.3821430000
C -0.3329980000 -1.9782970000 0.4740060000
O 2.2265030000 -0.9236710000 0.0916180000
H -1.3223450000 -2.2059850000 0.8570000000
H 0.4362030000 -2.2656850000 1.1981930000
H -0.1353450000 -2.5975350000 -0.4114100000
H 2.0872340000 1.8412450000 -0.5098760000
B 3.6496300000 -0.3677090000 -0.0331620000
F 3.7695780000 0.1782640000 -1.3197720000
F 4.4966380000 -1.4256550000 0.1857210000
F 3.7781930000 0.6492480000 0.9259670000
H -2.7121630000 1.6557410000 -0.3810210000
C -3.5300260000 -0.3448650000 -0.0752530000
C -0.3972100000 2.9140740000 0.6267010000
H -0.3864710000 2.1589780000 -1.3916890000
H -0.2384170000 2.5578820000 1.6481080000
H -1.4095220000 3.3180350000 0.5487070000
H 0.3051990000 3.7279120000 0.4311170000
C -4.8189140000 0.4067990000 -0.4612640000
H -5.6836840000 -0.2584820000 -0.3818720000
H -4.9927820000 1.2631210000 0.1991650000
H -4.7701040000 0.7723100000 -1.4924850000
C -3.3717990000 -1.5335530000 -1.0419380000
H -3.3076100000 -1.1807170000 -2.0757280000
H -2.4872250000 -2.1354860000 -0.8393440000
H -4.2470030000 -2.1862200000 -0.9623550000
C -3.6743420000 -0.8122830000 1.3888040000
H -3.8648530000 0.0396690000 2.0486430000
H -4.5223800000 -1.4998000000 1.4707880000
H -2.7848450000 -1.3230920000 1.7602610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.287574 (Hartree/Particle)
Thermal correction to Energy= 0.306258
Thermal correction to Enthalpy= 0.307202
Thermal correction to Gibbs (Free) Energy= 0.240352
Sum of electronic and zero-point Energies= -867.379574
Sum of electronic and thermal Energies= -867.360890
Sum of electronic and thermal Enthalpies= -867.359945
Sum of electronic and thermal (Free) Energies= -867.426796

ccRT

C -2.3283440000 -1.2972040000 -0.7653780000
C -1.1281190000 -1.3920390000 -0.2688150000
C -3.5833910000 -0.7674130000 -0.0868750000
H -2.4613900000 -1.6707990000 -1.7829500000
C 0.0871560000 -1.6369660000 0.1936130000
C -3.2954900000 -0.2386880000 1.3213350000
C -4.5810680000 -1.9371660000 -0.0028930000
C -4.1731310000 0.3515520000 -0.9601260000
C 1.1964170000 -0.7070770000 -0.0707110000

C 0.4324210000 -2.9451060000 0.8706600000
H -2.7992890000 -0.9936170000 1.9398370000
H -2.6627010000 0.6530340000 1.2921350000
H -4.2323650000 0.0399950000 1.8136870000
H -5.5283910000 -1.5934480000 0.4258750000
H -4.7909510000 -2.3523060000 -0.9942630000
H -4.1902020000 -2.7414990000 0.6279900000
H -4.4110990000 -0.0140020000 -1.9646740000
H -5.0969050000 0.7334450000 -0.5126870000
H -3.4707090000 1.1840590000 -1.0585710000
C 1.0185110000 0.6991470000 -0.4138430000
O 2.3421700000 -1.2167770000 0.0042140000
H -0.4686480000 -3.5406940000 1.0226990000
H 0.9094990000 -2.7613040000 1.8373120000
H 1.1414150000 -3.5117350000 0.2616990000
C 0.0481680000 1.4587420000 0.1114670000
H 1.8044170000 1.1394900000 -1.0195350000
B 3.7510350000 -0.4431340000 -0.1762620000
H -0.6725110000 1.0101860000 0.7934380000
C -0.0789540000 2.9362640000 -0.1000870000
F 4.6729630000 -1.4122090000 0.0877390000
F 3.7212810000 0.5840140000 0.7451620000
F 3.7570120000 0.0060130000 -1.4841410000
C -1.4759330000 3.2811230000 -0.6324620000
C 0.2074570000 3.6674730000 1.2206370000
H 0.6684940000 3.2463910000 -0.8394300000
H -1.6761220000 2.7768150000 -1.5825920000
H -1.5652780000 4.3596720000 -0.7930480000
H -2.2505900000 2.9855240000 0.0851810000
H -0.5131640000 3.3737830000 1.9928060000
H 0.1258350000 4.7494100000 1.0787820000
H 1.2126160000 3.4412710000 1.5859330000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.285211 (Hartree/Particle)
Thermal correction to Energy= 0.305257
Thermal correction to Enthalpy= 0.306201
Thermal correction to Gibbs (Free) Energy= 0.236134
Sum of electronic and zero-point Energies= -867.374806
Sum of electronic and thermal Energies= -867.354761
Sum of electronic and thermal Enthalpies= -867.353817
Sum of electronic and thermal (Free) Energies= -867.423883

ccTS

C 2.2888960000 0.6565060000 -0.5889360000
C 1.0341850000 0.5397890000 -0.1719740000
C -0.1556810000 1.2007790000 -0.0502670000
C -1.3148090000 0.3557480000 -0.0506900000
C -0.9453530000 -1.0118720000 -0.0532050000
C 0.3279450000 -1.3261730000 0.4096740000
H -1.5843640000 -1.7467210000 -0.5332190000
C -0.2894030000 2.6791420000 0.1419280000
O -2.4872500000 0.8542080000 -0.1241700000
H 0.6654570000 3.1910550000 0.0187530000
H -0.6989520000 2.9043340000 1.1316620000
H -1.0106830000 3.0624670000 -0.5868040000
B -3.7427340000 -0.0694590000 -0.0210700000
F -4.8149020000 0.7799300000 0.0299160000
F -3.5733780000 -0.8304900000 1.1348240000
F -3.7265230000 -0.8808460000 -1.1565640000
C 3.5955240000 0.1275420000 -0.0327400000
H 2.4009680000 1.2679850000 -1.4889630000
H 0.6334760000 -0.9444650000 1.3816580000
C 4.1502620000 -0.9700190000 -0.9590910000
H 3.4888980000 -1.8387690000 -0.9937240000
H 4.2711060000 -0.5966530000 -1.9811070000
H 5.1315550000 -1.3001950000 -0.6024110000
C 3.4705690000 -0.3830390000 1.4079180000
H 4.4629960000 -0.6259500000 1.7998870000
H 3.0288900000 0.3793210000 2.0577930000
H 2.8664180000 -1.2885560000 1.4802340000
C 4.5704170000 1.3239730000 -0.0413450000
H 4.2085650000 2.1336340000 0.6003930000
H 5.5506570000 1.0078490000 0.3294810000
H 4.7059040000 1.7217600000 -1.0525540000
C 0.9660450000 -2.6169870000 -0.0302580000
H 1.0621730000 -2.6575600000 -1.1179270000
H 0.3233950000 -3.4487020000 0.2788030000
H 1.9468590000 -2.7768830000 0.4170910000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.284446 (Hartree/Particle)
Thermal correction to Energy= 0.303488
Thermal correction to Enthalpy= 0.304433
Thermal correction to Gibbs (Free) Energy= 0.237108
Sum of electronic and zero-point Energies= -867.340042
Sum of electronic and thermal Energies= -867.321000
Sum of electronic and thermal Enthalpies= -867.320055
Sum of electronic and thermal (Free) Energies= -867.387379

ccPT

C 2.2592440000 0.7331060000 -0.0791930000
C 1.0049090000 0.2262560000 -0.0591580000
C -0.1571820000 1.0589970000 -0.2286730000
C -1.3444310000 0.3082200000 -0.0063570000
C -0.9625410000 -0.9989820000 0.2556060000
C 0.5089730000 -1.1880400000 0.1851350000
C -0.2367100000 2.4997070000 -0.5426330000
O -2.5193130000 0.8534730000 -0.0714080000
H 0.7152540000 2.9565650000 -0.8114480000
H -0.6659990000 3.0226060000 0.3207720000
H -0.9632020000 2.6389280000 -1.3505810000
H -1.6613100000 -1.8064220000 0.4407880000
B -3.7502730000 -0.0335890000 0.1275370000
F -4.8441520000 0.7862730000 -0.0046150000
F -3.6457430000 -0.6104720000 1.4030670000
F -3.6961900000 -1.0402280000 -0.8504140000
C 3.6118540000 0.1122450000 0.1740270000
H 2.3269730000 1.7920010000 -0.3286410000
H 0.8804920000 -1.5791660000 1.1404480000
C 0.8585730000 -2.1829610000 -0.9418500000
H 0.5205020000 -1.7941990000 -1.9062960000
H 0.3607400000 -3.1396050000 -0.7651160000
H 1.9329230000 -2.3649390000 -0.9993660000
C 4.4965140000 1.1975790000 0.8202550000
H 5.5067970000 0.8101520000 0.9825030000
H 4.5757220000 2.0826300000 0.1801580000
H 4.0946080000 1.5099530000 1.7895660000
C 3.5899870000 -1.1094300000 1.1037660000
H 3.1041310000 -0.8722900000 2.0553840000
H 3.0859150000 -1.9693560000 0.6604870000
H 4.6180570000 -1.4148340000 1.3208720000
C 4.2108330000 -0.2673300000 -1.1989830000
H 4.2705040000 0.6026350000 -1.8605330000
H 5.2247560000 -0.6565740000 -1.0600490000
H 3.6136500000 -1.0342810000 -1.6993510000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.287776 (Hartree/Particle)
Thermal correction to Energy= 0.306415
Thermal correction to Enthalpy= 0.307359
Thermal correction to Gibbs (Free) Energy= 0.240840
Sum of electronic and zero-point Energies= -867.387089
Sum of electronic and thermal Energies= -867.368450
Sum of electronic and thermal Enthalpies= -867.367506
Sum of electronic and thermal (Free) Energies= -867.434024

3c

c/s RT

C -2.5378930000 -0.3579100000 -0.7337210000
C -1.3196230000 -0.7664170000 -0.9390140000
C -0.0926690000 -1.2330280000 -1.0981830000
C 1.0145210000 -0.6135990000 -0.3518170000
C 0.9481220000 0.7362380000 0.1979450000
C 0.2899310000 1.7369230000 -0.4039030000
H 1.5520120000 0.9184760000 1.0813840000
H -0.2298690000 1.5538250000 -1.3442890000
C 0.2461310000 3.1483450000 0.0942650000
C 0.2156150000 -2.4697340000 -1.9092950000
O 2.0282280000 -1.3388000000 -0.1974540000
H -0.6804910000 -2.8164050000 -2.4256030000
H 0.5871260000 -3.2647580000 -1.2575310000
H 0.9972060000 -2.2618530000 -2.6451680000
C -1.2148470000 3.5780030000 0.2927450000
C 0.9698230000 4.0749910000 -0.8937320000
H 0.7631520000 3.1934410000 1.0597660000

H -1.7645420000 3.5387040000 -0.6552010000
H -1.2611330000 4.6062710000 0.6636850000
H -1.7276660000 2.9311770000 1.0105430000
H 0.4875350000 4.0493530000 -1.8777390000
H 2.0152450000 3.7801270000 -1.0169670000
H 0.9422860000 5.1076320000 -0.5328600000
B 3.4034670000 -0.9118780000 0.5385270000
F 4.2005960000 -2.0044280000 0.3664020000
F 3.0505610000 -0.6676670000 1.8537690000
F 3.8336940000 0.2205990000 -0.1217510000
C -3.4456560000 -0.8297490000 0.3951000000
C -3.7320080000 0.3820210000 1.2989950000
C -2.7838280000 -1.9431900000 1.2126200000
C -4.7562340000 -1.3388240000 -0.2265450000
H -5.2454420000 -0.5572370000 -0.8179740000
H -5.4510110000 -1.6499110000 0.5606350000
H -4.5731390000 -2.1975980000 -0.8798420000
H -2.8098370000 0.7468760000 1.7621940000
H -4.4280600000 0.1020360000 2.0967480000
H -4.1811540000 1.2051110000 0.7324320000
H -1.8485080000 -1.6019280000 1.6676600000
H -2.5608290000 -2.8149850000 0.5890030000
H -3.4527520000 -2.2641020000 2.0170780000
H -2.9452510000 0.4045700000 -1.3995100000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342456 (Hartree/Particle)
Thermal correction to Energy= 0.365181
Thermal correction to Enthalpy= 0.366125
Thermal correction to Gibbs (Free) Energy= 0.288826
Sum of electronic and zero-point Energies= -945.932977
Sum of electronic and thermal Energies= -945.910253
Sum of electronic and thermal Enthalpies= -945.909308
Sum of electronic and thermal (Free) Energies= -945.986607

c/s TS

C -2.3662260000 -0.0971330000 -0.4454920000
C -1.0580190000 -0.2712330000 -0.5526680000
H -2.8037540000 0.7920790000 -0.8932900000
C -3.3388150000 -0.9724220000 0.3263490000
C 0.0085510000 -1.1139940000 -0.6760880000
C -4.0279840000 -0.0792680000 1.3753000000
C -2.6485190000 -2.1468940000 1.0248110000
C -4.3868560000 -1.4934950000 -0.6745690000
C 1.2421520000 -0.5609260000 -0.2025050000
C -0.0228910000 -2.4548420000 -1.3417240000
H -4.5378220000 0.7680830000 0.9037740000
H -4.7769200000 -0.6564420000 1.9273440000
H -3.3017210000 0.3126800000 2.0944760000
H -2.1998320000 -2.8375540000 0.3057690000
H -1.8630910000 -1.8028600000 1.7047620000
H -3.3814780000 -2.7094010000 1.6110400000
H -5.1446360000 -2.0831870000 -0.1482220000
H -4.8960610000 -0.6692060000 -1.1850940000
H -3.9237890000 -2.1318320000 -1.4334150000
C 1.0930610000 0.8105960000 0.1155760000
O 2.2827040000 -1.2912530000 -0.0715430000
H 0.1959200000 -3.2268190000 -0.5959680000
H 0.7593680000 -2.5225430000 -2.1027410000
H -0.9956950000 -2.6580910000 -1.7912580000
C 0.0081310000 1.4811960000 -0.4433420000
H 1.7277130000 1.2687720000 0.8678140000
B 3.6484620000 -0.6429910000 0.3051640000
H -0.1501910000 1.4223210000 -1.5222650000
C -0.4346020000 2.7948000000 0.1730660000
F 3.8477680000 0.4052490000 -0.5949300000
F 4.5735940000 -1.6463390000 0.1931530000
F 3.5096770000 -0.1554680000 1.6064050000
C -1.8862500000 3.1781400000 -0.1248500000
C 0.5210330000 3.8857250000 -0.3470680000
H -0.3127400000 2.7189540000 1.2595520000
H -2.5934970000 2.5415210000 0.4113010000
H -2.0679520000 4.2098630000 0.1894080000
H -2.1013800000 3.1198480000 -1.1988770000
H 1.5654330000 3.6473450000 -0.1296730000
H 0.4200860000 4.0038950000 -1.4317810000
H 0.2821520000 4.8450830000 0.1214450000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342359 (Hartree/Particle)
Thermal correction to Energy= 0.363727
Thermal correction to Enthalpy= 0.364671
Thermal correction to Gibbs (Free) Energy= 0.291585
Sum of electronic and zero-point Energies= -945.901633
Sum of electronic and thermal Energies= -945.880266
Sum of electronic and thermal Enthalpies= -945.879321
Sum of electronic and thermal (Free) Energies= -945.952408

c/s PT

C 2.3588560000 0.1838090000 0.3148410000
C 1.0179400000 0.1458170000 0.1272370000
H 2.7104100000 1.1478160000 0.6817570000
C 3.4794710000 -0.8290080000 0.1781110000
C 0.1132940000 -0.8843660000 -0.3144670000
C 4.6963470000 -0.2665790000 0.9392300000
C 3.8669670000 -0.9655850000 -1.3097470000
C 3.1284920000 -2.1937340000 0.7948310000
C -1.2157570000 -0.5493380000 0.0654030000
C 0.3284550000 -2.1241430000 -1.0912140000
H 4.4711530000 -0.1373720000 2.0031330000
H 5.5453730000 -0.9515000000 0.8561320000
H 5.0058870000 0.7028470000 0.5338950000
H 3.0453170000 -1.3423120000 -1.9220040000
H 4.1731000000 0.0007340000 -1.7228000000
H 4.7100790000 -1.6573940000 -1.4071570000
H 4.0071760000 -2.8454950000 0.7592160000
H 2.8356150000 -2.0795170000 1.8429100000
H 2.3207830000 -2.7037720000 0.2726650000
C -1.1826600000 0.6923800000 0.6887550000
O -2.2169650000 -1.3363800000 -0.1769970000
H -0.4393710000 -2.1682520000 -1.8718360000
H 0.1257190000 -2.9912510000 -0.4497340000
H 1.3182200000 -2.2121230000 -1.5293380000
C 0.1485480000 1.3181150000 0.5845540000
H -2.0496960000 1.1550240000 1.1428530000
B -3.6306580000 -0.8028700000 0.0703040000
H 0.4766750000 1.7187920000 1.5547380000
C 0.1153250000 2.5107540000 -0.4365040000
F -3.7537950000 -0.5549170000 1.4448970000
F -4.4957810000 -1.7660590000 -0.3849500000
F -3.7356210000 0.4097150000 -0.6367360000
C 1.4656320000 3.2235550000 -0.5447620000
C -0.9873570000 3.5083440000 -0.0658440000
H -0.1279450000 2.0718790000 -1.4126790000
H 2.2406370000 2.5814070000 -0.9701320000
H 1.3702480000 4.0962070000 -1.1974420000
H 1.8053730000 3.5812960000 0.4348100000
H -1.9853390000 3.0726760000 -0.1574410000
H -0.8599710000 3.8706740000 0.9613700000
H -0.9449780000 4.3762440000 -0.7298960000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344954 (Hartree/Particle)
Thermal correction to Energy= 0.366174
Thermal correction to Enthalpy= 0.367118
Thermal correction to Gibbs (Free) Energy= 0.294693
Sum of electronic and zero-point Energies= -945.934740
Sum of electronic and thermal Energies= -945.913520
Sum of electronic and thermal Enthalpies= -945.912576
Sum of electronic and thermal (Free) Energies= -945.985002

cc/s RT

C -2.4027470000 -1.0900310000 -0.8495150000
C -1.2169260000 -1.2987370000 -0.3530740000
C -3.6544240000 -0.6262250000 -0.1191370000
H -2.5254100000 -1.3018480000 -1.9138420000
C -0.0202550000 -1.6550400000 0.0846180000
C -3.3776400000 -0.3282010000 1.3571520000
C -4.6907140000 -1.7596340000 -0.2293470000
C -4.1900950000 0.6314530000 -0.8218290000
C 1.1256560000 -0.7393430000 -0.0289260000
C 0.2668330000 -3.0623830000 0.5599140000
H -2.9307430000 -1.1902360000 1.8629850000
H -2.7034980000 0.5252720000 1.4726340000
H -4.3123650000 -0.0814120000 1.8701380000
H -5.6343810000 -1.4527310000 0.2340610000
H -4.8951140000 -2.0107290000 -1.2754830000

H -4.3380650000 -2.6641070000 0.2759420000
H -4.4207280000 0.4290370000 -1.8731230000
H -5.1092280000 0.9743840000 -0.3350280000
H -3.4589020000 1.4438220000 -0.7847030000
C 1.0099390000 0.7093940000 -0.1468670000
O 2.2501440000 -1.3000470000 -0.0364520000
H -0.6577820000 -3.6385430000 0.6136660000
H 0.7371850000 -3.0442470000 1.5469690000
H 0.9623800000 -3.5583900000 -0.1217930000
C 0.0766090000 1.4174710000 0.5039740000
H 1.8181430000 1.1942040000 -0.6825940000
B 3.6888570000 -0.5651640000 -0.1056460000
H -0.6617610000 0.8874840000 1.1022440000
C -0.0211170000 2.9153250000 0.5377440000
F 4.5709410000 -1.5995990000 -0.0021560000
F 3.7040840000 0.3084300000 0.9626850000
F 3.7118440000 0.0805880000 -1.3287800000
C 1.0505540000 3.6326490000 -0.2807010000
C -1.4362070000 3.3467290000 0.1180970000
H 0.1041390000 3.1966590000 1.5940960000
H 2.0581930000 3.3718200000 0.0547450000
H 0.9327720000 4.7154330000 -0.1824350000
H 0.9673770000 3.3829110000 -1.3442260000
H -1.6224980000 3.0849630000 -0.9291370000
H -1.5495560000 4.4295540000 0.2222310000
H -2.2042160000 2.8675570000 0.7341410000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342651 (Hartree/Particle)
Thermal correction to Energy= 0.365257
Thermal correction to Enthalpy= 0.366201
Thermal correction to Gibbs (Free) Energy= 0.290020
Sum of electronic and zero-point Energies= -945.931812
Sum of electronic and thermal Energies= -945.909205
Sum of electronic and thermal Enthalpies= -945.908261
Sum of electronic and thermal (Free) Energies= -945.984443

cc/s TS

C -2.0957380000 -1.0695510000 -0.5925110000
C -0.8366460000 -0.7667690000 -0.2789990000
C -3.4156450000 -0.8096400000 0.0982300000
H -2.1826560000 -1.7388010000 -1.4544240000
C 0.3706120000 -1.4105330000 -0.1883020000
C -3.3166300000 0.1470110000 1.2864140000
C -3.8431430000 -2.2020910000 0.6244350000
C -4.4718000000 -0.3293630000 -0.9115600000
C 1.5153650000 -0.5571870000 -0.1307680000
C 0.5205380000 -2.8913740000 -0.0265490000
H -2.5713060000 -0.1941140000 2.0128210000
H -3.0571680000 1.1580610000 0.9728030000
H -4.2814400000 0.1983670000 1.7998890000
H -4.8213040000 -2.1241290000 1.1104390000
H -3.9287100000 -2.9305820000 -0.1883760000
H -3.1247280000 -2.5845740000 1.3557780000
H -4.5736910000 -1.0396590000 -1.7387020000
H -5.4461570000 -0.2444950000 -0.4201100000
H -4.2209900000 0.6453400000 -1.3360510000
C 1.1297640000 0.8017020000 -0.1119270000
O 2.6998390000 -1.0379400000 -0.1603030000
H 0.7659270000 -3.1423450000 1.0107710000
H 1.3641680000 -3.2276830000 -0.6361370000
H -0.3855360000 -3.4259610000 -0.3159370000
C -0.1783300000 1.1112500000 0.2655240000
H 1.8041370000 1.5533150000 -0.5091180000
B 3.9298050000 -0.1061780000 0.0503980000
H -0.5401950000 0.7568540000 1.2313500000
C -0.7302230000 2.4534990000 -0.2025340000
F 5.0122430000 -0.9418630000 0.1280180000
F 3.6867110000 0.6057330000 1.2258070000
F 3.9694400000 0.7545500000 -1.0489120000
C -1.7890590000 2.3458580000 -1.3064210000
C -1.2011730000 3.3149980000 0.9739040000
H 0.1229270000 2.9685270000 -0.6602280000
H -1.4525300000 1.6944710000 -2.1174280000
H -1.9875430000 3.3387180000 -1.7205900000
H -2.7317280000 1.9545720000 -0.9209360000
H -2.0588830000 2.8717450000 1.4896820000
H -1.5027940000 4.3053330000 0.6200340000
H -0.4004260000 3.4487990000 1.7070730000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341946 (Hartree/Particle)
Thermal correction to Energy= 0.363522
Thermal correction to Enthalpy= 0.364466
Thermal correction to Gibbs (Free) Energy= 0.291570
Sum of electronic and zero-point Energies= -945.889723
Sum of electronic and thermal Energies= -945.868147
Sum of electronic and thermal Enthalpies= -945.867203
Sum of electronic and thermal (Free) Energies= -945.940098

cc/s PT

C -2.1645700000 -0.9830150000 -0.2742140000
C -0.9407050000 -0.4070830000 -0.2306360000
C -3.5009790000 -0.6724930000 0.3557060000
H -2.1955470000 -1.9338220000 -0.8079960000
C 0.2200210000 -1.1553580000 -0.6559470000
C -3.4957530000 0.4505970000 1.3965900000
C -3.9447970000 -1.9779960000 1.0556200000
C -4.5071990000 -0.3568180000 -0.7710610000
C 1.3941730000 -0.6048640000 -0.0777740000
C 0.2875790000 -2.3728350000 -1.4895160000
H -2.8095510000 0.2250780000 2.2187960000
H -3.2248750000 1.4143550000 0.9665440000
H -4.4989790000 0.5511790000 1.8221160000
H -4.9280520000 -1.8348060000 1.5144360000
H -4.0226960000 -2.8085740000 0.3463580000
H -3.2404750000 -2.2635100000 1.8432980000
H -4.5265400000 -1.1525150000 -1.5229390000
H -5.5134560000 -0.2686020000 -0.3489150000
H -4.2682630000 0.5834080000 -1.2746470000
C 1.0106490000 0.5211670000 0.6347710000
O 2.5656420000 -1.1411640000 -0.2440640000
H -0.6295910000 -2.5858720000 -2.0386590000
H 0.5425730000 -3.2279460000 -0.8509790000
H 1.1287140000 -2.2702150000 -2.1829300000
C -0.4146020000 0.8728530000 0.4003640000
H 1.6977160000 1.1198040000 1.2190900000
B 3.7840560000 -0.3639090000 0.2500860000
H -0.9235910000 1.1582400000 1.3254040000
C -0.4493930000 2.0889090000 -0.6001310000
F 4.8902610000 -1.0747530000 -0.1453820000
F 3.6755390000 -0.2451880000 1.6443440000
F 3.7174020000 0.9163760000 -0.3338360000
C -1.8623850000 2.5702060000 -0.9191630000
C 0.4052560000 3.2529720000 -0.0868710000
H 0.0016710000 1.7158210000 -1.5288500000
H -2.5015790000 1.7573800000 -1.2713600000
H -1.8204400000 3.3255680000 -1.7095480000
H -2.3314630000 3.0380550000 -0.0467560000
H 0.0972920000 3.5491790000 0.9230620000
H 0.2788430000 4.1220940000 -0.7387420000
H 1.4702810000 3.0091840000 -0.0672660000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345226 (Hartree/Particle)
Thermal correction to Energy= 0.366358
Thermal correction to Enthalpy= 0.367302
Thermal correction to Gibbs (Free) Energy= 0.295344
Sum of electronic and zero-point Energies= -945.938207
Sum of electronic and thermal Energies= -945.917076
Sum of electronic and thermal Enthalpies= -945.916131
Sum of electronic and thermal (Free) Energies= -945.988090

c/d RT

C -2.7103160000 -0.0646160000 -0.7503590000
C -1.5568100000 -0.6406310000 -0.9256920000
C -0.4039510000 -1.2754040000 -1.0533550000
C 0.7900180000 -0.7467440000 -0.3748180000
C 0.9124140000 0.6326240000 0.0827390000
C 0.3827150000 1.6713600000 -0.5795480000
H 1.5577910000 0.7792580000 0.9416230000
H -0.1784310000 1.4865930000 -1.4941890000
C 0.5500750000 3.1181100000 -0.2182040000
C -0.2771550000 -2.6078080000 -1.7543480000
O 1.7097400000 -1.5817920000 -0.1860410000
H -1.2223790000 -2.8777690000 -2.2270590000
H 0.0042160000 -3.3851380000 -1.0391830000

H 0.5072180000 -2.5681670000 -2.5151140000
C 1.2319630000 3.8546870000 -1.3846520000
C 1.2852850000 3.3562440000 1.0992360000
H -0.4701270000 3.5224250000 -0.1271990000
H 2.2524110000 3.4840960000 -1.5241090000
H 1.2822300000 4.9274630000 -1.1773100000
H 0.6872410000 3.7161530000 -2.3239910000
H 2.3179420000 2.9957860000 1.0453240000
H 0.7910270000 2.8535990000 1.9361190000
H 1.3169530000 4.4266550000 1.3209890000
B 3.1435480000 -1.2836880000 0.4967450000
F 3.7935690000 -2.4775280000 0.3907010000
F 2.8564630000 -0.9073020000 1.7972220000
F 3.6986480000 -0.2621160000 -0.2467800000
C -3.6435030000 -0.3073450000 0.4291300000
C -3.7991820000 1.0274660000 1.1785680000
C -3.0790690000 -1.3724510000 1.3741150000
C -5.0058320000 -0.7587070000 -0.1220650000
H -5.4238590000 -0.0137470000 -0.8077900000
H -5.7173380000 -0.8974980000 0.6987520000
H -4.9162100000 -1.7069690000 -0.6610610000
H -2.8363710000 1.3681050000 1.5725120000
H -4.4914360000 0.9099850000 2.0189370000
H -4.1973230000 1.8082340000 0.5212440000
H -2.1099740000 -1.0690880000 1.7830800000
H -2.9469480000 -2.3302110000 0.8604050000
H -3.7650350000 -1.5296390000 2.2121620000
H -3.0352840000 0.6744620000 -1.4843180000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342612 (Hartree/Particle)
Thermal correction to Energy= 0.365215
Thermal correction to Enthalpy= 0.366159
Thermal correction to Gibbs (Free) Energy= 0.288965
Sum of electronic and zero-point Energies= -945.932200
Sum of electronic and thermal Energies= -945.909597
Sum of electronic and thermal Enthalpies= -945.908653
Sum of electronic and thermal (Free) Energies= -945.985847

c/d TS

C -2.3839400000 -0.0535950000 -0.5622670000
C -1.1046790000 -0.3439660000 -0.7080090000
H -2.7728930000 0.8339270000 -1.0619940000
C -3.3828980000 -0.7921460000 0.3150620000
C -0.0410830000 -1.1945620000 -0.7376060000
C -3.9004880000 0.1962830000 1.3757390000
C -2.7616780000 -2.0101230000 1.0040350000
C -4.5481940000 -1.2353520000 -0.5884450000
C 1.1816670000 -0.6053870000 -0.2678570000
C -0.0651350000 -2.5909740000 -1.2781100000
H -4.3198780000 1.0962390000 0.9130230000
H -4.6881140000 -0.2731400000 1.9742800000
H -3.0967790000 0.5013540000 2.0528140000
H -2.4299240000 -2.7569460000 0.2767730000
H -1.9031680000 -1.7275430000 1.6212000000
H -3.5028060000 -2.4850800000 1.6540020000
H -5.3161380000 -1.7362630000 0.0101580000
H -5.0150260000 -0.3786570000 -1.0861670000
H -4.2057410000 -1.9334570000 -1.3586460000
C 1.0411290000 0.7960530000 -0.0827110000
O 2.2010690000 -1.3315100000 -0.0176130000
H 0.0960210000 -3.2936360000 -0.4533400000
H 0.7524150000 -2.7429270000 -1.9878410000
H -1.0191160000 -2.8180240000 -1.7559530000
C 0.0134290000 1.4157160000 -0.7788380000
H 1.6349340000 1.3036140000 0.6703760000
B 3.5590360000 -0.6688860000 0.3739550000
H -0.0934340000 1.2030730000 -1.8423350000
C -0.5757780000 2.7386130000 -0.3560920000
F 3.8324010000 0.2775190000 -0.6128460000
F 4.4646060000 -1.6944200000 0.4200620000
F 3.3524610000 -0.0511440000 1.6092190000
C 0.2753010000 3.8802010000 -0.9400070000
C -0.7362150000 2.8649290000 1.1590180000
H -1.5700100000 2.8040740000 -0.8173280000
H 0.3615700000 3.8036460000 -2.0279640000
H -0.1790530000 4.8460970000 -0.7008870000
H 1.2851930000 3.8631180000 -0.5187360000
H -1.2915750000 2.0148970000 1.5670690000
H 0.2344940000 2.9091710000 1.6624880000
H -1.2785450000 3.7812300000 1.4087430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342035 (Hartree/Particle)
Thermal correction to Energy= 0.363592
Thermal correction to Enthalpy= 0.364536
Thermal correction to Gibbs (Free) Energy= 0.290938
Sum of electronic and zero-point Energies= -945.905825
Sum of electronic and thermal Energies= -945.884268
Sum of electronic and thermal Enthalpies= -945.883324
Sum of electronic and thermal (Free) Energies= -945.956922

c/d PT

C -2.4102300000 0.3148770000 -0.3442460000
C -1.0655060000 0.1654360000 -0.2757430000
H -2.7069920000 1.3224560000 -0.6427640000
C -3.5962090000 -0.6013460000 -0.1198140000
C -0.1973630000 -0.9149310000 0.1100880000
C -4.8398110000 0.1034500000 -0.6961450000
C -3.8157580000 -0.7933730000 1.3961920000
C -3.4407250000 -1.9495940000 -0.8450940000
C 1.1516490000 -0.5780320000 -0.1951480000
C -0.4562030000 -2.2128470000 0.7711590000
H -4.7313210000 0.2794640000 -1.7715800000
H -5.7297810000 -0.5145880000 -0.5450070000
H -5.0135000000 1.0675580000 -0.2061710000
H -2.9638610000 -1.2675180000 1.8868730000
H -3.9879040000 0.1689310000 1.8882940000
H -4.6977070000 -1.4206810000 1.5619290000
H -4.3507010000 -2.5428090000 -0.7098530000
H -3.2962530000 -1.7936220000 -1.9184720000
H -2.6034020000 -2.5398650000 -0.4763790000
C 1.1666750000 0.6986520000 -0.7443340000
O 2.1314210000 -1.3908780000 0.0503820000
H 0.3325830000 -2.3801150000 1.5120620000
H -0.3317940000 -3.0179690000 0.0350160000
H -1.4358210000 -2.2946950000 1.2321430000
C -0.1696830000 1.3145540000 -0.7285820000
H 2.0668160000 1.1833390000 -1.1022670000
B 3.5607300000 -0.8541110000 -0.0581850000
H -0.4466460000 1.6406460000 -1.7428300000
C -0.2459400000 2.5756340000 0.1927750000
F 3.7821150000 -0.5034820000 -1.3975160000
F 4.3880130000 -1.8569110000 0.3817850000
F 3.6201860000 0.3001970000 0.7458680000
C 0.6052570000 3.7107790000 -0.3799220000
C 0.1481730000 2.2605610000 1.6362580000
H -1.2937250000 2.9020770000 0.1798010000
H 0.3419570000 3.9299920000 -1.4199470000
H 0.4562680000 4.6239030000 0.2036870000
H 1.6718670000 3.4669250000 -0.3398430000
H -0.4490220000 1.4435790000 2.0542110000
H 1.2037190000 1.9781430000 1.7073470000
H -0.0085860000 3.1412750000 2.2657080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.344920 (Hartree/Particle)
Thermal correction to Energy= 0.366151
Thermal correction to Enthalpy= 0.367095
Thermal correction to Gibbs (Free) Energy= 0.294696
Sum of electronic and zero-point Energies= -945.938832
Sum of electronic and thermal Energies= -945.917601
Sum of electronic and thermal Enthalpies= -945.916657
Sum of electronic and thermal (Free) Energies= -945.989056

cc/d RT

C -2.4956000000 -1.0959360000 -0.8864290000
C -1.3066340000 -1.3685570000 -0.4322710000
C -3.6563690000 -0.5068520000 -0.0936290000
H -2.6832250000 -1.2968360000 -1.9426420000
C -0.1131700000 -1.7273200000 0.0099430000
C -3.3813680000 -0.5324880000 1.4139360000
C -4.9052590000 -1.3505010000 -0.4002630000
C -3.8825550000 0.9395570000 -0.5668190000
C 1.0366010000 -0.8148840000 -0.1059540000
C 0.1606740000 -3.1169990000 0.5396220000
H -3.2046400000 -1.5537620000 1.7656550000

H -2.5087360000 0.0708210000 1.6829140000
H -4.2415740000 -0.1288460000 1.9570330000
H -5.7736830000 -0.9463000000 0.1302070000
H -5.1330410000 -1.3466510000 -1.4715380000
H -4.7653330000 -2.3891370000 -0.0846370000
H -4.0640980000 0.9807050000 -1.6457720000
H -4.7523300000 1.3710410000 -0.0600080000
H -3.0138270000 1.5671550000 -0.3456300000
C 0.9310970000 0.6154930000 -0.3729450000
O 2.1592330000 -1.3661120000 0.0161910000
H -0.7658920000 -3.6902250000 0.5912040000
H 0.6075530000 -3.0642180000 1.5361430000
H 0.8718590000 -3.6373310000 -0.1069200000
C -0.0750490000 1.3788350000 0.0752580000
H 1.7895930000 1.0507950000 -0.8720050000
B 3.5996850000 -0.6319350000 -0.0060570000
H -0.8718820000 0.9142380000 0.6511750000
C -0.1889200000 2.8669760000 -0.0801470000
F 4.4693010000 -1.6472960000 0.2614220000
F 3.5309630000 0.3357090000 0.9757940000
F 3.7205540000 -0.1004790000 -1.2773860000
C -0.3616370000 3.5066870000 1.3077850000
C 0.9592580000 3.5072480000 -0.8576080000
H -1.1233390000 3.0393530000 -0.6372250000
H -1.2110210000 3.0742190000 1.8471480000
H -0.5343890000 4.5823650000 1.2116190000
H 0.5385370000 3.3572920000 1.9124550000
H 1.9122750000 3.3683840000 -0.3363540000
H 0.7866120000 4.5821070000 -0.9613240000
H 1.0545270000 3.0844360000 -1.8620900000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342981 (Hartree/Particle)
Thermal correction to Energy= 0.365384
Thermal correction to Enthalpy= 0.366328
Thermal correction to Gibbs (Free) Energy= 0.291076
Sum of electronic and zero-point Energies= -945.931212
Sum of electronic and thermal Energies= -945.908810
Sum of electronic and thermal Enthalpies= -945.907866
Sum of electronic and thermal (Free) Energies= -945.983117

cc/d TS

C -2.0762360000 -1.0249500000 -0.6262810000
C -0.8222680000 -0.7813780000 -0.2498630000
C -3.4033560000 -0.7934410000 0.0648420000
H -2.1572990000 -1.5673470000 -1.5732430000
C 0.3928690000 -1.4071470000 -0.1987760000
C -3.2406500000 -0.3742920000 1.5297170000
C -4.1109250000 -2.1673380000 0.0297310000
C -4.2636670000 0.2147680000 -0.7154890000
C 1.5231050000 -0.5359320000 -0.0754230000
C 0.5731060000 -2.8928610000 -0.1673750000
H -2.6404110000 -1.1068650000 2.0793070000
H -2.7686440000 0.6020000000 1.6333820000
H -4.2225570000 -0.3146840000 2.0094360000
H -5.0857690000 -2.0920830000 0.5221160000
H -4.2778790000 -2.5060880000 -0.9981200000
H -3.5236200000 -2.9289760000 0.5524180000
H -4.3776440000 -0.0913760000 -1.7606310000
H -5.2622090000 0.2756590000 -0.2706130000
H -3.8280280000 1.2156910000 -0.7041280000
C 1.1122760000 0.8086570000 0.0372300000
O 2.7143530000 -0.9932750000 -0.1501950000
H -0.3355810000 -3.4183740000 -0.4640310000
H 0.8683470000 -3.2234490000 0.8338200000
H 1.3952840000 -3.1604400000 -0.8377330000
C -0.2009370000 1.0655380000 0.4399600000
H 1.7625420000 1.5982230000 -0.3265620000
B 3.9333780000 -0.0523590000 0.0872450000
H -0.5451390000 0.6472910000 1.3853300000
C -0.7849470000 2.4066880000 0.0133300000
F 5.0313180000 -0.8711390000 0.0882400000
F 3.7084260000 0.5846700000 1.3074740000
F 3.9293610000 0.8713680000 -0.9609270000
C -1.1324250000 2.4304180000 -1.4819120000
C -1.9244170000 2.9381250000 0.8831660000
H 0.0550100000 3.1026940000 0.1475000000
H -0.2777240000 2.1207650000 -2.0901970000
H -1.4175520000 3.4415160000 -1.7867910000
H -1.9647230000 1.7580160000 -1.7057050000
H -2.8697340000 2.4266790000 0.6889210000
H -2.0846210000 3.9991610000 0.6710840000
H -1.6948910000 2.8447680000 1.9495610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341803 (Hartree/Particle)
Thermal correction to Energy= 0.363346
Thermal correction to Enthalpy= 0.364290
Thermal correction to Gibbs (Free) Energy= 0.291731
Sum of electronic and zero-point Energies= -945.891193
Sum of electronic and thermal Energies= -945.869650
Sum of electronic and thermal Enthalpies= -945.868706
Sum of electronic and thermal (Free) Energies= -945.941265

cc/d PT

C -2.1345670000 -0.9098250000 -0.3118840000
C -0.9162200000 -0.3422710000 -0.1507350000
C -3.4970320000 -0.6877450000 0.2981290000
H -2.1393900000 -1.7769920000 -0.9735020000
C 0.2568200000 -1.0345640000 -0.6327080000
C -3.5197370000 0.2166240000 1.5333110000
C -4.0058850000 -2.0866470000 0.7146300000
C -4.4320490000 -0.1335130000 -0.7974080000
C 1.4181670000 -0.5488060000 0.0238150000
C 0.3517040000 -2.1387210000 -1.6092650000
H -2.8595130000 -0.1686200000 2.3167560000
H -3.2305320000 1.2403300000 1.3016980000
H -4.5351280000 0.2468460000 1.9403530000
H -5.0101170000 -2.0029220000 1.1413700000
H -4.0605290000 -2.7666290000 -0.1419530000
H -3.3529380000 -2.5364220000 1.4693480000
H -4.4365440000 -0.7794740000 -1.6814270000
H -5.4559270000 -0.0813440000 -0.4131920000
H -4.1348580000 0.8704720000 -1.1104900000
C 1.0202630000 0.5031650000 0.8333990000
O 2.5958310000 -1.0536220000 -0.1941920000
H -0.5464410000 -2.2781560000 -2.2110350000
H 0.5859490000 -3.0686550000 -1.0762090000
H 1.2153920000 -1.9513020000 -2.2556630000
C -0.4121580000 0.8479720000 0.6502900000
H 1.7026530000 1.0854500000 1.4419060000
B 3.8105840000 -0.2716080000 0.2985420000
H -0.9224280000 0.9705580000 1.6101340000
C -0.4606930000 2.2312850000 -0.1107940000
F 4.9201590000 -0.9463080000 -0.1481610000
F 3.7369570000 -0.2004200000 1.6981960000
F 3.7031280000 1.0249640000 -0.2426960000
C 0.1430750000 2.1566570000 -1.5157070000
C -1.8586930000 2.8421710000 -0.1549370000
H 0.1695700000 2.9003400000 0.4878760000
H 1.1912090000 1.8481770000 -1.5056270000
H 0.0948410000 3.1435720000 -1.9842880000
H -0.4182430000 1.4641210000 -2.1540910000
H -2.5485750000 2.2109160000 -0.7236200000
H -1.8192990000 3.8164930000 -0.6508580000
H -2.2688850000 3.0014470000 0.8464650000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345547 (Hartree/Particle)
Thermal correction to Energy= 0.366587
Thermal correction to Enthalpy= 0.367532
Thermal correction to Gibbs (Free) Energy= 0.295865
Sum of electronic and zero-point Energies= -945.938597
Sum of electronic and thermal Energies= -945.917556
Sum of electronic and thermal Enthalpies= -945.916612
Sum of electronic and thermal (Free) Energies= -945.988279

c/u RT

C -2.5472430000 -0.4938630000 -0.7306640000
C -1.3297500000 -0.9235490000 -0.8927590000
C -0.1006100000 -1.3997460000 -0.9965280000
C 1.0145680000 -0.6425760000 -0.4049430000
C 0.9455910000 0.7842590000 -0.1101670000
C 0.2609750000 1.6491650000 -0.8726950000
H 1.5700980000 1.1203840000 0.7098930000
H -0.2766770000 1.2758720000 -1.7426880000
C 0.1687580000 3.1313000000 -0.6596570000

C 0.2057910000 -2.7622360000 -1.5726830000
O 2.0401590000 -1.3187870000 -0.1421610000
H -0.6970720000 -3.2067490000 -1.9934060000
H 0.6031970000 -3.4194610000 -0.7948550000
H 0.9673450000 -2.6867160000 -2.3536760000
C 0.9711550000 3.6471280000 0.5327430000
C -1.3165310000 3.5220240000 -0.5549080000
H 0.5649560000 3.5962140000 -1.5744150000
H 0.6021840000 3.2187110000 1.4712310000
H 0.8783160000 4.7344500000 0.6040370000
H 2.0335310000 3.4044860000 0.4404670000
H -1.7654330000 3.0868900000 0.3441140000
H -1.8880250000 3.1748650000 -1.4221070000
H -1.4198850000 4.6092080000 -0.4951440000
B 3.4195930000 -0.7529230000 0.4815210000
F 4.2278730000 -1.8507660000 0.4981450000
F 3.0820570000 -0.2772660000 1.7366100000
F 3.8282760000 0.2459680000 -0.3781030000
C -3.4156180000 -0.7531190000 0.4939110000
C -3.6858450000 0.6039410000 1.1669050000
C -2.7181620000 -1.6933580000 1.4816340000
C -4.7394240000 -1.3737070000 0.0191250000
H -5.2539250000 -0.7172440000 -0.6910500000
H -5.4070050000 -1.5362340000 0.8717970000
H -4.5679230000 -2.3379840000 -0.4693440000
H -2.7533250000 1.0514910000 1.5249410000
H -4.3547580000 0.4739050000 2.0241920000
H -4.1594250000 1.3064740000 0.4723740000
H -1.7733070000 -1.2696880000 1.8367390000
H -2.5048250000 -2.6641710000 1.0226590000
H -3.3595190000 -1.8634610000 2.3518870000
H -2.9835460000 0.1282660000 -1.5137020000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342618 (Hartree/Particle)
Thermal correction to Energy= 0.365185
Thermal correction to Enthalpy= 0.366130
Thermal correction to Gibbs (Free) Energy= 0.289507
Sum of electronic and zero-point Energies= -945.932840
Sum of electronic and thermal Energies= -945.910272
Sum of electronic and thermal Enthalpies= -945.909328
Sum of electronic and thermal (Free) Energies= -945.985950

c/u TS

C -2.1977380000 -1.0684190000 -0.5670750000
C -0.9426670000 -0.9280100000 -0.1579120000
C -3.5159610000 -0.6186980000 0.0307650000
H -2.3007790000 -1.6470570000 -1.4897210000
C 0.2653920000 -1.5591050000 -0.0677280000
C -3.3871940000 -0.1468330000 1.4846830000
C -4.4275500000 -1.8646520000 0.0069670000
C -4.1508180000 0.4711290000 -0.8522350000
C 1.4013470000 -0.6834540000 -0.0413250000
C 0.4399980000 -3.0394800000 0.0705000000
H -2.8924490000 -0.9053550000 2.0999230000
H -2.8306790000 0.7872020000 1.5769410000
H -4.3828310000 0.0290070000 1.9034960000
H -5.4144560000 -1.6109220000 0.4070430000
H -4.5645190000 -2.2404980000 -1.0123980000
H -4.0097550000 -2.6717120000 0.6172110000
H -4.2761360000 0.1174980000 -1.8807990000
H -5.1395970000 0.7375890000 -0.4644630000
H -3.5408750000 1.3770220000 -0.8817140000
C 0.9958950000 0.6717590000 0.0003980000
O 2.5874660000 -1.1465940000 -0.1355690000
H 1.1761010000 -3.3749460000 -0.6668680000
H -0.4993460000 -3.5730800000 -0.0778870000
H 0.8495150000 -3.2899540000 1.0541710000
C -0.2835930000 0.9398010000 0.4740680000
H 1.6199330000 1.4314640000 -0.4591110000
B 3.8136170000 -0.1899340000 -0.0087490000
H -0.5723510000 0.5231750000 1.4383130000
C -0.9737820000 2.2321050000 0.0966630000
F 4.9124940000 -1.0062070000 0.0074500000
F 3.6303870000 0.5284840000 1.1724120000
F 3.7660980000 0.6592730000 -1.1165600000
C -0.3748840000 3.3826410000 0.9249590000
C -0.9113240000 2.5177520000 -1.4052090000
H -2.0251140000 2.1434270000 0.3841140000
H -0.4479960000 3.1852270000 1.9986170000
H -0.9091620000 4.3130860000 0.7114050000
H 0.6814700000 3.5318460000 0.6812500000
H 0.1133320000 2.7154470000 -1.7347530000
H -1.5112650000 3.3998340000 -1.6479410000
H -1.2943770000 1.6709580000 -1.9833580000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341716 (Hartree/Particle)
Thermal correction to Energy= 0.363326
Thermal correction to Enthalpy= 0.364270
Thermal correction to Gibbs (Free) Energy= 0.290499
Sum of electronic and zero-point Energies= -945.903990
Sum of electronic and thermal Energies= -945.882380
Sum of electronic and thermal Enthalpies= -945.881436
Sum of electronic and thermal (Free) Energies= -945.955208

c/u PT

C -2.3277210000 0.1341090000 -0.4178080000
C -0.9786840000 0.1328230000 -0.2890330000
H -2.7098400000 1.0547960000 -0.8575220000
C -3.4264340000 -0.8668700000 -0.1182690000
C -0.0334400000 -0.8367140000 0.2037080000
C -4.7044950000 -0.3671740000 -0.8202600000
C -3.6958800000 -0.8922140000 1.4014560000
C -3.1112470000 -2.2719740000 -0.6602960000
C 1.2822580000 -0.4697650000 -0.1941930000
C -0.1924520000 -2.0428330000 1.0446010000
H -4.5652170000 -0.3174450000 -1.9053710000
H -5.5382140000 -1.0464340000 -0.6192870000
H -4.9896770000 0.6290020000 -0.4649980000
H -2.8248700000 -1.2121870000 1.9762840000
H -3.9833920000 0.1007990000 1.7611020000
H -4.5190550000 -1.5813400000 1.6167770000
H -3.9716250000 -2.9277220000 -0.4929620000
H -2.9200820000 -2.2348300000 -1.7370480000
H -2.2485400000 -2.7319520000 -0.1814260000
C 1.2031230000 0.7344800000 -0.8825700000
O 2.3144450000 -1.1946410000 0.1084150000
H 0.6010220000 -2.0315290000 1.8000610000
H 0.0110470000 -2.9338230000 0.4366090000
H -1.1652900000 -2.1368900000 1.5171970000
C -0.1603900000 1.2892940000 -0.8565960000
H 2.0600210000 1.2382620000 -1.3149830000
B 3.7043110000 -0.5851880000 -0.0840810000
H -0.4958310000 1.5533930000 -1.8695800000
C -0.1814460000 2.6084420000 -0.0026690000
F 3.8809250000 -0.3506480000 -1.4550020000
F 4.6013790000 -1.4879630000 0.4297800000
F 3.7035380000 0.6422380000 0.6068290000
C 0.2803380000 2.3791920000 1.4374600000
C -1.5394640000 3.3128090000 -0.0401050000
H 0.5459980000 3.2675360000 -0.4925740000
H 1.3078080000 2.0091510000 1.4896610000
H 0.2321980000 3.3191460000 1.9947600000
H -0.3699320000 1.6603750000 1.9503520000
H -1.9260650000 3.4091500000 -1.0606290000
H -2.2808510000 2.7806210000 0.5654280000
H -1.4437070000 4.3207220000 0.3742370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345099 (Hartree/Particle)
Thermal correction to Energy= 0.366227
Thermal correction to Enthalpy= 0.367171
Thermal correction to Gibbs (Free) Energy= 0.295136
Sum of electronic and zero-point Energies= -945.936767
Sum of electronic and thermal Energies= -945.915639
Sum of electronic and thermal Enthalpies= -945.914695
Sum of electronic and thermal (Free) Energies= -945.986730

cc/u RT

C -2.4956000000 -1.0959360000 -0.8864290000
C -1.3066340000 -1.3685570000 -0.4322710000
C -3.6563690000 -0.5068520000 -0.0936290000
H -2.6832250000 -1.2968360000 -1.9426420000
C -0.1131700000 -1.7273200000 0.0099430000
C -3.3813680000 -0.5324880000 1.4139360000
C -4.9052590000 -1.3505010000 -0.4002630000

C -3.8825550000 0.9395570000 -0.5668190000
C 1.0366010000 -0.8148840000 -0.1059540000
C 0.1606740000 -3.1169990000 0.5396220000
H -3.2046400000 -1.5537620000 1.7656550000
H -2.5087360000 0.0708210000 1.6829140000
H -4.2415740000 -0.1288460000 1.9570330000
H -5.7736830000 -0.9463000000 0.1302070000
H -5.1330410000 -1.3466510000 -1.4715380000
H -4.7653330000 -2.3891370000 -0.0846370000
H -4.0640980000 0.9807050000 -1.6457720000
H -4.7523300000 1.3710410000 -0.0600080000
H -3.0138270000 1.5671550000 -0.3456300000
C 0.9310970000 0.6154930000 -0.3729450000
O 2.1592330000 -1.3661120000 0.0161910000
H -0.7658920000 -3.6902250000 0.5912040000
H 0.6075530000 -3.0642180000 1.5361430000
H 0.8718590000 -3.6373310000 -0.1069200000
C -0.0750490000 1.3788350000 0.0752580000
H 1.7895930000 1.0507950000 -0.8720050000
B 3.5996850000 -0.6319350000 -0.0060570000
H -0.8718820000 0.9142380000 0.6511750000
C -0.1889200000 2.8669760000 -0.0801470000
F 4.4693010000 -1.6472960000 0.2614220000
F 3.5309630000 0.3357090000 0.9757940000
F 3.7205540000 -0.1004790000 -1.2773860000
C -0.3616370000 3.5066870000 1.3077850000
C 0.9592580000 3.5072480000 -0.8576080000
H -1.1233390000 3.0393530000 -0.6372250000
H -1.2110210000 3.0742190000 1.8471480000
H -0.5343890000 4.5823650000 1.2116190000
H 0.5385370000 3.3572920000 1.9124550000
H 1.9122750000 3.3683840000 -0.3363540000
H 0.7866120000 4.5821070000 -0.9613240000
H 1.0545270000 3.0844360000 -1.8620900000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342688 (Hartree/Particle)
Thermal correction to Energy= 0.365264
Thermal correction to Enthalpy= 0.366208
Thermal correction to Gibbs (Free) Energy= 0.289713
Sum of electronic and zero-point Energies= -945.932126
Sum of electronic and thermal Energies= -945.909550
Sum of electronic and thermal Enthalpies= -945.908606
Sum of electronic and thermal (Free) Energies= -945.985101

cc/u TS

C -2.1977380000 -1.0684190000 -0.5670750000
C -0.9426670000 -0.9280100000 -0.1579120000
C -3.5159610000 -0.6186980000 0.0307650000
H -2.3007790000 -1.6470570000 -1.4897210000
C 0.2653920000 -1.5591050000 -0.0677280000
C -3.3871940000 -0.1468330000 1.4846830000
C -4.4275500000 -1.8646520000 0.0069670000
C -4.1508180000 0.4711290000 -0.8522350000
C 1.4013470000 -0.6834540000 -0.0413250000
C 0.4399980000 -3.0394800000 0.0705000000
H -2.8924490000 -0.9053550000 2.0999230000
H -2.8306790000 0.7872020000 1.5769410000
H -4.3828310000 0.0290070000 1.9034960000
H -5.4144560000 -1.6109220000 0.4070430000
H -4.5645190000 -2.2404980000 -1.0123980000
H -4.0097550000 -2.6717120000 0.6172110000
H -4.2761360000 0.1174980000 -1.8807990000
H -5.1395970000 0.7375890000 -0.4644630000
H -3.5408750000 1.3770220000 -0.8817140000
C 0.9958950000 0.6717590000 0.0003980000
O 2.5874660000 -1.1465940000 -0.1355690000
H 1.1761010000 -3.3749460000 -0.6668680000
H -0.4993460000 -3.5730800000 -0.0778870000
H 0.8495150000 -3.2899540000 1.0541710000
C -0.2835930000 0.9398010000 0.4740680000
H 1.6199330000 1.4314640000 -0.4591110000
B 3.8136170000 -0.1899340000 -0.0087490000
H -0.5723510000 0.5231750000 1.4383130000
C -0.9737820000 2.2321050000 0.0966630000
F 4.9124940000 -1.0062070000 0.0074500000
F 3.6303870000 0.5284840000 1.1724120000
F 3.7660980000 0.6592730000 -1.1165600000
C -0.3748840000 3.3826410000 0.9249590000
C -0.9113240000 2.5177520000 -1.4052090000
H -2.0251140000 2.1434270000 0.3841140000
H -0.4479960000 3.1852270000 1.9986170000
H -0.9091620000 4.3130860000 0.7114050000
H 0.6814700000 3.5318460000 0.6812500000
H 0.1133320000 2.7154470000 -1.7347530000
H -1.5112650000 3.3998340000 -1.6479410000
H -1.2943770000 1.6709580000 -1.9833580000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342103 (Hartree/Particle)
Thermal correction to Energy= 0.363610
Thermal correction to Enthalpy= 0.364554
Thermal correction to Gibbs (Free) Energy= 0.292141
Sum of electronic and zero-point Energies= -945.898421
Sum of electronic and thermal Energies= -945.876914
Sum of electronic and thermal Enthalpies= -945.875970
Sum of electronic and thermal (Free) Energies= -945.948383

cc/u PT

C 2.2217660000 -1.0613770000 0.0981770000
C 0.9696250000 -0.5686740000 -0.0366760000
C 3.5827420000 -0.4911300000 -0.2234310000
H 2.2826360000 -2.0624730000 0.5251700000
C -0.1986350000 -1.3537200000 0.2691100000
C 3.5918040000 0.5672750000 -1.3359610000
C 4.4738060000 -1.6682850000 -0.6694190000
C 4.1551720000 0.0990270000 1.0849800000
C -1.3743720000 -0.6596270000 -0.1228950000
C -0.2910390000 -2.6983500000 0.8727780000
H 3.1249250000 0.1837990000 -2.2485660000
H 3.0867140000 1.4904530000 -1.0473780000
H 4.6274050000 0.8275440000 -1.5752250000
H 5.4901970000 -1.3153410000 -0.8683410000
H 4.5328640000 -2.4410250000 0.1043700000
H 4.0904070000 -2.1290150000 -1.5856370000
H 4.1950420000 -0.6556800000 1.8768610000
H 5.1743820000 0.4585480000 0.9090700000
H 3.5524690000 0.9373810000 1.4450410000
C -0.9783720000 0.5563790000 -0.6597330000
O -2.5598320000 -1.1626090000 0.0431590000
H 0.6579730000 -3.0998500000 1.2268330000
H -0.7322680000 -3.3845890000 0.1399790000
H -1.0122010000 -2.6577510000 1.6966790000
C 0.4841370000 0.7728720000 -0.5534540000
H -1.6735400000 1.2859860000 -1.0565670000
B -3.7649530000 -0.2525900000 -0.1880580000
H 0.9062040000 0.9949740000 -1.5412690000
C 0.8074800000 1.9797470000 0.3892520000
F -4.8773360000 -0.9798430000 0.1569740000
F -3.7557680000 0.1321410000 -1.5376130000
F -3.5791480000 0.8835370000 0.6235630000
C 0.3880410000 3.2986430000 -0.2623120000
C 0.1827930000 1.8168150000 1.7760210000
H 1.8954490000 1.9978030000 0.5092510000
H 0.8353190000 3.4179830000 -1.2550100000
H 0.7099680000 4.1424510000 0.3548660000
H -0.6995450000 3.3665380000 -0.3662120000
H -0.9106550000 1.8480630000 1.7305030000
H 0.5166130000 2.6271090000 2.4306500000
H 0.4736410000 0.8708270000 2.2450070000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345208 (Hartree/Particle)
Thermal correction to Energy= 0.366424
Thermal correction to Enthalpy= 0.367368
Thermal correction to Gibbs (Free) Energy= 0.295049
Sum of electronic and zero-point Energies= -945.946493
Sum of electronic and thermal Energies= -945.925276
Sum of electronic and thermal Enthalpies= -945.924332
Sum of electronic and thermal (Free) Energies= -945.996651

3d

cRT

C -0.0232600000 2.7905060000 -0.6815450000
C -0.8697060000 1.8227820000 -0.8828110000
C -1.7637430000 0.8602800000 -1.0314980000

C -1.5164910000 -0.4582680000 -0.4229560000
C -0.1971370000 -0.9404900000 -0.0485120000
C 0.9259550000 -0.5946230000 -0.7050740000
H -0.1874410000 -1.6679880000 0.7548600000
O -2.5485940000 -1.1446610000 -0.2072650000
B -2.5913750000 -2.6284020000 0.4214410000
F -3.9161290000 -2.9485320000 0.3830790000
F -2.0766740000 -2.4988690000 1.7015110000
F -1.7911370000 -3.3991600000 -0.3972420000
H 0.7456660000 2.9690650000 -1.4351100000
C 0.0191130000 3.6807550000 0.5536410000
H 0.8503210000 0.0839240000 -1.5508020000
C 2.2791630000 -1.0623990000 -0.4043480000
C 3.3549320000 -0.4597600000 -1.0716780000
C 2.5450480000 -2.0769620000 0.5284680000
C 3.8526810000 -2.4627180000 0.7908410000
C 4.6648250000 -0.8431140000 -0.8042750000
C 4.9154910000 -1.8453320000 0.1295750000
H 3.1592040000 0.3191510000 -1.8041250000
H 5.4869420000 -0.3644480000 -1.3262600000
H 5.9355850000 -2.1518690000 0.3378220000
H 1.7297740000 -2.5800260000 1.0378180000
H 4.0451830000 -3.2526210000 1.5093720000
C -0.1072770000 5.1432590000 0.0972150000
H -1.0707050000 5.3202240000 -0.3909720000
H -0.0317250000 5.8147490000 0.9589720000
H 0.6876240000 5.4097290000 -0.6078620000
C -1.1110770000 3.3332080000 1.5271570000
H -2.0928160000 3.4679410000 1.0615710000
H -1.0363150000 2.2964080000 1.8704380000
H -1.0607580000 3.9839920000 2.4055210000
C 1.3821650000 3.4602130000 1.2330010000
H 2.2079800000 3.7003390000 0.5543730000
H 1.4726300000 4.1042300000 2.1141040000
H 1.4955980000 2.4201460000 1.5543700000
C -3.1127410000 1.0901590000 -1.6720960000
H -3.2929930000 0.3555070000 -2.4616670000
H -3.9074970000 0.9714520000 -0.9311360000
H -3.1628150000 2.0934660000 -2.0971270000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.339303 (Hartree/Particle)
Thermal correction to Energy= 0.362376
Thermal correction to Enthalpy= 0.363320
Thermal correction to Gibbs (Free) Energy= 0.283612
Sum of electronic and zero-point Energies= -1059.004133
Sum of electronic and thermal Energies= -1058.981061
Sum of electronic and thermal Enthalpies= -1058.980116
Sum of electronic and thermal (Free) Energies= -1059.059825

cTS

C 1.6530910000 1.4112880000 -0.5676530000
C 0.3700690000 1.1442990000 -0.7246080000
H 2.3745560000 0.7811060000 -1.0895740000
C 2.2550040000 2.4115830000 0.4031490000
C -0.9578700000 1.4488340000 -0.7189990000
C 1.1913470000 3.2887880000 1.0684610000
C 3.2484660000 3.2877830000 -0.3795740000
C 3.0092390000 1.5996710000 1.4736780000
C -1.7981410000 0.3607010000 -0.2979150000
C -1.5510020000 2.7466480000 -1.1711970000
H 0.6568630000 3.8966470000 0.3320000000
H 1.6654810000 3.9693860000 1.7821160000
H 0.4580700000 2.6868330000 1.6142100000
H 4.0222330000 2.6796610000 -0.8601300000
H 3.7446790000 3.9887840000 0.2995150000
H 2.7375620000 3.8674420000 -1.1548250000
H 2.3194160000 0.9696070000 2.0436900000
H 3.5138920000 2.2764610000 2.1712460000
H 3.7658030000 0.9495040000 1.0218030000
C -1.0662530000 -0.8484220000 -0.1926090000
O -3.0283970000 0.5644570000 -0.0195790000
H -0.8009460000 3.3893730000 -1.6336890000
H -1.9753490000 3.2625170000 -0.3029020000
H -2.3749120000 2.5707740000 -1.8679040000
C 0.1453420000 -0.8981020000 -0.8841850000
H -1.3896130000 -1.6323050000 0.4836850000
B -3.9641750000 -0.6296910000 0.3387020000
C 1.2687590000 -1.7497710000 -0.4633150000
H 0.1520370000 -0.6341520000 -1.9413250000
F -3.8460080000 -1.5496300000 -0.7014420000
F -5.2167560000 -0.0883360000 0.4562010000
F -3.4761100000 -1.1659360000 1.5334500000
C 2.1882360000 -2.2116720000 -1.4118370000
C 1.4671770000 -2.0597790000 0.8882200000
C 3.2746820000 -2.9888330000 -1.0218370000
H 2.0431810000 -1.9705040000 -2.4618760000
C 2.5512200000 -2.8363210000 1.2779670000
H 0.7756660000 -1.6782370000 1.6342630000
C 3.4560690000 -3.3023110000 0.3235690000
H 3.9767420000 -3.3508480000 -1.7657630000
H 2.6961580000 -3.0737340000 2.3267600000
H 4.3037890000 -3.9067030000 0.6300670000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.338649 (Hartree/Particle)
Thermal correction to Energy= 0.360594
Thermal correction to Enthalpy= 0.361538
Thermal correction to Gibbs (Free) Energy= 0.285852
Sum of electronic and zero-point Energies= -1058.979590
Sum of electronic and thermal Energies= -1058.957645
Sum of electronic and thermal Enthalpies= -1058.956701
Sum of electronic and thermal (Free) Energies= -1059.032387

cPT

C -1.9713230000 -0.9965390000 -0.4366990000
C -0.6446940000 -0.7202490000 -0.4691280000
C 0.5373610000 -1.4330190000 -0.0785200000
C 1.6764120000 -0.5775790000 -0.1631810000
C 1.2661950000 0.6398410000 -0.6910370000
C -0.1812440000 0.6499790000 -0.9834980000
C -0.9240950000 1.8455270000 -0.4176650000
C 0.7602210000 -2.8399760000 0.3188410000
O 2.8518940000 -0.9871340000 0.1921770000
H -0.0727640000 -3.5042790000 0.1111550000
H 0.9926220000 -2.8669840000 1.3917430000
H 1.6700440000 -3.1966840000 -0.1752870000
C -1.8478650000 2.5412190000 -1.1971160000
C -0.7076540000 2.2452830000 0.9044710000
H -0.3119210000 0.6481150000 -2.0778530000
H 1.9240370000 1.4814940000 -0.8703020000
B 4.0381880000 -0.0210830000 0.0810300000
F 4.1341410000 0.3616780000 -1.2646650000
F 5.1382280000 -0.7117490000 0.5258100000
F 3.7309180000 1.0956920000 0.8728600000
H -2.5758750000 -0.1894030000 -0.8546590000
C -2.8063710000 -2.1386230000 0.1038060000
C -2.7144680000 -3.3517360000 -0.8459330000
H -3.0616720000 -3.0865070000 -1.8492830000
H -1.6977250000 -3.7375390000 -0.9390350000
H -3.3521400000 -4.1582840000 -0.4697620000
C -4.2717190000 -1.6613890000 0.1308440000
H -4.9217960000 -2.4550700000 0.5107710000
H -4.3897690000 -0.7876180000 0.7800650000
H -4.6202120000 -1.3923260000 -0.8720130000
C -2.4056660000 -2.5133090000 1.5422800000
H -2.4801200000 -1.6421940000 2.2001620000
H -3.0871560000 -3.2819360000 1.9203280000
H -1.3920480000 -2.9046290000 1.6157610000
C -1.4126870000 3.3185310000 1.4377520000
C -2.3418020000 4.0051680000 0.6559500000
C -2.5571190000 3.6163440000 -0.6627760000
H -2.0112280000 2.2478530000 -2.2313320000
H -2.8882840000 4.8451960000 1.0723700000
H -3.2707490000 4.1521650000 -1.2805380000
H 0.0215570000 1.7190760000 1.5157470000
H -1.2313720000 3.6246370000 2.4630080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341035 (Hartree/Particle)
Thermal correction to Energy= 0.362880
Thermal correction to Enthalpy= 0.363825
Thermal correction to Gibbs (Free) Energy= 0.288333
Sum of electronic and zero-point Energies= -1059.006585
Sum of electronic and thermal Energies= -1058.984740
Sum of electronic and thermal Enthalpies= -1058.983796
Sum of electronic and thermal (Free) Energies= -1059.059288

ccRT

C -1.5535780000 -2.3864900000 -0.8893180000
C -0.3850920000 -2.2139370000 -0.3414780000
C -2.9160780000 -2.2129140000 -0.2319810000
H -1.5624320000 -2.6683230000 -1.9439710000
C 0.8356620000 -2.1149690000 0.1576930000
C -2.8015410000 -2.1032660000 1.2921470000
C -3.7693110000 -3.4413160000 -0.5905250000
C -3.5668220000 -0.9443210000 -0.8110340000
C 1.5943420000 -0.8613180000 0.0040640000
C 1.5673720000 -3.2993690000 0.7470480000
H -2.3170040000 -2.9877690000 1.7174110000
H -2.2249910000 -1.2252740000 1.5980590000
H -3.7980680000 -2.0136260000 1.7358970000
H -4.7734610000 -3.3404890000 -0.1656420000
H -3.8723590000 -3.5487820000 -1.6755350000
H -3.3225240000 -4.3599390000 -0.1972140000
H -3.6679530000 -1.0138600000 -1.8990320000
H -4.5674960000 -0.8062500000 -0.3870780000
H -2.9725900000 -0.0539220000 -0.5858040000
C 0.9775690000 0.4378850000 -0.2089420000
O 2.8448670000 -0.9920980000 0.0415770000
H 1.9504990000 -3.0559800000 1.7419430000
H 2.4259020000 -3.5622280000 0.1238770000
H 0.8985400000 -4.1578990000 0.8202100000
C -0.2223410000 0.7642060000 0.3060500000
H 1.5992390000 1.1640730000 -0.7195240000
B 3.9330960000 0.1942660000 -0.0599160000
H -0.7485820000 0.0214900000 0.8984120000
C -0.8965770000 2.0574640000 0.1946320000
F 5.1216870000 -0.4561160000 0.0927130000
F 3.6204110000 1.0656740000 0.9631060000
F 3.7508250000 0.7543050000 -1.3139180000
C -0.4023380000 3.1089440000 -0.5923580000
C -2.0936890000 2.2468910000 0.8996150000
C -1.0909270000 4.3120250000 -0.6679950000
H 0.5227440000 2.9898280000 -1.1465600000
C -2.7825920000 3.4525500000 0.8244270000
H -2.4844210000 1.4396730000 1.5140380000
C -2.2817110000 4.4874420000 0.0386950000
H -0.6980500000 5.1181550000 -1.2787480000
H -3.7064690000 3.5843130000 1.3780080000
H -2.8153390000 5.4304510000 -0.0233190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.339869 (Hartree/Particle)
Thermal correction to Energy= 0.362720
Thermal correction to Enthalpy= 0.363664
Thermal correction to Gibbs (Free) Energy= 0.286042
Sum of electronic and zero-point Energies= -1059.003937
Sum of electronic and thermal Energies= -1058.981086
Sum of electronic and thermal Enthalpies= -1058.980142
Sum of electronic and thermal (Free) Energies= -1059.057764

ccTS

C -1.4209460000 -1.9060980000 -0.6231580000
C -0.2498970000 -1.4642550000 -0.1799940000
C -2.8170380000 -1.8557010000 -0.0361450000
H -1.3583660000 -2.4232950000 -1.5850920000
C 1.0866220000 -1.7502630000 -0.1335940000
C -2.8137940000 -1.5428420000 1.4642840000
C -3.4086470000 -3.2654110000 -0.2446990000
C -3.6807240000 -0.8345750000 -0.8002880000
C 1.9460130000 -0.6051840000 -0.0384240000
C 1.6574910000 -3.1332700000 -0.1136640000
H -2.1560650000 -2.2277830000 2.0095170000
H -2.4994930000 -0.5182250000 1.6625440000
H -3.8258630000 -1.6533600000 1.8662300000
H -4.4276680000 -3.3027770000 0.1532940000
H -3.4532730000 -3.5267830000 -1.3073350000
H -2.8139610000 -4.0260920000 0.2716520000
H -3.6780530000 -1.0430240000 -1.8752210000
H -4.7161480000 -0.8923240000 -0.4480500000
H -3.3247540000 0.1865820000 -0.6486860000
C 1.1922410000 0.5808900000 0.1202480000
O 3.2102870000 -0.7261570000 -0.1718990000
H 2.1401610000 -3.3371730000 0.8474590000
H 2.4426880000 -3.1974280000 -0.8736930000
H 0.8948940000 -3.8888230000 -0.3047970000
C -0.1086090000 0.4392450000 0.6135360000
H 1.5722840000 1.5308670000 -0.2399420000
B 4.1441690000 0.5087920000 0.0237230000
H -0.2523440000 -0.0904570000 1.5540050000
C -1.1220740000 1.4625790000 0.2903510000
F 5.4191310000 0.0124840000 -0.0355100000
F 3.8130660000 1.0583140000 1.2612910000
F 3.8429450000 1.3959510000 -1.0112590000
C -1.2272550000 1.9442750000 -1.0195320000
C -1.9799070000 1.9652780000 1.2743000000
C -2.1790100000 2.9048690000 -1.3417410000
H -0.5734290000 1.5424800000 -1.7887710000
C -2.9292970000 2.9299290000 0.9539680000
H -1.8927640000 1.6115390000 2.2981010000
C -3.0340610000 3.3957740000 -0.3557290000
H -2.2583440000 3.2667410000 -2.3615150000
H -3.5856420000 3.3195560000 1.7251170000
H -3.7799190000 4.1428800000 -0.6072570000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.338564 (Hartree/Particle)
Thermal correction to Energy= 0.360418
Thermal correction to Enthalpy= 0.361362
Thermal correction to Gibbs (Free) Energy= 0.287364
Sum of electronic and zero-point Energies= -1058.972919
Sum of electronic and thermal Energies= -1058.951065
Sum of electronic and thermal Enthalpies= -1058.950121
Sum of electronic and thermal (Free) Energies= -1059.024119

ccPT

C -1.6182460000 -1.8569850000 -0.2399720000
C -0.4859900000 -1.1582610000 0.0087230000
C 0.7998610000 -1.5745890000 -0.4787330000
C 1.8186010000 -0.6872840000 -0.0311450000
C 1.2063180000 0.2975420000 0.7299100000
C -0.2695080000 0.1212960000 0.8036570000
C 1.1507140000 -2.7516960000 -1.2982950000
O 3.0640030000 -0.8707690000 -0.3403770000
H 0.2952530000 -3.3147550000 -1.6699830000
H 1.7938860000 -3.4106530000 -0.7023390000
H 1.7782030000 -2.4207470000 -2.1330210000
C -0.9732520000 1.3587500000 0.2542580000
H 1.7280570000 1.1293560000 1.1875530000
C -0.8990650000 1.6612840000 -1.1074320000
C -1.6575420000 2.2242880000 1.1061630000
H -0.5711140000 -0.0238610000 1.8486890000
B 4.1038610000 0.1324950000 0.1680860000
F 5.3193290000 -0.3006830000 -0.3030480000
F 4.0259360000 0.1344070000 1.5693880000
F 3.7384460000 1.3927590000 -0.3283250000
C -3.0474620000 -1.6524850000 0.2003280000
H -1.4943900000 -2.7171950000 -0.8975090000
C -3.1822720000 -1.0425850000 1.6033590000
H -2.6045410000 -1.6091530000 2.3408280000
H -2.8660320000 0.0004590000 1.6258670000
H -4.2330630000 -1.0685990000 1.9080930000
C -3.7335980000 -3.0318580000 0.1918260000
H -4.7872830000 -2.9288140000 0.4674770000
H -3.6908980000 -3.4931030000 -0.8007880000
H -3.2626940000 -3.7135910000 0.9080180000
C -3.7352950000 -0.7380150000 -0.8393970000
H -3.6587500000 -1.1549960000 -1.8487690000
H -4.7979020000 -0.6479320000 -0.5905500000
H -3.2956870000 0.2624780000 -0.8433470000
C -1.5293410000 2.7925760000 -1.6130450000
C -2.2317710000 3.6428220000 -0.7594090000
C -2.2889640000 3.3601860000 0.6020880000
H -0.3459430000 1.0084140000 -1.7774980000
H -1.4657780000 3.0153410000 -2.6731610000
H -2.7222790000 4.5267260000 -1.1538200000
H -1.7008610000 2.0127650000 2.1716330000
H -2.8220380000 4.0232720000 1.2757770000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.341275 (Hartree/Particle)
Thermal correction to Energy= 0.363074
Thermal correction to Enthalpy= 0.364018
Thermal correction to Gibbs (Free) Energy= 0.289187

Sum of electronic and zero-point Energies= -1059.015469
Sum of electronic and thermal Energies= -1058.993671
Sum of electronic and thermal Enthalpies= -1058.992727
Sum of electronic and thermal (Free) Energies= -1059.067558

4a

cRT

C -2.5602800000 -0.3311520000 0.7641860000
C -1.3554250000 0.1474560000 0.6576570000
C -0.1511410000 0.6578170000 0.4563400000
C 0.9661050000 -0.2968490000 0.3800810000
C 0.9610960000 -1.5731370000 1.1096920000
C 0.3761000000 -1.7237580000 2.3009210000
H 1.5541600000 -2.3674880000 0.6695610000
C 0.0701030000 2.1608830000 0.1884660000
O 1.9400000000 0.0178160000 -0.3421810000
B 3.3191710000 -0.8125800000 -0.5550610000
F 4.0423790000 0.0131050000 -1.3636210000
F 2.9370300000 -2.0005920000 -1.1465690000
F 3.8368950000 -0.9764520000 0.7104550000
C -3.4269400000 -0.7884370000 -0.4024550000
H -2.9938950000 -0.4248360000 1.7606170000
H -0.1564520000 -0.9154000000 2.7912760000
H 0.4534010000 -2.6653250000 2.8343460000
C 1.2495780000 2.6690650000 1.0370270000
H 2.1904030000 2.1887380000 0.7607620000
H 1.3689180000 3.7465800000 0.8858140000
H 1.0676650000 2.4979040000 2.1037410000
C 0.3478070000 2.3969350000 -1.3085620000
H 0.4463320000 3.4721060000 -1.4928240000
H 1.2669920000 1.9079800000 -1.6331410000
H -0.4809370000 2.0236790000 -1.9193890000
C -1.1928320000 2.9388850000 0.5830700000
H -2.0554670000 2.6440670000 -0.0226220000
H -1.4484140000 2.7849830000 1.6368880000
H -1.0217810000 4.0083260000 0.4278540000
C -2.7133130000 -0.5789770000 -1.7414060000
H -2.4811890000 0.4783530000 -1.9061770000
H -1.7767610000 -1.1436990000 -1.7889600000
H -3.3531400000 -0.9162800000 -2.5625420000
C -4.7298320000 0.0278930000 -0.3688670000
H -5.3994710000 -0.2979750000 -1.1717340000
H -5.2561700000 -0.1024570000 0.5828380000
H -4.5279990000 1.0952130000 -0.5040380000
C -3.7398490000 -2.2808890000 -0.2020760000
H -4.2446720000 -2.4558530000 0.7541960000
H -4.3980820000 -2.6388870000 -1.0006970000
H -2.8230950000 -2.8783250000 -0.2198460000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342221 (Hartree/Particle)
Thermal correction to Energy= 0.364533
Thermal correction to Enthalpy= 0.365477
Thermal correction to Gibbs (Free) Energy= 0.290216
Sum of electronic and zero-point Energies= -945.924205
Sum of electronic and thermal Energies= -945.901893
Sum of electronic and thermal Enthalpies= -945.900949
Sum of electronic and thermal (Free) Energies= -945.976211

cTS

C 2.4084600000 -0.7205210000 -0.7630660000
C 1.1491920000 -0.3159910000 -0.7217290000
C 3.4234240000 -0.7006870000 0.3690460000
H 2.7521670000 -1.2113740000 -1.6735790000
C 0.0934490000 0.4519580000 -0.3324470000
C 4.6236010000 0.1541940000 -0.0766350000
C 3.8843470000 -2.1564640000 0.5797040000
C 2.8383820000 -0.1634950000 1.6773550000
C -1.1312490000 -0.3119740000 -0.2067520000
C 0.1168900000 1.9740720000 -0.1901390000
H 5.0590440000 -0.2270200000 -1.0064050000
H 4.3328440000 1.1959550000 -0.2394510000
H 5.4020320000 0.1327530000 0.6931280000
H 4.6557650000 -2.1962650000 1.3555460000
H 3.0502620000 -2.7906400000 0.8960210000
H 4.3088440000 -2.5775440000 -0.3380570000
H 1.9537050000 -0.7310380000 1.9822690000
H 3.5840450000 -0.2426940000 2.4741370000
H 2.5544180000 0.8880170000 1.5947630000
C -0.9924120000 -1.6109240000 -0.7693530000
O -2.1496360000 0.1502450000 0.4046360000
C -0.9845550000 2.5743420000 -1.0883360000
C -0.1570800000 2.3432720000 1.2823910000
C 1.4670680000 2.5564780000 -0.6262050000
C 0.0538550000 -1.7702540000 -1.6573680000
H -1.5752970000 -2.4399740000 -0.3833480000
B -3.5181660000 -0.6077570000 0.3858580000
H -1.9785720000 2.2315480000 -0.7964340000
H -0.9628160000 3.6655200000 -1.0049290000
H -0.8171430000 2.3137780000 -2.1390130000
H -1.1310350000 1.9747120000 1.6086800000
H 0.6110430000 1.9342980000 1.9454120000
H -0.1473870000 3.4334630000 1.3834420000
H 1.6998290000 2.3015290000 -1.6650120000
H 1.4298810000 3.6468250000 -0.5453520000
H 2.2896570000 2.2056650000 0.0016430000
H 0.2044860000 -1.0958040000 -2.4961090000
H 0.4829210000 -2.7607240000 -1.8015390000
F -4.4050740000 0.2555910000 0.9726980000
F -3.3250660000 -1.7857610000 1.1047010000
F -3.7955270000 -0.8740760000 -0.9519520000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342271 (Hartree/Particle)
Thermal correction to Energy= 0.363268
Thermal correction to Enthalpy= 0.364212
Thermal correction to Gibbs (Free) Energy= 0.293434
Sum of electronic and zero-point Energies= -945.895696
Sum of electronic and thermal Energies= -945.874699
Sum of electronic and thermal Enthalpies= -945.873755
Sum of electronic and thermal (Free) Energies= -945.944532

cPT

C 2.3681060000 -0.9800240000 -0.6000690000
C 1.0426710000 -0.7321560000 -0.7246040000
C 3.4529020000 -0.5526130000 0.3653550000
H 2.7016890000 -1.8123950000 -1.2237180000
C 0.0975840000 0.2518390000 -0.2580560000
C 4.5124660000 0.2911950000 -0.3718540000
C 4.1254600000 -1.8712620000 0.8186610000
C 2.9329640000 0.1500590000 1.6242760000
C -1.1738190000 -0.3945800000 -0.0814340000
C 0.1984680000 1.7619090000 -0.2392710000
H 4.9123480000 -0.2516080000 -1.2346310000
H 4.1098610000 1.2406730000 -0.7281980000
H 5.3454840000 0.5042260000 0.3058460000
H 4.9368310000 -1.6497520000 1.5187440000
H 3.4104040000 -2.5267300000 1.3262700000
H 4.5525450000 -2.4170590000 -0.0291640000
H 2.1524850000 -0.4455970000 2.1085840000
H 3.7531880000 0.2740210000 2.3378190000
H 2.5274170000 1.1393160000 1.4259530000
C -1.1263540000 -1.6183650000 -0.7370930000
O -2.1747730000 0.1656350000 0.5214010000
C -0.9132760000 2.2695580000 -1.2045510000
C -0.0897580000 2.3123550000 1.1760200000
C 1.5276040000 2.3054440000 -0.7777070000
C 0.1932080000 -1.8593680000 -1.3305840000
H -1.9705610000 -2.2926470000 -0.8126190000
B -3.5771080000 -0.4366980000 0.3860350000
H -1.9090650000 1.9642500000 -0.8846660000
H -0.8745620000 3.3627870000 -1.2210670000
H -0.7383180000 1.9089530000 -2.2233230000
H -1.0812700000 2.0113570000 1.5167260000
H 0.6498050000 1.9692880000 1.9038220000
H -0.0468220000 3.4053450000 1.1368610000
H 1.7913030000 1.8484190000 -1.7366940000
H 1.4265020000 3.3826080000 -0.9374340000
H 2.3575940000 2.1638560000 -0.0887000000
H 0.1677180000 -1.7178650000 -2.4203890000
H 0.5667740000 -2.8717330000 -1.1399530000
F -4.4204870000 0.4252100000 1.0454660000
F -3.5486470000 -1.7184290000 0.9485020000
F -3.8471970000 -0.5218090000 -0.9890790000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.344771 (Hartree/Particle)
Thermal correction to Energy= 0.365781
Thermal correction to Enthalpy= 0.366725
Thermal correction to Gibbs (Free) Energy= 0.295547
Sum of electronic and zero-point Energies= -945.919611
Sum of electronic and thermal Energies= -945.898601
Sum of electronic and thermal Enthalpies= -945.897657
Sum of electronic and thermal (Free) Energies= -945.968835

ccRT

C 2.4147030000 -0.2046140000 -0.9571580000
C 1.2657990000 0.1783460000 -0.4809100000
C 3.6458770000 -0.6349500000 -0.1698990000
H 2.4998720000 -0.2438830000 -2.0447610000
C 0.0831690000 0.6262090000 -0.0876300000
C 3.5778300000 -0.1681630000 1.2879430000
C 4.8771410000 -0.0104790000 -0.8466140000
C 3.7404830000 -2.1691480000 -0.2333540000
C -1.0068240000 -0.3607620000 -0.0294140000
C -0.1958770000 2.1268520000 0.1408870000
H 3.5235440000 0.9228720000 1.3486030000
H 2.7085270000 -0.5794560000 1.8088930000
H 4.4722510000 -0.4955160000 1.8271240000
H 5.7899290000 -0.3115850000 -0.3223550000
H 4.9644810000 -0.3359830000 -1.8887090000
H 4.8211170000 1.0827650000 -0.8331890000
H 3.7858340000 -2.5206650000 -1.2692410000
H 4.6433980000 -2.5138970000 0.2820280000
H 2.8725450000 -2.6354260000 0.2432210000
C -0.7744440000 -1.7855130000 0.2524060000
O -2.1663490000 0.0574470000 -0.2516980000
C -0.9440160000 2.7163510000 -1.0696920000
C -1.0256260000 2.3102480000 1.4248590000
C 1.1350290000 2.8728330000 0.3115340000
C 0.1509400000 -2.2086650000 1.1160940000
H -1.4801430000 -2.4736460000 -0.2006660000
B -3.5493650000 -0.7945730000 -0.1990660000
H -1.9188210000 2.2474650000 -1.2103430000
H -1.0988780000 3.7892900000 -0.9134340000
H -0.3573190000 2.5886470000 -1.9855530000
H -2.0185650000 1.8650370000 1.3406760000
H -0.5146860000 1.8694120000 2.2880860000
H -1.1548300000 3.3790770000 1.6224420000
H 0.9340960000 3.9330650000 0.4921270000
H 1.7018750000 2.4861690000 1.1651170000
H 1.7629780000 2.7959680000 -0.5810750000
H 0.8073850000 -1.5213240000 1.6380470000
H 0.2410430000 -3.2632070000 1.3546840000
F -4.4952240000 0.1600990000 -0.4276950000
F -3.5812140000 -1.3450740000 1.0627650000
F -3.4316870000 -1.7353770000 -1.2025280000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342238 (Hartree/Particle)
Thermal correction to Energy= 0.364487
Thermal correction to Enthalpy= 0.365432
Thermal correction to Gibbs (Free) Energy= 0.291028
Sum of electronic and zero-point Energies= -945.922891
Sum of electronic and thermal Energies= -945.900642
Sum of electronic and thermal Enthalpies= -945.899698
Sum of electronic and thermal (Free) Energies= -945.974102

ccTS

C 2.3938250000 -0.0469580000 -0.6307970000
C 1.1563770000 -0.0173450000 -0.1662070000
C 3.6686990000 -0.6626240000 -0.0885800000
H 2.5167610000 0.4634610000 -1.5894490000
C -0.0483520000 0.6206700000 -0.0751110000
C 3.5781970000 -1.0647130000 1.3889600000
C 4.7610000000 0.4153400000 -0.2406550000
C 4.0364460000 -1.8859230000 -0.9478730000
C -1.1730440000 -0.2841450000 -0.0632540000
C -0.2095710000 2.1347910000 0.0584260000
H 3.1826140000 -0.2475140000 2.0013000000
H 2.9573660000 -1.9499860000 1.5417340000
H 4.5774300000 -1.3095370000 1.7617470000
H 5.7264620000 0.0205270000 0.0911930000
H 4.8676150000 0.7309830000 -1.2838180000
H 4.5275110000 1.2990860000 0.3617740000
H 4.1365810000 -1.6141170000 -2.0035750000
H 4.9906310000 -2.3070340000 -0.6141720000
H 3.2724850000 -2.6657350000 -0.8707200000
C -0.7456910000 -1.6375200000 0.0720810000
O -2.3686430000 0.1194120000 -0.2401510000
C -0.8991460000 2.6521010000 -1.2224260000
C -1.0769290000 2.4532680000 1.2915220000
C 1.1467930000 2.8357660000 0.2138300000
C 0.4984250000 -1.8262630000 0.6343920000
H -1.3169890000 -2.4371210000 -0.3871520000
B -3.5817250000 -0.8571550000 -0.0773110000
H -1.8863460000 2.2056010000 -1.3529410000
H -1.0171970000 3.7382760000 -1.1507120000
H -0.2936500000 2.4343260000 -2.1086350000
H -2.0718010000 2.0119280000 1.2123000000
H -0.6014700000 2.0862900000 2.2075480000
H -1.1918030000 3.5380230000 1.3834000000
H 0.9804080000 3.9096720000 0.3399910000
H 1.6919990000 2.4723630000 1.0911410000
H 1.7836450000 2.6979840000 -0.6650320000
H 0.7837320000 -1.3235860000 1.5522760000
H 1.0387610000 -2.7499770000 0.4376350000
F -4.6889980000 -0.0533720000 -0.1295220000
F -3.4048420000 -1.4918030000 1.1493600000
F -3.4971760000 -1.7650590000 -1.1302740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342041 (Hartree/Particle)
Thermal correction to Energy= 0.363123
Thermal correction to Enthalpy= 0.364067
Thermal correction to Gibbs (Free) Energy= 0.292320
Sum of electronic and zero-point Energies= -945.892119
Sum of electronic and thermal Energies= -945.871037
Sum of electronic and thermal Enthalpies= -945.870093
Sum of electronic and thermal (Free) Energies= -945.941840

ccPT

C 2.4205750000 0.1476520000 0.0207640000
C 1.1359440000 -0.2688000000 -0.0836270000
C 3.7211730000 -0.6198230000 0.0315330000
H 2.5767770000 1.2058970000 0.1799670000
C -0.0490370000 0.5637090000 -0.0277990000
C 3.7070840000 -1.9790920000 -0.6811350000
C 4.1043050000 -0.8141030000 1.5167740000
C 4.7770020000 0.2768670000 -0.6473450000
C -1.2060800000 -0.2912250000 -0.0050300000
C -0.2180640000 2.0682010000 -0.0245430000
H 3.1092790000 -2.7254590000 -0.1550990000
H 3.3364490000 -1.8893590000 -1.7069500000
H 4.7297380000 -2.3650620000 -0.7305960000
H 5.0890410000 -1.2884680000 1.5818390000
H 4.1537270000 0.1423160000 2.0469150000
H 3.3792020000 -1.4527230000 2.0300810000
H 4.8543570000 1.2502500000 -0.1515640000
H 5.7602410000 -0.2010290000 -0.6026270000
H 4.5314620000 0.4476110000 -1.7005910000
C -0.7819410000 -1.6065810000 -0.0975000000
O -2.4243660000 0.1525210000 0.0798640000
C -1.0799630000 2.4297270000 -1.2643740000
C -0.9714280000 2.4575360000 1.2735800000
C 1.0606170000 2.9150000000 -0.0962910000
C 0.6812520000 -1.7064010000 -0.1840180000
H -1.4550830000 -2.4543840000 -0.1065770000
B -3.6007310000 -0.8214090000 0.0436290000
H -2.0422680000 1.9188990000 -1.2552410000
H -1.2593990000 3.5092060000 -1.2548390000
H -0.5483470000 2.1818910000 -2.1888990000
H -1.9397470000 1.9628960000 1.3438280000
H -0.3744000000 2.2067090000 2.1565360000
H -1.1309630000 3.5402870000 1.2679750000
H 0.7627590000 3.9651180000 -0.1658420000
H 1.6768630000 2.8239770000 0.8035370000
H 1.6641260000 2.6929290000 -0.9818580000
H 1.0848840000 -2.3338960000 0.6203510000
H 0.9896500000 -2.1689120000 -1.1294180000
F -4.7326400000 -0.0450010000 0.1351970000
F -3.4534300000 -1.7037600000 1.1241510000
F -3.5204180000 -1.5309970000 -1.1642280000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.345388 (Hartree/Particle)
Thermal correction to Energy= 0.366260
Thermal correction to Enthalpy= 0.367204
Thermal correction to Gibbs (Free) Energy= 0.294005
Sum of electronic and zero-point Energies= -945.936102
Sum of electronic and thermal Energies= -945.915231
Sum of electronic and thermal Enthalpies= -945.914287
Sum of electronic and thermal (Free) Energies= -945.987486

4b

cRT

C -2.5711590000 -0.3965540000 0.5306050000
C -1.3770730000 0.1194920000 0.5718820000
C -0.1830480000 0.6857570000 0.5327540000
C 0.9492700000 -0.1825550000 0.1587550000
C 0.9921570000 -1.6026480000 0.4911010000
C 0.4007940000 -2.1193580000 1.5788310000
H 1.6244420000 -2.2167590000 -0.1419910000
C 0.0174490000 2.2003300000 0.7433920000
O 1.8869120000 0.3574650000 -0.4785390000
B 3.2752870000 -0.3242150000 -0.9347100000
F 3.9538040000 0.7168290000 -1.4998240000
F 2.9240530000 -1.3224310000 -1.8246120000
F 3.8410180000 -0.8102550000 0.2259220000
C -3.4409000000 -0.4941860000 -0.7161250000
H -0.1578400000 -1.4651140000 2.2449430000
C 0.4906050000 -3.5534560000 1.9765750000
H 1.0674340000 -4.1408900000 1.2595400000
H -0.5140890000 -3.9829910000 2.0623710000
H 0.9582590000 -3.6434320000 2.9630620000
C 0.2634070000 2.8959580000 -0.6092140000
H 0.3501440000 3.9762330000 -0.4500910000
H 1.1791330000 2.5435150000 -1.0852510000
H -0.5746720000 2.7204740000 -1.2919290000
C 1.2091780000 2.4360700000 1.6886260000
H 2.1483590000 2.0797080000 1.2604220000
H 1.3160360000 3.5085670000 1.8798920000
H 1.0507780000 1.9375360000 2.6513540000
C -1.2448370000 2.7965110000 1.3815150000
H -2.1169490000 2.6893550000 0.7289270000
H -1.4761420000 2.3187490000 2.3395820000
H -1.0888870000 3.8641570000 1.5632540000
C -2.7507390000 0.1411960000 -1.9268860000
C -4.7653630000 0.2315450000 -0.4264570000
C -3.7103680000 -1.9839110000 -0.9881550000
H -2.5493230000 1.2037750000 -1.7558500000
H -3.3918040000 0.0564180000 -2.8097340000
H -1.7996890000 -0.3523870000 -2.1507780000
H -2.7776110000 -2.5178730000 -1.1949150000
H -4.3694710000 -2.0967400000 -1.8554350000
H -4.1971560000 -2.4621870000 -0.1311230000
H -4.5944780000 1.2936750000 -0.2242980000
H -5.2755000000 -0.2031950000 0.4399730000
H -5.4364650000 0.1509430000 -1.2880880000
H -2.9923570000 -0.8026000000 1.4514360000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.370102 (Hartree/Particle)
Thermal correction to Energy= 0.394155
Thermal correction to Enthalpy= 0.395099
Thermal correction to Gibbs (Free) Energy= 0.315364
Sum of electronic and zero-point Energies= -985.211440
Sum of electronic and thermal Energies= -985.187387
Sum of electronic and thermal Enthalpies= -985.186443
Sum of electronic and thermal (Free) Energies= -985.266178

cTS

C 2.3903220000 -0.5997380000 -0.5232210000
C 1.1167200000 -0.2458980000 -0.5848280000
H 2.7700650000 -1.2545210000 -1.3077340000
C 3.3797500000 -0.3382130000 0.6006820000
C 0.0475940000 0.5688830000 -0.3418770000
C 2.7594210000 0.4271920000 1.7715120000
C 4.5761520000 0.4376610000 0.0211650000
C 3.8578100000 -1.7178470000 1.0952730000
C -1.1581520000 -0.1870220000 -0.0846850000
C 0.0375490000 2.0888880000 -0.4866950000
H 1.8756280000 -0.0870610000 2.1616570000
H 3.4882950000 0.5138390000 2.5830130000
H 2.4633720000 1.4385530000 1.4849210000
H 5.3383230000 0.5801450000 0.7943540000
H 5.0372780000 -0.1068640000 -0.8097500000
H 4.2727200000 1.4226050000 -0.3450610000
H 4.3073570000 -2.2996900000 0.2832130000
H 4.6129340000 -1.5949890000 1.8784360000
H 3.0261050000 -2.2948130000 1.5120300000
C -0.9879230000 -1.5506940000 -0.4200200000
O -2.1936990000 0.3519850000 0.4377830000
C -0.2686040000 2.7212780000 0.8870930000
C -1.0659560000 2.4806000000 -1.4919100000
C 1.3790740000 2.6139750000 -1.0125260000
C 0.0774170000 -1.8454850000 -1.2675060000
H -1.5739050000 -2.3188140000 0.0746330000
B -3.5342840000 -0.4310270000 0.5460280000
H -1.2380610000 2.3929910000 1.2658410000
H 0.4986260000 2.4662210000 1.6239400000
H -0.2878400000 3.8108210000 0.7801550000
H -1.0722740000 3.5682440000 -1.6151260000
H -0.8777550000 2.0318740000 -2.4733230000
H -2.0548320000 2.1714480000 -1.1491960000
H 1.6313660000 2.1749520000 -1.9830630000
H 1.3149320000 3.6989050000 -1.1379270000
H 2.2017510000 2.4081350000 -0.3237710000
C 0.6914940000 -3.2165560000 -1.2860460000
H 0.1625890000 -1.2991080000 -2.2055830000
F -3.8056880000 -0.9262410000 -0.7288520000
F -4.4509590000 0.4902080000 0.9830620000
F -3.3186080000 -1.4727800000 1.4494020000
H 0.8362550000 -3.6074970000 -0.2766930000
H 1.6483620000 -3.2243090000 -1.8125310000
H 0.0210210000 -3.8946490000 -1.8258080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.370200 (Hartree/Particle)
Thermal correction to Energy= 0.392936
Thermal correction to Enthalpy= 0.393880
Thermal correction to Gibbs (Free) Energy= 0.319224
Sum of electronic and zero-point Energies= -985.182421
Sum of electronic and thermal Energies= -985.159684
Sum of electronic and thermal Enthalpies= -985.158740
Sum of electronic and thermal (Free) Energies= -985.233397

cPT

C -2.3596690000 0.7900770000 -0.4243420000
C -1.0336720000 0.6107970000 -0.6074450000
H -2.7519780000 1.6680420000 -0.9376260000
C -3.3900400000 0.2217670000 0.5289630000
C -0.0653590000 -0.3992510000 -0.2535350000
C -2.8114770000 -0.6439570000 1.6527830000
C -4.4831250000 -0.5236210000 -0.2618270000
C -4.0374250000 1.4630690000 1.1902000000
C 1.1835450000 0.2495100000 0.0237440000
C -0.1237970000 -1.8977110000 -0.4570390000
H -1.9852480000 -0.1321460000 2.1570180000
H -3.5884190000 -0.8409350000 2.3976620000
H -2.4508540000 -1.6092560000 1.3048360000
H -5.2801930000 -0.8375160000 0.4199020000
H -4.9283120000 0.1269720000 -1.0218470000
H -4.0937600000 -1.4111350000 -0.7643900000
H -4.4997250000 2.1205420000 0.4464460000
H -4.8173600000 1.1451700000 1.8890100000
H -3.2970720000 2.0437480000 1.7500460000
C 1.1148060000 1.5263830000 -0.5132400000
O 2.1909960000 -0.3512820000 0.5757970000
C 0.1917630000 -2.6495230000 0.8557420000
C 0.9997760000 -2.2152720000 -1.4887390000
C -1.4389980000 -2.3931540000 -1.0709250000
C -0.1976120000 1.8136700000 -1.1204930000
H 1.9481670000 2.2196570000 -0.5193870000
B 3.5830430000 0.2824970000 0.4996880000
H 1.1739930000 -2.3700600000 1.2386540000
H -0.5547310000 -2.4504070000 1.6281940000
H 0.1866850000 -3.7239810000 0.6471740000
H 0.9953320000 -3.2934780000 -1.6741560000

H 0.8108530000 -1.7071800000 -2.4399410000
H 1.9865830000 -1.9311410000 -1.1234820000
H -1.7116800000 -1.8164920000 -1.9602130000
H -1.3127220000 -3.4364280000 -1.3738590000
H -2.2739010000 -2.3629360000 -0.3737450000
C -0.6985100000 3.2315190000 -0.8487670000
H -0.1121180000 1.6642330000 -2.2083660000
F 3.8546750000 0.4912870000 -0.8624250000
F 4.4395290000 -0.6197340000 1.0840420000
F 3.5340990000 1.5102760000 1.1711090000
H -0.8892210000 3.3813660000 0.2177840000
H -1.6131220000 3.4562950000 -1.4028740000
H 0.0596660000 3.9525660000 -1.1666870000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.373256 (Hartree/Particle)
Thermal correction to Energy= 0.395685
Thermal correction to Enthalpy= 0.396629
Thermal correction to Gibbs (Free) Energy= 0.322621
Sum of electronic and zero-point Energies= -985.199712
Sum of electronic and thermal Energies= -985.177283
Sum of electronic and thermal Enthalpies= -985.176339
Sum of electronic and thermal (Free) Energies= -985.250347

ccRT

C 2.3757750000 0.1804270000 -1.0686720000
C 1.2336960000 0.4714270000 -0.5144430000
C 0.0514550000 0.8318640000 -0.0445610000
C -1.0209360000 -0.1793700000 -0.1185090000
C -0.7780610000 -1.6052030000 0.0768170000
C 0.1633270000 -2.0697300000 0.9109480000
H -1.4867860000 -2.2769790000 -0.3968390000
C -0.2586580000 2.2752460000 0.4032130000
O -2.1732080000 0.2462010000 -0.3775740000
B -3.5395950000 -0.6119880000 -0.4260020000
F -4.4897900000 0.3422670000 -0.6477850000
F -3.6247440000 -1.2252900000 0.8071310000
F -3.3798310000 -1.5079980000 -1.4659870000
C 3.6316830000 -0.3423610000 -0.3848320000
H 0.7990280000 -1.3601670000 1.4351350000
C 0.3666700000 -3.5124470000 1.2284860000
H -0.2822940000 -4.1565750000 0.6319720000
H 0.1607270000 -3.6937820000 2.2892340000
H 1.4101410000 -3.7993990000 1.0566280000
C -0.9878890000 3.0332340000 -0.7218360000
H -1.1711790000 4.0659050000 -0.4057860000
H -0.3748450000 3.0594410000 -1.6289030000
H -1.9469930000 2.5720210000 -0.9617540000
C 1.0559050000 3.0010860000 0.7224300000
H 1.7076060000 3.0662910000 -0.1539570000
H 0.8358200000 4.0197720000 1.0558400000
H 1.6056850000 2.4942810000 1.5227880000
C -1.1240430000 2.2466130000 1.6760390000
H -2.1062800000 1.8053150000 1.4960350000
H -0.6280890000 1.6844130000 2.4753050000
H -1.2785120000 3.2697590000 2.0330210000
C 3.5960710000 -0.1043360000 1.1282670000
C 4.8387780000 0.3951760000 -0.9871180000
C 3.7422090000 -1.8480050000 -0.6817840000
H 3.5121730000 0.9624080000 1.3564990000
H 4.5154140000 -0.4807780000 1.5878490000
H 2.7551190000 -0.6191740000 1.6014360000
H 2.8863620000 -2.3894490000 -0.2671350000
H 4.6579610000 -2.2563030000 -0.2405170000
H 3.7701690000 -2.0386380000 -1.7595150000
H 4.7732050000 1.4722150000 -0.8022970000
H 4.9001320000 0.2372060000 -2.0691740000
H 5.7685690000 0.0283480000 -0.5401190000
H 2.4338930000 0.3016470000 -2.1520400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.370599 (Hartree/Particle)
Thermal correction to Energy= 0.394490
Thermal correction to Enthalpy= 0.395435
Thermal correction to Gibbs (Free) Energy= 0.316919
Sum of electronic and zero-point Energies= -985.209893
Sum of electronic and thermal Energies= -985.186001
Sum of electronic and thermal Enthalpies= -985.185057
Sum of electronic and thermal (Free) Energies= -985.263572

ccTS

C 2.3230460000 0.1239030000 -0.6615830000
C 1.0713650000 0.0463800000 -0.2241420000
H 2.4324820000 0.6698870000 -1.6018930000
C 3.6384550000 -0.3357120000 -0.0653390000
C -0.1211090000 0.7083810000 -0.1155060000
C 3.5226030000 -0.7514430000 1.4062140000
C 4.2433170000 -1.4679200000 -0.9143320000
C 4.5699890000 0.8939660000 -0.1452140000
C -0.2608350000 2.2209930000 0.0532750000
C -1.2602180000 -0.1761320000 -0.0948550000
H 2.9631280000 -1.6783040000 1.5394170000
H 4.5216150000 -0.9173110000 1.8209250000
H 3.0386740000 0.0324860000 1.9981230000
H 3.6200990000 -2.3646030000 -0.8941450000
H 5.2353770000 -1.7324560000 -0.5335360000
H 4.3550370000 -1.1575760000 -1.9582650000
H 5.5576250000 0.6383250000 0.2517890000
H 4.1721540000 1.7297960000 0.4387850000
H 4.6997170000 1.2300940000 -1.1793160000
C -0.9730370000 2.7708870000 -1.2018250000
C 1.1006420000 2.9143550000 0.1968350000
C -1.0991370000 2.5216590000 1.3114500000
C -0.8552020000 -1.5278220000 -0.0115350000
O -2.4572110000 0.2542750000 -0.2239140000
H -0.3876850000 2.5674280000 -2.1049220000
H -1.0811490000 3.8561750000 -1.1048890000
H -1.9660590000 2.3342850000 -1.3206660000
H 1.7192310000 2.7998060000 -0.6980300000
H 0.9391550000 3.9850750000 0.3533060000
H 1.6624860000 2.5289680000 1.0541060000
H -1.1999090000 3.6054190000 1.4288850000
H -2.0997210000 2.0920210000 1.2444380000
H -0.6077480000 2.1298800000 2.2086940000
C 0.4316660000 -1.7787150000 0.4549160000
H -1.4787530000 -2.3077150000 -0.4376530000
B -3.6759780000 -0.6990300000 -0.0481560000
C 1.0976900000 -3.0728670000 0.0667940000
H 0.7309340000 -1.3476760000 1.4080360000
F -3.6360140000 -1.5996220000 -1.1132840000
F -4.7744240000 0.1210480000 -0.0665540000
F -3.4905290000 -1.3568580000 1.1669870000
H 1.2291730000 -3.1357280000 -1.0161810000
H 2.0644210000 -3.2152350000 0.5488100000
H 0.4505750000 -3.9026850000 0.3710020000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.370549 (Hartree/Particle)
Thermal correction to Energy= 0.393097
Thermal correction to Enthalpy= 0.394041
Thermal correction to Gibbs (Free) Energy= 0.319859
Sum of electronic and zero-point Energies= -985.174855
Sum of electronic and thermal Energies= -985.152308
Sum of electronic and thermal Enthalpies= -985.151364
Sum of electronic and thermal (Free) Energies= -985.225545

ccPT

C -2.3400580000 0.2962360000 -0.1478290000
C -1.0788720000 -0.1671350000 0.0208450000
H -2.4481870000 1.3716350000 -0.1808690000
C -3.6775440000 -0.3930790000 -0.3004490000
C 0.1147080000 0.6606330000 0.0319830000
C -3.6453490000 -1.8313350000 -0.8347340000
C -4.3576300000 -0.3562950000 1.0872750000
C -4.5066700000 0.4629080000 -1.2810460000
C 0.3002290000 2.1543730000 0.1938670000
C 1.2593620000 -0.1954820000 -0.1194750000
H -3.1928870000 -2.5359920000 -0.1354910000
H -4.6716830000 -2.1684850000 -1.0096490000
H -3.1115200000 -1.8885590000 -1.7883580000
H -3.8052850000 -0.9511720000 1.8199120000
H -5.3717520000 -0.7618160000 1.0089430000
H -4.4316650000 0.6678120000 1.4668840000
H -5.5132810000 0.0466460000 -1.3845260000
H -4.0454660000 0.4836650000 -2.2738050000
H -4.6052900000 1.4946920000 -0.9273610000
C 1.2299670000 2.3518740000 1.4233950000

C -0.9606930000 2.9947530000 0.4461640000
C 0.9920140000 2.6958410000 -1.0824520000
C 0.8260340000 -1.5075270000 -0.0626250000
O 2.4767420000 0.2445480000 -0.2437540000
H 0.7381040000 2.0042690000 2.3377910000
H 1.4310510000 3.4219720000 1.5319020000
H 2.1799810000 1.8319700000 1.3060890000
H -1.5462950000 2.6305560000 1.2960980000
H -0.6411650000 4.0128380000 0.6863770000
H -1.6017330000 3.0715620000 -0.4372150000
H 1.1598200000 3.7699420000 -0.9551930000
H 1.9518030000 2.2104770000 -1.2583210000
H 0.3510100000 2.5535250000 -1.9587450000
C -0.6358450000 -1.6148720000 0.1067560000
H 1.4945720000 -2.3599020000 -0.0843430000
B 3.6457690000 -0.7367590000 -0.2389980000
C -0.9712890000 -2.2727110000 1.4636870000
H -1.0588710000 -2.2218190000 -0.7012870000
F 3.5834780000 -1.4526840000 0.9676680000
F 4.7821540000 0.0312180000 -0.3467670000
F 3.4730950000 -1.6135190000 -1.3200990000
H -0.5670810000 -1.6710970000 2.2825340000
H -2.0489990000 -2.3700500000 1.6053770000
H -0.5266800000 -3.2694920000 1.5188850000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.374010 (Hartree/Particle)
Thermal correction to Energy= 0.396269
Thermal correction to Enthalpy= 0.397213
Thermal correction to Gibbs (Free) Energy= 0.322821
Sum of electronic and zero-point Energies= -985.213246
Sum of electronic and thermal Energies= -985.190986
Sum of electronic and thermal Enthalpies= -985.190042
Sum of electronic and thermal (Free) Energies= -985.264434

4c

c/s RT

C 2.5412360000 -0.0373450000 0.3240590000
C 1.3264000000 -0.4698780000 0.4968130000
C 3.4202580000 -0.3473490000 -0.8801120000
H 2.9685230000 0.6194630000 1.0832340000
C 0.1011110000 -0.9556870000 0.6069490000
C 4.7372270000 -0.9512380000 -0.3660070000
C 3.7009760000 0.9796520000 -1.6062430000
C 2.7312110000 -1.3283320000 -1.8335020000
C -0.9743780000 -0.1790690000 -0.0376870000
C -0.1876040000 -2.3183160000 1.2672960000
H 5.2466580000 -0.2666660000 0.3208780000
H 4.5567460000 -1.8928560000 0.1621950000
H 5.4130980000 -1.1530420000 -1.2036970000
H 4.3722750000 0.8125910000 -2.4552510000
H 2.7727240000 1.4193730000 -1.9848180000
H 4.1769000000 1.7053850000 -0.9375170000
H 1.7864000000 -0.9239230000 -2.2104010000
H 3.3780390000 -1.5324320000 -2.6923140000
H 2.5183110000 -2.2802570000 -1.3359420000
C -0.8929290000 1.2674450000 -0.2096250000
O -1.9664930000 -0.8249070000 -0.4577100000
C -1.3837110000 -2.1857520000 2.2270540000
C -0.4836590000 -3.3762440000 0.1869770000
C 1.0420050000 -2.7653940000 2.0700670000
C -0.2469890000 2.0704470000 0.6479680000
H -1.4662080000 1.6790670000 -1.0343810000
B -3.3042300000 -0.2188970000 -1.1195240000
H -2.3039640000 -1.9244750000 1.7008480000
H -1.5497090000 -3.1407080000 2.7358100000
H -1.1893750000 -1.4266640000 2.9928140000
H -1.3808930000 -3.1324950000 -0.3830870000
H 0.3584320000 -3.4648630000 -0.5076170000
H -0.6325800000 -4.3504350000 0.6650660000
H 1.3076500000 -2.0339200000 2.8407760000
H 0.8248720000 -3.7167230000 2.5651200000
H 1.9144690000 -2.9119970000 1.4255690000
H 0.2434660000 1.6425660000 1.5224910000
C -0.1588470000 3.5591510000 0.5205670000
F -4.0847910000 -1.3248760000 -1.2977260000
F -2.8968570000 0.3828390000 -2.2962640000
F -3.7946730000 0.6812960000 -0.1956410000
H -0.6801730000 3.8631380000 -0.3943950000
C 1.3180880000 3.9680520000 0.4078570000
C -0.8346720000 4.2355180000 1.7214750000
H 1.4038060000 5.0532970000 0.2983040000
H 1.8722570000 3.6773140000 1.3082440000
H 1.7976830000 3.4961710000 -0.4549000000
H -1.8901580000 3.9585320000 1.7877620000
H -0.3445400000 3.9471770000 2.6585940000
H -0.7690750000 5.3238290000 1.6291670000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.427595 (Hartree/Particle)
Thermal correction to Energy= 0.454239
Thermal correction to Enthalpy= 0.455183
Thermal correction to Gibbs (Free) Energy= 0.369299
Sum of electronic and zero-point Energies= -1063.768946
Sum of electronic and thermal Energies= -1063.742302
Sum of electronic and thermal Enthalpies= -1063.741358
Sum of electronic and thermal (Free) Energies= -1063.827242

c/s TS

C 2.3576220000 0.1284350000 0.2261160000
C 1.0630710000 -0.0933480000 0.3929430000
C 3.2825160000 -0.4511680000 -0.8313020000
H 2.8119850000 0.9194600000 0.8226910000
C -0.0580950000 -0.8796190000 0.3477620000
C 4.4532640000 -1.1539220000 -0.1213460000
C 3.8215210000 0.7469100000 -1.6387880000
C 2.5731280000 -1.4159660000 -1.7837200000
C -1.2216110000 -0.1206010000 -0.0365310000
C -0.1539030000 -2.3256630000 0.8275120000
H 4.9788850000 -0.4673900000 0.5509560000
H 4.1070970000 -2.0077250000 0.4681450000
H 5.1738090000 -1.5186240000 -0.8608450000
H 4.5377850000 0.4009550000 -2.3910640000
H 3.0098500000 1.2675420000 -2.1574550000
H 4.3348650000 1.4668490000 -0.9918830000
H 1.7032830000 -0.9464510000 -2.2535160000
H 3.2619420000 -1.7246540000 -2.5759530000
H 2.2349720000 -2.3190040000 -1.2715820000
C -0.9592210000 1.2695420000 -0.0015470000
O -2.3133980000 -0.6838970000 -0.3990000000
C -1.2442940000 -2.4097160000 1.9170150000
C -0.5468240000 -3.2251880000 -0.3629200000
C 1.1692740000 -2.8103170000 1.4326420000
C 0.1619040000 1.6624000000 0.7307110000
H -1.5485220000 1.9492550000 -0.6054340000
B -3.6040300000 0.1503950000 -0.6217640000
H -2.2235470000 -2.1182010000 1.5336890000
H -1.3123720000 -3.4400110000 2.2804360000
H -0.9951370000 -1.7680360000 2.7691590000
H -1.5068260000 -2.9232570000 -0.7851770000
H 0.2076830000 -3.1938380000 -1.1541700000
H -0.6305340000 -4.2597130000 -0.0140940000
H 1.4788710000 -2.1855330000 2.2764800000
H 1.0424590000 -3.8338320000 1.7977230000
H 1.9809630000 -2.8174480000 0.7017480000
H 0.2368720000 1.3089110000 1.7600330000
C 0.9002830000 2.9667920000 0.4749500000
F -4.5981450000 -0.7723130000 -0.8241560000
F -3.3716900000 0.9678870000 -1.7301890000
F -3.7831280000 0.9181830000 0.5298490000
H 1.6660280000 2.7558450000 -0.2832650000
C 1.6020610000 3.4459570000 1.7495320000
C -0.0128770000 4.0624860000 -0.0935260000
H 2.2116350000 4.3313350000 1.5493240000
H 0.8661710000 3.7106890000 2.5170490000
H 2.2580950000 2.6755440000 2.1696060000
H -0.4123190000 3.7984260000 -1.0757930000
H -0.8545850000 4.2639520000 0.5765360000
H 0.5576910000 4.9882660000 -0.2090850000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.427640 (Hartree/Particle)
Thermal correction to Energy= 0.452921
Thermal correction to Enthalpy= 0.453865
Thermal correction to Gibbs (Free) Energy= 0.373393
Sum of electronic and zero-point Energies= -1063.737414
Sum of electronic and thermal Energies= -1063.712133

Sum of electronic and thermal Enthalpies= -1063.711188
Sum of electronic and thermal (Free) Energies= -1063.791660

c/s PT

C 2.3335840000 0.2881790000 0.1176070000
C 1.0154930000 0.2563430000 0.4011300000
C 3.2494980000 -0.5363330000 -0.7636150000
H 2.8272410000 1.2095250000 0.4198600000
C -0.0230430000 -0.7413430000 0.2651760000
C 4.3671730000 -1.1677770000 0.0885510000
C 3.8959880000 0.4968600000 -1.7189530000
C 2.5439360000 -1.5818400000 -1.6324850000
C -1.2314200000 -0.0849780000 -0.1282750000
C -0.0519270000 -2.1599740000 0.7912120000
H 4.9052950000 -0.4024480000 0.6576660000
H 3.9765530000 -1.9015220000 0.7969080000
H 5.0887460000 -1.6710720000 -0.5631380000
H 4.6051100000 -0.0066810000 -2.3833550000
H 3.1392650000 0.9871780000 -2.3401380000
H 4.4419090000 1.2694290000 -1.1672550000
H 1.6872840000 -1.1463320000 -2.1574120000
H 3.2412930000 -1.9595740000 -2.3863670000
H 2.1949450000 -2.4410220000 -1.0638910000
C -1.0777340000 1.2610660000 0.1666820000
O -2.2893030000 -0.7146660000 -0.5377570000
C -1.1509210000 -2.1521490000 1.8968680000
C -0.4752700000 -3.1618670000 -0.3058990000
C 1.2523400000 -2.6004580000 1.4672240000
C 0.2593200000 1.5829640000 0.7084340000
H -1.8899680000 1.9723080000 0.0884040000
B -3.6323650000 0.0160120000 -0.5807800000
H -2.1311950000 -1.8880710000 1.4994640000
H -1.2085760000 -3.1573170000 2.3250550000
H -0.8916350000 -1.4558750000 2.7010500000
H -1.4495680000 -2.8987950000 -0.7194420000
H 0.2503400000 -3.2043820000 -1.1211400000
H -0.5395770000 -4.1578200000 0.1435140000
H 1.5880390000 -1.8700900000 2.2097590000
H 1.0762740000 -3.5482380000 1.9839280000
H 2.0640570000 -2.7668280000 0.7617080000
H 0.1562590000 1.5990370000 1.8068200000
C 0.8796100000 2.9329160000 0.2706070000
F -4.5571220000 -0.9157310000 -0.9876940000
F -3.5089350000 1.0932000000 -1.4686790000
F -3.8735690000 0.4934460000 0.7185750000
H 1.4587930000 2.7508710000 -0.6430840000
C 1.8165200000 3.4786550000 1.3562730000
C -0.1816390000 3.9882510000 -0.0624530000
H 2.3577520000 4.3580200000 0.9954380000
H 1.2353380000 3.7823720000 2.2349940000
H 2.5554310000 2.7463100000 1.6955650000
H -0.7857660000 3.7099100000 -0.9300020000
H -0.8556660000 4.1588120000 0.7848220000
H 0.3058480000 4.9402350000 -0.2920960000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.430811 (Hartree/Particle)
Thermal correction to Energy= 0.455798
Thermal correction to Enthalpy= 0.456742
Thermal correction to Gibbs (Free) Energy= 0.377268
Sum of electronic and zero-point Energies= -1063.752051
Sum of electronic and thermal Energies= -1063.727064
Sum of electronic and thermal Enthalpies= -1063.726120
Sum of electronic and thermal (Free) Energies= -1063.805594

cc/s RT

C -1.0832870000 -0.9648890000 -0.5228880000
C 0.1187280000 -1.1516340000 -0.0037220000
C 1.1408940000 -0.1202220000 -0.2637080000
C 0.8354070000 1.3024200000 -0.3530400000
C -0.1418150000 1.8811900000 0.3585050000
C 0.5009600000 -2.4671140000 0.7106480000
O 2.3174050000 -0.5314310000 -0.4199050000
H 1.5327350000 1.9000850000 -0.9313760000
B 3.6457850000 0.3628780000 -0.6068840000
F 3.4791720000 1.0387690000 -1.8008230000
F 4.6408780000 -0.5716510000 -0.6257420000
F 3.6745200000 1.2017970000 0.4891180000
H -0.7716470000 1.2650270000 0.9987540000
C -0.4016250000 3.3561470000 0.3943510000
H 0.3392870000 3.8530220000 -0.2423990000
C -0.2431790000 3.8754610000 1.8305170000
H -0.9669260000 3.3961380000 2.5000900000
H 0.7615930000 3.6779680000 2.2135590000
H -0.4181940000 4.9549720000 1.8641720000
C -1.8023630000 3.6626730000 -0.1555940000
H -1.9863560000 4.7410870000 -0.1368350000
H -1.9073050000 3.3161270000 -1.1878370000
H -2.5785320000 3.1813540000 0.4504590000
C 1.3096500000 -3.3738160000 -0.2361990000
H 2.2512940000 -2.9100260000 -0.5325000000
H 1.5343620000 -4.3190420000 0.2697790000
H 0.7318270000 -3.6011790000 -1.1383180000
C 1.3206480000 -2.1448370000 1.9734390000
H 1.5309950000 -3.0715700000 2.5166890000
H 2.2770580000 -1.6756080000 1.7345740000
H 0.7626690000 -1.4820280000 2.6444170000
C -0.7747570000 -3.2096540000 1.1337050000
H -1.3905710000 -2.5992040000 1.8032170000
H -1.3846760000 -3.4939500000 0.2712130000
H -0.5001470000 -4.1238330000 1.6685830000
C -2.2503360000 -0.9250930000 -1.1005170000
H -2.2889590000 -1.2819620000 -2.1319670000
C -3.5818120000 -0.4949270000 -0.5039140000
C -3.4382440000 -0.0141860000 0.9425070000
H -2.9593120000 -0.7717150000 1.5709230000
H -2.8481850000 0.9041200000 0.9987060000
H -4.4251900000 0.2009550000 1.3639540000
C -4.5107660000 -1.7221350000 -0.5453390000
H -5.5060520000 -1.4545560000 -0.1747580000
H -4.6222180000 -2.1017940000 -1.5665070000
H -4.1175600000 -2.5309170000 0.0786740000
C -4.1670320000 0.6283810000 -1.3747600000
H -5.1474960000 0.9324830000 -0.9928610000
H -3.5123810000 1.5048100000 -1.3743140000
H -4.2958300000 0.2994840000 -2.4113500000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.427900 (Hartree/Particle)
Thermal correction to Energy= 0.454383
Thermal correction to Enthalpy= 0.455327
Thermal correction to Gibbs (Free) Energy= 0.370718
Sum of electronic and zero-point Energies= -1063.767411
Sum of electronic and thermal Energies= -1063.740928
Sum of electronic and thermal Enthalpies= -1063.739984
Sum of electronic and thermal (Free) Energies= -1063.824593

cc/s TS

C 2.1270920000 0.7316610000 -0.5964930000
C 0.8875530000 0.3865930000 -0.2392380000
C 3.4946600000 0.5139930000 0.0146270000
H 2.1583230000 1.3985330000 -1.4617790000
C -0.3658710000 0.9522810000 -0.1473620000
C 4.4955080000 0.0659350000 -1.0659970000
C 3.5054130000 -0.4321040000 1.2146180000
C 3.9351250000 1.9151190000 0.5073970000
C -1.4278750000 -0.0141560000 -0.1409820000
C -0.6642560000 2.4420520000 0.0475660000
H 4.2271630000 -0.8948210000 -1.5084550000
H 5.4959450000 -0.0261930000 -0.6315710000
H 4.5483140000 0.8029240000 -1.8743480000
H 3.2796530000 -1.4579950000 0.9292730000
H 2.7835850000 -0.1164050000 1.9755780000
H 4.4973080000 -0.4293740000 1.6766100000
H 3.8892180000 2.6606030000 -0.2927820000
H 4.9698900000 1.8630090000 0.8615350000
H 3.3083390000 2.2601010000 1.3336720000
C -0.9220800000 -1.3251100000 -0.0728010000
O -2.6625610000 0.3157850000 -0.2444890000
C -1.5349230000 2.6334250000 1.3068230000
C -1.4277660000 2.9263310000 -1.2059330000
C 0.5974680000 3.2963820000 0.2132390000
C 0.4086450000 -1.5067140000 0.3170570000
H -1.5254340000 -2.1472320000 -0.4427670000
B -3.7919520000 -0.7244440000 -0.0239960000
H -1.7466220000 3.6994110000 1.4389340000
H -2.4854960000 2.1048510000 1.2323200000

H -1.0059140000 2.2823960000 2.1995470000
H -2.3638470000 2.3823600000 -1.3402070000
H -1.6592050000 3.9905200000 -1.0923460000
H -0.8160740000 2.8065960000 -2.1067250000
H 1.1889380000 2.9781130000 1.0761410000
H 1.2370280000 3.2779730000 -0.6730870000
H 0.2986960000 4.3358450000 0.3783020000
H 0.7245260000 -1.1262770000 1.2893480000
C 1.0414600000 -2.8301220000 -0.1187420000
F -4.9530950000 0.0062670000 -0.0035370000
F -3.5154030000 -1.3618260000 1.1870320000
F -3.7258470000 -1.6295000000 -1.0853780000
C 1.5574530000 -3.6363430000 1.0781850000
C 2.0775810000 -2.7208270000 -1.2427180000
H 0.2103520000 -3.4009960000 -0.5488420000
H 2.3920330000 -3.1410870000 1.5837450000
H 1.9066590000 -4.6189130000 0.7469160000
H 0.7639460000 -3.7928140000 1.8148090000
H 1.7269820000 -2.0672460000 -2.0461540000
H 2.2627670000 -3.7135330000 -1.6632490000
H 3.0311520000 -2.3392370000 -0.8770440000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.428216 (Hartree/Particle)
Thermal correction to Energy= 0.453269
Thermal correction to Enthalpy= 0.454213
Thermal correction to Gibbs (Free) Energy= 0.374580
Sum of electronic and zero-point Energies= -1063.721793
Sum of electronic and thermal Energies= -1063.696739
Sum of electronic and thermal Enthalpies= -1063.695795
Sum of electronic and thermal (Free) Energies= -1063.775428

cc/s PT

C -2.2178620000 0.6568280000 -0.2735180000
C -1.0155710000 0.0842230000 -0.0408890000
C -3.5507830000 0.1572280000 -0.7818000000
H -2.2427530000 1.7329830000 -0.1442850000
C 0.1904180000 0.8785360000 0.1404530000
C -4.5753140000 0.3365260000 0.3593570000
C -3.5930870000 -1.2823120000 -1.3009870000
C -3.9383210000 1.1013000000 -1.9425640000
C 1.2969280000 0.1214150000 -0.3655190000
C 0.3897920000 2.2341080000 0.7742980000
H -4.3711650000 -0.3425260000 1.1917240000
H -5.5825560000 0.1233420000 -0.0132540000
H -4.5685720000 1.3616130000 0.7443280000
H -3.3623190000 -2.0112330000 -0.5240890000
H -2.9038450000 -1.4249280000 -2.1388160000
H -4.6018470000 -1.5007290000 -1.6652220000
H -3.9884230000 2.1443550000 -1.6129180000
H -4.9228380000 0.8248740000 -2.3328150000
H -3.2163700000 1.0352460000 -2.7626260000
C 0.8483920000 -1.1616180000 -0.6218700000
O 2.5040610000 0.5951590000 -0.4923210000
C 0.9772500000 3.1998800000 -0.2820310000
C 1.4223820000 2.0154260000 1.9165650000
C -0.8556550000 2.8781010000 1.4055130000
C -0.5586560000 -1.3556970000 -0.2068990000
H 1.4914870000 -1.9504830000 -0.9909910000
B 3.6650820000 -0.3801770000 -0.6452230000
H 1.1536390000 4.1697210000 0.1938760000
H 1.9204720000 2.8276550000 -0.6832060000
H 0.2711360000 3.3483400000 -1.1057800000
H 2.3534520000 1.5840400000 1.5497870000
H 1.6432540000 2.9875220000 2.3677010000
H 1.0060010000 1.3665970000 2.6940870000
H -1.5312260000 3.3136070000 0.6639440000
H -1.4157280000 2.1780370000 2.0330040000
H -0.5251000000 3.7027990000 2.0433330000
H -1.1239560000 -1.9357270000 -0.9398110000
C -0.5726970000 -2.1218260000 1.1688790000
F 4.8115820000 0.3770180000 -0.5826800000
F 3.5169200000 -1.0507880000 -1.8674810000
F 3.5656570000 -1.3040750000 0.4140640000
C 0.2248190000 -3.4265370000 1.0845900000
C -1.9834280000 -2.3889440000 1.6884010000
H -0.0656340000 -1.4546950000 1.8788350000
H -0.1450320000 -4.0588960000 0.2685450000
H 0.1158200000 -3.9911310000 2.0151260000
H 1.2918050000 -3.2484640000 0.9289220000
H -2.5034480000 -3.1264850000 1.0674060000
H -2.5839710000 -1.4766790000 1.7292460000
H -1.9292550000 -2.7983700000 2.7016190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.431554 (Hartree/Particle)
Thermal correction to Energy= 0.456275
Thermal correction to Enthalpy= 0.457219
Thermal correction to Gibbs (Free) Energy= 0.377874
Sum of electronic and zero-point Energies= -1063.766168
Sum of electronic and thermal Energies= -1063.741447
Sum of electronic and thermal Enthalpies= -1063.740502
Sum of electronic and thermal (Free) Energies= -1063.819847

c/d RT

C 2.5596610000 0.7843780000 0.3762840000
C 1.5345800000 -0.0041880000 0.5204120000
C 3.4884290000 0.8017590000 -0.8308470000
H 2.7751740000 1.5035460000 1.1678130000
C 0.5241870000 -0.8534480000 0.5985800000
C 4.9217200000 0.5575960000 -0.3304540000
C 3.3910200000 2.1935290000 -1.4786950000
C 3.0988720000 -0.2755480000 -1.8475500000
C -0.7427940000 -0.4276130000 -0.0243210000
C 0.6785190000 -2.2652720000 1.1984460000
H 5.2209030000 1.3143010000 0.4029160000
H 5.0105300000 -0.4269810000 0.1395850000
H 5.6267120000 0.6020360000 -1.1673220000
H 4.0754280000 2.2629430000 -2.3308280000
H 2.3752690000 2.3861700000 -1.8380540000
H 3.6584780000 2.9821970000 -0.7668880000
H 2.0784240000 -0.1288100000 -2.2155510000
H 3.7762670000 -0.2417130000 -2.7063790000
H 3.1599730000 -1.2763270000 -1.4075120000
C -1.1484600000 0.9707320000 -0.1002470000
O -1.4678100000 -1.3333300000 -0.5072030000
C -0.5041290000 -2.5579470000 2.1392400000
C 0.7381570000 -3.3157030000 0.0729760000
C 1.9817400000 -2.3350520000 2.0064120000
C -0.8196660000 1.8754620000 0.8342860000
H -1.8318720000 1.2134300000 -0.9060000000
B -2.9298590000 -1.1568010000 -1.1575110000
H -1.4565420000 -2.5766320000 1.6054670000
H -0.3642070000 -3.5378420000 2.6067030000
H -0.5639830000 -1.8102720000 2.9379170000
H -0.1860760000 -3.3425140000 -0.5052980000
H 1.5699330000 -3.1055980000 -0.6077090000
H 0.9005150000 -4.3066530000 0.5105750000
H 1.9979470000 -1.5907810000 2.8098040000
H 2.0740610000 -3.3265530000 2.4599400000
H 2.8592880000 -2.1707720000 1.3732330000
H -0.2035380000 1.5647860000 1.6769510000
C -1.2845990000 3.3009800000 0.8763060000
F -3.3033160000 -2.4427240000 -1.4244140000
F -2.7461210000 -0.3748070000 -2.2836010000
F -3.6904900000 -0.5333930000 -0.1884610000
H -0.3692020000 3.9116390000 0.9173920000
C -2.0540050000 3.5417860000 2.1872690000
C -2.1020490000 3.7327490000 -0.3395360000
H -2.3246550000 4.5975650000 2.2786600000
H -2.9743570000 2.9494800000 2.2027800000
H -1.4567760000 3.2678410000 3.0627840000
H -1.5490980000 3.5872270000 -1.2723830000
H -3.0382840000 3.1685550000 -0.4054110000
H -2.3562960000 4.7934800000 -0.2611000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.428013 (Hartree/Particle)
Thermal correction to Energy= 0.454479
Thermal correction to Enthalpy= 0.455423
Thermal correction to Gibbs (Free) Energy= 0.369872
Sum of electronic and zero-point Energies= -1063.767853
Sum of electronic and thermal Energies= -1063.741388
Sum of electronic and thermal Enthalpies= -1063.740444
Sum of electronic and thermal (Free) Energies= -1063.825995

c/d TS

C 2.3669990000 0.2345820000 0.3725890000
C 1.0842150000 -0.0736140000 0.4754030000
C 3.3732370000 -0.2538550000 -0.6579090000
H 2.7536010000 1.0026180000 1.0429510000
C -0.0012410000 -0.8960760000 0.3509210000
C 4.5038750000 -0.9860610000 0.0887730000
C 3.9562590000 0.9923450000 -1.3520760000
C 2.7445580000 -1.1660870000 -1.7134660000
C -1.1896180000 -0.1651410000 -0.0236250000
C -0.0509820000 -2.3727600000 0.7379700000
H 4.9755470000 -0.3331020000 0.8309110000
H 4.1323940000 -1.8746820000 0.6063430000
H 5.2757250000 -1.3011460000 -0.6212130000
H 4.7539210000 0.6974170000 -2.0415850000
H 3.1895250000 1.5181550000 -1.9287540000
H 4.3813070000 1.6940050000 -0.6260710000
H 1.9005610000 -0.6771220000 -2.2100560000
H 3.4888050000 -1.4170860000 -2.4753600000
H 2.3858640000 -2.1026370000 -1.2816050000
C -0.9995620000 1.2279680000 0.1214250000
O -2.2347920000 -0.7537730000 -0.4709270000
C -1.1703330000 -2.5692060000 1.7823090000
C -0.3652000000 -3.2116990000 -0.5181940000
C 1.2723640000 -2.8403510000 1.3553400000
C 0.0667090000 1.6230850000 0.9265730000
H -1.5845140000 1.9241840000 -0.4699230000
B -3.5592720000 0.0302630000 -0.6844520000
H -2.1484780000 -2.2922990000 1.3854560000
H -1.2076960000 -3.6225720000 2.0776340000
H -0.9744420000 -1.9744430000 2.6811490000
H -1.3253290000 -2.9285430000 -0.9525790000
H 0.4104240000 -3.0951330000 -1.2807490000
H -0.4088920000 -4.2691190000 -0.2372080000
H 1.5375280000 -2.2494320000 2.2378540000
H 1.1743040000 -3.8853060000 1.6641420000
H 2.1010540000 -2.7816760000 0.6462920000
H 0.1384720000 1.2047890000 1.9305630000
C 0.6991010000 2.9883060000 0.7948030000
F -4.4948960000 -0.9235020000 -0.9932910000
F -3.3293650000 0.9381940000 -1.7202110000
F -3.8203700000 0.6995810000 0.5117190000
H 1.7017150000 2.9230920000 1.2365460000
C -0.1041210000 3.9940730000 1.6384480000
C 0.8352480000 3.4464030000 -0.6572390000
H 0.3750700000 4.9768100000 1.6046850000
H -1.1228300000 4.0972970000 1.2521380000
H -0.1689780000 3.6822940000 2.6851900000
H 1.3250160000 2.6811820000 -1.2667820000
H -0.1414870000 3.6584380000 -1.1028700000
H 1.4291310000 4.3629540000 -0.7136440000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.427772 (Hartree/Particle)
Thermal correction to Energy= 0.453027
Thermal correction to Enthalpy= 0.453971
Thermal correction to Gibbs (Free) Energy= 0.373872
Sum of electronic and zero-point Energies= -1063.740470
Sum of electronic and thermal Energies= -1063.715215
Sum of electronic and thermal Enthalpies= -1063.714270
Sum of electronic and thermal (Free) Energies= -1063.794370

c/d PT

C -2.3429590000 0.4225290000 -0.3779490000
C -1.0105090000 0.2717820000 -0.5461850000
C -3.3899660000 -0.2162020000 0.5110060000
H -2.7325120000 1.3306910000 -0.8378750000
C -0.0418040000 -0.7610600000 -0.2678400000
C -4.4436770000 -0.9432290000 -0.3481370000
C -4.0920810000 0.9723490000 1.2125110000
C -2.8195730000 -1.1198670000 1.6090450000
C 1.2144360000 -0.1359950000 0.0280790000
C -0.0999560000 -2.2466720000 -0.5581230000
H -4.8809620000 -0.2626730000 -1.0861910000
H -4.0242660000 -1.7960460000 -0.8840010000
H -5.2527480000 -1.3058710000 0.2941550000
H -4.8872360000 0.5980270000 1.8646490000
H -3.3901630000 1.5421880000 1.8294310000
H -4.5454570000 1.6565390000 0.4875510000
H -2.0362440000 -0.6015840000 2.1719180000
H -3.6149970000 -1.3902630000 2.3101370000
H -2.4010990000 -2.0471590000 1.2249080000
C 1.1504210000 1.1642580000 -0.4447360000
O 2.2261580000 -0.7697440000 0.5349060000
C 1.0144220000 -2.5050340000 -1.6155310000
C 0.2265030000 -3.0690400000 0.7092290000
C -1.4179020000 -2.7146950000 -1.1866060000
C -0.1795000000 1.5126610000 -0.9759180000
H 1.9997950000 1.8362900000 -0.4374120000
B 3.6018350000 -0.1007930000 0.5566330000
H 2.0035590000 -2.2340100000 -1.2467980000
H 1.0148690000 -3.5724550000 -1.8553430000
H 0.8114940000 -1.9504850000 -2.5374640000
H 1.2135820000 -2.8140760000 1.0965710000
H -0.5111530000 -2.9082920000 1.4992390000
H 0.2140740000 -4.1309070000 0.4438940000
H -1.7170260000 -2.0754090000 -2.0229930000
H -1.2805620000 -3.7286820000 -1.5727420000
H -2.2385470000 -2.7560330000 -0.4734390000
H -0.1436830000 1.4622400000 -2.0763320000
C -0.6525030000 2.9240630000 -0.5667250000
F 4.4608180000 -1.0213080000 1.1079150000
F 3.4943580000 1.0737990000 1.3145900000
F 3.9208550000 0.2169020000 -0.7733890000
H -1.6856720000 3.0442710000 -0.9141610000
C 0.1791820000 3.9984360000 -1.2758390000
C -0.6204980000 3.1127000000 0.9523020000
H -0.2103910000 4.9928280000 -1.0395340000
H 1.2265010000 3.9753640000 -0.9580100000
H 0.1520970000 3.8762460000 -2.3635230000
H -1.1696950000 2.3194420000 1.4694850000
H 0.4084570000 3.1046390000 1.3271070000
H -1.0689580000 4.0706490000 1.2308260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.430507 (Hartree/Particle)
Thermal correction to Energy= 0.455639
Thermal correction to Enthalpy= 0.456584
Thermal correction to Gibbs (Free) Energy= 0.376715
Sum of electronic and zero-point Energies= -1063.757493
Sum of electronic and thermal Energies= -1063.732360
Sum of electronic and thermal Enthalpies= -1063.731416
Sum of electronic and thermal (Free) Energies= -1063.811285

cc/d RT

C -2.3440600000 -0.6771790000 -1.0970800000
C -1.1921890000 -0.8596980000 -0.5162320000
C -3.6470630000 -0.2039910000 -0.4718600000
H -2.3905600000 -0.9197430000 -2.1608740000
C -0.0121830000 -1.1799610000 -0.0129760000
C -4.0819500000 1.0909330000 -1.1770640000
C -3.5058230000 0.0389680000 1.0329340000
C -4.6947730000 -1.3050070000 -0.7157260000
C 1.0794300000 -0.2002510000 -0.1710990000
C 0.2757590000 -2.5840190000 0.5637700000
H -3.3419970000 1.8828690000 -1.0300120000
H -5.0407140000 1.4376150000 -0.7766640000
H -4.2027620000 0.9334970000 -2.2540180000
H -2.8012780000 0.8483210000 1.2406130000
H -3.1585720000 -0.8602520000 1.5511090000
H -4.4732130000 0.3239620000 1.4583290000
H -4.8137660000 -1.5102070000 -1.7848900000
H -5.6681290000 -0.9933460000 -0.3221950000
H -4.4062860000 -2.2368030000 -0.2190110000
C 0.8853710000 1.2420640000 -0.0936160000
O 2.2215390000 -0.6750050000 -0.3922800000
C 1.1281360000 -2.4507210000 1.8387810000
C 1.0054520000 -3.4501530000 -0.4800740000
C -1.0492440000 -3.2666250000 0.9326150000
C -0.0321030000 1.8089740000 0.7032370000
H 1.6297800000 1.8362000000 -0.6107140000
B 3.6086820000 0.1375620000 -0.5042330000
H 1.2692370000 -3.4395100000 2.2866430000
H 2.1164700000 -2.0359180000 1.6315250000
H 0.6294210000 -1.8154040000 2.5794080000
H 1.9766930000 -3.0303940000 -0.7449720000
H 1.1632280000 -4.4547570000 -0.0728060000
H 0.4041980000 -3.5438490000 -1.3906230000
H -1.6074600000 -2.6824980000 1.6722800000

H -1.6888580000 -3.4132900000 0.0573530000
H -0.8412480000 -4.2492980000 1.3666470000
H -0.7076120000 1.1653870000 1.2638240000
C -0.1886370000 3.2831130000 0.9423820000
F 4.5339520000 -0.8570470000 -0.6400140000
F 3.7093500000 0.8501430000 0.6743580000
F 3.4810960000 0.9497890000 -1.6155340000
C -1.6139520000 3.7206500000 0.5627210000
C 0.8618230000 4.1469190000 0.2465960000
H -0.0853810000 3.4194510000 2.0290790000
H -1.7695660000 3.6175380000 -0.5164120000
H -1.7694010000 4.7702550000 0.8281360000
H -2.3756830000 3.1269870000 1.0778600000
H 0.7851890000 4.0618900000 -0.8429390000
H 1.8766480000 3.8653450000 0.5410580000
H 0.7123570000 5.1981390000 0.5085190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.428239 (Hartree/Particle)
Thermal correction to Energy= 0.454547
Thermal correction to Enthalpy= 0.455491
Thermal correction to Gibbs (Free) Energy= 0.371315
Sum of electronic and zero-point Energies= -1063.766731
Sum of electronic and thermal Energies= -1063.740423
Sum of electronic and thermal Enthalpies= -1063.739479
Sum of electronic and thermal (Free) Energies= -1063.823656

cc/d TS

C 2.1166960000 0.6559990000 -0.6234550000
C 0.8778730000 0.3753980000 -0.2152780000
C 3.4709020000 0.4897450000 0.0356660000
H 2.1585130000 1.1940490000 -1.5738450000
C -0.3721130000 0.9344530000 -0.1380910000
C 4.3638910000 -0.4838700000 -0.7521880000
C 3.3656810000 0.0945010000 1.5123140000
C 4.1207820000 1.8918610000 -0.0400140000
C -1.4306660000 -0.0397770000 -0.0623750000
C -0.6603920000 2.4335800000 -0.0359770000
H 3.9880580000 -1.5071490000 -0.7173830000
H 5.3754060000 -0.4815600000 -0.3332710000
H 4.4339900000 -0.1868900000 -1.8039110000
H 2.9435410000 -0.8996540000 1.6513610000
H 2.7449900000 0.8108810000 2.0608630000
H 4.3609830000 0.0929230000 1.9675440000
H 4.2305810000 2.2268950000 -1.0768140000
H 5.1181380000 1.8563970000 0.4098520000
H 3.5295940000 2.6365450000 0.5000400000
C -0.9141370000 -1.3401350000 0.0673970000
O -2.6648830000 0.2826960000 -0.1830770000
C -1.5259070000 2.7069210000 1.2110750000
C -1.4227610000 2.8493960000 -1.3135370000
C 0.6161290000 3.2761940000 0.0756600000
C 0.4210160000 -1.4849240000 0.4622180000
H -1.5005470000 -2.1851070000 -0.2792260000
B -3.7930560000 -0.7561200000 0.0580870000
H -1.7290320000 3.7804770000 1.2802940000
H -2.4805910000 2.1816120000 1.1685320000
H -0.9984510000 2.4046390000 2.1223750000
H -2.3641760000 2.3064110000 -1.4111200000
H -1.6444320000 3.9205780000 -1.2647380000
H -0.8160930000 2.6687440000 -2.2074950000
H 1.2091150000 2.9930050000 0.9513290000
H 1.2490970000 3.1949020000 -0.8123200000
H 0.3371260000 4.3284070000 0.1854290000
H 0.7297650000 -1.0598060000 1.4169210000
C 1.0882000000 -2.7873540000 0.0291030000
F -4.9583790000 -0.0328080000 0.0236180000
F -3.5383860000 -1.3419120000 1.2982690000
F -3.6982010000 -1.7017240000 -0.9655980000
C 2.2596390000 -3.2608560000 0.8901910000
C 1.4116660000 -2.7983290000 -1.4714240000
H 0.2906800000 -3.5294460000 0.1745800000
H 3.1790550000 -2.7058530000 0.6954580000
H 2.4687970000 -4.3127790000 0.6749310000
H 2.0301420000 -3.1821000000 1.9578570000
H 0.5266550000 -2.5511620000 -2.0648390000
H 1.7571920000 -3.7906860000 -1.7754110000
H 2.1919510000 -2.0740560000 -1.7171330000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.428056 (Hartree/Particle)
Thermal correction to Energy= 0.453042
Thermal correction to Enthalpy= 0.453987
Thermal correction to Gibbs (Free) Energy= 0.374937
Sum of electronic and zero-point Energies= -1063.724810
Sum of electronic and thermal Energies= -1063.699824
Sum of electronic and thermal Enthalpies= -1063.698880
Sum of electronic and thermal (Free) Energies= -1063.777930

cc/d PT

C -2.2024220000 0.6057950000 -0.2894170000
C -1.0084980000 0.0014780000 -0.0953380000
C -3.5576920000 0.1539990000 -0.7827230000
H -2.1987470000 1.6774680000 -0.1270030000
C 0.2129720000 0.7787720000 0.0602660000
C -4.5363970000 0.2431540000 0.4078150000
C -3.6222160000 -1.2379190000 -1.4160260000
C -3.9844870000 1.1886310000 -1.8483320000
C 1.2957970000 0.0110960000 -0.4803330000
C 0.4488120000 2.1295210000 0.6935100000
H -4.2983830000 -0.4961580000 1.1771890000
H -5.5576500000 0.0561100000 0.0599260000
H -4.5137490000 1.2360160000 0.8690450000
H -3.3937180000 -2.0282470000 -0.7021750000
H -2.9401260000 -1.3195990000 -2.2679750000
H -4.6363030000 -1.4163040000 -1.7871510000
H -4.0162630000 2.2021000000 -1.4346230000
H -4.9845800000 0.9470910000 -2.2214820000
H -3.2950070000 1.1869290000 -2.6985670000
C 0.8319660000 -1.2719310000 -0.6997320000
O 2.5041670000 0.4741760000 -0.6397590000
C 0.9836470000 3.0942350000 -0.3919680000
C 1.5372620000 1.9163150000 1.7839210000
C -0.7622550000 2.7735570000 1.3892900000
C -0.5800910000 -1.4416170000 -0.2954300000
H 1.4702910000 -2.0876450000 -1.0202000000
B 3.6656630000 -0.5100960000 -0.6764590000
H 1.1834770000 4.0646700000 0.0733900000
H 1.9068540000 2.7203640000 -0.8364610000
H 0.2388750000 3.2416850000 -1.1812300000
H 2.4443530000 1.4685380000 1.3799250000
H 1.7908170000 2.8940310000 2.2046230000
H 1.1547930000 1.2862760000 2.5926150000
H -1.4670480000 3.2277400000 0.6872350000
H -1.2997890000 2.0670780000 2.0294890000
H -0.3964420000 3.5840540000 2.0259370000
H -1.1526300000 -1.9730150000 -1.0592460000
C -0.6159890000 -2.3079330000 1.0249040000
F 4.8126950000 0.2490920000 -0.6630620000
F 3.5444000000 -1.2992770000 -1.8284460000
F 3.5404560000 -1.3231870000 0.4689520000
C -2.0335830000 -2.7231340000 1.4117330000
C 0.0891860000 -1.6310720000 2.2019300000
H -0.0573880000 -3.2191620000 0.7787140000
H -2.6570310000 -1.8474840000 1.6204190000
H -2.0071180000 -3.3345390000 2.3185460000
H -2.5137970000 -3.3187320000 0.6301870000
H -0.4115190000 -0.6952630000 2.4791110000
H 1.1399630000 -1.4147610000 1.9943840000
H 0.0521740000 -2.2895060000 3.0743260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.431731 (Hartree/Particle)
Thermal correction to Energy= 0.456350
Thermal correction to Enthalpy= 0.457295
Thermal correction to Gibbs (Free) Energy= 0.378611
Sum of electronic and zero-point Energies= -1063.766956
Sum of electronic and thermal Energies= -1063.742337
Sum of electronic and thermal Enthalpies= -1063.741393
Sum of electronic and thermal (Free) Energies= -1063.820076

c/u RT

C -2.5467090000 -0.1090120000 -0.3724050000
C -1.3356270000 -0.5663500000 -0.5016530000
C -3.3894250000 -0.2021630000 0.8924240000
H -2.9975940000 0.4067060000 -1.2215010000
C -0.1110860000 -1.0630770000 -0.5595280000

C -4.7184840000 -0.8852060000 0.5315250000
C -3.6537940000 1.2323920000 1.3817100000
C -2.6688930000 -1.0007900000 1.9828650000
C 0.9758070000 -0.1868200000 -0.0839220000
C 0.1672080000 -2.5187620000 -0.9831290000
H -5.2499900000 -0.3317740000 -0.2502600000
H -4.5499870000 -1.9055260000 0.1726840000
H -5.3691160000 -0.9349190000 1.4109910000
H -4.2981220000 1.2183500000 2.2671600000
H -2.7163440000 1.7311200000 1.6478380000
H -4.1530520000 1.8293040000 0.6104420000
H -1.7154650000 -0.5369600000 2.2551390000
H -3.2898390000 -1.0502690000 2.8826370000
H -2.4660180000 -2.0254620000 1.6543550000
C 0.8889690000 1.2680370000 -0.1446760000
O 1.9845130000 -0.7518450000 0.4078720000
C 1.3369970000 -2.5528080000 -1.9830500000
C 0.4968980000 -3.3748110000 0.2548300000
C -1.0807240000 -3.0982760000 -1.6636900000
C 0.2191240000 1.9172250000 -1.1082840000
H 1.4794830000 1.8002950000 0.5923450000
B 3.3298910000 -0.0393170000 0.9325920000
H 2.2691170000 -2.2036250000 -1.5344470000
H 1.4948470000 -3.5811250000 -2.3236360000
H 1.1183260000 -1.9375290000 -2.8628300000
H 1.4072860000 -3.0359300000 0.7506140000
H -0.3265200000 -3.3434040000 0.9762650000
H 0.6386770000 -4.4165990000 -0.0523630000
H -1.3697420000 -2.5113820000 -2.5421260000
H -0.8720310000 -4.1209190000 -1.9921940000
H -1.9355020000 -3.1312600000 -0.9807980000
H -0.2850690000 1.3393540000 -1.8812570000
C 0.0858400000 3.4051700000 -1.2398360000
F 4.1296900000 -1.0975230000 1.2565180000
F 2.9437810000 0.7313860000 2.0145230000
F 3.7864870000 0.7150050000 -0.1291140000
H 0.4765160000 3.6642100000 -2.2346870000
C 0.8580030000 4.2025130000 -0.1911640000
C -1.4130770000 3.7586510000 -1.2295810000
H 0.7391370000 5.2742100000 -0.3736610000
H 0.4849750000 3.9928560000 0.8174030000
H 1.9268380000 3.9721190000 -0.2147820000
H -1.9611590000 3.2165030000 -2.0072610000
H -1.8592520000 3.5080770000 -0.2611540000
H -1.5517220000 4.8296330000 -1.4027980000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.427873 (Hartree/Particle)
Thermal correction to Energy= 0.454366
Thermal correction to Enthalpy= 0.455310
Thermal correction to Gibbs (Free) Energy= 0.369919
Sum of electronic and zero-point Energies= -1063.768657
Sum of electronic and thermal Energies= -1063.742164
Sum of electronic and thermal Enthalpies= -1063.741220
Sum of electronic and thermal (Free) Energies= -1063.826611

c/u TS

C 2.3038890000 0.0193710000 0.2554970000
C 0.9955520000 -0.1128280000 0.4187560000
C 3.1913980000 -0.6335230000 -0.7941400000
H 2.8192920000 0.7393760000 0.8874920000
C -0.1742170000 -0.8206580000 0.3337220000
C 4.2595570000 -1.4633600000 -0.0567660000
C 3.8907710000 0.4948270000 -1.5774090000
C 2.4133040000 -1.5077700000 -1.7797320000
C -1.2869790000 0.0262810000 -0.0210910000
C -0.3799290000 -2.2706750000 0.7692930000
H 4.8456100000 -0.8372910000 0.6246220000
H 3.8087020000 -2.2700440000 0.5275110000
H 4.9493340000 -1.9094610000 -0.7807880000
H 4.6302710000 0.0683950000 -2.2629490000
H 3.1711360000 1.0659950000 -2.1714250000
H 4.4140960000 1.1861100000 -0.9074000000
H 1.6022820000 -0.9473450000 -2.2550970000
H 3.0862260000 -1.8640400000 -2.5656550000
H 1.9804230000 -2.3850250000 -1.2958050000
C -0.9580750000 1.3890980000 0.1369640000
O -2.3981360000 -0.4529510000 -0.4429470000
C -1.4805540000 -2.2990780000 1.8521620000
C -0.8347170000 -3.1069850000 -0.4449360000
C 0.8966940000 -2.8722790000 1.3685890000
C 0.1739580000 1.6705750000 0.9063900000
H -1.5051080000 2.1576740000 -0.3994670000
B -3.6431280000 0.4572460000 -0.6151430000
H -2.4324940000 -1.9227420000 1.4739190000
H -1.6302990000 -3.3304530000 2.1868040000
H -1.1875540000 -1.7021360000 2.7227490000
H -1.7688320000 -2.7243760000 -0.8594540000
H -0.0786860000 -3.1108920000 -1.2351840000
H -0.9943290000 -4.1412690000 -0.1227960000
H 1.2566630000 -2.2878860000 2.2213860000
H 0.6837370000 -3.8865540000 1.7190430000
H 1.7050440000 -2.9388780000 0.6377080000
H 0.2401300000 1.2381240000 1.9046170000
C 0.8597170000 3.0174470000 0.7663320000
F -4.6744730000 -0.3964730000 -0.9133810000
F -3.3511880000 1.3551960000 -1.6443680000
F -3.8119910000 1.1309730000 0.5957650000
H 0.0447270000 3.7342340000 0.9486890000
C 1.3907690000 3.2828530000 -0.6459240000
C 1.9235450000 3.2699420000 1.8377090000
H 1.6967470000 4.3281050000 -0.7449300000
H 2.2614640000 2.6563330000 -0.8554580000
H 0.6324240000 3.0798420000 -1.4071800000
H 1.5366450000 3.0742260000 2.8426520000
H 2.8118830000 2.6482170000 1.6869640000
H 2.2519620000 4.3124440000 1.8040840000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.427615 (Hartree/Particle)
Thermal correction to Energy= 0.452909
Thermal correction to Enthalpy= 0.453853
Thermal correction to Gibbs (Free) Energy= 0.373665
Sum of electronic and zero-point Energies= -1063.737674
Sum of electronic and thermal Energies= -1063.712380
Sum of electronic and thermal Enthalpies= -1063.711436
Sum of electronic and thermal (Free) Energies= -1063.791623

c/u PT

C -2.2917480000 0.1831800000 -0.3463790000
C -0.9499270000 0.1929980000 -0.5203760000
C -3.2489860000 -0.5505280000 0.5701120000
H -2.7915580000 1.0116190000 -0.8419440000
C 0.1301460000 -0.7253930000 -0.2491680000
C -4.2205340000 -1.4132020000 -0.2609260000
C -4.0838960000 0.5641340000 1.2486070000
C -2.5724560000 -1.3521750000 1.6868260000
C 1.3254590000 0.0308400000 -0.0122360000
C 0.2243460000 -2.2167500000 -0.5058620000
H -4.7426460000 -0.8026280000 -1.0050890000
H -3.7128100000 -2.2226360000 -0.7869100000
H -4.9743710000 -1.8535190000 0.3997240000
H -4.8389110000 0.1121570000 1.8993220000
H -3.4564980000 1.2149190000 1.8650760000
H -4.6037520000 1.1845310000 0.5109450000
H -1.8456830000 -0.7335050000 2.2235330000
H -3.3268600000 -1.6854700000 2.4060090000
H -2.0584500000 -2.2402330000 1.3268410000
C 1.1154660000 1.2940010000 -0.5366790000
O 2.4097240000 -0.4797810000 0.4820600000
C 1.3371610000 -2.3872320000 -1.5822110000
C 0.6610470000 -2.9652130000 0.7743410000
C -1.0476810000 -2.8394770000 -1.0927230000
C -0.2680440000 1.5049860000 -1.0000160000
H 1.8899430000 2.0500080000 -0.5990260000
B 3.7060130000 0.3331750000 0.4598350000
H 2.3010170000 -2.0073420000 -1.2444980000
H 1.4426290000 -3.4549130000 -1.7962550000
H 1.0585460000 -1.8808820000 -2.5120730000
H 1.6248340000 -2.5998190000 1.1306240000
H -0.0716960000 -2.8584370000 1.5779850000
H 0.7524040000 -4.0298870000 0.5371040000
H -1.4324050000 -2.2567490000 -1.9354240000
H -0.8085080000 -3.8412660000 -1.4605610000
H -1.8428080000 -2.9536210000 -0.3595080000
H -0.2896600000 1.4508810000 -2.1003610000
C -0.7704450000 2.9074490000 -0.5702990000
F 4.6673290000 -0.4747790000 1.0188250000

F 3.4835490000 1.5091080000 1.1895170000
F 3.9683450000 0.6455970000 -0.8834400000
H 0.0242480000 3.5781470000 -0.9248680000
C -0.8437880000 3.0575460000 0.9513450000
C -2.0617430000 3.3820360000 -1.2478180000
H -1.1000190000 4.0864390000 1.2201450000
H -1.6121220000 2.4027950000 1.3744690000
H 0.1106640000 2.8151490000 1.4283850000
H -2.0964320000 3.1041490000 -2.3067010000
H -2.9570160000 2.9875750000 -0.7568090000
H -2.1291840000 4.4723680000 -1.1891300000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.430287 (Hartree/Particle)
Thermal correction to Energy= 0.455533
Thermal correction to Enthalpy= 0.456477
Thermal correction to Gibbs (Free) Energy= 0.375620
Sum of electronic and zero-point Energies= -1063.754191
Sum of electronic and thermal Energies= -1063.728946
Sum of electronic and thermal Enthalpies= -1063.728001
Sum of electronic and thermal (Free) Energies= -1063.808858

cc/u RT

C -2.4077930000 -0.6982530000 -1.1322030000
C -1.2781930000 -0.9398490000 -0.5308730000
C -3.6363200000 -0.0073130000 -0.5572450000
H -2.4744170000 -1.0013630000 -2.1788550000
C -0.1059380000 -1.2537350000 -0.0056110000
C -3.6897990000 1.4174460000 -1.1362450000
C -3.5960900000 0.0479980000 0.9732360000
C -4.8763670000 -0.7979030000 -1.0056240000
C 0.9912890000 -0.2978380000 -0.2496590000
C 0.1628390000 -2.6042700000 0.6874180000
H -2.8052020000 1.9902860000 -0.8406450000
H -4.5804890000 1.9419700000 -0.7734040000
H -3.7287110000 1.3994750000 -2.2303080000
H -2.7427520000 0.6280000000 1.3352250000
H -3.5319790000 -0.9565390000 1.4023330000
H -4.5050240000 0.5246080000 1.3538120000
H -4.9387950000 -0.8513970000 -2.0977860000
H -5.7875640000 -0.3133590000 -0.6397310000
H -4.8528100000 -1.8201190000 -0.6144590000
C 0.7777640000 1.1441360000 -0.2914370000
O 2.1337630000 -0.7856660000 -0.4353510000
C 1.0260930000 -2.3759050000 1.9412690000
C 0.8741360000 -3.5655660000 -0.2830070000
C -1.1721530000 -3.2277840000 1.1182600000
C -0.1212280000 1.7494590000 0.4982060000
H 1.4793770000 1.7081910000 -0.8956020000
B 3.5095210000 0.0333750000 -0.6204410000
H 1.1554860000 -3.3246010000 2.4717280000
H 2.0188730000 -1.9955730000 1.6925590000
H 0.5426880000 -1.6714030000 2.6274850000
H 1.8457160000 -3.1782390000 -0.5931490000
H 1.0291560000 -4.5316950000 0.2094350000
H 0.2629130000 -3.7336270000 -1.1759790000
H -1.7108920000 -2.5740110000 1.8126480000
H -1.8223030000 -3.4280130000 0.2613560000
H -0.9816920000 -4.1777330000 1.6269050000
H -0.7325160000 1.1333690000 1.1548550000
C -0.3170230000 3.2293850000 0.6416180000
F 4.4491350000 -0.9551790000 -0.6761710000
F 3.6029270000 0.8443930000 0.4934830000
F 3.3656880000 0.7472970000 -1.7956190000
C 0.4815470000 4.0667740000 -0.3549650000
C -0.0109170000 3.6343110000 2.0947600000
H -1.3896030000 3.4118920000 0.4730390000
H 1.5584080000 3.9472960000 -0.1961620000
H 0.2417540000 5.1263840000 -0.2299310000
H 0.2552160000 3.7890240000 -1.3888650000
H 1.0460690000 3.4643330000 2.3224330000
H -0.6108730000 3.0605300000 2.8083390000
H -0.2285650000 4.6956130000 2.2451010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.427742 (Hartree/Particle)
Thermal correction to Energy= 0.454296
Thermal correction to Enthalpy= 0.455240
Thermal correction to Gibbs (Free) Energy= 0.369688
Sum of electronic and zero-point Energies= -1063.767505
Sum of electronic and thermal Energies= -1063.740950
Sum of electronic and thermal Enthalpies= -1063.740006
Sum of electronic and thermal (Free) Energies= -1063.825558

cc/u TS

C -2.2208180000 -0.6283390000 -0.6264410000
C -0.9737660000 -0.4696730000 -0.1966160000
C -3.5617410000 -0.2789270000 -0.0117870000
H -2.2991590000 -1.1701460000 -1.5724060000
C 0.2594110000 -1.0541220000 -0.1032740000
C -4.2751800000 0.7965030000 -0.8505860000
C -3.4631130000 0.1364980000 1.4616350000
C -4.3873730000 -1.5832160000 -0.0850860000
C 1.3401070000 -0.0990250000 -0.0793390000
C 0.4975470000 -2.5564300000 0.0487910000
H -3.7331480000 1.7447630000 -0.8471780000
H -5.2792220000 0.9761330000 -0.4522940000
H -4.3786590000 0.4738460000 -1.8917110000
H -2.9765010000 1.1034020000 1.5984130000
H -2.9125460000 -0.6114720000 2.0417470000
H -4.4677440000 0.2191430000 1.8876540000
H -4.5004430000 -1.9269000000 -1.1186530000
H -5.3883200000 -1.4123020000 0.3240260000
H -3.9139110000 -2.3837700000 0.4916870000
C 0.8509150000 1.2218280000 0.0158510000
O 2.5624010000 -0.4500780000 -0.2194490000
C 1.3652140000 -2.8149600000 1.2963920000
C 1.2314410000 -3.0467030000 -1.2183570000
C -0.8145450000 -3.3381190000 0.1976970000
C -0.4468510000 1.3901170000 0.4883880000
H 1.4276960000 2.0371130000 -0.4083500000
B 3.7144000000 0.5807610000 -0.0463220000
H 1.5366200000 -3.8911000000 1.4017170000
H 2.3352810000 -2.3208390000 1.2254910000
H 0.8577040000 -2.4645110000 2.2017270000
H 2.1928160000 -2.5453990000 -1.3420720000
H 1.4108270000 -4.1235980000 -1.1339590000
H 0.6251600000 -2.8727220000 -2.1138050000
H -1.3915930000 -2.9978210000 1.0638960000
H -1.4481110000 -3.2559930000 -0.6901860000
H -0.5823470000 -4.3974900000 0.3423440000
H -0.7098400000 0.9374980000 1.4437750000
C -1.2093770000 2.6503910000 0.1404450000
F 4.8661850000 -0.1625690000 -0.0745300000
F 3.4937670000 1.2217920000 1.1724720000
F 3.6092860000 1.4823770000 -1.1072650000
C -1.1583320000 2.9785330000 -1.3530760000
C -0.6776210000 3.8100920000 1.0012560000
H -2.2543990000 2.4971760000 0.4212420000
H -0.1457690000 3.2433220000 -1.6724880000
H -1.8074760000 3.8306420000 -1.5755580000
H -1.4903220000 2.1265770000 -1.9547330000
H 0.3693900000 4.0250400000 0.7667900000
H -0.7432240000 3.5806930000 2.0690690000
H -1.2626100000 4.7144420000 0.8095660000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.427659 (Hartree/Particle)
Thermal correction to Energy= 0.452873
Thermal correction to Enthalpy= 0.453817
Thermal correction to Gibbs (Free) Energy= 0.373812
Sum of electronic and zero-point Energies= -1063.733796
Sum of electronic and thermal Energies= -1063.708582
Sum of electronic and thermal Enthalpies= -1063.707637
Sum of electronic and thermal (Free) Energies= -1063.787643

cc/u PT

C -2.2990650000 0.6638220000 -0.2752220000
C -1.0463190000 0.1556510000 -0.2214920000
C -3.6590990000 0.0331130000 -0.4786810000
H -2.3806300000 1.7345180000 -0.1430500000
C 0.1666870000 0.9425030000 -0.0815880000
C -4.2887810000 -0.1122920000 0.9256550000
C -3.6877880000 -1.3165220000 -1.2088210000
C -4.4974950000 1.0373980000 -1.2967770000
C 1.2805260000 0.1147130000 -0.4461050000
C 0.3938200000 2.3541640000 0.4122030000

H -3.7275450000 -0.8193340000 1.5432920000
H -5.3167150000 -0.4778940000 0.8314310000
H -4.3185520000 0.8484160000 1.4498280000
H -3.2262820000 -2.1215140000 -0.6343970000
H -3.1956020000 -1.2512030000 -2.1840780000
H -4.7294850000 -1.6033420000 -1.3830510000
H -4.5552010000 2.0107380000 -0.7980600000
H -5.5183870000 0.6631940000 -1.4197510000
H -4.0698870000 1.1882020000 -2.2933450000
C 0.8122820000 -1.1666830000 -0.6720410000
O 2.5131660000 0.5337450000 -0.4957900000
C 1.1036640000 3.1571310000 -0.7055580000
C 1.3273080000 2.2328590000 1.6493580000
C -0.8455940000 3.1438910000 0.8579940000
C -0.6325630000 -1.2894430000 -0.4167850000
H 1.4599110000 -1.9923460000 -0.9406260000
B 3.6431650000 -0.4868470000 -0.4426140000
H 1.3024010000 4.1673230000 -0.3339870000
H 2.0493890000 2.6975670000 -0.9926810000
H 0.4615180000 3.2402330000 -1.5886430000
H 2.2597820000 1.7224120000 1.4107040000
H 1.5634660000 3.2422060000 2.0001100000
H 0.8232550000 1.6995240000 2.4618490000
H -1.4854790000 3.4345320000 0.0193510000
H -1.4397650000 2.6071440000 1.6041950000
H -0.5021180000 4.0723470000 1.3232460000
H -1.1305350000 -1.7523470000 -1.2749140000
C -0.9179510000 -2.1843680000 0.8397580000
F 4.8063930000 0.2369870000 -0.3218170000
F 3.5970900000 -1.2583930000 -1.6121800000
F 3.3975080000 -1.3097580000 0.6751740000
C -0.2047730000 -1.6768450000 2.0936340000
C -0.5638740000 -3.6429480000 0.5462880000
H -1.9970820000 -2.1277710000 1.0187600000
H 0.8831110000 -1.7519690000 1.9972540000
H -0.5113200000 -2.2720790000 2.9586980000
H -0.4525880000 -0.6316090000 2.3079330000
H 0.5144900000 -3.7716210000 0.4089080000
H -1.0704740000 -4.0074960000 -0.3539370000
H -0.8656640000 -4.2799520000 1.3828500000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.431694 (Hartree/Particle)
Thermal correction to Energy= 0.456429
Thermal correction to Enthalpy= 0.457373
Thermal correction to Gibbs (Free) Energy= 0.377951
Sum of electronic and zero-point Energies= -1063.773301
Sum of electronic and thermal Energies= -1063.748565
Sum of electronic and thermal Enthalpies= -1063.747621
Sum of electronic and thermal (Free) Energies= -1063.827043

4d

cRT

C 0.8403960000 2.5350990000 0.1701120000
C 1.1290240000 1.2962600000 0.4461340000
C 1.4742230000 0.0387780000 0.6608600000
C 0.6325480000 -0.9934530000 0.0235460000
C -0.7983660000 -0.8312470000 -0.1653520000
C -1.5577830000 -0.0544750000 0.6316620000
H -1.2326100000 -1.4470740000 -0.9438660000
H -1.0760940000 0.4857640000 1.4432530000
C -3.0047600000 0.1304460000 0.5344430000
C 2.7540550000 -0.3489960000 1.4278290000
O 1.2217170000 -2.0318830000 -0.3740480000
C -3.8050490000 -0.5791360000 -0.3750760000
C -3.6142660000 1.0650010000 1.3838630000
B 0.5437850000 -3.3362220000 -1.0195180000
F 1.6003400000 -4.1849970000 -1.1856040000
F -0.0331720000 -2.9124590000 -2.2052570000
F -0.3899440000 -3.7628120000 -0.0957670000
C 1.3173770000 3.2940890000 -1.0609760000
C 3.8536680000 -0.7835940000 0.4402290000
H 4.7713240000 -1.0071120000 0.9950910000
H 3.5650750000 -1.6731190000 -0.1208930000
H 4.0741260000 0.0202760000 -0.2699850000
C 2.4387500000 -1.4908700000 2.4105280000
H 2.1276900000 -2.4012870000 1.8937810000
H 3.3341960000 -1.7280390000 2.9937700000
H 1.6489850000 -1.1985910000 3.1114950000
C 3.2561010000 0.8642100000 2.2228080000
H 3.5289390000 1.6943450000 1.5637780000
H 2.4994130000 1.2242870000 2.9281150000
H 4.1452920000 0.5806440000 2.7940310000
C 0.0743410000 3.7054960000 -1.8684520000
C 2.2387510000 2.4280950000 -1.9252270000
C 2.0695550000 4.5477030000 -0.5845090000
H 1.4307910000 5.1802600000 0.0414750000
H 2.3941460000 5.1431260000 -1.4444320000
H 2.9559480000 4.2757600000 -0.0025650000
H 1.7290270000 1.5236030000 -2.2720430000
H 3.1313980000 2.1224380000 -1.3696060000
H 2.5642860000 2.9914010000 -2.8052070000
H -0.4772680000 2.8249290000 -2.2120110000
H 0.3701090000 4.2899830000 -2.7461420000
H -0.6040750000 4.3203380000 -1.2669750000
H 0.1932460000 3.0820090000 0.8576030000
C -4.9837700000 1.2986230000 1.3215900000
C -5.7650510000 0.5921330000 0.4106950000
C -5.1725300000 -0.3480030000 -0.4339660000
H -3.3631730000 -1.3234120000 -1.0291410000
H -3.0050980000 1.6130780000 2.0979510000
H -5.4402560000 2.0266020000 1.9841900000
H -5.7814420000 -0.9061750000 -1.1374790000
H -6.8349500000 0.7675970000 0.3609990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.424383 (Hartree/Particle)
Thermal correction to Energy= 0.451373
Thermal correction to Enthalpy= 0.452318
Thermal correction to Gibbs (Free) Energy= 0.363959
Sum of electronic and zero-point Energies= -1176.840231
Sum of electronic and thermal Energies= -1176.813240
Sum of electronic and thermal Enthalpies= -1176.812296
Sum of electronic and thermal (Free) Energies= -1176.900655

cTS

C -1.5291570000 1.4662530000 0.2816970000
C -0.3335930000 0.9229910000 0.4427480000
C -1.9934660000 2.4093660000 -0.8135740000
H -2.3342300000 1.0938220000 0.9166440000
C 1.0310440000 0.8906790000 0.3712840000
C -0.8895250000 2.7469000000 -1.8178480000
C -3.1421900000 1.6867240000 -1.5458340000
C -2.5327850000 3.6904390000 -0.1527220000
C 1.5241950000 -0.4275330000 0.0378330000
C 1.9656540000 2.0333440000 0.7592430000
H -1.3022030000 3.3529570000 -2.6301180000
H -0.0813530000 3.3194150000 -1.3573460000
H -0.4575430000 1.8413360000 -2.2552480000
H -3.9513410000 1.4214310000 -0.8570540000
H -3.5566640000 2.3357860000 -2.3242170000
H -2.7876290000 0.7656730000 -2.0189350000
H -2.9430790000 4.3595520000 -0.9162900000
H -3.3320660000 3.4623160000 0.5603510000
H -1.7423060000 4.2256690000 0.3816040000
C 0.5085190000 -1.3996990000 0.1549100000
O 2.7283270000 -0.6139310000 -0.3579030000
C 2.7592370000 2.4736390000 -0.4889270000
C 2.9437320000 1.5272710000 1.8402830000
C 1.1889690000 3.2269080000 1.3288480000
C -0.6241280000 -1.0131050000 0.8842570000
H 0.5687040000 -2.3385770000 -0.3841200000
B 3.2926660000 -2.0459260000 -0.5612480000
H 3.4381740000 3.2859120000 -0.2092880000
H 3.3511480000 1.6498200000 -0.8912660000
H 2.0939750000 2.8426150000 -1.2749580000
H 3.5567720000 0.7009910000 1.4765890000
H 1.8967810000 4.0068970000 1.6247600000
H 0.5030290000 3.6610860000 0.5976060000
H 0.6073860000 2.9440200000 2.2120770000
H 3.6101860000 2.3443240000 2.1343350000
H 2.4020250000 1.1967760000 2.7332000000
C -1.9541990000 -1.5922680000 0.6246780000
H -0.4864660000 -0.6548800000 1.9042440000
F 3.0616330000 -2.7379860000 0.6269800000
F 4.6239960000 -1.8695470000 -0.8420640000
F 2.5754460000 -2.6160320000 -1.6161680000

C -2.8964750000 -1.6700440000 1.6558280000
C -2.3107160000 -2.0189360000 -0.6606090000
C -4.1673120000 -2.1831690000 1.4137480000
H -2.6275430000 -1.3370480000 2.6551720000
C -3.5785840000 -2.5325990000 -0.9027250000
H -1.5940690000 -1.9341050000 -1.4729420000
C -4.5087750000 -2.6150790000 0.1339660000
H -4.8883940000 -2.2480760000 2.2219660000
H -3.8457870000 -2.8631650000 -1.9010720000
H -5.4997970000 -3.0138810000 -0.0574670000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.424523 (Hartree/Particle)
Thermal correction to Energy= 0.450118
Thermal correction to Enthalpy= 0.451062
Thermal correction to Gibbs (Free) Energy= 0.369022
Sum of electronic and zero-point Energies= -1176.814350
Sum of electronic and thermal Energies= -1176.788755
Sum of electronic and thermal Enthalpies= -1176.787811
Sum of electronic and thermal (Free) Energies= -1176.869852

cPT

C -1.6881580000 1.2826660000 0.3231600000
C -0.5170580000 0.6476080000 0.5458720000
C -2.1529190000 2.3521330000 -0.6401990000
H -2.5399550000 0.7747850000 0.7774870000
C 0.8752460000 0.8922720000 0.2907590000
C -1.1185590000 2.7690720000 -1.6903980000
C -3.3379360000 1.6939660000 -1.3905810000
C -2.6891080000 3.5667060000 0.1419240000
C 1.5207890000 -0.3636970000 0.0252640000
C 1.6902840000 2.1375420000 0.5611490000
H -1.6090350000 3.3624790000 -2.4678870000
H -0.3172660000 3.3810370000 -1.2808180000
H -0.6702820000 1.8928960000 -2.1703600000
H -4.1359260000 1.3986330000 -0.7017910000
H -3.7564730000 2.4027430000 -2.1119390000
H -3.0135490000 0.8011710000 -1.9346600000
H -3.1332220000 4.2848790000 -0.5548760000
H -3.4649780000 3.2637430000 0.8526180000
H -1.8995870000 4.0752570000 0.6998910000
C 0.6799500000 -1.3706970000 0.4741020000
O 2.7189650000 -0.4527380000 -0.4592880000
C 2.4241420000 2.5959990000 -0.7199080000
C 2.7561720000 1.7280560000 1.6184990000
C 0.8748970000 3.2831250000 1.1731420000
C -0.5884410000 -0.8422420000 1.0101680000
H 0.9314810000 -2.4243570000 0.4588000000
B 3.4278590000 -1.8109500000 -0.4867350000
H 3.0413150000 3.4651050000 -0.4714570000
H 3.0701150000 1.8040370000 -1.1016190000
H 1.7257650000 2.8888940000 -1.5069760000
H 3.4197140000 0.9455980000 1.2505340000
H 1.5605320000 4.0784560000 1.4791630000
H 0.1638460000 3.7217190000 0.4764040000
H 0.3251500000 2.9536360000 2.0603340000
H 3.3572780000 2.6109560000 1.8556230000
H 2.2784690000 1.3860620000 2.5423700000
C -1.8113200000 -1.6329050000 0.6134610000
H -0.5225540000 -0.7998700000 2.1078160000
F 3.4481280000 -2.2853660000 0.8334440000
F 4.6844380000 -1.5671500000 -0.9881600000
F 2.6695640000 -2.6676220000 -1.2942570000
C -2.8096680000 -1.9219440000 1.5433090000
C -1.9667930000 -2.0585340000 -0.7093380000
C -3.9529310000 -2.6215550000 1.1589770000
H -2.6933390000 -1.6021570000 2.5759970000
C -3.1048920000 -2.7575620000 -1.0946490000
H -1.1892900000 -1.8408540000 -1.4385570000
C -4.1026970000 -3.0381460000 -0.1606420000
H -4.7214770000 -2.8445590000 1.8921580000
H -3.2126470000 -3.0880360000 -2.1227360000
H -4.9902770000 -3.5855300000 -0.4611990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.426834 (Hartree/Particle)
Thermal correction to Energy= 0.452471
Thermal correction to Enthalpy= 0.453416
Thermal correction to Gibbs (Free) Energy= 0.370928
Sum of electronic and zero-point Energies= -1176.828355
Sum of electronic and thermal Energies= -1176.802717
Sum of electronic and thermal Enthalpies= -1176.801773
Sum of electronic and thermal (Free) Energies= -1176.884261

ccRT

C -0.5837310000 1.7348740000 -0.5483790000
C -1.4749860000 0.9566790000 0.0411890000
C -2.6951060000 1.5152630000 0.8014020000
C -1.3378510000 -0.4952230000 -0.1953740000
O -2.4080940000 -1.1389110000 -0.3452450000
C -0.0496360000 -1.1613070000 -0.2827580000
B -2.5574690000 -2.7297850000 -0.5210730000
C 1.0379520000 -0.7122960000 0.3718670000
H -0.0484060000 -2.0985630000 -0.8265520000
F -1.9145340000 -3.0406730000 -1.7072670000
F -3.9099520000 -2.9118440000 -0.5545450000
F -1.9354360000 -3.2792290000 0.5824930000
H 0.9416950000 0.1921200000 0.9660680000
C 2.3599280000 -1.3361820000 0.3993760000
C 2.6521900000 -2.5338220000 -0.2716340000
C 3.3806840000 -0.6988160000 1.1193840000
H 1.8778310000 -3.0549120000 -0.8246320000
C 3.9321870000 -3.0691200000 -0.2246430000
C 4.6629580000 -1.2346380000 1.1645200000
H 3.1643620000 0.2278430000 1.6447910000
H 4.1453840000 -3.9973170000 -0.7444740000
C 4.9406000000 -2.4213780000 0.4906870000
H 5.4423260000 -0.7289800000 1.7250890000
H 5.9392350000 -2.8450310000 0.5245700000
C 0.2217520000 2.5209030000 -1.2044850000
H -0.0466150000 2.7351440000 -2.2406870000
C 1.5162600000 3.1488660000 -0.7046140000
C 1.5852540000 3.1633480000 0.8261360000
H 0.7612950000 3.7442120000 1.2514210000
H 1.5367690000 2.1546950000 1.2460070000
H 2.5272660000 3.6143990000 1.1541150000
C 1.5714590000 4.5940460000 -1.2263820000
H 2.5001410000 5.0774660000 -0.9057690000
H 1.5387710000 4.6208360000 -2.3208210000
H 0.7309680000 5.1828880000 -0.8449030000
C 2.6935310000 2.3439000000 -1.2831230000
H 3.6449710000 2.7981430000 -0.9849220000
H 2.6802530000 1.3100670000 -0.9261090000
H 2.6570420000 2.3224580000 -2.3771750000
C -2.4105680000 2.9644490000 1.2205700000
H -1.5306690000 3.0248470000 1.8700680000
H -2.2433580000 3.6123590000 0.3549300000
H -3.2683640000 3.3568150000 1.7752690000
C -3.9407180000 1.4910940000 -0.1038640000
H -3.7724980000 2.0881780000 -1.0063270000
H -4.2015350000 0.4745350000 -0.4018460000
H -4.7913840000 1.9220010000 0.4352960000
C -2.9400820000 0.6766250000 2.0687390000
H -3.7590450000 1.1189690000 2.6447180000
H -3.2171970000 -0.3528720000 1.8331560000
H -2.0502950000 0.6620360000 2.7082220000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.424528 (Hartree/Particle)
Thermal correction to Energy= 0.451427
Thermal correction to Enthalpy= 0.452371
Thermal correction to Gibbs (Free) Energy= 0.365730
Sum of electronic and zero-point Energies= -1176.840274
Sum of electronic and thermal Energies= -1176.813375
Sum of electronic and thermal Enthalpies= -1176.812431
Sum of electronic and thermal (Free) Energies= -1176.899073

ccTS

C 1.2938040000 1.7352270000 -0.6350040000
C 0.2387960000 1.0689360000 -0.1783420000
C 2.6594900000 2.0178770000 -0.0421440000
H 1.1258930000 2.2137900000 -1.6030420000
C -1.1293210000 1.0620860000 -0.1121840000
C 3.7531550000 1.2326920000 -0.7891870000
C 2.7218300000 1.7358730000 1.4630400000
C 2.8903170000 3.5283970000 -0.2654050000
C -1.6891530000 -0.2657270000 -0.0420750000

C -1.9999100000 2.3156440000 -0.0356110000
H 3.6632480000 0.1575230000 -0.6220790000
H 4.7400530000 1.5524030000 -0.4379520000
H 3.7028150000 1.4177770000 -1.8672520000
H 2.6732000000 0.6688110000 1.6783010000
H 1.9087070000 2.2427100000 1.9935630000
H 3.6701520000 2.1033910000 1.8675860000
H 2.8791190000 3.7808180000 -1.3311120000
H 3.8657390000 3.8179550000 0.1383140000
H 2.1220880000 4.1255530000 0.2364550000
C -0.6781280000 -1.2347210000 0.1321320000
O -2.9392430000 -0.4841020000 -0.2048990000
C -2.9157440000 2.2280760000 1.2013710000
C -2.8518500000 2.3751820000 -1.3226740000
C -1.1622530000 3.5973930000 0.0667930000
C 0.5532560000 -0.7810480000 0.6178160000
H -0.8214980000 -2.2528080000 -0.2132980000
B -3.5430130000 -1.9011660000 0.0160190000
H -3.5439850000 3.1232790000 1.2503590000
H -3.5689810000 1.3552080000 1.1615320000
H -2.3225990000 2.1821780000 2.1211700000
H -3.4981690000 1.5007060000 -1.4142720000
H -3.4813720000 3.2705610000 -1.2926520000
H -2.2147150000 2.4382050000 -2.2113680000
H -0.5048480000 3.5827320000 0.9423080000
H -0.5456550000 3.7605220000 -0.8217920000
H -1.8355840000 4.4542220000 0.1644300000
H 0.5713790000 -0.2386830000 1.5617980000
C 1.7746110000 -1.5449320000 0.2909200000
F -4.9008870000 -1.7252420000 -0.0643930000
F -3.1092030000 -2.3250850000 1.2711690000
F -3.0283660000 -2.7172510000 -0.9921580000
C 1.9857270000 -1.9830570000 -1.0212260000
C 2.7203370000 -1.8516040000 1.2745460000
C 3.1279110000 -2.7055070000 -1.3466310000
H 1.2590900000 -1.7324150000 -1.7893010000
C 3.8611190000 -2.5788420000 0.9511580000
H 2.5545170000 -1.5340380000 2.3004860000
C 4.0693530000 -3.0003040000 -0.3611650000
H 3.2871320000 -3.0340740000 -2.3683430000
H 4.5861160000 -2.8184150000 1.7220350000
H 4.9631990000 -3.5609230000 -0.6151110000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.424311 (Hartree/Particle)
Thermal correction to Energy= 0.449839
Thermal correction to Enthalpy= 0.450783
Thermal correction to Gibbs (Free) Energy= 0.369276
Sum of electronic and zero-point Energies= -1176.807963
Sum of electronic and thermal Energies= -1176.782435
Sum of electronic and thermal Enthalpies= -1176.781490
Sum of electronic and thermal (Free) Energies= -1176.862997

ccPT

C -1.6053250000 1.6962040000 -0.2408430000
C -0.5601270000 0.8365510000 -0.3152510000
C -3.0495770000 1.5843390000 -0.6747520000
H -1.4042920000 2.6444210000 0.2362290000
C 0.8006460000 1.1246350000 0.0958030000
C -3.8498170000 1.0261640000 0.5248890000
C -3.2979950000 0.7170080000 -1.9169970000
C -3.5344020000 3.0167320000 -0.9771750000
C 1.6376580000 0.0180610000 -0.2855790000
C 1.4100360000 2.3159140000 0.8063010000
H -3.5555770000 -0.0002140000 0.7574160000
H -4.9170790000 1.0333050000 0.2794590000
H -3.7050340000 1.6400090000 1.4199290000
H -3.1641140000 -0.3446920000 -1.7105010000
H -2.6449440000 1.0096000000 -2.7455980000
H -4.3333300000 0.8519050000 -2.2451600000
H -3.4159700000 3.6712540000 -0.1068280000
H -4.5949400000 3.0062100000 -1.2457280000
H -2.9788210000 3.4544050000 -1.8134790000
C 0.8389900000 -0.9595700000 -0.8499930000
O 2.9232580000 -0.0103270000 -0.0962090000
C 2.4895130000 2.9227000000 -0.1270340000
C 2.0721600000 1.7721810000 2.1018680000
C 0.4660760000 3.4523110000 1.2251570000
C -0.5868770000 -0.5738490000 -0.8800570000
H 1.2066350000 -1.9207070000 -1.1877510000
B 3.7309940000 -1.2422340000 -0.5009660000
H 2.9654820000 3.7589400000 0.3945170000
H 3.2560920000 2.1943460000 -0.3894420000
H 2.0319270000 3.3102400000 -1.0431800000
H 2.8162470000 1.0052350000 1.8904800000
H 2.5666070000 2.6054700000 2.6103570000
H 1.3142690000 1.3644190000 2.7792740000
H 0.0291740000 3.9759820000 0.3694940000
H -0.3281180000 3.1145750000 1.8982980000
H 1.0576710000 4.1897320000 1.7752640000
H -0.9478050000 -0.5735940000 -1.9150910000
C -1.4086180000 -1.5762290000 -0.0700040000
F 5.0390870000 -0.9500690000 -0.1893420000
F 3.5285580000 -1.4468220000 -1.8741860000
F 3.2265570000 -2.3317500000 0.2229770000
C -1.3267940000 -1.5923520000 1.3239650000
C -2.2057940000 -2.5209690000 -0.7142200000
C -2.0596200000 -2.5146980000 2.0622150000
H -0.6875090000 -0.8786130000 1.8368780000
C -2.9401350000 -3.4481190000 0.0234020000
H -2.2569860000 -2.5355010000 -1.8000510000
C -2.8740050000 -3.4424050000 1.4134640000
H -1.9891830000 -2.5146400000 3.1451120000
H -3.5604300000 -4.1749410000 -0.4910980000
H -3.4447640000 -4.1632440000 1.9897090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.427912 (Hartree/Particle)
Thermal correction to Energy= 0.453226
Thermal correction to Enthalpy= 0.454170
Thermal correction to Gibbs (Free) Energy= 0.372014
Sum of electronic and zero-point Energies= -1176.841141
Sum of electronic and thermal Energies= -1176.815827
Sum of electronic and thermal Enthalpies= -1176.814883
Sum of electronic and thermal (Free) Energies= -1176.897039

5a

cRT

C -1.9612520000 -1.3871540000 0.2888460000
C -0.7335080000 -1.1367680000 0.6607930000
C 0.4751280000 -0.8258520000 1.0918830000
C 1.5246140000 -0.4552600000 0.1257910000
C 1.4734830000 -0.8175230000 -1.2958930000
C 0.9540680000 -1.9674940000 -1.7336920000
H 1.9744760000 -0.1325160000 -1.9714840000
C 0.8108490000 -0.7051350000 2.5614020000
H -2.2336580000 -2.4279880000 0.1159430000
C -3.0141690000 -0.3743490000 0.0700710000
O 2.4739570000 0.2114260000 0.5943230000
H -0.0413280000 -1.0091820000 3.1699910000
H 1.0783990000 0.3265070000 2.8032120000
H 1.6726590000 -1.3311860000 2.8082340000
C -4.3052630000 -0.7979040000 -0.2599070000
C -2.7546440000 0.9974840000 0.1814670000
C -3.7696650000 1.9222100000 -0.0285360000
H -1.7540700000 1.3396170000 0.4303540000
C -5.0564690000 1.4922130000 -0.3545390000
H -3.5563990000 2.9826290000 0.0592480000
C -5.3214580000 0.1304770000 -0.4700410000
H -4.5160500000 -1.8600150000 -0.3507670000
H -5.8469240000 2.2172270000 -0.5191930000
H -6.3193510000 -0.2117230000 -0.7247150000
B 3.7878000000 0.7475700000 -0.2228150000
F 4.5245930000 1.3443610000 0.7526070000
F 3.2781070000 1.6127890000 -1.1695550000
F 4.3494580000 -0.3851180000 -0.7646780000
H 0.9899690000 -2.2173790000 -2.7887030000
H 0.5219110000 -2.7031970000 -1.0638630000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.225846 (Hartree/Particle)
Thermal correction to Energy= 0.243344
Thermal correction to Enthalpy= 0.244288
Thermal correction to Gibbs (Free) Energy= 0.177696
Sum of electronic and zero-point Energies= -901.877159
Sum of electronic and thermal Energies= -901.859661
Sum of electronic and thermal Enthalpies= -901.858717

Sum of electronic and thermal (Free) Energies= -901.925310

cTS

C 1.8638360000 1.3436650000 0.3812550000
C 0.6054430000 0.9760270000 0.5794480000
C 2.9537250000 0.4251160000 0.0188310000
H 2.1167990000 2.3988310000 0.4594610000
C -0.3585490000 0.1162070000 0.9830450000
C 4.2636420000 0.9195950000 -0.0309320000
C 2.7262430000 -0.9282730000 -0.2685030000
C -1.5971500000 0.2159660000 0.2485770000
C -0.2176630000 -0.8335890000 2.1347670000
C 5.3254120000 0.0775770000 -0.3441060000
H 4.4501270000 1.9684540000 0.1829850000
C 3.7886530000 -1.7664310000 -0.5824630000
H 1.7140580000 -1.3213010000 -0.2598010000
C -1.5902670000 1.3357780000 -0.6418690000
O -2.4975880000 -0.6678760000 0.3819970000
H 0.8006500000 -0.8403880000 2.5251270000
H -0.4838720000 -1.8395030000 1.7957360000
H -0.9174300000 -0.5740280000 2.9345260000
C 5.0908800000 -1.2677590000 -0.6190830000
H 6.3354540000 0.4729170000 -0.3758470000
H 3.5997140000 -2.8112210000 -0.8063670000
C -0.7266650000 2.3611630000 -0.3357220000
H -2.1277690000 1.2789930000 -1.5823780000
B -3.8917640000 -0.5137550000 -0.3411430000
H 5.9179500000 -1.9249040000 -0.8671950000
H -0.6378060000 2.7585880000 0.6716110000
H -0.3946560000 3.0374790000 -1.1206660000
F -4.6569070000 -1.5339540000 0.1494750000
F -3.6231330000 -0.6136880000 -1.7030380000
F -4.3531760000 0.7540460000 -0.0072050000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.225101 (Hartree/Particle)
Thermal correction to Energy= 0.241608
Thermal correction to Enthalpy= 0.242553
Thermal correction to Gibbs (Free) Energy= 0.178892
Sum of electronic and zero-point Energies= -901.852575
Sum of electronic and thermal Energies= -901.836068
Sum of electronic and thermal Enthalpies= -901.835124
Sum of electronic and thermal (Free) Energies= -901.898785

cPT

C -1.8021200000 1.4347160000 0.0728570000
C -0.4727100000 1.1563760000 0.0662030000
C 0.2308420000 -0.0625570000 -0.1944110000
C 1.6314950000 0.1410360000 -0.0114400000
C 1.8353670000 1.4810430000 0.3084490000
C 0.5656200000 2.2296270000 0.3164310000
C -0.2615730000 -1.3663160000 -0.6935330000
C -2.9412100000 0.5184500000 0.0746430000
O 2.4814590000 -0.8221370000 -0.1670490000
H -1.2687170000 -1.3180400000 -1.1051650000
H -0.2458270000 -2.1004840000 0.1215650000
H 0.4511920000 -1.7395490000 -1.4354370000
C -4.0985690000 0.8637080000 -0.6407630000
C -2.9355500000 -0.6640980000 0.8286180000
C -4.0445260000 -1.5015740000 0.8315380000
H -2.0694000000 -0.9079960000 1.4350940000
C -5.1720950000 -1.1703950000 0.0818770000
H -4.0322330000 -2.4094160000 1.4254770000
C -5.1983030000 0.0149390000 -0.6527170000
H -4.1234200000 1.7920940000 -1.2044500000
H -6.0358830000 -1.8271290000 0.0825500000
H -6.0797990000 0.2810210000 -1.2264460000
B 3.9797050000 -0.5179620000 -0.0451330000
F 4.2717440000 0.4842110000 -0.9832540000
F 4.6333710000 -1.6988400000 -0.2961990000
F 4.1991890000 -0.0310210000 1.2516740000
H 0.5449380000 2.9790160000 -0.4879280000
H 0.4058620000 2.7726300000 1.2570450000
H -2.0632100000 2.4931270000 0.1125050000
H 2.8075680000 1.9127550000 0.5107440000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227836 (Hartree/Particle)
Thermal correction to Energy= 0.243942
Thermal correction to Enthalpy= 0.244886
Thermal correction to Gibbs (Free) Energy= 0.182438
Sum of electronic and zero-point Energies= -901.899642
Sum of electronic and thermal Energies= -901.883537
Sum of electronic and thermal Enthalpies= -901.882592
Sum of electronic and thermal (Free) Energies= -901.945040

ccRT

C 1.8420590000 0.9172970000 -1.1311560000
C 0.6620410000 1.0638360000 -0.5887090000
C 3.0269010000 0.3629750000 -0.4462860000
H 1.9523150000 1.1956340000 -2.1786790000
C -0.5249930000 1.2471520000 -0.0426830000
C 4.1513960000 0.0136180000 -1.2010380000
C 3.0511240000 0.1654390000 0.9407140000
C -1.5463120000 0.1870400000 -0.1342900000
C -0.9377250000 2.5530880000 0.5976740000
C 5.2732980000 -0.5341260000 -0.5851490000
H 4.1450530000 0.1672930000 -2.2765180000
C 4.1714270000 -0.3828110000 1.5538160000
H 2.1939470000 0.4573220000 1.5420970000
C -1.2322250000 -1.2133960000 -0.4430360000
O -2.7233310000 0.5606740000 0.0655200000
H -0.0910900000 3.2393860000 0.6370340000
H -1.3110280000 2.3800550000 1.6106040000
H -1.7485680000 3.0125740000 0.0267310000
C 5.2854510000 -0.7365800000 0.7925510000
H 6.1381150000 -0.8027420000 -1.1831680000
H 4.1786420000 -0.5285630000 2.6292340000
C -0.0997220000 -1.8144870000 -0.0671550000
H -2.0286040000 -1.7707270000 -0.9245380000
B -4.0626680000 -0.3817360000 0.0826490000
H 6.1601290000 -1.1624810000 1.2731630000
H 0.6854470000 -1.3073860000 0.4841440000
H 0.0528590000 -2.8675080000 -0.2788780000
F -4.1505800000 -0.8871430000 -1.1980660000
F -5.0444440000 0.4999960000 0.4135390000
F -3.8009260000 -1.3421680000 1.0322880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.225883 (Hartree/Particle)
Thermal correction to Energy= 0.243324
Thermal correction to Enthalpy= 0.244268
Thermal correction to Gibbs (Free) Energy= 0.178520
Sum of electronic and zero-point Energies= -901.878694
Sum of electronic and thermal Energies= -901.861254
Sum of electronic and thermal Enthalpies= -901.860310
Sum of electronic and thermal (Free) Energies= -901.926058

ccTS

C -1.7825800000 1.0963480000 0.7002770000
C -0.5566690000 0.8874160000 0.2318900000
C -3.0106090000 0.4072930000 0.2821520000
H -1.8668370000 1.8076900000 1.5230030000
C 0.6919940000 1.3046390000 -0.0942060000
C -4.0434360000 0.2182290000 1.2101750000
C -3.1836660000 -0.0582030000 -1.0290370000
C 1.7102790000 0.2920900000 0.0442520000
C 1.0339970000 2.6669540000 -0.6163700000
C -5.2062760000 -0.4512280000 0.8458680000
H -3.9255010000 0.5870060000 2.2252390000
C -4.3474100000 -0.7283540000 -1.3911570000
H -2.4206770000 0.1391260000 -1.7765250000
C 1.1394050000 -0.9770370000 0.3721920000
O 2.9391590000 0.5971220000 -0.0425680000
H 0.1544420000 3.3090510000 -0.6689080000
H 1.4977770000 2.5949160000 -1.6043530000
H 1.7762550000 3.1219160000 0.0473150000
C -5.3583690000 -0.9320340000 -0.4537670000
H -5.9949340000 -0.5981300000 1.5765540000
H -4.4709250000 -1.0796710000 -2.4104240000
C -0.1805120000 -1.1574880000 0.0263990000
H 1.6847250000 -1.6651550000 1.0093900000
B 4.0479680000 -0.5226970000 0.0098990000
H -6.2672090000 -1.4518860000 -0.7386170000
H -0.5514810000 -0.9190110000 -0.9668780000
H -0.7893220000 -1.8830470000 0.5611520000

F 4.0005540000 -1.0421880000 1.3003110000
F 5.2157800000 0.1224360000 -0.2856950000
F 3.6707430000 -1.4733650000 -0.9321610000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.224754 (Hartree/Particle)
Thermal correction to Energy= 0.241284
Thermal correction to Enthalpy= 0.242228
Thermal correction to Gibbs (Free) Energy= 0.178687
Sum of electronic and zero-point Energies= -901.851303
Sum of electronic and thermal Energies= -901.834773
Sum of electronic and thermal Enthalpies= -901.833829
Sum of electronic and thermal (Free) Energies= -901.897370

ccPT

C 1.7576480000 0.8592360000 -0.0000010000
C 0.5182040000 0.2981110000 -0.0000010000
C -0.6871860000 1.0676640000 -0.0000010000
C -1.8259810000 0.2080270000 0.0000000000
C -1.3640960000 -1.0998730000 0.0000000000
C 0.1175900000 -1.1568400000 0.0000000000
C -0.8624660000 2.5344100000 -0.0000020000
O -3.0318230000 0.6828920000 0.0000000000
H 0.0683750000 3.1009940000 -0.0000020000
H -1.4673990000 2.8135900000 0.8703150000
H -1.4673990000 2.8135890000 -0.8703190000
H -2.0073420000 -1.9707470000 0.0000010000
C 3.0844350000 0.2601570000 0.0000000000
H 1.7787840000 1.9471510000 -0.0000010000
C 4.1813290000 1.1414150000 0.0000010000
C 5.4860260000 0.6658110000 0.0000020000
C 5.7218330000 -0.7068690000 0.0000010000
C 4.6472610000 -1.5968490000 -0.0000010000
C 3.3429120000 -1.1231120000 -0.0000020000
H 4.0023050000 2.2130520000 0.0000020000
H 6.3164860000 1.3636590000 0.0000030000
H 6.7391270000 -1.0844380000 0.0000010000
H 4.8285910000 -2.6664500000 -0.0000020000
H 2.5314560000 -1.8381800000 -0.0000030000
B -4.2106980000 -0.2946800000 0.0000010000
F -5.3488630000 0.4746060000 0.0000000000
F -4.0868750000 -1.0934200000 1.1473350000
F -4.0868750000 -1.0934210000 -1.1473330000
H 0.4917730000 -1.6897820000 0.8836830000
H 0.4917720000 -1.6897820000 -0.8836830000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227719 (Hartree/Particle)
Thermal correction to Energy= 0.244148
Thermal correction to Enthalpy= 0.245092
Thermal correction to Gibbs (Free) Energy= 0.178146
Sum of electronic and zero-point Energies= -901.904092
Sum of electronic and thermal Energies= -901.887663
Sum of electronic and thermal Enthalpies= -901.886719
Sum of electronic and thermal (Free) Energies= -901.953665

5b

cRT

C 2.0058900000 0.6519350000 1.1891470000
C 0.7895380000 0.1872100000 1.3092740000
C -0.4067950000 -0.3571660000 1.4235020000
C -1.4669930000 -0.0071220000 0.4562410000
C -1.4706210000 1.2262390000 -0.3201010000
C -0.9612430000 2.3816030000 0.1334850000
H -2.0056200000 1.1872400000 -1.2635540000
H -0.5097130000 2.4174300000 1.1224470000
C -1.0136130000 3.6683220000 -0.6177240000
C -0.7161330000 -1.4422010000 2.4301680000
H 2.2655590000 1.5440210000 1.7587250000
C 3.0624830000 0.0740960000 0.3333900000
O -2.3702230000 -0.8680160000 0.3287520000
H 0.1404190000 -1.6066790000 3.0847280000
H -0.9625910000 -2.3738200000 1.9148920000
H -1.5844030000 -1.1651500000 3.0344120000
C 4.3463150000 0.6270140000 0.3716970000
C 2.8127280000 -1.0089490000 -0.5188790000
C 3.8299730000 -1.5280550000 -1.3097120000
H 1.8174980000 -1.4420740000 -0.5639400000
C 5.1095130000 -0.9733450000 -1.2637100000
H 3.6238330000 -2.3664280000 -1.9672250000
C 5.3648150000 0.1053850000 -0.4216030000
H 4.5497880000 1.4686370000 1.0283120000
H 5.9016640000 -1.3802890000 -1.8837860000
H 6.3570260000 0.5432160000 -0.3809960000
B -3.6849630000 -0.7577100000 -0.6195250000
F -4.3645860000 -1.9035040000 -0.3344800000
F -3.1922970000 -0.6921040000 -1.9089590000
F -4.3170170000 0.4006050000 -0.2222250000
H -1.4799860000 3.5498690000 -1.5976500000
H -0.0012540000 4.0659970000 -0.7512670000
H -1.5756650000 4.4159330000 -0.0475600000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.253812 (Hartree/Particle)
Thermal correction to Energy= 0.273010
Thermal correction to Enthalpy= 0.273955
Thermal correction to Gibbs (Free) Energy= 0.203359
Sum of electronic and zero-point Energies= -941.164361
Sum of electronic and thermal Energies= -941.145163
Sum of electronic and thermal Enthalpies= -941.144219
Sum of electronic and thermal (Free) Energies= -941.214815

cTS

C 1.8643930000 1.0416290000 0.6757360000
C 0.6060590000 0.6430560000 0.8009920000
C 2.9563620000 0.2177300000 0.1363740000
H 2.1166820000 2.0638760000 0.9522140000
C -0.3363220000 -0.3060150000 1.0234260000
C 4.2653180000 0.7151080000 0.1853450000
C 2.7320280000 -1.0509140000 -0.4170700000
C -1.5781420000 -0.0666750000 0.3331550000
C -0.1696730000 -1.4737670000 1.9471600000
C 5.3288130000 -0.0444800000 -0.2906190000
H 4.4497590000 1.6999610000 0.6058750000
C 3.7959990000 -1.8065810000 -0.8933980000
H 1.7206190000 -1.4395560000 -0.4876900000
C -1.5922290000 1.2187670000 -0.2797690000
O -2.4683460000 -0.9737900000 0.2678000000
H 0.8536340000 -1.5488790000 2.3170250000
H -0.4296220000 -2.3892700000 1.4065820000
H -0.8624800000 -1.3988500000 2.7905740000
C 5.0971820000 -1.3079490000 -0.8297290000
H 6.3380050000 0.3515020000 -0.2425390000
H 3.6090090000 -2.7854810000 -1.3226250000
C -0.7310170000 2.1729360000 0.2351160000
H -2.1556570000 1.3771850000 -1.1940970000
B -3.8592000000 -0.6808440000 -0.3971810000
H 5.9254830000 -1.9001170000 -1.2048370000
C -0.2874980000 3.3617260000 -0.5633210000
H -0.6788610000 2.3056160000 1.3147820000
F -4.3454810000 0.4698680000 0.2170820000
F -4.6118520000 -1.7975890000 -0.1580030000
F -3.6005520000 -0.4573980000 -1.7485840000
H -0.2788430000 3.1528120000 -1.6344850000
H 0.7127920000 3.6827610000 -0.2599620000
H -0.9644210000 4.2016200000 -0.3721560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.253042 (Hartree/Particle)
Thermal correction to Energy= 0.271259
Thermal correction to Enthalpy= 0.272203
Thermal correction to Gibbs (Free) Energy= 0.204663
Sum of electronic and zero-point Energies= -941.139494
Sum of electronic and thermal Energies= -941.121277
Sum of electronic and thermal Enthalpies= -941.120333
Sum of electronic and thermal (Free) Energies= -941.187872

cPT

C -1.8128840000 1.2431930000 -0.2865980000
C -0.4850760000 0.9667840000 -0.2374300000
C 0.2002440000 -0.2906140000 -0.2536020000
C 1.6023760000 -0.0778210000 -0.1049550000
C 1.8233670000 1.2942980000 -0.0572010000
C 0.5701970000 2.0645430000 -0.2112850000
C 0.3809980000 3.1559050000 0.8512390000

C -0.3102600000 -1.6567030000 -0.5082950000
C -2.9512390000 0.3468040000 -0.0872620000
O 2.4379640000 -1.0657210000 -0.0632860000
H -1.3170270000 -1.6716610000 -0.9230970000
H -0.3036110000 -2.2294270000 0.4273980000
H 0.3974800000 -2.1688610000 -1.1676650000
C -4.1110490000 0.5284390000 -0.8564770000
C -2.9409620000 -0.6468540000 0.9022870000
C -4.0477560000 -1.4665390000 1.0878580000
H -2.0722920000 -0.7539720000 1.5439530000
C -5.1781970000 -1.3056740000 0.2884080000
H -4.0313280000 -2.2263530000 1.8621820000
C -5.2089020000 -0.3051800000 -0.6828210000
H -4.1395570000 1.3142050000 -1.6061940000
H -6.0403940000 -1.9486140000 0.4323260000
H -6.0924700000 -0.1696980000 -1.2976670000
H 0.5812090000 2.5410700000 -1.2055980000
B 3.9389130000 -0.7620090000 -0.0002960000
F 4.2446650000 0.0298350000 -1.1183090000
F 4.5787190000 -1.9768470000 -0.0089830000
F 4.1647380000 -0.0287720000 1.1743220000
H 1.2291620000 3.8450420000 0.8354770000
H 0.3141950000 2.7145480000 1.8493540000
H -0.5254840000 3.7375760000 0.6663430000
H -2.0776280000 2.2861080000 -0.4631720000
H 2.8012280000 1.7444200000 0.0676560000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256403 (Hartree/Particle)
Thermal correction to Energy= 0.273992
Thermal correction to Enthalpy= 0.274936
Thermal correction to Gibbs (Free) Energy= 0.209239
Sum of electronic and zero-point Energies= -941.179141
Sum of electronic and thermal Energies= -941.161552
Sum of electronic and thermal Enthalpies= -941.160607
Sum of electronic and thermal (Free) Energies= -941.226304

ccRT

C -1.7898670000 -1.1280420000 -1.1456440000
C -0.6180720000 -1.2847430000 -0.5867470000
C -2.9844390000 -0.5888200000 -0.4650360000
H -1.8838320000 -1.3770620000 -2.2020340000
C 0.5676980000 -1.4544050000 -0.0362030000
C -4.0777860000 -0.1706380000 -1.2308740000
C -3.0462170000 -0.4659360000 0.9294390000
C 1.5642700000 -0.3637810000 -0.1041230000
C 1.0115520000 -2.7640270000 0.5739500000
C -5.2032420000 0.3739380000 -0.6185090000
H -4.0434590000 -0.2673870000 -2.3124910000
C -4.1699930000 0.0793200000 1.5393730000
H -2.2159350000 -0.8151440000 1.5378710000
C 1.2060640000 1.0340500000 -0.3055890000
O 2.7575750000 -0.7303740000 0.0154520000
H 1.8343440000 -3.1883790000 -0.0068440000
H 0.1827150000 -3.4726170000 0.5959970000
H 1.3796600000 -2.6056970000 1.5913080000
C -5.2512960000 0.5038370000 0.7672810000
H -6.0431640000 0.6962220000 -1.2255200000
H -4.2062630000 0.1657450000 2.6206670000
C 0.0486560000 1.5659950000 0.1179810000
H 1.9785740000 1.6591220000 -0.7419370000
B 4.0649270000 0.2335300000 0.0543050000
H -6.1290630000 0.9265030000 1.2451570000
C -0.3178260000 3.0025350000 -0.0319090000
H -0.6775730000 0.9433180000 0.6355780000
F 5.0849590000 -0.6426460000 0.2734720000
F 3.8289560000 1.1120120000 1.0898820000
F 4.0965310000 0.8486940000 -1.1823780000
H -0.4655510000 3.4581080000 0.9532930000
H -1.2719660000 3.0872080000 -0.5641380000
H 0.4452430000 3.5671800000 -0.5711670000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.254019 (Hartree/Particle)
Thermal correction to Energy= 0.273113
Thermal correction to Enthalpy= 0.274057
Thermal correction to Gibbs (Free) Energy= 0.204341
Sum of electronic and zero-point Energies= -941.166173
Sum of electronic and thermal Energies= -941.147079
Sum of electronic and thermal Enthalpies= -941.146135
Sum of electronic and thermal (Free) Energies= -941.215850

ccTS

C 1.7084080000 1.1596410000 -0.7832690000
C 0.4820530000 0.9427230000 -0.3111230000
C 2.9504450000 0.5619470000 -0.2818970000
H 1.7840920000 1.7944210000 -1.6670460000
C -0.7659480000 1.4072790000 -0.0446250000
C 4.0059470000 0.3098730000 -1.1692660000
C 3.1103020000 0.2334130000 1.0722500000
C -1.7829970000 0.3880580000 -0.0614920000
C -1.1007630000 2.8216880000 0.3151930000
C 5.1768740000 -0.2912930000 -0.7212230000
H 3.8971410000 0.5718230000 -2.2179650000
C 4.2821670000 -0.3682430000 1.5182680000
H 2.3254430000 0.4798950000 1.7813570000
C -1.2146460000 -0.9033860000 -0.2259000000
O -3.0159870000 0.7026730000 -0.0103950000
H -0.2210950000 3.4649830000 0.2807390000
H -1.5536280000 2.8689980000 1.3098840000
H -1.8522490000 3.1940440000 -0.3885330000
C 5.3149550000 -0.6384550000 0.6220770000
H 5.9826000000 -0.4900250000 -1.4203560000
H 4.3945350000 -0.6148890000 2.5690390000
C 0.1249770000 -1.0507250000 0.1073010000
H -1.7747920000 -1.6820800000 -0.7340560000
B -4.1171600000 -0.4085720000 0.0804490000
H 6.2298360000 -1.1055490000 0.9717070000
C 0.9588830000 -2.1472540000 -0.4859080000
H 0.4653020000 -0.7013240000 1.0820950000
F -5.2908890000 0.2650950000 0.2820670000
F -3.7499310000 -1.2305320000 1.1432830000
F -4.0697910000 -1.1019030000 -1.1282720000
H 0.8925630000 -3.0348890000 0.1530140000
H 2.0118720000 -1.8582600000 -0.5243310000
H 0.6236220000 -2.4112090000 -1.4906660000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.253147 (Hartree/Particle)
Thermal correction to Energy= 0.271186
Thermal correction to Enthalpy= 0.272131
Thermal correction to Gibbs (Free) Energy= 0.205692
Sum of electronic and zero-point Energies= -941.139014
Sum of electronic and thermal Energies= -941.120974
Sum of electronic and thermal Enthalpies= -941.120030
Sum of electronic and thermal (Free) Energies= -941.186469

ccPT

C -1.7027630000 1.0430150000 -0.0672420000
C -0.4770130000 0.4551090000 -0.0869000000
C 0.7439820000 1.2008710000 -0.0764490000
C 1.8627930000 0.3192150000 -0.0677750000
C 1.3694460000 -0.9779330000 -0.0533790000
C -0.1140680000 -1.0188610000 -0.0543940000
C 0.9464630000 2.6644080000 -0.0935680000
O 3.0797450000 0.7642070000 -0.0660890000
H 0.0271780000 3.2473150000 -0.0417290000
H 1.4964640000 2.9296520000 -1.0042900000
H 1.6121470000 2.9361150000 0.7330470000
C -0.6606630000 -1.7808190000 1.1661150000
H 1.9937370000 -1.8628280000 -0.0177940000
C -3.0296380000 0.4414000000 -0.1181040000
H -0.4484600000 -1.5213260000 -0.9729220000
H -1.7143560000 2.1268760000 0.0322340000
C -4.0961320000 1.1623980000 0.4474100000
C -5.3833860000 0.6421280000 0.4557460000
C -5.6351830000 -0.5980730000 -0.1291950000
C -4.5953870000 -1.3098450000 -0.7255630000
C -3.3039880000 -0.7978110000 -0.7209970000
H -3.9041510000 2.1325100000 0.8974000000
H -6.1914110000 1.2053160000 0.9104820000
H -6.6420140000 -1.0027000000 -0.1330920000
H -4.7928580000 -2.2635590000 -1.2035400000
H -2.5148830000 -1.3475630000 -1.2193830000
B 4.2329270000 -0.2432410000 -0.0408830000
F 5.3908600000 0.4955870000 -0.0497500000
F 4.0936310000 -1.0611990000 -1.1729870000

F 4.0824230000 -1.0157350000 1.1213250000
H -0.3303420000 -1.2989580000 2.0902610000
H -0.2897170000 -2.8087500000 1.1635080000
H -1.7529320000 -1.8086370000 1.1574180000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.256372 (Hartree/Particle)
Thermal correction to Energy= 0.274168
Thermal correction to Enthalpy= 0.275113
Thermal correction to Gibbs (Free) Energy= 0.208566
Sum of electronic and zero-point Energies= -941.184091
Sum of electronic and thermal Energies= -941.166294
Sum of electronic and thermal Enthalpies= -941.165350
Sum of electronic and thermal (Free) Energies= -941.231897

5c

c/s RT

C 2.0234600000 0.1607440000 1.2710960000
C 0.8318360000 -0.3712900000 1.3505410000
C -0.3456570000 -0.9638660000 1.4099860000
C -1.4030800000 -0.5791310000 0.4529070000
C -1.4056520000 0.6900690000 -0.2623900000
C -0.9226960000 1.8261340000 0.2614540000
H -1.9080790000 0.6891010000 -1.2247220000
H -0.5116390000 1.8247690000 1.2708900000
C -0.9331890000 3.1536470000 -0.4297710000
C -0.6337560000 -2.1222140000 2.3374150000
H 2.2323240000 1.0265810000 1.8991240000
C 3.1111370000 -0.2988800000 0.3839760000
O -2.2945840000 -1.4431220000 0.2721660000
H 0.2209110000 -2.3078880000 2.9887760000
H -0.8504190000 -3.0231380000 1.7580880000
H -1.5147160000 -1.9098350000 2.9494270000
C 0.5080210000 3.6715470000 -0.5534580000
C -1.8180950000 4.1438210000 0.3408770000
H -1.3482600000 3.0197190000 -1.4352910000
H 0.9544390000 3.8197630000 0.4369760000
H 0.5203840000 4.6344260000 -1.0728370000
H 1.1374900000 2.9716780000 -1.1106470000
H -1.4392650000 4.2962350000 1.3581420000
H -2.8478200000 3.7830060000 0.4091820000
H -1.8256520000 5.1147730000 -0.1634630000
C 4.3609760000 0.3233480000 0.4627550000
C 2.9227850000 -1.3337230000 -0.5409070000
C 3.9671060000 -1.7382130000 -1.3628070000
H 1.9539800000 -1.8192000000 -0.6176570000
C 5.2126370000 -1.1151690000 -1.2760500000
H 3.8087340000 -2.5403260000 -2.0764380000
C 5.4065970000 -0.0832630000 -0.3619220000
H 4.5161410000 1.1288630000 1.1754850000
H 6.0260550000 -1.4327100000 -1.9203670000
H 6.3719340000 0.4073430000 -0.2893180000
B -3.5967970000 -1.2900160000 -0.6837820000
F -4.2781440000 -2.4493430000 -0.4637160000
F -3.0896580000 -1.1606810000 -1.9631080000
F -4.2378060000 -0.1532500000 -0.2393950000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311346 (Hartree/Particle)
Thermal correction to Energy= 0.333167
Thermal correction to Enthalpy= 0.334111
Thermal correction to Gibbs (Free) Energy= 0.256843
Sum of electronic and zero-point Energies= -1019.721603
Sum of electronic and thermal Energies= -1019.699782
Sum of electronic and thermal Enthalpies= -1019.698838
Sum of electronic and thermal (Free) Energies= -1019.776106

c/s TS

C 1.9056470000 0.6509770000 0.7128180000
C 0.6473890000 0.2256540000 0.7594030000
C -0.2236250000 -0.8005880000 0.9366170000
C -1.5013740000 -0.6008810000 0.3098730000
C -1.6195900000 0.7136370000 -0.2120600000
C -0.7826860000 1.6933480000 0.3041920000
C -0.5744890000 2.9821960000 -0.4618090000
C 0.0509330000 -2.0102560000 1.7769190000
H 2.1326540000 1.6474460000 1.0813410000
C 3.0275170000 -0.1144010000 0.1533900000
O -2.3429240000 -1.5548660000 0.2239140000
H 1.0942440000 -2.0519720000 2.0923570000
H -0.1900360000 -2.9045910000 1.1939170000
H -0.6007450000 -2.0228800000 2.6557260000
C 0.7587020000 3.6715080000 -0.1607540000
C -1.7524700000 3.9147080000 -0.1222440000
H -0.6121460000 2.7530550000 -1.5326380000
H 0.9004650000 3.8064720000 0.9186630000
H 0.7746260000 4.6641230000 -0.6195720000
H 1.6048820000 3.1078240000 -0.5603130000
H -1.7448320000 4.1786890000 0.9412650000
H -2.7146180000 3.4472210000 -0.3477890000
H -1.6745250000 4.8398110000 -0.7010300000
C 4.3281460000 0.3829640000 0.3137760000
C 2.8429340000 -1.3268980000 -0.5267390000
C 3.9367830000 -2.0310750000 -1.0141180000
H 1.8396530000 -1.7096380000 -0.6873870000
C 5.2284200000 -1.5348950000 -0.8372970000
H 3.7809670000 -2.9666870000 -1.5411910000
C 5.4212120000 -0.3249320000 -0.1739460000
H 4.4812100000 1.3262230000 0.8311950000
H 6.0800640000 -2.0863750000 -1.2221280000
H 6.4230760000 0.0693680000 -0.0384600000
H -0.6905200000 1.7981000000 1.3870880000
H -2.2543210000 0.8965490000 -1.0739790000
B -3.7748130000 -1.2958930000 -0.3499080000
F -4.2904450000 -0.2153810000 0.3638910000
F -4.4594240000 -2.4644620000 -0.1543150000
F -3.6027250000 -0.9669060000 -1.6947940000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310701 (Hartree/Particle)
Thermal correction to Energy= 0.331351
Thermal correction to Enthalpy= 0.332295
Thermal correction to Gibbs (Free) Energy= 0.259106
Sum of electronic and zero-point Energies= -1019.694388
Sum of electronic and thermal Energies= -1019.673738
Sum of electronic and thermal Enthalpies= -1019.672794
Sum of electronic and thermal (Free) Energies= -1019.745983

c/s PT

C 1.8354860000 0.8254890000 0.5334800000
C 0.5224080000 0.5462310000 0.3227990000
C -0.0967930000 -0.7266300000 0.0803590000
C -1.5140760000 -0.5861040000 0.1170920000
C -1.8029710000 0.7338940000 0.4346300000
C -0.5845130000 1.5719750000 0.5191880000
C -0.6195960000 2.7446780000 -0.5117710000
C 0.4964830000 -2.0767690000 -0.0525350000
H 2.0531400000 1.7954710000 0.9778690000
C 3.0159740000 0.0166570000 0.2268750000
O -2.3065230000 -1.5937960000 -0.0730560000
H 1.4878500000 -2.1547510000 0.3927920000
H 0.5781670000 -2.3352280000 -1.1158320000
H -0.1939800000 -2.8037460000 0.3832860000
C 0.6178630000 3.6437950000 -0.4293320000
C -1.8893950000 3.5855280000 -0.3308500000
H -0.6477470000 2.2863530000 -1.5088650000
H 0.7621850000 4.0268520000 0.5885030000
H 0.4935410000 4.5073590000 -1.0890410000
H 1.5293430000 3.1284020000 -0.7416580000
H -1.9596600000 3.9730640000 0.6925540000
H -2.7992710000 3.0214680000 -0.5473770000
H -1.8693440000 4.4431650000 -1.0089850000
C 4.0865040000 -0.0144870000 1.1334980000
C 3.1379050000 -0.6645170000 -0.9925560000
C 4.2859010000 -1.3933880000 -1.2801480000
H 2.3373290000 -0.5988740000 -1.7225720000
C 5.3253690000 -1.4530040000 -0.3535360000
H 4.3720030000 -1.9103970000 -2.2301310000
C 5.2245230000 -0.7608890000 0.8531990000
H 4.0131970000 0.5334210000 2.0687160000
H 6.2193560000 -2.0259360000 -0.5771770000
H 6.0373770000 -0.7963370000 1.5709150000
H -0.5018160000 2.0119040000 1.5262710000
H -2.8110870000 1.0978710000 0.5837370000
B -3.8177340000 -1.3652070000 0.0021700000
F -4.1016240000 -0.8751960000 1.2867490000

F -4.4066050000 -2.5792730000 -0.2530060000
F -4.1368980000 -0.3875770000 -0.9550500000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.313554 (Hartree/Particle)
Thermal correction to Energy= 0.333848
Thermal correction to Enthalpy= 0.334792
Thermal correction to Gibbs (Free) Energy= 0.262513
Sum of electronic and zero-point Energies= -1019.733479
Sum of electronic and thermal Energies= -1019.713186
Sum of electronic and thermal Enthalpies= -1019.712242
Sum of electronic and thermal (Free) Energies= -1019.784521

cc/s RT

C -1.5291630000 -1.7638430000 -0.9948800000
C -0.3558450000 -1.7878740000 -0.4174800000
C 0.8397720000 -1.7954990000 0.1378800000
C 1.7345230000 -0.6364550000 -0.0765790000
C 1.2339500000 0.6925670000 -0.3993660000
C 0.0464980000 1.1430010000 0.0351540000
C 1.3958900000 -2.9756880000 0.8995020000
O 2.9594960000 -0.8805310000 0.0362810000
H 2.2534150000 -3.3941380000 0.3665820000
H 0.6332540000 -3.7466160000 1.0162840000
H 1.7475640000 -2.6620600000 1.8862590000
H 1.9180960000 1.3428950000 -0.9351250000
B 4.1637700000 0.2030160000 -0.0645800000
F 4.1036320000 0.6917340000 -1.3556080000
F 5.2721260000 -0.5429850000 0.2037550000
F 3.8678910000 1.1551560000 0.8879870000
C -2.7480530000 -1.1866680000 -0.3940700000
C -3.8179910000 -0.8374970000 -1.2241470000
C -2.8425460000 -0.9279800000 0.9794100000
C -4.9477270000 -0.2171860000 -0.6983370000
H -3.7572550000 -1.0373810000 -2.2903000000
C -3.9707810000 -0.3074770000 1.5035320000
H -2.0308430000 -1.2230180000 1.6392510000
C -5.0249670000 0.0555450000 0.6653830000
H -5.7668610000 0.0559050000 -1.3557490000
H -4.0307960000 -0.1119670000 2.5694690000
H -5.9048580000 0.5402980000 1.0755830000
H -1.6007090000 -2.1408380000 -2.0144080000
H -0.5815550000 0.5054910000 0.6560310000
C -0.5063790000 2.5082420000 -0.2246800000
H 0.1903140000 3.0545640000 -0.8708890000
C -0.6542850000 3.2689040000 1.1013860000
H -1.3403170000 2.7421090000 1.7748300000
H 0.3092990000 3.3774300000 1.6064790000
H -1.0630410000 4.2674020000 0.9194750000
C -1.8609070000 2.3797230000 -0.9398370000
H -2.2708210000 3.3726990000 -1.1479560000
H -1.7622710000 1.8429750000 -1.8878700000
H -2.5822140000 1.8373820000 -0.3177260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311545 (Hartree/Particle)
Thermal correction to Energy= 0.333117
Thermal correction to Enthalpy= 0.334061
Thermal correction to Gibbs (Free) Energy= 0.259303
Sum of electronic and zero-point Energies= -1019.725567
Sum of electronic and thermal Energies= -1019.703995
Sum of electronic and thermal Enthalpies= -1019.703051
Sum of electronic and thermal (Free) Energies= -1019.777809

cc/s TS

C -1.5877010000 -1.4036090000 -0.8426760000
C -0.3440220000 -1.0800270000 -0.4707130000
C 0.8907250000 -1.5965750000 -0.2237720000
C 1.9356890000 -0.6165350000 -0.1419370000
C 1.4150600000 0.6935500000 -0.2683320000
C 0.0545450000 0.8844460000 -0.0403720000
O 3.1571370000 -0.9685480000 -0.0345450000
H 2.0391040000 1.4791270000 -0.6837720000
B 4.2686810000 0.1050690000 0.1963940000
F 4.3227310000 0.8714720000 -0.9681950000
F 5.4135770000 -0.6047230000 0.4392480000
F 3.8462400000 0.8763840000 1.2788480000
C -2.8299540000 -0.9480380000 -0.2206310000
C -4.0039720000 -0.8688450000 -0.9820240000
C -2.8766300000 -0.5974820000 1.1368460000
C -5.1816480000 -0.3980660000 -0.4153110000
H -3.9815450000 -1.1526430000 -2.0305310000
C -4.0568030000 -0.1290810000 1.7036620000
H -1.9929310000 -0.7218010000 1.7555830000
C -5.2082480000 -0.0170860000 0.9264810000
H -6.0804830000 -0.3260970000 -1.0189030000
H -4.0808870000 0.1383960000 2.7550250000
H -6.1288250000 0.3495330000 1.3687670000
H -1.6804910000 -2.0575440000 -1.7112950000
H -0.3770620000 0.5646930000 0.9107730000
C -0.5732190000 2.1441300000 -0.6196310000
H 0.0294160000 2.4299100000 -1.4893840000
C -0.4441220000 3.2508940000 0.4416390000
H -1.0401890000 3.0056890000 1.3283000000
H 0.5937710000 3.3911510000 0.7562520000
H -0.8126180000 4.1996550000 0.0402350000
C -2.0236950000 2.0224910000 -1.0872340000
H -2.3415880000 2.9814690000 -1.5070720000
H -2.1375270000 1.2612120000 -1.8621580000
H -2.6994180000 1.7801040000 -0.2622510000
C 1.1736700000 -3.0382940000 0.0670510000
H 1.9791220000 -3.3770950000 -0.5921760000
H 1.5384890000 -3.1596710000 1.0915380000
H 0.2921790000 -3.6624810000 -0.0819120000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310904 (Hartree/Particle)
Thermal correction to Energy= 0.331333
Thermal correction to Enthalpy= 0.332277
Thermal correction to Gibbs (Free) Energy= 0.260314
Sum of electronic and zero-point Energies= -1019.690094
Sum of electronic and thermal Energies= -1019.669665
Sum of electronic and thermal Enthalpies= -1019.668721
Sum of electronic and thermal (Free) Energies= -1019.740684

cc/s PT

C -1.6200970000 -1.3061230000 -0.2403220000
C -0.4141980000 -0.6869390000 -0.1760890000
C 0.8133510000 -1.4025250000 -0.3862450000
C 1.9174230000 -0.6109380000 0.0303230000
C 1.4132100000 0.6119880000 0.4512110000
C -0.0440500000 0.7399050000 0.2009960000
C 1.0161150000 -2.7788760000 -0.8844690000
O 3.1367760000 -1.0512740000 -0.0089640000
H 0.1286860000 -3.2266750000 -1.3317630000
H 1.3639940000 -3.4074990000 -0.0554680000
H 1.8389450000 -2.7703460000 -1.6067380000
C -0.3017420000 1.7787030000 -0.9477100000
H 2.0320180000 1.4007280000 0.8590320000
C -2.9438420000 -0.8070420000 0.1299960000
C -1.7887440000 2.0095070000 -1.2164470000
H -2.3020170000 1.1022750000 -1.5409300000
H -1.9028810000 2.7562320000 -2.0079220000
H -2.3010130000 2.3876940000 -0.3249080000
C 0.3954280000 3.1089850000 -0.6411100000
H 0.1534830000 1.3514170000 -1.8507830000
H 0.0776240000 3.5034200000 0.3316290000
H 0.1308780000 3.8504740000 -1.4001420000
H 1.4843390000 3.0174730000 -0.6378630000
H -0.5598860000 1.1006390000 1.0983100000
H -1.6180380000 -2.3304850000 -0.6097330000
C -4.0498520000 -1.2364630000 -0.6207380000
C -5.3259540000 -0.7689340000 -0.3337440000
C -5.5231220000 0.1050090000 0.7348000000
C -4.4402370000 0.5003260000 1.5176430000
C -3.1595540000 0.0509950000 1.2180100000
H -3.8993470000 -1.9233760000 -1.4490770000
H -6.1682050000 -1.0923580000 -0.9363500000
H -6.5209280000 0.4624650000 0.9673880000
H -4.5942410000 1.1555100000 2.3687090000
H -2.3307560000 0.3382360000 1.8541720000
B 4.2678090000 -0.0813190000 0.3370050000
F 5.4420120000 -0.7644650000 0.1379500000
F 4.0839990000 0.3217240000 1.6685770000
F 4.1283540000 1.0311300000 -0.5129160000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.313532 (Hartree/Particle)
Thermal correction to Energy= 0.333927
Thermal correction to Enthalpy= 0.334871
Thermal correction to Gibbs (Free) Energy= 0.262587
Sum of electronic and zero-point Energies= -1019.736991
Sum of electronic and thermal Energies= -1019.716596
Sum of electronic and thermal Enthalpies= -1019.715652
Sum of electronic and thermal (Free) Energies= -1019.787935

c/d RT

C 2.1681420000 0.3189350000 1.2852300000
C 1.0229970000 -0.3082710000 1.3548230000
C -0.0956770000 -1.0057750000 1.4067850000
C -1.2065460000 -0.6726850000 0.4924790000
C -1.3618720000 0.6292160000 -0.1407460000
C -0.9979930000 1.7768400000 0.4517740000
H -1.8940570000 0.6254040000 -1.0852370000
H -0.5522240000 1.7431920000 1.4447200000
C -1.2168820000 3.1542900000 -0.1004930000
C -0.2551830000 -2.2301160000 2.2792650000
H 2.3231820000 1.1645440000 1.9549790000
C 3.2722260000 -0.0142540000 0.3619700000
O -2.0126040000 -1.6099220000 0.2753850000
H 0.6280050000 -2.3676630000 2.9040160000
H -0.4018990000 -3.1176140000 1.6587660000
H -1.1372110000 -2.1304910000 2.9179370000
C -2.0910090000 3.9575440000 0.8789860000
C -1.7920640000 3.1807910000 -1.5151610000
H -0.2235090000 3.6286120000 -0.1178780000
H -3.0932840000 3.5219300000 0.9406100000
H -2.1878110000 4.9920820000 0.5375900000
H -1.6622490000 3.9718810000 1.8861000000
H -2.7958520000 2.7437090000 -1.5411220000
H -1.1605730000 2.6313540000 -2.2196010000
H -1.8688760000 4.2132930000 -1.8671150000
C 4.4768810000 0.6888730000 0.4610900000
C 3.1436910000 -1.0105200000 -0.6140720000
C 4.2023390000 -1.2979240000 -1.4663590000
H 2.2099530000 -1.5579350000 -0.7067000000
C 5.4027130000 -0.5945830000 -1.3592620000
H 4.0902440000 -2.0710920000 -2.2195890000
C 5.5370030000 0.3995210000 -0.3939860000
H 4.5857250000 1.4651280000 1.2137170000
H 6.2273750000 -0.8206120000 -2.0274420000
H 6.4669130000 0.9519800000 -0.3052200000
B -3.3478000000 -1.5337100000 -0.6418430000
F -3.9023280000 -2.7680900000 -0.4814640000
F -2.8926350000 -1.2752190000 -1.9213990000
F -4.0902150000 -0.4979200000 -0.1145090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311256 (Hartree/Particle)
Thermal correction to Energy= 0.332964
Thermal correction to Enthalpy= 0.333908
Thermal correction to Gibbs (Free) Energy= 0.257128
Sum of electronic and zero-point Energies= -1019.721211
Sum of electronic and thermal Energies= -1019.699503
Sum of electronic and thermal Enthalpies= -1019.698559
Sum of electronic and thermal (Free) Energies= -1019.775339

c/d TS

C -1.8943950000 0.5685590000 -0.9587820000
C -0.6587460000 0.0941800000 -1.0241720000
C 0.2564640000 -0.9017340000 -1.0799240000
C 1.4945320000 -0.5958420000 -0.4052360000
C 1.5428620000 0.7644450000 0.0084170000
C 0.7290230000 1.6587980000 -0.6645890000
C 0.2912870000 2.9752080000 -0.0739240000
C 0.0678240000 -2.1943590000 -1.8142130000
H -2.1015280000 1.5424140000 -1.3988890000
C -3.0128550000 -0.0957950000 -0.2727430000
O 2.3489300000 -1.5118990000 -0.1788440000
H -0.9512220000 -2.2962670000 -2.1893710000
H 0.2897740000 -3.0213170000 -1.1325200000
H 0.7758550000 -2.2718680000 -2.6446150000
C 1.3967680000 4.0226820000 -0.2980020000
C -0.1018050000 2.8643430000 1.3999950000
H -0.5886370000 3.3001940000 -0.6443750000
H 2.3036530000 3.7495990000 0.2502130000
H 1.0621560000 5.0009020000 0.0591510000
H 1.6567250000 4.1159600000 -1.3565860000
H 0.7615610000 2.6213210000 2.0271930000
H -0.8594010000 2.0885320000 1.5484680000
H -0.5092650000 3.8150370000 1.7553870000
C -4.2955340000 0.4574420000 -0.3793870000
C -2.8374920000 -1.2639980000 0.4824690000
C -3.9244170000 -1.8692970000 1.1007430000
H -1.8455230000 -1.6906690000 0.5967820000
C -5.1998150000 -1.3174430000 0.9797860000
H -3.7751900000 -2.7713390000 1.6851810000
C -5.3822050000 -0.1515960000 0.2394150000
H -4.4411900000 1.3666940000 -0.9563420000
H -6.0459910000 -1.7917450000 1.4660960000
H -6.3708870000 0.2857340000 0.1451500000
H 0.7062230000 1.6235100000 -1.7535860000
H 2.0943330000 1.0301040000 0.9044620000
B 3.7314870000 -1.1678960000 0.4765480000
F 4.2796720000 -0.1430560000 -0.2896150000
F 4.4464710000 -2.3334770000 0.4362460000
F 3.4472680000 -0.7296560000 1.7697130000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310650 (Hartree/Particle)
Thermal correction to Energy= 0.331394
Thermal correction to Enthalpy= 0.332338
Thermal correction to Gibbs (Free) Energy= 0.259019
Sum of electronic and zero-point Energies= -1019.697390
Sum of electronic and thermal Energies= -1019.676646
Sum of electronic and thermal Enthalpies= -1019.675702
Sum of electronic and thermal (Free) Energies= -1019.749021

c/d PT

C -1.8687210000 0.9116490000 -0.5959150000
C -0.5601360000 0.5663310000 -0.5003080000
C 0.0433290000 -0.7174460000 -0.2970550000
C 1.4599000000 -0.5771940000 -0.2360730000
C 1.7686220000 0.7575400000 -0.4723430000
C 0.5587210000 1.5807900000 -0.6836060000
C 0.4842470000 2.8421280000 0.2179340000
C -0.5616920000 -2.0684510000 -0.2677050000
H -2.0709410000 1.9223800000 -0.9519840000
C -3.0574290000 0.1371390000 -0.2386140000
O 2.2371170000 -1.5921170000 -0.0259260000
H -1.5738090000 -2.0964990000 -0.6689860000
H -0.5822840000 -2.4359590000 0.7658950000
H 0.0983240000 -2.7531570000 -0.8088700000
C 1.5748550000 3.8477670000 -0.1583960000
C 0.5523320000 2.4780360000 1.7027100000
H -0.4860750000 3.3156230000 0.0201260000
H 2.5735230000 3.4564900000 0.0615260000
H 1.4525020000 4.7702680000 0.4164820000
H 1.5371280000 4.1062970000 -1.2217170000
H 1.5234170000 2.0386480000 1.9553840000
H -0.2254670000 1.7592320000 1.9804330000
H 0.4176590000 3.3710010000 2.3197270000
C -4.2069900000 0.2294820000 -1.0380980000
C -3.1015580000 -0.6397960000 0.9278560000
C -4.2538040000 -1.3408110000 1.2635350000
H -2.2370060000 -0.6694030000 1.5834180000
C -5.3756820000 -1.2762790000 0.4389750000
H -4.2786960000 -1.9322980000 2.1727800000
C -5.3510570000 -0.4881560000 -0.7115170000
H -4.1920050000 0.8513670000 -1.9287710000
H -6.2734000000 -1.8270440000 0.7001710000
H -6.2272350000 -0.4266960000 -1.3484300000
H 0.5421120000 1.9177990000 -1.7335340000
H 2.7818860000 1.1389800000 -0.4964190000
B 3.7492370000 -1.3606400000 0.0298560000
F 4.1338400000 -0.8193510000 -1.2065460000
F 4.3197060000 -2.5834690000 0.2836080000
F 3.9850790000 -0.4219890000 1.0487840000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.313141 (Hartree/Particle)
Thermal correction to Energy= 0.333530
Thermal correction to Enthalpy= 0.334474
Thermal correction to Gibbs (Free) Energy= 0.262156

Sum of electronic and zero-point Energies= -1019.738244
Sum of electronic and thermal Energies= -1019.717855
Sum of electronic and thermal Enthalpies= -1019.716911
Sum of electronic and thermal (Free) Energies= -1019.789229

cc/d RT

C -1.6454270000 -1.4894630000 -1.2115530000
C -0.4750420000 -1.6677170000 -0.6561230000
C 0.7173050000 -1.8318980000 -0.1183950000
C 1.6542640000 -0.6874400000 -0.0942040000
C 1.2118820000 0.6988760000 -0.1439270000
C 0.0478290000 1.1076390000 0.3863280000
C 1.2281910000 -3.1643280000 0.3776750000
O 2.8688920000 -0.9958520000 -0.0357200000
H 2.0712870000 -3.4933710000 -0.2349800000
H 0.4375580000 -3.9144660000 0.3350730000
H 1.5884380000 -3.0762290000 1.4063450000
H 1.9306550000 1.4032020000 -0.5471250000
B 4.1137690000 0.0387640000 0.0728200000
F 4.0782890000 0.7722980000 -1.0981020000
F 5.1917110000 -0.7871610000 0.1864490000
F 3.8523440000 0.7989380000 1.1933390000
C -2.8503830000 -1.0234470000 -0.4971120000
C -3.9090880000 -0.4765510000 -1.2289520000
C -2.9427190000 -1.0686820000 0.8998530000
C -5.0260490000 0.0396110000 -0.5781290000
H -3.8495690000 -0.4403810000 -2.3131410000
C -4.0587420000 -0.5530000000 1.5489550000
H -2.1392920000 -1.5181880000 1.4775030000
C -5.1017990000 0.0083190000 0.8123190000
H -5.8365420000 0.4687840000 -1.1583570000
H -4.1178730000 -0.5940230000 2.6319180000
H -5.9720600000 0.4110960000 1.3201620000
H -1.7249610000 -1.6412350000 -2.2873470000
H -0.6045230000 0.3803870000 0.8662610000
C -0.4655690000 2.5159060000 0.4128000000
H -0.5719250000 2.7772710000 1.4763720000
C -1.8773000000 2.5391200000 -0.2024170000
H -1.8394480000 2.2636720000 -1.2617210000
H -2.5528550000 1.8421270000 0.3033600000
H -2.3032400000 3.5437280000 -0.1265460000
C 0.4589000000 3.5358500000 -0.2479490000
H 0.0290580000 4.5380400000 -0.1656370000
H 1.4462200000 3.5536610000 0.2223800000
H 0.5904870000 3.3154750000 -1.3130620000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311828 (Hartree/Particle)
Thermal correction to Energy= 0.333244
Thermal correction to Enthalpy= 0.334188
Thermal correction to Gibbs (Free) Energy= 0.259905
Sum of electronic and zero-point Energies= -1019.725046
Sum of electronic and thermal Energies= -1019.703630
Sum of electronic and thermal Enthalpies= -1019.702686
Sum of electronic and thermal (Free) Energies= -1019.776969

cc/d TS

C -1.5129670000 -1.2345640000 -0.9958560000
C -0.2856520000 -1.0324050000 -0.5143310000
C 0.9679080000 -1.5310420000 -0.3518100000
C 1.9696000000 -0.5288520000 -0.1136210000
C 1.3898810000 0.7592570000 -0.0032640000
C 0.0289530000 0.8394620000 0.2809200000
C 1.3152220000 -2.9872040000 -0.3185470000
O 3.2062270000 -0.8383860000 -0.0903220000
H 0.4483000000 -3.6139780000 -0.5294070000
H 1.7388430000 -3.2595630000 0.6526980000
H 2.0944000000 -3.1786950000 -1.0633050000
H 1.9698580000 1.6328850000 -0.2842190000
B 4.2859910000 0.2308940000 0.2795410000
F 4.2615150000 1.1806510000 -0.7424060000
F 5.4652170000 -0.4595680000 0.3577550000
F 3.8812120000 0.7907850000 1.4895670000
C -2.7666890000 -0.8717960000 -0.3298140000
C -3.8756170000 -0.4719140000 -1.0874170000
C -2.8831280000 -0.9351760000 1.0659740000
C -5.0585940000 -0.0983160000 -0.4603210000
H -3.7996280000 -0.4350130000 -2.1706560000
C -4.0701740000 -0.5696650000 1.6910790000
H -2.0471120000 -1.2966980000 1.6575910000
C -5.1561680000 -0.1405290000 0.9306080000
H -5.9062910000 0.2249460000 -1.0555530000
H -4.1494150000 -0.6242080000 2.7718790000
H -6.0814220000 0.1475920000 1.4187890000
H -1.5838720000 -1.6752300000 -1.9913090000
H -0.3642400000 0.3158970000 1.1545240000
C -0.7170740000 2.0979620000 -0.1365310000
H 0.0000900000 2.9051260000 0.0696760000
C -1.9755100000 2.3903000000 0.6824220000
H -2.7944020000 1.7146810000 0.4256840000
H -1.7837790000 2.3045420000 1.7566760000
H -2.3147700000 3.4113780000 0.4848160000
C -0.9969050000 2.1348200000 -1.6461830000
H -1.3425330000 3.1307710000 -1.9376220000
H -0.0975360000 1.9031160000 -2.2243670000
H -1.7762720000 1.4162240000 -1.9151180000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310337 (Hartree/Particle)
Thermal correction to Energy= 0.330903
Thermal correction to Enthalpy= 0.331847
Thermal correction to Gibbs (Free) Energy= 0.260181
Sum of electronic and zero-point Energies= -1019.694037
Sum of electronic and thermal Energies= -1019.673471
Sum of electronic and thermal Enthalpies= -1019.672527
Sum of electronic and thermal (Free) Energies= -1019.744193

cc/d PT

C 1.6035050000 -1.2294360000 0.2787700000
C 0.4009930000 -0.6258870000 0.1054960000
C -0.8363020000 -1.3113270000 0.3521210000
C -1.9282020000 -0.5401590000 -0.1294990000
C -1.4077550000 0.6467620000 -0.6273310000
C 0.0543120000 0.7602900000 -0.4147060000
C -1.0614440000 -2.6385340000 0.9613970000
O -3.1541550000 -0.9572870000 -0.0498650000
H -0.1794910000 -3.0672410000 1.4372530000
H -1.4295400000 -3.3253300000 0.1894690000
H -1.8775620000 -2.5538560000 1.6866480000
C 0.3373300000 1.9496100000 0.5722540000
H -2.0163010000 1.4414310000 -1.0432620000
C 2.9353810000 -0.7611240000 -0.1035260000
C -0.3248030000 1.7429410000 1.9365540000
H -1.4109020000 1.6424810000 1.8605450000
H -0.1129770000 2.6001690000 2.5818300000
H 0.0694290000 0.8504460000 2.4364860000
C 1.8245690000 2.2659510000 0.7242280000
H -0.1370770000 2.8174110000 0.0966320000
H 2.3510550000 1.4783260000 1.2713880000
H 1.9421050000 3.1963100000 1.2880380000
H 2.3203030000 2.3938130000 -0.2424460000
H 0.5617720000 0.9925790000 -1.3580370000
H 1.5927440000 -2.2057110000 0.7612610000
C 4.0160560000 -1.0482850000 0.7448280000
C 5.2947390000 -0.6009010000 0.4377090000
C 5.5206710000 0.1045070000 -0.7439100000
C 4.4643740000 0.3521630000 -1.6181920000
C 3.1798610000 -0.0738890000 -1.3007770000
H 3.8429720000 -1.6047740000 1.6618620000
H 6.1172490000 -0.8097740000 1.1137050000
H 6.5212040000 0.4443840000 -0.9907210000
H 4.6421120000 0.8738600000 -2.5528560000
H 2.3704630000 0.0960950000 -2.0015560000
B -4.2748710000 0.0262830000 -0.3872160000
F -5.4565870000 -0.6293220000 -0.1446450000
F -4.1193920000 0.4025050000 -1.7300180000
F -4.0906540000 1.1501690000 0.4398050000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.313194 (Hartree/Particle)
Thermal correction to Energy= 0.333641
Thermal correction to Enthalpy= 0.334585
Thermal correction to Gibbs (Free) Energy= 0.262169
Sum of electronic and zero-point Energies= -1019.739078
Sum of electronic and thermal Energies= -1019.718632
Sum of electronic and thermal Enthalpies= -1019.717687
Sum of electronic and thermal (Free) Energies= -1019.790103

c/u RT

C -2.0363990000 -0.1186310000 -1.3539370000
C -0.8309380000 -0.6245000000 -1.3665980000
C 0.3645770000 -1.1825420000 -1.3438130000
C 1.4281550000 -0.5866260000 -0.5094570000
C 1.3999510000 0.7941980000 -0.0467940000
C 0.8691730000 1.7929040000 -0.7681600000
H 1.9182060000 0.9819450000 0.8868240000
H 0.4430040000 1.5721110000 -1.7452550000
C 0.8053130000 3.2348900000 -0.3614730000
C 0.6714410000 -2.4913910000 -2.0347060000
H -2.2900410000 0.6006410000 -2.1324060000
C -3.0830900000 -0.4201240000 -0.3565650000
O 2.3539080000 -1.3715670000 -0.1909390000
H -0.1901850000 -2.8254190000 -2.6137390000
H 0.9303370000 -3.2548270000 -1.2968890000
H 1.5316120000 -2.3779620000 -2.7002660000
C 1.4697120000 3.5416160000 0.9787530000
C -0.6698610000 3.6773860000 -0.3776610000
H 1.3256960000 3.8004050000 -1.1482590000
H 0.9679900000 3.0144230000 1.7975510000
H 1.4111090000 4.6133780000 1.1879130000
H 2.5250070000 3.2543020000 0.9819970000
H -1.2429390000 3.1313050000 0.3789830000
H -1.1345610000 3.4972400000 -1.3526690000
H -0.7465250000 4.7464370000 -0.1598410000
C -4.3517420000 0.1476880000 -0.5101570000
C -2.8367580000 -1.2487700000 0.7454670000
C -3.8428050000 -1.5057180000 1.6682960000
H -1.8528110000 -1.6890480000 0.8802280000
C -5.1072930000 -0.9381350000 1.5068570000
H -3.6395830000 -2.1483940000 2.5188110000
C -5.3588660000 -0.1106040000 0.4159890000
H -4.5517880000 0.7939870000 -1.3605500000
H -5.8905940000 -1.1396120000 2.2303790000
H -6.3393050000 0.3357270000 0.2841930000
B 3.6642400000 -0.9980370000 0.6894390000
F 4.3835500000 -2.1553170000 0.6775400000
F 3.1727490000 -0.6452510000 1.9327020000
F 4.2580880000 0.0545950000 0.0260990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311523 (Hartree/Particle)
Thermal correction to Energy= 0.333193
Thermal correction to Enthalpy= 0.334137
Thermal correction to Gibbs (Free) Energy= 0.257460
Sum of electronic and zero-point Energies= -1019.721400
Sum of electronic and thermal Energies= -1019.699730
Sum of electronic and thermal Enthalpies= -1019.698786
Sum of electronic and thermal (Free) Energies= -1019.775463

c/u TS

C -1.8357610000 0.5173340000 -0.8733420000
C -0.5565310000 0.1705360000 -0.9431900000
C 0.4172730000 -0.7626930000 -1.0665900000
C 1.6448460000 -0.4248770000 -0.3912920000
C 1.6204810000 0.9060930000 0.1030380000
C 0.7215160000 1.7893860000 -0.4758740000
C 0.2614730000 3.0287040000 0.2620370000
C 0.2960830000 -2.0149960000 -1.8804360000
H -2.1354490000 1.4861890000 -1.2642780000
C -2.8885980000 -0.2908950000 -0.2423710000
O 2.5595480000 -1.2988760000 -0.2414160000
H -0.7220830000 -2.1596240000 -2.2437980000
H 0.5863770000 -2.8673270000 -1.2583500000
H 0.9896390000 -1.9920720000 -2.7262630000
C -0.4853920000 2.6895140000 1.5593710000
C -0.5404680000 3.9788950000 -0.6298970000
H 1.1914830000 3.5447640000 0.5431420000
H -1.4386780000 2.1967960000 1.3437880000
H -0.6938660000 3.6023420000 2.1244870000
H 0.1019330000 2.0240030000 2.1977650000
H -1.5077420000 3.5473360000 -0.9080720000
H 0.0025800000 4.2221840000 -1.5484380000
H -0.7434960000 4.9151900000 -0.1030180000
C -4.2197880000 0.1332500000 -0.3503850000
C -2.6059110000 -1.4696910000 0.4623790000
C -3.6349430000 -2.2127530000 1.0271060000
H -1.5770500000 -1.7959340000 0.5804730000
C -4.9582920000 -1.7893660000 0.9034470000
H -3.4033890000 -3.1216930000 1.5726860000
C -5.2479940000 -0.6134000000 0.2148750000
H -4.4485910000 1.0499490000 -0.8872530000
H -5.7590430000 -2.3709460000 1.3484930000
H -6.2748570000 -0.2756410000 0.1198950000
H 0.6623430000 1.8402340000 -1.5633890000
H 2.1952970000 1.1621480000 0.9876560000
B 3.9315960000 -0.9166830000 0.4104520000
F 4.4080030000 0.1814460000 -0.3005170000
F 4.7100940000 -2.0354260000 0.2887080000
F 3.6499320000 -0.5730990000 1.7329510000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310336 (Hartree/Particle)
Thermal correction to Energy= 0.331158
Thermal correction to Enthalpy= 0.332102
Thermal correction to Gibbs (Free) Energy= 0.258608
Sum of electronic and zero-point Energies= -1019.696127
Sum of electronic and thermal Energies= -1019.675304
Sum of electronic and thermal Enthalpies= -1019.674360
Sum of electronic and thermal (Free) Energies= -1019.747854

c/u PT

C -1.8209920000 0.7736120000 -0.6643310000
C -0.4906030000 0.5482250000 -0.5043520000
C 0.1943720000 -0.6843910000 -0.2412710000
C 1.6027050000 -0.4649020000 -0.2489280000
C 1.8233140000 0.8654750000 -0.5800720000
C 0.5622120000 1.6203400000 -0.7409020000
C 0.5377120000 2.8645820000 0.1974900000
C -0.3266880000 -2.0638180000 -0.1045500000
H -2.0947960000 1.7233160000 -1.1210610000
C -2.9523170000 -0.0661830000 -0.2722200000
O 2.4435370000 -1.4219700000 -0.0113360000
H -1.3301720000 -2.1870830000 -0.5099790000
H -0.3447530000 -2.3414230000 0.9568610000
H 0.3802530000 -2.7501420000 -0.5791730000
C 0.6366670000 2.4687330000 1.6730060000
C -0.6616910000 3.7830920000 -0.0470470000
H 1.4419620000 3.4298720000 -0.0626230000
H -0.2254220000 1.8624420000 1.9748130000
H 0.6473250000 3.3628840000 2.3028820000
H 1.5459380000 1.8986050000 1.8842580000
H -1.5846950000 3.3509110000 0.3544010000
H -0.8083360000 3.9924660000 -1.1124170000
H -0.5076700000 4.7398840000 0.4603910000
C -4.0799680000 -0.1383800000 -1.1044970000
C -2.9711250000 -0.7392990000 0.9578700000
C -4.0737690000 -1.5006250000 1.3267990000
H -2.1269200000 -0.6410130000 1.6331230000
C -5.1707530000 -1.6002470000 0.4726160000
H -4.0802370000 -2.0109490000 2.2842510000
C -5.1729380000 -0.9162110000 -0.7429700000
H -4.0865440000 0.4033410000 -2.0461780000
H -6.0296590000 -2.1977880000 0.7602220000
H -6.0309580000 -0.9825020000 -1.4036490000
H 0.4753860000 1.9780970000 -1.7788920000
H 2.8082180000 1.3083870000 -0.6706750000
B 3.9381670000 -1.0953040000 0.0127300000
F 4.2768160000 -0.5876570000 -1.2510640000
F 4.5869750000 -2.2675820000 0.3135890000
F 4.1245560000 -0.0988780000 0.9864360000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.313749 (Hartree/Particle)
Thermal correction to Energy= 0.333933
Thermal correction to Enthalpy= 0.334877
Thermal correction to Gibbs (Free) Energy= 0.263285
Sum of electronic and zero-point Energies= -1019.736000
Sum of electronic and thermal Energies= -1019.715816
Sum of electronic and thermal Enthalpies= -1019.714872
Sum of electronic and thermal (Free) Energies= -1019.786464

cc/u RT

C -1.7474080000 -1.6291190000 -1.1286400000

C -0.5779760000 -1.7528620000 -0.5563090000
C 0.6055710000 -1.8713190000 0.0118850000
C 1.5787040000 -0.7623770000 -0.1008640000
C 1.1910350000 0.6131610000 -0.3775250000
C 0.0101590000 1.1270740000 0.0025360000
C 1.0677220000 -3.1346120000 0.7004350000
O 2.7788000000 -1.0936240000 0.0557340000
H 1.9080650000 -3.5722840000 0.1557510000
H 0.2541150000 -3.8592770000 0.7506330000
H 1.4171170000 -2.9117430000 1.7123020000
H 1.9587960000 1.2307780000 -0.8296270000
B 4.0554770000 -0.0935720000 0.0694070000
F 4.0955290000 0.4624820000 -1.1952680000
F 5.0966160000 -0.9268450000 0.3502400000
F 3.7774140000 0.8297480000 1.0556840000
C -2.9391010000 -1.0419860000 -0.4830460000
C -4.0189710000 -0.6403810000 -1.2763680000
C -3.0061730000 -0.8459760000 0.9028770000
C -5.1345950000 -0.0387780000 -0.7004630000
H -3.9807690000 -0.7930980000 -2.3513850000
C -4.1199130000 -0.2435060000 1.4763680000
H -2.1870790000 -1.1811090000 1.5339510000
C -5.1867110000 0.1653920000 0.6762360000
H -5.9635430000 0.2705970000 -1.3289160000
H -4.1597030000 -0.1000650000 2.5515180000
H -6.0565680000 0.6332470000 1.1256070000
H -1.8389460000 -1.9345820000 -2.1702000000
H -0.6974840000 0.5005720000 0.5414180000
C -0.4443040000 2.5416330000 -0.1921800000
H -1.3594650000 2.4680550000 -0.8007310000
C 0.5589160000 3.4328550000 -0.9208650000
H 1.4846180000 3.5354760000 -0.3446560000
H 0.8135560000 3.0348480000 -1.9076200000
H 0.1386230000 4.4326560000 -1.0608900000
C -0.8535040000 3.1332460000 1.1675310000
H -1.2750420000 4.1334610000 1.0334900000
H -1.6065460000 2.5117120000 1.6627930000
H 0.0157370000 3.2144580000 1.8280960000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311363 (Hartree/Particle)
Thermal correction to Energy= 0.333047
Thermal correction to Enthalpy= 0.333991
Thermal correction to Gibbs (Free) Energy= 0.257614
Sum of electronic and zero-point Energies= -1019.723702
Sum of electronic and thermal Energies= -1019.702018
Sum of electronic and thermal Enthalpies= -1019.701073
Sum of electronic and thermal (Free) Energies= -1019.777451

cc/u TS

C -1.5861270000 -1.4414340000 -0.8566330000
C -0.3679520000 -1.2623780000 -0.3517300000
C 0.8985630000 -1.7038350000 -0.1448770000
C 1.8750770000 -0.6489610000 -0.0518170000
C 1.2576490000 0.6292660000 -0.0604620000
C -0.0786680000 0.6900770000 0.3077400000
C 1.2918380000 -3.1361620000 0.0459060000
O 3.1203740000 -0.9180150000 -0.0508840000
H 2.0518240000 -3.3929280000 -0.6991150000
H 0.4379230000 -3.8056730000 -0.0611580000
H 1.7537510000 -3.2813490000 1.0268500000
H 1.7876510000 1.4764140000 -0.4839420000
B 4.1767430000 0.2200990000 0.1505610000
F 4.0754050000 1.0480420000 -0.9677640000
F 5.3814690000 -0.4209390000 0.2510740000
F 3.8014510000 0.8979440000 1.3081360000
C -2.8398440000 -0.9344080000 -0.2873050000
C -3.8804540000 -0.5433620000 -1.1399950000
C -3.0167830000 -0.8166190000 1.0986260000
C -5.0549490000 -0.0097670000 -0.6208620000
H -3.7564150000 -0.6400200000 -2.2149720000
C -4.1926650000 -0.2838230000 1.6159740000
H -2.2386540000 -1.1674930000 1.7703440000
C -5.2109900000 0.1278750000 0.7577560000
H -5.8492530000 0.3003580000 -1.2920290000
H -4.3186480000 -0.1992370000 2.6905110000
H -6.1284980000 0.5425220000 1.1623650000
H -1.6455500000 -1.9543410000 -1.8175070000
H -0.3850990000 0.2099250000 1.2380830000
C -0.9764430000 1.8208340000 -0.1315590000
H -2.0074490000 1.4977230000 0.0470110000
C -0.8259790000 2.1570900000 -1.6157140000
H 0.1672110000 2.5575780000 -1.8424420000
H -0.9837560000 1.2690030000 -2.2360230000
H -1.5616010000 2.9122860000 -1.9068770000
C -0.7153870000 3.0435600000 0.7658320000
H -1.4073060000 3.8498580000 0.5057680000
H -0.8556120000 2.8023610000 1.8237650000
H 0.3065340000 3.4134870000 0.6353340000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310367 (Hartree/Particle)
Thermal correction to Energy= 0.331106
Thermal correction to Enthalpy= 0.332051
Thermal correction to Gibbs (Free) Energy= 0.259227
Sum of electronic and zero-point Energies= -1019.697690
Sum of electronic and thermal Energies= -1019.676951
Sum of electronic and thermal Enthalpies= -1019.676007
Sum of electronic and thermal (Free) Energies= -1019.748830

cc/u PT

C 1.6783560000 -1.3200300000 0.0026180000
C 0.4548540000 -0.7477970000 -0.1474960000
C -0.7674420000 -1.4750540000 0.0172840000
C -1.8820460000 -0.6172500000 -0.1983830000
C -1.3862660000 0.6424120000 -0.5034980000
C 0.0935980000 0.6952840000 -0.4466320000
C -0.9723030000 -2.9010530000 0.3463150000
O -3.1035750000 -1.0414950000 -0.0971900000
H -0.0537370000 -3.4564730000 0.5342390000
H -1.5256000000 -3.3746190000 -0.4730910000
H -1.6351290000 -2.9667090000 1.2163580000
C 0.6136210000 1.7242460000 0.6033960000
H -2.0169020000 1.4953170000 -0.7214600000
C 3.0108340000 -0.7473980000 -0.1531500000
C 0.3545770000 3.1554790000 0.1293100000
H 0.7948770000 3.3390510000 -0.8568920000
H 0.7949370000 3.8700120000 0.8307590000
H -0.7168120000 3.3732050000 0.0705400000
C 0.0180660000 1.4784030000 1.9918460000
H 1.6984640000 1.5830210000 0.6655080000
H -1.0608070000 1.6643340000 2.0055550000
H 0.4846330000 2.1475840000 2.7204370000
H 0.1875750000 0.4508880000 2.3298130000
H 0.4741280000 0.9952420000 -1.4330900000
H 1.6847030000 -2.3622330000 0.3165460000
C 4.0669800000 -1.3598690000 0.5438850000
C 5.3597860000 -0.8585550000 0.4662010000
C 5.6276700000 0.2498400000 -0.3352570000
C 4.5980410000 0.8483710000 -1.0602320000
C 3.3018650000 0.3573530000 -0.9715480000
H 3.8628710000 -2.2285910000 1.1637250000
H 6.1591490000 -1.3356770000 1.0232200000
H 6.6384050000 0.6383270000 -0.4058950000
H 4.8073210000 1.6967400000 -1.7033000000
H 2.5216260000 0.8165940000 -1.5659090000
B -4.2374360000 -0.0192780000 -0.1870620000
F -5.4046460000 -0.7132560000 0.0178130000
F -4.1680530000 0.5780320000 -1.4551460000
F -3.9945300000 0.9503420000 0.8026460000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.313351 (Hartree/Particle)
Thermal correction to Energy= 0.333896
Thermal correction to Enthalpy= 0.334841
Thermal correction to Gibbs (Free) Energy= 0.261979
Sum of electronic and zero-point Energies= -1019.743152
Sum of electronic and thermal Energies= -1019.722607
Sum of electronic and thermal Enthalpies= -1019.721663
Sum of electronic and thermal (Free) Energies= -1019.794524

5d

cRT

C 2.2898460000 0.1859590000 1.2746630000
C 1.3185520000 -0.6868300000 1.3458330000
C 0.3853300000 -1.6177510000 1.3900900000

C -0.8110980000 -1.4958380000 0.5300820000
C -1.3190030000 -0.2307700000 0.0347070000
C -1.1599510000 0.9327420000 0.6958840000
H -1.9163430000 -0.2978200000 -0.8667840000
H -0.6159900000 0.9290920000 1.6371420000
C -1.6810490000 2.2361390000 0.2876470000
C 0.5426490000 -2.8952890000 2.1833710000
H 2.2845510000 1.0090020000 1.9891790000
C 3.3956620000 0.1611070000 0.2956330000
O -1.3570200000 -2.5876450000 0.2298080000
H 1.4586400000 -2.8634080000 2.7743300000
H 0.5760590000 -3.7544510000 1.5089980000
H -0.3123140000 -3.0375710000 2.8502630000
C -1.3281340000 3.3609580000 1.0469500000
C -2.5113150000 2.4089870000 -0.8311630000
C 4.4079380000 1.1209950000 0.3907360000
C 3.4559970000 -0.7928440000 -0.7280450000
C 4.5114730000 -0.7860960000 -1.6312180000
H 2.6712050000 -1.5386260000 -0.8176320000
C 5.5198840000 0.1728460000 -1.5280250000
H 4.5464910000 -1.5293840000 -2.4211920000
C 5.4651050000 1.1264430000 -0.5152950000
H 4.3683790000 1.8671910000 1.1797290000
H 6.3422070000 0.1761280000 -2.2361440000
H 6.2444810000 1.8767840000 -0.4293290000
B -2.6988620000 -2.7752500000 -0.6520280000
F -3.6667760000 -2.0377800000 -0.0021840000
F -2.9008180000 -4.1228530000 -0.6297670000
F -2.3883280000 -2.2676160000 -1.9020840000
C -1.7778950000 4.6287550000 0.6947860000
C -2.5959090000 4.7869660000 -0.4210370000
C -2.9628340000 3.6743820000 -1.1798150000
H -0.6928520000 3.2371990000 1.9201220000
H -1.4937810000 5.4897980000 1.2907770000
H -2.9528750000 5.7737770000 -0.6979740000
H -3.6077920000 3.7948780000 -2.0439260000
H -2.8177840000 1.5538950000 -1.4242810000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.308398 (Hartree/Particle)
Thermal correction to Energy= 0.330480
Thermal correction to Enthalpy= 0.331424
Thermal correction to Gibbs (Free) Energy= 0.252461
Sum of electronic and zero-point Energies= -1132.792413
Sum of electronic and thermal Energies= -1132.770331
Sum of electronic and thermal Enthalpies= -1132.769387
Sum of electronic and thermal (Free) Energies= -1132.848350

cTS

C -1.7218110000 -0.3541660000 -0.9717220000
C -0.4164220000 -0.5756260000 -1.0231560000
H -2.1098430000 0.5521850000 -1.4346070000
C -2.6927640000 -1.1986960000 -0.2621220000
C 0.6833260000 -1.3678890000 -1.0235980000
C -4.0558840000 -0.8927640000 -0.3679090000
C -2.3016850000 -2.3000610000 0.5126770000
C 1.8316950000 -0.7729470000 -0.3860520000
C 0.7670320000 -2.7146370000 -1.6747120000
C -5.0088260000 -1.6794010000 0.2705260000
H -4.3680650000 -0.0354310000 -0.9578800000
C -3.2554410000 -3.0831000000 1.1505540000
H -1.2476430000 -2.5346730000 0.6267650000
C 1.6157970000 0.5985390000 -0.0882560000
O 2.8518900000 -1.4843360000 -0.1053300000
H 1.1413000000 -3.4359180000 -0.9413810000
H 1.4890210000 -2.6996580000 -2.4966540000
H -0.2054190000 -3.0423850000 -2.0441910000
C -4.6112450000 -2.7775500000 1.0299070000
H -6.0615330000 -1.4329350000 0.1773740000
H -2.9402090000 -3.9310340000 1.7498610000
C 0.6118700000 1.2446530000 -0.8050990000
H 2.1433390000 1.0687380000 0.7345710000
B 4.1370640000 -0.8329150000 0.5045570000
H -5.3533480000 -3.3901740000 1.5314620000
H 0.5927110000 1.1349730000 -1.8889110000
C -0.1103660000 2.4206910000 -0.3021870000
F 4.4957420000 0.2018770000 -0.3546750000
F 5.0572000000 -1.8443410000 0.5677170000
F 3.7652710000 -0.3383610000 1.7559110000
C -0.6567740000 3.3383910000 -1.2076100000
C -0.2994990000 2.6197810000 1.0717180000
C -1.3578610000 4.4493090000 -0.7498940000
H -0.5175110000 3.1871180000 -2.2751070000
C -0.9992070000 3.7295780000 1.5285850000
H 0.0909900000 1.8945360000 1.7796890000
C -1.5275720000 4.6461780000 0.6190770000
H -1.7684410000 5.1609610000 -1.4586140000
H -1.1401590000 3.8774900000 2.5940980000
H -2.0757250000 5.5111990000 0.9784330000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.307375 (Hartree/Particle)
Thermal correction to Energy= 0.328452
Thermal correction to Enthalpy= 0.329396
Thermal correction to Gibbs (Free) Energy= 0.254283
Sum of electronic and zero-point Energies= -1132.770435
Sum of electronic and thermal Energies= -1132.749358
Sum of electronic and thermal Enthalpies= -1132.748414
Sum of electronic and thermal (Free) Energies= -1132.823527

cPT

C -1.8340030000 0.1616360000 -0.7439050000
C -0.5029370000 -0.0911800000 -0.6706380000
C 0.2050200000 -1.2871030000 -0.3414540000
C 1.6043540000 -1.0156210000 -0.2570690000
C 1.8062810000 0.3118340000 -0.6164260000
C 0.5400240000 0.9803090000 -0.9931670000
C 0.3124150000 2.3303610000 -0.3432020000
C -0.2815650000 -2.6788110000 -0.2089580000
C -2.9498670000 -0.6415240000 -0.2491950000
O 2.4509600000 -1.9360500000 0.0757880000
H -1.3002900000 -2.8171350000 -0.5676780000
H -0.2271920000 -2.9841450000 0.8432720000
H 0.4163200000 -3.3370310000 -0.7364240000
C 0.5719750000 2.5070560000 1.0188970000
C -0.1828010000 3.4013340000 -1.0870300000
C -4.1501190000 -0.6700870000 -0.9763300000
C -2.8776640000 -1.3296350000 0.9707560000
C -3.9640240000 -2.0650760000 1.4289380000
H -1.9765720000 -1.2595550000 1.5715140000
C -5.1358190000 -2.1229330000 0.6762500000
H -3.8996930000 -2.5861190000 2.3784190000
C -5.2280340000 -1.4220370000 -0.5261170000
H -4.2261790000 -0.1147590000 -1.9069110000
H -5.9823990000 -2.6998800000 1.0339290000
H -6.1440540000 -1.4543230000 -1.1065900000
H 0.5346320000 1.1134490000 -2.0871910000
B 3.9417480000 -1.5824470000 0.1382490000
F 4.3094830000 -1.1174810000 -1.1330160000
F 4.5951470000 -2.7343340000 0.5011580000
F 4.0788880000 -0.5514180000 1.0799510000
H -2.1117410000 1.1201600000 -1.1837170000
H 2.7733230000 0.7995730000 -0.6341470000
C -0.4269220000 4.6317610000 -0.4789970000
C 0.3313830000 3.7348840000 1.6261300000
C -0.1716830000 4.7995950000 0.8790290000
H -0.8084200000 5.4589780000 -1.0690300000
H -0.3556820000 5.7581590000 1.3533270000
H -0.3711970000 3.2785480000 -2.1509760000
H 0.9720700000 1.6823940000 1.6039590000
H 0.5429040000 3.8628350000 2.6828070000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.309933 (Hartree/Particle)
Thermal correction to Energy= 0.330674
Thermal correction to Enthalpy= 0.331618
Thermal correction to Gibbs (Free) Energy= 0.257218
Sum of electronic and zero-point Energies= -1132.805613
Sum of electronic and thermal Energies= -1132.784872
Sum of electronic and thermal Enthalpies= -1132.783927
Sum of electronic and thermal (Free) Energies= -1132.858328

ccRT

C -1.0704570000 -2.2613740000 -1.2423540000
H -1.1142450000 -2.4597160000 -2.3122810000
C 0.1037420000 -2.2211690000 -0.6675550000
C -2.3389080000 -1.9624730000 -0.5446500000

C 1.2874950000 -2.1392960000 -0.0941090000
C -3.4378330000 -1.5126280000 -1.2839490000
C -2.4531540000 -2.0640540000 0.8479160000
C 2.0161900000 -3.3315560000 0.4802040000
C 2.0010930000 -0.8403700000 -0.0971630000
H -3.3600230000 -1.4293240000 -2.3641860000
C -4.6193510000 -1.1499150000 -0.6433000000
H -1.6137500000 -2.4356350000 1.4295630000
C -3.6346610000 -1.7028230000 1.4866780000
H 2.9271590000 -3.5243260000 -0.0918620000
H 1.3790170000 -4.2164130000 0.4521830000
H 2.3162050000 -3.1339950000 1.5130510000
O 3.2517480000 -0.9244030000 -0.0095450000
C 1.3216490000 0.4357640000 -0.2097400000
H -5.4610220000 -0.7944270000 -1.2289640000
C -4.7203590000 -1.2399650000 0.7434150000
H -3.7097010000 -1.7868080000 2.5661040000
B 4.2839230000 0.3166340000 0.0878660000
C 0.0514380000 0.6223520000 0.2026710000
H 1.9256850000 1.2505180000 -0.5920270000
H -5.6420320000 -0.9590900000 1.2426720000
F 4.1416190000 1.0052450000 -1.1038960000
F 5.4926320000 -0.2942140000 0.2415460000
F 3.8674770000 1.0487400000 1.1807720000
H -0.4868330000 -0.2104670000 0.6461430000
C -0.7140340000 1.8643160000 0.1277850000
C -0.1301560000 3.1041270000 -0.1748630000
C -2.0971720000 1.7988270000 0.3535120000
H 0.9419340000 3.1818540000 -0.3242500000
C -0.9171220000 4.2448660000 -0.2593680000
C -2.8837570000 2.9414380000 0.2587790000
H -2.5568650000 0.8426510000 0.5907620000
H -0.4559390000 5.2005510000 -0.4858460000
C -2.2946560000 4.1659650000 -0.0475510000
H -3.9537230000 2.8755050000 0.4273720000
H -2.9049380000 5.0610540000 -0.1153490000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.308200 (Hartree/Particle)
Thermal correction to Energy= 0.330172
Thermal correction to Enthalpy= 0.331116
Thermal correction to Gibbs (Free) Energy= 0.254300
Sum of electronic and zero-point Energies= -1132.797660
Sum of electronic and thermal Energies= -1132.775688
Sum of electronic and thermal Enthalpies= -1132.774744
Sum of electronic and thermal (Free) Energies= -1132.851560

44BA45DA

C -0.9991140000 -1.7236210000 -1.1096240000
C 0.1888810000 -1.4780720000 -0.5626580000
C -2.2953860000 -1.5230290000 -0.4491580000
H -1.0079760000 -2.0209600000 -2.1589090000
C 1.5140130000 -1.7531780000 -0.4445960000
C -3.3668150000 -0.9752000000 -1.1655170000
C -2.4767600000 -1.8598610000 0.8982390000
C 2.3208880000 -0.6056900000 -0.1155460000
C -4.5820100000 -0.7341540000 -0.5363580000
H -3.2332480000 -0.7110430000 -2.2105090000
C -3.6992220000 -1.6315340000 1.5223940000
H -1.6629340000 -2.3256130000 1.4471280000
C 1.5176240000 0.5290280000 0.1572830000
O 3.5932140000 -0.6780520000 -0.1648760000
C -4.7503040000 -1.0597880000 0.8092360000
H -5.3994480000 -0.2901230000 -1.0949920000
H -3.8322260000 -1.9047730000 2.5643850000
C 0.1831670000 0.2863650000 0.4920970000
H 1.8998570000 1.5292580000 -0.0154190000
B 4.4770490000 0.5336920000 0.2776770000
H -5.7027030000 -0.8781780000 1.2969210000
H -0.0372680000 -0.3988630000 1.3118780000
C -0.8722390000 1.2736350000 0.2139260000
F 5.7663000000 0.0753480000 0.2290170000
F 4.0518660000 0.8800030000 1.5578420000
F 4.2152790000 1.5596400000 -0.6313220000
C -0.8511060000 2.0097080000 -0.9770140000
C -1.9269410000 1.4579830000 1.1138140000
C -1.8637040000 2.9194220000 -1.2573700000
H -0.0470960000 1.8500800000 -1.6904590000
C -2.9376690000 2.3705640000 0.8360270000
H -1.9557960000 0.8806460000 2.0327020000
C -2.9082820000 3.1000840000 -0.3508810000
H -1.8421170000 3.4843170000 -2.1835920000
H -3.7504380000 2.5077670000 1.5415350000
H -3.7009670000 3.8078570000 -0.5720800000
C 2.1263470000 -3.1137280000 -0.5644980000
H 1.3821750000 -3.8699310000 -0.8158810000
H 2.8943260000 -3.0835750000 -1.3442850000
H 2.6356920000 -3.3894410000 0.3636100000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.307107 (Hartree/Particle)
Thermal correction to Energy= 0.328029
Thermal correction to Enthalpy= 0.328973
Thermal correction to Gibbs (Free) Energy= 0.255670
Sum of electronic and zero-point Energies= -1132.771269
Sum of electronic and thermal Energies= -1132.750347
Sum of electronic and thermal Enthalpies= -1132.749403
Sum of electronic and thermal (Free) Energies= -1132.822706

ccPT

C 1.1998770000 -1.8578850000 0.1651770000
C 0.0453820000 -1.1947750000 -0.1155040000
C -1.2446540000 -1.6802540000 0.2564400000
C -2.2476200000 -0.7104450000 -0.0378410000
C -1.6155390000 0.3823150000 -0.6130880000
C -0.1468890000 0.1758700000 -0.7457870000
C -1.6154130000 -2.9816540000 0.8495290000
O -3.4970690000 -0.9267210000 0.2274380000
H -0.7697800000 -3.6335130000 1.0675290000
H -2.3025910000 -3.4922030000 0.1644770000
H -2.1995860000 -2.8009100000 1.7586200000
C 0.6422330000 1.3169850000 -0.1231120000
H -2.1189910000 1.2890900000 -0.9250080000
C 2.5762680000 -1.4836290000 -0.1162370000
C 1.2455040000 2.2792410000 -0.9321100000
C 0.7330390000 1.4399630000 1.2645460000
H 0.0935000000 0.1240610000 -1.8178780000
H 1.0970490000 -2.7752890000 0.7418520000
C 3.5776910000 -2.0017080000 0.7248930000
C 4.9082270000 -1.6490760000 0.5481500000
C 5.2664020000 -0.7929370000 -0.4927570000
C 4.2905730000 -0.3006380000 -1.3575080000
C 2.9572750000 -0.6415120000 -1.1736230000
H 3.2999760000 -2.6704550000 1.5349820000
H 5.6664640000 -2.0438320000 1.2160340000
H 6.3067270000 -0.5201430000 -0.6374820000
H 4.5696770000 0.3489770000 -2.1802410000
H 2.2165510000 -0.2772070000 -1.8734700000
B -4.5287620000 0.1426320000 -0.1479290000
F -5.7531860000 -0.3588980000 0.2224600000
F -4.4173970000 0.3548020000 -1.5308550000
F -4.1824170000 1.3133870000 0.5413060000
C 1.4360800000 2.4967400000 1.8325490000
C 2.0471490000 3.4492120000 1.0182200000
C 1.9462460000 3.3415390000 -0.3658880000
H 1.1691910000 2.1998200000 -2.0139880000
H 2.4116640000 4.0834050000 -1.0069170000
H 1.5012400000 2.5810460000 2.9124840000
H 2.5937070000 4.2748580000 1.4622550000
H 0.2515850000 0.7051670000 1.9044070000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310038 (Hartree/Particle)
Thermal correction to Energy= 0.330941
Thermal correction to Enthalpy= 0.331886
Thermal correction to Gibbs (Free) Energy= 0.257242
Sum of electronic and zero-point Energies= -1132.810091
Sum of electronic and thermal Energies= -1132.789188
Sum of electronic and thermal Enthalpies= -1132.788244
Sum of electronic and thermal (Free) Energies= -1132.862887

6a

cRT

C -2.0518950000 0.4080010000 1.2703990000
C -0.8197750000 0.6432870000 0.9024660000
C 0.3884800000 0.8901100000 0.4318520000

C 1.3643070000 -0.2163040000 0.4953470000
C 1.3538170000 -1.2076710000 1.5783280000
C 0.9515800000 -0.9190290000 2.8193230000
H 1.7859440000 -2.1725690000 1.3364200000
C 0.7450740000 2.2191040000 -0.2679330000
H -2.3342090000 0.6535010000 2.2934290000
C -3.1000710000 -0.1674040000 0.4029720000
O 2.2100610000 -0.2808520000 -0.4241440000
C -0.3192930000 3.2712570000 0.0724100000
C 0.7718270000 2.0159310000 -1.7949640000
C 2.1137140000 2.7155880000 0.2308450000
C -4.3925960000 -0.3265470000 0.9120230000
C -2.8357210000 -0.5561920000 -0.9166140000
C -3.8460780000 -1.0897110000 -1.7064800000
H -1.8343840000 -0.4428880000 -1.3228060000
C -5.1341140000 -1.2436790000 -1.1921490000
H -3.6281900000 -1.3892560000 -2.7265490000
C -5.4044710000 -0.8609430000 0.1186400000
H -4.6075730000 -0.0293430000 1.9348880000
H -5.9210470000 -1.6616230000 -1.8115420000
H -6.4032500000 -0.9785520000 0.5266160000
B 3.4442080000 -1.3389160000 -0.5607690000
F 4.0825950000 -0.9029840000 -1.6824610000
F 2.8442750000 -2.5746030000 -0.6847450000
F 4.1607360000 -1.1927970000 0.6051670000
H 2.9226450000 2.0338530000 -0.0397260000
H 2.1121680000 2.8446310000 1.3188140000
H 2.3328780000 3.6880900000 -0.2209920000
H -0.2018990000 1.6665180000 -2.1543480000
H 1.5360280000 1.2980780000 -2.0957850000
H 0.9877230000 2.9724770000 -2.2827340000
H -1.3086990000 2.9796990000 -0.2929350000
H -0.0519130000 4.2212220000 -0.3999920000
H -0.3885650000 3.4378230000 1.1527320000
H 1.0169100000 -1.6658520000 3.6035020000
H 0.5867420000 0.0642650000 3.0975810000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311098 (Hartree/Particle)
Thermal correction to Energy= 0.332450
Thermal correction to Enthalpy= 0.333394
Thermal correction to Gibbs (Free) Energy= 0.258697
Sum of electronic and zero-point Energies= -1019.712851
Sum of electronic and thermal Energies= -1019.691498
Sum of electronic and thermal Enthalpies= -1019.690554
Sum of electronic and thermal (Free) Energies= -1019.765252

cTS

C 1.8868480000 -0.8102920000 -1.2678690000
C 0.6363560000 -0.4171400000 -1.0657170000
H 2.1305840000 -1.3134960000 -2.2010340000
C 2.9784450000 -0.6484870000 -0.2957360000
C -0.3367260000 0.3802820000 -0.5600250000
C 4.2998090000 -0.8304070000 -0.7228120000
C 2.7362680000 -0.3122620000 1.0430650000
C -1.5494150000 -0.3458390000 -0.2344840000
C -0.2255730000 1.9012190000 -0.4358620000
C 5.3581030000 -0.6536760000 0.1625730000
H 4.4979880000 -1.1014990000 -1.7561950000
C 3.7947470000 -0.1391290000 1.9259890000
H 1.7146660000 -0.2011940000 1.3934870000
C -1.5135720000 -1.6845710000 -0.7316430000
O -2.4683470000 0.1720740000 0.4745270000
C 1.1007600000 2.4095380000 -1.0155650000
C -0.2988620000 2.2772780000 1.0591930000
C -1.3933130000 2.5556410000 -1.1991940000
C 5.1086310000 -0.3048330000 1.4881210000
H 6.3777700000 -0.7906100000 -0.1825440000
H 3.5939510000 0.1178320000 2.9609770000
C -0.6447690000 -1.9359930000 -1.7678030000
H -2.0353050000 -2.4707500000 -0.1965530000
B -3.8421220000 -0.5593100000 0.6992680000
H 1.9642800000 1.9993040000 -0.4836210000
H 1.1365570000 3.4988900000 -0.9207020000
H 1.1993370000 2.1608600000 -2.0770050000
H 0.5474960000 1.8569040000 1.6115780000
H -1.2281890000 1.9336650000 1.5164690000
H -0.2507950000 3.3671060000 1.1520730000
H -2.3616690000 2.2606350000 -0.7906810000
H -1.3633460000 2.2891830000 -2.2611450000
H -1.3094260000 3.6443920000 -1.1234810000
H 5.9335850000 -0.1706350000 2.1801510000
H -0.2841860000 -2.9495840000 -1.9319970000
H -0.5774380000 -1.2865150000 -2.6360960000
F -4.6266850000 0.3660500000 1.3322800000
F -3.5599270000 -1.6810600000 1.4728700000
F -4.2972660000 -0.9152700000 -0.5651090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310764 (Hartree/Particle)
Thermal correction to Energy= 0.330945
Thermal correction to Enthalpy= 0.331889
Thermal correction to Gibbs (Free) Energy= 0.260950
Sum of electronic and zero-point Energies= -1019.689355
Sum of electronic and thermal Energies= -1019.669174
Sum of electronic and thermal Enthalpies= -1019.668229
Sum of electronic and thermal (Free) Energies= -1019.739168

cPT

C 1.7864560000 1.6625910000 0.4815290000
C 0.4695210000 1.3472090000 0.5574050000
C -0.2514490000 0.1092070000 0.4184440000
C -1.5899320000 0.4249800000 -0.0075830000
C -1.7795710000 1.7937250000 0.1358530000
C -0.5638420000 2.4615290000 0.6243070000
C 0.1158120000 -1.2898770000 0.8661400000
C 2.8710810000 0.8647730000 -0.0815670000
O -2.4430900000 -0.4748110000 -0.3857270000
C 1.4852500000 -1.4211020000 1.5479270000
C 0.0260650000 -2.2757980000 -0.3208210000
C -0.9588230000 -1.6758430000 1.9262640000
C 4.1576320000 0.9287840000 0.4727370000
C 2.6532940000 0.0693200000 -1.2154840000
C 3.6878980000 -0.6897420000 -1.7505820000
H 1.6744920000 0.0667220000 -1.6849370000
C 4.9501760000 -0.6590160000 -1.1618020000
H 3.5097290000 -1.3005860000 -2.6294240000
C 5.1845230000 0.1549400000 -0.0522240000
H 4.3399800000 1.5626430000 1.3358480000
H 5.7568090000 -1.2548610000 -1.5762690000
H 6.1710770000 0.1889230000 0.3980700000
B -3.9142230000 -0.0982480000 -0.5820680000
F -4.3585200000 0.4518760000 0.6300910000
F -4.5596940000 -1.2671720000 -0.9092820000
F -3.9758770000 0.8662790000 -1.5961350000
H 2.0521280000 2.6815890000 0.7650280000
H -2.7183020000 2.2929510000 -0.0695970000
H -0.6815140000 2.7776300000 1.6707190000
H -0.3054820000 3.3543270000 0.0427890000
H -0.9048970000 -1.0085700000 2.7925300000
H -0.7475900000 -2.6929750000 2.2688600000
H -1.9687190000 -1.6516290000 1.5177410000
H 1.6454170000 -0.6401810000 2.2981260000
H 2.3144220000 -1.4015060000 0.8416740000
H 1.5200670000 -2.3857060000 2.0623330000
H 0.1984520000 -3.2878030000 0.0587440000
H 0.7975100000 -2.0614470000 -1.0658320000
H -0.9554680000 -2.2427220000 -0.7955740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.313500 (Hartree/Particle)
Thermal correction to Energy= 0.333376
Thermal correction to Enthalpy= 0.334320
Thermal correction to Gibbs (Free) Energy= 0.264458
Sum of electronic and zero-point Energies= -1019.725140
Sum of electronic and thermal Energies= -1019.705265
Sum of electronic and thermal Enthalpies= -1019.704320
Sum of electronic and thermal (Free) Energies= -1019.774183

ccRT

C 1.9262540000 0.2185440000 -1.3492450000
C 0.7599020000 0.4599840000 -0.8109420000
C 3.1499700000 -0.1157860000 -0.5942440000
H 1.9966990000 0.2435360000 -2.4359700000
C -0.4176050000 0.7341390000 -0.2822780000
C 4.2456170000 -0.6611510000 -1.2715190000
C 3.2433590000 0.0940650000 0.7879280000

C -1.3668930000 -0.3907660000 -0.1495470000
C -0.8348190000 2.1706650000 0.0977010000
C 5.4041310000 -1.0052310000 -0.5807080000
H 4.1869850000 -0.8221100000 -2.3443630000
C 4.4001620000 -0.2510590000 1.4768350000
H 2.4107250000 0.5457100000 1.3211040000
C -0.9266170000 -1.7819170000 0.0182480000
O -2.5851000000 -0.1102330000 -0.1928710000
C 0.4080040000 3.0720530000 0.1125580000
C -1.4592720000 2.1675090000 1.5049110000
C -1.8364160000 2.7244500000 -0.9331590000
C 5.4837960000 -0.8044420000 0.7951280000
H 6.2451380000 -1.4305560000 -1.1188350000
H 4.4600380000 -0.0803460000 2.5470000000
C 0.2045560000 -2.1265360000 0.6402520000
H -1.6331060000 -2.5342010000 -0.3156260000
B -3.8479790000 -1.1220730000 0.0134350000
H 0.8766370000 3.1341470000 -0.8740950000
H 1.1597690000 2.7139230000 0.8241790000
H 0.1168440000 4.0834150000 0.4113930000
H -1.6920500000 3.1956350000 1.7994600000
H -0.7613540000 1.7574040000 2.2434310000
H -2.3866490000 1.5927580000 1.5426780000
H -1.4000590000 2.7187640000 -1.9374340000
H -2.0818770000 3.7605160000 -0.6766780000
H -2.7619360000 2.1478190000 -0.9505690000
H 6.3874540000 -1.0706600000 1.3336310000
H 0.8977580000 -1.3992600000 1.0495640000
H 0.4505760000 -3.1733540000 0.7836700000
F -4.9138210000 -0.2750490000 -0.0408500000
F -3.6347460000 -1.7021480000 1.2431720000
F -3.7687290000 -2.0136960000 -1.0354620000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.311094 (Hartree/Particle)
Thermal correction to Energy= 0.332424
Thermal correction to Enthalpy= 0.333368
Thermal correction to Gibbs (Free) Energy= 0.259204
Sum of electronic and zero-point Energies= -1019.714208
Sum of electronic and thermal Energies= -1019.692878
Sum of electronic and thermal Enthalpies= -1019.691933
Sum of electronic and thermal (Free) Energies= -1019.766097

ccTS

C 1.9218330000 0.5302240000 -0.9463460000
C 0.7043480000 0.3693750000 -0.4384650000
C 3.1774080000 0.0007670000 -0.3975960000
H 1.9818450000 1.0699450000 -1.8918970000
C -0.5653560000 0.7793150000 -0.1857360000
C 4.2208290000 -0.3431060000 -1.2672890000
C 3.3671720000 -0.1528650000 0.9829040000
C -1.5148230000 -0.3147480000 -0.1496410000
C -0.9609150000 2.2266890000 0.1063480000
C 5.4114350000 -0.8621620000 -0.7710960000
H 4.0896050000 -0.2144910000 -2.3380380000
C 4.5588040000 -0.6728110000 1.4774440000
H 2.5924320000 0.1713900000 1.6720340000
C -0.8577210000 -1.5813150000 -0.2129260000
O -2.7700320000 -0.1136820000 -0.1529160000
C 0.2710520000 3.1392200000 0.1659040000
C -1.6997890000 2.2941510000 1.4564660000
C -1.8875760000 2.7072850000 -1.0305500000
C 5.5809420000 -1.0343710000 0.6019570000
H 6.2084440000 -1.1325030000 -1.4560980000
H 4.6946850000 -0.7825780000 2.5484690000
C 0.4640150000 -1.6044910000 0.1674190000
H -1.3490780000 -2.4167250000 -0.7003890000
B -3.7868100000 -1.2978110000 0.0315060000
H 0.8065550000 3.1655240000 -0.7881520000
H 0.9742240000 2.8233950000 0.9433470000
H -0.0504600000 4.1593130000 0.3957680000
H -1.9805520000 3.3315880000 1.6641980000
H -1.0541660000 1.9505860000 2.2719260000
H -2.6092890000 1.6907800000 1.4514810000
H -1.3748340000 2.6659480000 -1.9972970000
H -2.1729760000 3.7474200000 -0.8422890000
H -2.7962130000 2.1058750000 -1.0887040000
H 6.5115550000 -1.4363040000 0.9890420000
H 0.8030090000 -1.1516130000 1.0951370000
H 1.1270010000 -2.3786710000 -0.2125200000
F -5.0046880000 -0.6897990000 0.1730290000
F -3.3670160000 -1.9901250000 1.1620230000
F -3.6791220000 -2.0819990000 -1.1131630000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.310416 (Hartree/Particle)
Thermal correction to Energy= 0.330648
Thermal correction to Enthalpy= 0.331592
Thermal correction to Gibbs (Free) Energy= 0.260474
Sum of electronic and zero-point Energies= -1019.686975
Sum of electronic and thermal Energies= -1019.666743
Sum of electronic and thermal Enthalpies= -1019.665799
Sum of electronic and thermal (Free) Energies= -1019.736917

ccPT

C 1.9299740000 0.6102410000 0.0152180000
C 0.7063310000 0.0266070000 0.1354060000
C -0.5756850000 0.6852050000 0.0800070000
C -1.5994830000 -0.3214120000 -0.0339920000
C -0.9963610000 -1.5677930000 0.0018940000
C 0.4609700000 -1.4626590000 0.1802320000
C -0.9479500000 2.1496130000 0.1633300000
O -2.8637630000 -0.0456440000 -0.1480380000
C 0.2089150000 3.1443980000 0.3350920000
C -1.8793130000 2.3062800000 1.3955260000
C -1.7163060000 2.5265980000 -1.1284700000
H -1.5410470000 -2.5004000000 -0.0726910000
C 3.2521180000 -0.0114990000 0.0059560000
H 1.9567820000 1.6758930000 -0.1646510000
C 4.2744860000 0.6744690000 -0.6733790000
C 5.5580860000 0.1500960000 -0.7536890000
C 5.8532370000 -1.0599170000 -0.1290930000
C 4.8600600000 -1.7360110000 0.5786040000
C 3.5720290000 -1.2206060000 0.6465150000
H 4.0502760000 1.6222820000 -1.1549810000
H 6.3289820000 0.6879650000 -1.2952470000
H 6.8569430000 -1.4689480000 -0.1813600000
H 5.0926050000 -2.6655730000 1.0874980000
H 2.8274120000 -1.7459630000 1.2304620000
B -3.8937270000 -1.1741860000 -0.1734490000
F -5.1210970000 -0.5595110000 -0.2636230000
F -3.7361690000 -1.9097360000 1.0111670000
F -3.6056720000 -1.9867780000 -1.2795740000
H -1.0743540000 2.4109480000 -2.0079710000
H -2.0123470000 3.5780790000 -1.0599190000
H -2.6118010000 1.9192670000 -1.2579240000
H -2.2062000000 3.3493310000 1.4486420000
H -1.3404510000 2.0716180000 2.3192610000
H -2.7615210000 1.6709200000 1.3229720000
H 0.8345900000 3.2189080000 -0.5598430000
H 0.8337690000 2.9178220000 1.2045290000
H -0.2216390000 4.1368020000 0.4963020000
H 0.7412230000 -1.8891370000 1.1528180000
H 1.0253210000 -2.0111920000 -0.5830230000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.313864 (Hartree/Particle)
Thermal correction to Energy= 0.333862
Thermal correction to Enthalpy= 0.334806
Thermal correction to Gibbs (Free) Energy= 0.263379
Sum of electronic and zero-point Energies= -1019.731027
Sum of electronic and thermal Energies= -1019.711030
Sum of electronic and thermal Enthalpies= -1019.710086
Sum of electronic and thermal (Free) Energies= -1019.781512

6b

cRT

C 2.0745490000 -0.2311700000 -1.2123330000
C 0.8592600000 0.2099280000 -1.0144690000
C -0.3289990000 0.7081180000 -0.7347060000
C -1.3250050000 -0.2261200000 -0.1632960000
C -1.4104760000 -1.6218530000 -0.5713130000
C -1.0282770000 -2.0548610000 -1.7832040000
H -1.8940550000 -2.2919110000 0.1319830000
C -0.6475250000 2.2121400000 -0.8702060000
H 2.3325960000 -0.5918560000 -2.2074360000

C 3.1357860000 -0.2758720000 -0.1855090000
O -2.0944260000 0.2441990000 0.7084420000
C 0.4004480000 2.8711150000 -1.7775640000
C -0.5994230000 2.8848640000 0.5149410000
C -2.0385640000 2.3901360000 -1.5037050000
C 4.4162740000 -0.7059220000 -0.5468960000
C 2.8948320000 0.1021640000 1.1416900000
C 3.9160650000 0.0526830000 2.0819380000
H 1.9025510000 0.4315240000 1.4372780000
C 5.1920700000 -0.3751880000 1.7131770000
H 3.7157330000 0.3458040000 3.1074840000
C 5.4391730000 -0.7544150000 0.3967420000
H 4.6134180000 -1.0025280000 -1.5736090000
H 5.9875290000 -0.4138140000 2.4503370000
H 6.4284740000 -1.0895040000 0.1018770000
B -3.3379690000 -0.5066780000 1.4228720000
F -3.8773560000 0.4770200000 2.1989560000
F -2.7801640000 -1.5517160000 2.1326540000
F -4.1454990000 -0.9249740000 0.3862430000
H -2.8334520000 1.9938790000 -0.8683990000
H -2.0916310000 1.8970550000 -2.4807540000
H -2.2342900000 3.4561900000 -1.6560300000
H 0.3909700000 2.7647620000 0.9666710000
H -1.3471190000 2.4708640000 1.1926940000
H -0.7918370000 3.9573020000 0.4028480000
H 1.4062790000 2.7993000000 -1.3527400000
H 0.1597590000 3.9318140000 -1.8969280000
H 0.4152520000 2.4127970000 -2.7722810000
C -1.1650090000 -3.4645160000 -2.2472990000
H -0.6194480000 -1.3453500000 -2.4996800000
H -1.5834670000 -4.1110250000 -1.4736190000
H -0.1867590000 -3.8564920000 -2.5479470000
H -1.8091490000 -3.5093770000 -3.1322370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.339276 (Hartree/Particle)
Thermal correction to Energy= 0.362305
Thermal correction to Enthalpy= 0.363249
Thermal correction to Gibbs (Free) Energy= 0.284238
Sum of electronic and zero-point Energies= -1059.000012
Sum of electronic and thermal Energies= -1058.976982
Sum of electronic and thermal Enthalpies= -1058.976038
Sum of electronic and thermal (Free) Energies= -1059.055050

cTS

C -1.8786320000 1.0041870000 -0.8878690000
C -0.6264740000 0.5701170000 -0.8339040000
C -2.9686700000 0.5327020000 -0.0210080000
H -2.1257830000 1.7952370000 -1.5933950000
C 0.3255130000 -0.3732120000 -0.6083120000
C -4.2916840000 0.8350920000 -0.3673370000
C -2.7233590000 -0.2126060000 1.1401850000
C 1.5419410000 0.1954560000 -0.0672170000
C 0.1935460000 -1.8489970000 -0.9817370000
C -5.3480360000 0.3780300000 0.4138860000
H -4.4925350000 1.4213670000 -1.2599460000
C -3.7798320000 -0.6651340000 1.9207170000
H -1.7005570000 -0.4230660000 1.4373750000
C 1.5280400000 1.6150890000 -0.1309740000
O 2.4506100000 -0.5321800000 0.4535630000
C -1.1332500000 -2.1254630000 -1.7003140000
C 0.2519330000 -2.6890340000 0.3119290000
C 1.3609840000 -2.2373160000 -1.9100290000
C -5.0951850000 -0.3756420000 1.5581340000
H -6.3688910000 0.6123840000 0.1300350000
H -3.5762210000 -1.2383420000 2.8193840000
C 0.6606450000 2.1982750000 -1.0408660000
H 2.0771990000 2.1958980000 0.6036420000
B 3.8212770000 0.0760820000 0.8958000000
H -1.2209230000 -1.5441500000 -2.6237370000
H -1.9964870000 -1.8993980000 -1.0676300000
H -1.1810240000 -3.1861170000 -1.9645680000
H 0.1965050000 -3.7499110000 0.0469110000
H -0.5963660000 -2.4627120000 0.9654820000
H 1.1797430000 -2.5186380000 0.8605610000
H 1.3431800000 -1.6419090000 -2.8292410000
H 1.2651230000 -3.2910940000 -2.1903450000
H 2.3284730000 -2.1014310000 -1.4229800000
H -5.9185810000 -0.7289250000 2.1702370000
H 0.6369430000 1.8194300000 -2.0613400000
C 0.1865020000 3.6127240000 -0.8870280000
F 4.3000160000 0.7935270000 -0.1975040000
F 4.5947450000 -1.0044480000 1.2282270000
F 3.5491340000 0.9205280000 1.9708300000
H -0.7718940000 3.7646780000 -1.3899540000
H 0.9078710000 4.2859400000 -1.3636140000
H 0.0840110000 3.8956930000 0.1621140000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.338769 (Hartree/Particle)
Thermal correction to Energy= 0.360651
Thermal correction to Enthalpy= 0.361595
Thermal correction to Gibbs (Free) Energy= 0.286814
Sum of electronic and zero-point Energies= -1058.976256
Sum of electronic and thermal Energies= -1058.954374
Sum of electronic and thermal Enthalpies= -1058.953430
Sum of electronic and thermal (Free) Energies= -1059.028211

cPT

C 1.7865210000 1.4923500000 0.4978540000
C 0.4727680000 1.1767890000 0.5873270000
C -0.2257070000 -0.0746960000 0.4346070000
C -1.5610740000 0.2166700000 -0.0109450000
C -1.7791280000 1.5754590000 0.1626380000
C -0.5910430000 2.2762830000 0.6900040000
C 0.1545360000 -1.4642260000 0.9009980000
C 2.8593210000 0.6926870000 -0.0876010000
O -2.3919120000 -0.6946500000 -0.4122980000
C 1.5196500000 -1.5740570000 1.5947540000
C 0.0835590000 -2.4681620000 -0.2720600000
C -0.9267480000 -1.8447460000 1.9570130000
C 4.1543560000 0.7487310000 0.4474460000
C 2.6221060000 -0.0965630000 -1.2215760000
C 3.6453350000 -0.8590800000 -1.7740850000
H 1.6372720000 -0.0922560000 -1.6783750000
C 4.9161750000 -0.8366620000 -1.2040870000
H 3.4512370000 -1.4658010000 -2.6524720000
C 5.1702460000 -0.0271620000 -0.0955370000
H 4.3520180000 1.3779560000 1.3106200000
H 5.7138110000 -1.4348550000 -1.6323630000
H 6.1634530000 0.0011800000 0.3403770000
B -3.8693440000 -0.3446270000 -0.6040050000
F -4.3282070000 0.1664560000 0.6202880000
F -4.4902560000 -1.5181260000 -0.9611250000
F -3.9498520000 0.6432460000 -1.5943380000
H 2.0655640000 2.5061890000 0.7814620000
H -2.7273610000 2.0602330000 -0.0386300000
H -0.7475820000 2.4522350000 1.7665180000
C -0.3088050000 3.6144690000 0.0040470000
H -0.0691660000 3.4678510000 -1.0528330000
H 0.5187930000 4.1465300000 0.4798500000
H -1.1916810000 4.2558570000 0.0703040000
H 1.6657590000 -0.7852410000 2.3394180000
H 2.3536690000 -1.5512960000 0.8941220000
H 1.5608990000 -2.5339890000 2.1174420000
H -0.8880490000 -1.1642590000 2.8138000000
H -0.7093040000 -2.8545780000 2.3168600000
H -1.9328980000 -1.8364690000 1.5382290000
H 0.2599020000 -3.4727860000 0.1249240000
H 0.8612220000 -2.2589330000 -1.0118050000
H -0.8931220000 -2.4499110000 -0.7572500000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.342045 (Hartree/Particle)
Thermal correction to Energy= 0.363363
Thermal correction to Enthalpy= 0.364307
Thermal correction to Gibbs (Free) Energy= 0.291563
Sum of electronic and zero-point Energies= -1059.005029
Sum of electronic and thermal Energies= -1058.983711
Sum of electronic and thermal Enthalpies= -1058.982767
Sum of electronic and thermal (Free) Energies= -1059.055511

ccRT

C 1.8383990000 0.6000490000 -1.3903310000
C 0.6813030000 0.7815040000 -0.8080060000
C 3.0795300000 0.2170910000 -0.6876950000
H 1.8851390000 0.7031830000 -2.4736400000

C -0.4953290000 0.9544480000 -0.2404220000
C 4.1381430000 -0.3345470000 -1.4173240000
C 3.2217190000 0.3740290000 0.6972530000
C -1.3817460000 -0.2330370000 -0.1857670000
C -0.9849040000 2.3260070000 0.2655910000
C 5.3046210000 -0.7405060000 -0.7750820000
H 4.0428360000 -0.4535510000 -2.4930330000
C 4.3863870000 -0.0330990000 1.3380560000
H 2.4209620000 0.8343970000 1.2700450000
C -0.8624270000 -1.5833950000 -0.0182840000
O -2.6114020000 -0.0167430000 -0.3026730000
C 0.2142490000 3.2763460000 0.3899930000
C -1.6311660000 2.1571560000 1.6523210000
C -1.9974280000 2.9276250000 -0.7268810000
C 5.4307920000 -0.5953460000 0.6044920000
H 6.1157600000 -1.1704340000 -1.3539580000
H 4.4838140000 0.0978100000 2.4111430000
C 0.3011310000 -1.8491930000 0.5973550000
H -1.5156210000 -2.3854030000 -0.3464600000
B -3.8097770000 -1.0957320000 -0.1638480000
H 0.7004750000 3.4447300000 -0.5755760000
H 0.9655530000 2.8889350000 1.0867220000
H -0.1279260000 4.2441810000 0.7685730000
H -1.9207500000 3.1389440000 2.0398990000
H -0.9264360000 1.7108490000 2.3630010000
H -2.5287390000 1.5363420000 1.6140740000
H -1.5445120000 3.0442980000 -1.7169080000
H -2.3036070000 3.9185180000 -0.3745810000
H -2.8886380000 2.3060010000 -0.8217840000
H 6.3408610000 -0.9095320000 1.1050730000
H 0.8997680000 -1.0309600000 0.9905340000
C 0.8439680000 -3.2181790000 0.8184180000
F -4.9270340000 -0.3213130000 -0.2792070000
F -3.6346440000 -1.6642250000 1.0804460000
F -3.6259900000 -1.9896240000 -1.2001630000
H 0.2043660000 -3.9900180000 0.3859800000
H 0.9570870000 -3.4102500000 1.8909980000
H 1.8452760000 -3.2906820000 0.3787150000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.339577 (Hartree/Particle)
Thermal correction to Energy= 0.362450
Thermal correction to Enthalpy= 0.363395
Thermal correction to Gibbs (Free) Energy= 0.285685
Sum of electronic and zero-point Energies= -1059.001731
Sum of electronic and thermal Energies= -1058.978858
Sum of electronic and thermal Enthalpies= -1058.977914
Sum of electronic and thermal (Free) Energies= -1059.055624

ccTS

C 1.8369480000 0.6772090000 -0.9346410000
C 0.6225500000 0.4520750000 -0.4347400000
C 3.1085570000 0.2150740000 -0.3694690000
H 1.8835730000 1.2200020000 -1.8789600000
C -0.6492160000 0.8721490000 -0.1997500000
C 4.1809040000 -0.0843140000 -1.2210450000
C 3.2818020000 0.0712820000 1.0147790000
C -1.5925600000 -0.2232390000 -0.1383490000
C -1.0500240000 2.3222130000 0.0644570000
C 5.3827610000 -0.5549470000 -0.7043040000
H 4.0612060000 0.0363930000 -2.2940530000
C 4.4847260000 -0.4000460000 1.5298930000
H 2.4800610000 0.3596950000 1.6885820000
C -0.9324410000 -1.4780550000 -0.1652040000
O -2.8531950000 -0.0271230000 -0.1432670000
C 0.1732080000 3.2473270000 0.1017950000
C -1.7856910000 2.4111650000 1.4154150000
C -1.9851310000 2.7720400000 -1.0786340000
C 5.5350490000 -0.7210770000 0.6718060000
H 6.2017390000 -0.7933070000 -1.3751000000
H 4.6068860000 -0.5046370000 2.6030830000
C 0.4116340000 -1.4962580000 0.1810810000
H -1.4337440000 -2.3431770000 -0.5879530000
B -3.8574680000 -1.2033620000 0.0769820000
H 0.7036670000 3.2628280000 -0.8552200000
H 0.8833610000 2.9526470000 0.8811840000
H -0.1575230000 4.2681450000 0.3150800000
H -2.0747400000 3.4502270000 1.6030190000
H -1.1345260000 2.0895740000 2.2355060000
H -2.6894270000 1.7992670000 1.4249660000
H -1.4753340000 2.7158870000 -2.0462630000
H -2.2791120000 3.8132110000 -0.9100100000
H -2.8879300000 2.1605420000 -1.1208810000
H 6.4740240000 -1.0862950000 1.0747460000
H 0.7195940000 -1.0329270000 1.1182660000
C 1.3174470000 -2.5908730000 -0.3007820000
F -5.0834680000 -0.6021210000 0.1920450000
F -3.4442070000 -1.8582150000 1.2346700000
F -3.7458190000 -2.0339570000 -1.0369440000
H 1.0379750000 -2.9359150000 -1.2980390000
H 1.2520270000 -3.4358690000 0.3939710000
H 2.3594230000 -2.2642140000 -0.3124850000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.338733 (Hartree/Particle)
Thermal correction to Energy= 0.360510
Thermal correction to Enthalpy= 0.361454
Thermal correction to Gibbs (Free) Energy= 0.287287
Sum of electronic and zero-point Energies= -1058.974678
Sum of electronic and thermal Energies= -1058.952901
Sum of electronic and thermal Enthalpies= -1058.951957
Sum of electronic and thermal (Free) Energies= -1059.026124

ccPT

C -1.8625500000 0.7798410000 0.0076240000
C -0.6524130000 0.1599610000 -0.0444530000
C 0.6442230000 0.7942010000 -0.0249820000
C 1.6514280000 -0.2324030000 -0.0078940000
C 1.0193170000 -1.4647030000 -0.0133630000
C -0.4480750000 -1.3467170000 -0.0406800000
C 1.0478380000 2.2534160000 -0.0684400000
O 2.9270180000 0.0120240000 0.0115310000
C -0.0868760000 3.2864760000 -0.1035780000
C 1.8994040000 2.4545160000 -1.3497380000
C 1.9088220000 2.5427940000 1.1883010000
H 1.5474460000 -2.4097050000 0.0271080000
C -3.1927030000 0.1792910000 -0.0898750000
H -1.8795820000 1.8457920000 0.1856410000
C -4.2230720000 0.7396650000 0.6838070000
C -5.5054390000 0.2069970000 0.6534600000
C -5.7907560000 -0.8728500000 -0.1811460000
C -4.7893790000 -1.4112660000 -0.9870180000
C -3.5005640000 -0.8925340000 -0.9423190000
H -4.0054070000 1.5873300000 1.3276790000
H -6.2847380000 0.6388340000 1.2725520000
H -6.7947170000 -1.2831660000 -0.2152720000
H -5.0141260000 -2.2331990000 -1.6586460000
H -2.7410510000 -1.2970620000 -1.6010200000
B 3.9290810000 -1.1409400000 -0.0199480000
F 5.1740160000 -0.5557280000 -0.0191460000
F 3.6753210000 -1.8851860000 -1.1821100000
F 3.6970800000 -1.9344270000 1.1132890000
H 1.3191350000 2.4048490000 2.1006060000
H 2.2356450000 3.5865970000 1.1500430000
H 2.7900020000 1.9034530000 1.2323030000
H 2.2415680000 3.4937610000 -1.3769780000
H 1.2972750000 2.2714920000 -2.2457350000
H 2.7720910000 1.8022060000 -1.3645950000
H -0.6823090000 3.2866450000 0.8149430000
H -0.7425650000 3.1629570000 -0.9708940000
H 0.3656390000 4.2790710000 -0.1832970000
H -0.8163840000 -1.7874950000 -0.9771820000
C -1.0935620000 -2.0849000000 1.1463870000
H -0.7523660000 -1.6512080000 2.0904480000
H -0.8054970000 -3.1390260000 1.1295260000
H -2.1832100000 -2.0262470000 1.1054030000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.343083 (Hartree/Particle)
Thermal correction to Energy= 0.364347
Thermal correction to Enthalpy= 0.365291
Thermal correction to Gibbs (Free) Energy= 0.291762
Sum of electronic and zero-point Energies= -1059.010204
Sum of electronic and thermal Energies= -1058.988940
Sum of electronic and thermal Enthalpies= -1058.987995
Sum of electronic and thermal (Free) Energies= -1059.061524

6c

c/s RT

C 2.0835830000 0.4688230000 0.9285580000
C 0.9095450000 -0.1068230000 0.9364760000
H 2.2594920000 1.2773050000 1.6374120000
C 3.1974930000 0.1116360000 0.0268720000
C -0.2391510000 -0.7541670000 0.8981970000
C 4.4219690000 0.7733330000 0.1613150000
C 3.0604030000 -0.8711410000 -0.9619350000
C -1.2473740000 -0.2593310000 -0.0655690000
C -0.4946190000 -2.0327660000 1.7227470000
C 5.4917730000 0.4584420000 -0.6726150000
H 4.5379440000 1.5381700000 0.9245420000
C 4.1284160000 -1.1838690000 -1.7932260000
H 2.1121400000 -1.3879760000 -1.0809440000
C -1.3674670000 1.1516100000 -0.4061570000
O -1.9886130000 -1.1225050000 -0.5944200000
C 0.5589770000 -2.1377000000 2.8339200000
C -0.3843740000 -3.2727670000 0.8149720000
C -1.8913150000 -1.9618960000 2.3651660000
C 5.3480790000 -0.5208040000 -1.6515680000
H 6.4367160000 0.9795240000 -0.5565650000
H 4.0088260000 -1.9456390000 -2.5568810000
C -1.0434680000 2.1384120000 0.4432480000
H -1.8224940000 1.3703530000 -1.3669420000
B -3.2309940000 -0.8540310000 -1.5935550000
H 0.5292410000 -1.2679320000 3.4989880000
H 1.5708950000 -2.2214310000 2.4257860000
H 0.3627830000 -3.0306250000 3.4351430000
H -0.5318560000 -4.1757330000 1.4171180000
H 0.6101180000 -3.3293820000 0.3596970000
H -1.1336100000 -3.2621960000 0.0223030000
H -1.9881110000 -1.0719830000 2.9969520000
H -2.0439500000 -2.8408550000 2.9993880000
H -2.6874300000 -1.9487540000 1.6179260000
H 6.1802840000 -0.7667790000 -2.3031530000
C -1.1853270000 3.5979750000 0.1453850000
H -0.6717140000 1.8943150000 1.4386200000
F -4.0643680000 0.0048380000 -0.9075730000
F -2.6795830000 -0.2859610000 -2.7255490000
F -3.7415250000 -2.1050900000 -1.7836820000
C -2.2010100000 4.2350910000 1.1046660000
H -1.5515100000 3.7111380000 -0.8813680000
C 0.1895610000 4.2744080000 0.2583370000
H -3.1839650000 3.7664110000 1.0078940000
H -2.3055760000 5.3025720000 0.8886450000
H -1.8725380000 4.1330850000 2.1454360000
H 0.5870870000 4.1806610000 1.2758970000
H 0.1055750000 5.3409870000 0.0295670000
H 0.9106590000 3.8300730000 -0.4338110000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.396578 (Hartree/Particle)
Thermal correction to Energy= 0.422268
Thermal correction to Enthalpy= 0.423213
Thermal correction to Gibbs (Free) Energy= 0.337750
Sum of electronic and zero-point Energies= -1137.557424
Sum of electronic and thermal Energies= -1137.531733
Sum of electronic and thermal Enthalpies= -1137.530789
Sum of electronic and thermal (Free) Energies= -1137.616251

c/s TS

C 1.8830120000 0.8593020000 0.6011170000
C 0.6320890000 0.4076230000 0.6003240000
H 2.1056740000 1.7698230000 1.1491400000
C 2.9959670000 0.2455200000 -0.1342990000
C -0.2463720000 -0.6323100000 0.5855840000
C 4.3086730000 0.6106300000 0.1917160000
C 2.7842460000 -0.6954150000 -1.1514550000
C -1.5003070000 -0.2786610000 -0.0390260000
C -0.0174860000 -1.9836280000 1.2628620000
C 5.3872580000 0.0230970000 -0.4610170000
H 4.4825830000 1.3486620000 0.9701230000
C 3.8630420000 -1.2781990000 -1.8043700000
H 1.7701920000 -0.9571780000 -1.4376160000
C -1.5884250000 1.1151940000 -0.2651700000
O -2.3625890000 -1.1596410000 -0.3759720000
C 1.3151070000 -2.0220210000 2.0215150000
C -0.0110760000 -3.0802320000 0.1763360000
C -1.1659910000 -2.2415970000 2.2589060000
C 5.1673130000 -0.9251030000 -1.4581630000
H 6.3996610000 0.3071260000 -0.1927430000
H 3.6861820000 -2.0037770000 -2.5916880000
C -0.7341770000 1.9438330000 0.4546340000
H -2.2118620000 1.4941780000 -1.0690630000
B -3.7763250000 -0.7472910000 -0.8855670000
H 1.3628890000 -1.2479450000 2.7940390000
H 2.1722690000 -1.8978280000 1.3543350000
H 1.4144800000 -2.9942550000 2.5135400000
H 0.1075230000 -4.0555640000 0.6595510000
H 0.8278850000 -2.9438550000 -0.5132350000
H -0.9426270000 -3.0885550000 -0.3920620000
H -1.1935840000 -1.4651570000 3.0310420000
H -1.0039120000 -3.2036700000 2.7552880000
H -2.1362610000 -2.2746510000 1.7602010000
H 6.0082510000 -1.3806760000 -1.9707970000
C -0.5003390000 3.3594710000 -0.0349560000
H -0.6749280000 1.8339440000 1.5392420000
F -4.2863830000 0.1499380000 0.0522290000
F -3.5907960000 -0.1254460000 -2.1204050000
F -4.4817950000 -1.9196730000 -0.9638980000
C -1.7108020000 4.1979730000 0.4201590000
H -0.4832760000 3.3437080000 -1.1303930000
C 0.8004710000 3.9953240000 0.4620040000
H -2.6539240000 3.7768580000 0.0623940000
H -1.6214890000 5.2183160000 0.0358150000
H -1.7567410000 4.2505880000 1.5137090000
H 0.9041640000 3.8918210000 1.5491710000
H 0.7991990000 5.0650430000 0.2345100000
H 1.6775410000 3.5584560000 -0.0204290000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.396690 (Hartree/Particle)
Thermal correction to Energy= 0.420928
Thermal correction to Enthalpy= 0.421873
Thermal correction to Gibbs (Free) Energy= 0.341930
Sum of electronic and zero-point Energies= -1137.530198
Sum of electronic and thermal Energies= -1137.505960
Sum of electronic and thermal Enthalpies= -1137.505016
Sum of electronic and thermal (Free) Energies= -1137.584958

c/s PT

C 1.7740470000 1.2367120000 0.3489130000
C 0.4847240000 0.8617630000 0.5141030000
C -0.1180200000 -0.4501410000 0.4567960000
C -1.4639250000 -0.2974060000 -0.0134140000
C -1.7895060000 1.0468390000 0.0805310000
C -0.6661210000 1.8808040000 0.5626050000
C 0.3583910000 -1.7600130000 1.0490600000
C 2.8640920000 0.4405090000 -0.2115010000
O -2.2249600000 -1.2948140000 -0.3457670000
C 1.7304480000 -1.7121020000 1.7358610000
C 0.3474420000 -2.8821130000 -0.0130940000
C -0.6944300000 -2.0975600000 2.1485750000
C 4.1720950000 0.6006610000 0.2685610000
C 2.6294720000 -0.4491570000 -1.2687140000
C 3.6704650000 -1.2073560000 -1.7943050000
H 1.6319820000 -0.5272950000 -1.6902790000
C 4.9565290000 -1.0792830000 -1.2753560000
H 3.4775240000 -1.8929590000 -2.6129240000
C 5.2067350000 -0.1690520000 -0.2466860000
H 4.3664500000 1.3076340000 1.0701750000
H 5.7680480000 -1.6735410000 -1.6825110000
H 6.2111950000 -0.0583150000 0.1485050000
B -3.7148050000 -1.0617490000 -0.5962940000
F -4.2464620000 -0.5086150000 0.5798430000
F -4.2450830000 -2.2944850000 -0.8949900000
F -3.8328410000 -0.1436690000 -1.6498140000
H 2.0150480000 2.2812790000 0.5304470000
H -2.7870970000 1.4217550000 -0.1076900000
H -0.8531890000 2.0697620000 1.6339940000
C -0.4721880000 3.2535680000 -0.1338540000
C -1.7839540000 3.8230890000 -0.6856630000
H 0.2038290000 3.0985970000 -0.9836680000
C 0.1593050000 4.2681540000 0.8278450000
H -0.5500400000 4.5236210000 1.6238880000
H 0.4162430000 5.1920080000 0.3017830000

H 1.0674760000 3.8965410000 1.3119170000
H -2.2041760000 3.2000570000 -1.4796270000
H -1.6069930000 4.8179470000 -1.1046860000
H -2.5371680000 3.9268390000 0.1038820000
H -0.6959020000 -1.3330810000 2.9323470000
H -0.4143350000 -3.0508920000 2.6060340000
H -1.7000200000 -2.1931940000 1.7386280000
H 0.5891230000 -3.8269470000 0.4838320000
H 1.1080890000 -2.7017160000 -0.7774330000
H -0.6294210000 -2.9760980000 -0.4887080000
H 1.8310650000 -0.8421140000 2.3923210000
H 2.5572430000 -1.7110290000 1.0259890000
H 1.8345770000 -2.6081780000 2.3544740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.399147 (Hartree/Particle)
Thermal correction to Energy= 0.423140
Thermal correction to Enthalpy= 0.424084
Thermal correction to Gibbs (Free) Energy= 0.345389
Sum of electronic and zero-point Energies= -1137.557850
Sum of electronic and thermal Energies= -1137.533858
Sum of electronic and thermal Enthalpies= -1137.532913
Sum of electronic and thermal (Free) Energies= -1137.611608

cc/s RT

C -1.5469480000 -1.2866420000 -1.3890530000
C -0.3853550000 -1.2679880000 -0.7877620000
C -2.8258100000 -0.9391150000 -0.7377640000
H -1.5703850000 -1.5289240000 -2.4506180000
C 0.7921870000 -1.2339690000 -0.1973060000
C -3.9135040000 -0.5504960000 -1.5265250000
C -2.9697000000 -0.9494090000 0.6555610000
C 1.5373470000 0.0457650000 -0.2831050000
C 1.4213830000 -2.4664260000 0.4822100000
C -5.1095470000 -0.1528470000 -0.9359130000
H -3.8157280000 -0.5440160000 -2.6085190000
C -4.1644620000 -0.5518650000 1.2450870000
H -2.1425970000 -1.2806180000 1.2777510000
C 0.8638040000 1.3363780000 -0.2945780000
O 2.7867000000 -0.0401620000 -0.3538200000
C 0.3376690000 -3.5306560000 0.7043820000
C 2.0011410000 -2.0552540000 1.8475400000
C 2.5264480000 -3.0592490000 -0.4120490000
C -5.2371510000 -0.1465210000 0.4512880000
H -5.9419670000 0.1546940000 -1.5606680000
H -4.2614910000 -0.5649380000 2.3260890000
C -0.3397930000 1.5390930000 0.2651340000
H 1.4304950000 2.1626840000 -0.7114810000
B 3.8491950000 1.1787310000 -0.3312130000
H -0.0976320000 -3.8699890000 -0.2403460000
H -0.4733710000 -3.1549880000 1.3376440000
H 0.7789730000 -4.3986200000 1.2033990000
H 2.3889930000 -2.9417020000 2.3592140000
H 1.2284070000 -1.6111730000 2.4851740000
H 2.8226350000 -1.3428860000 1.7470360000
H 2.1197840000 -3.3498000000 -1.3862900000
H 2.9360690000 -3.9555880000 0.0659810000
H 3.3406960000 -2.3511230000 -0.5708170000
H -6.1694280000 0.1636470000 0.9118750000
H -0.8560590000 0.7143840000 0.7544890000
C -1.0575510000 2.8505910000 0.3032340000
F 5.0506400000 0.5316620000 -0.3310820000
F 3.5739490000 1.8707530000 0.8300400000
F 3.5977420000 1.9130720000 -1.4733670000
C -2.3826250000 2.7261930000 -0.4670560000
H -0.4327630000 3.6084560000 -0.1832310000
C -1.3050390000 3.2685480000 1.7596580000
H -2.2130440000 2.4303060000 -1.5062510000
H -2.9076080000 3.6863180000 -0.4635920000
H -3.0368380000 1.9788580000 -0.0045000000
H -1.9257130000 2.5259530000 2.2745040000
H -1.8315890000 4.2270470000 1.7926750000
H -0.3653660000 3.3734910000 2.3088690000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397130 (Hartree/Particle)
Thermal correction to Energy= 0.422465
Thermal correction to Enthalpy= 0.423409
Thermal correction to Gibbs (Free) Energy= 0.340897
Sum of electronic and zero-point Energies= -1137.561337
Sum of electronic and thermal Energies= -1137.536002
Sum of electronic and thermal Enthalpies= -1137.535058
Sum of electronic and thermal (Free) Energies= -1137.617570

cc/s TS

C 1.6821220000 0.9979460000 -0.9406760000
C 0.4560780000 0.6235330000 -0.5513710000
C -0.8093010000 1.0618590000 -0.2999490000
C -1.7639470000 -0.0169250000 -0.1951660000
C -1.1265400000 -1.2738790000 -0.2732400000
C 0.2489580000 -1.3285530000 -0.0594350000
C -1.1928550000 2.5141800000 -0.0104270000
O -3.0219750000 0.1910840000 -0.1079610000
H -1.6793550000 -2.1304110000 -0.6467500000
B -4.0117410000 -0.9734390000 0.1940720000
F -4.0081180000 -1.8042560000 -0.9260830000
F -5.2189650000 -0.3636540000 0.4188320000
F -3.5075440000 -1.6397700000 1.3107180000
C 2.9407910000 0.6750290000 -0.2730830000
C 4.1357820000 0.6511220000 -1.0056730000
C 2.9848010000 0.4132550000 1.1044610000
C 5.3340450000 0.3147630000 -0.3897130000
H 4.1146660000 0.8704630000 -2.0695800000
C 4.1854960000 0.0774520000 1.7205430000
H 2.0805020000 0.5056840000 1.6989000000
C 5.3598510000 0.0155470000 0.9730360000
H 6.2500660000 0.2835880000 -0.9705280000
H 4.2067700000 -0.1235490000 2.7866580000
H 6.2967020000 -0.2465280000 1.4537780000
H 1.7479770000 1.6041610000 -1.8441360000
H 0.6585750000 -0.9528560000 0.8810120000
C 0.9715090000 -2.5517430000 -0.6101330000
H 0.4065040000 -2.8878910000 -1.4870720000
C 0.8857870000 -3.6478480000 0.4675510000
H 1.4470650000 -3.3530400000 1.3617310000
H -0.1477770000 -3.8465810000 0.7640240000
H 1.3195290000 -4.5783650000 0.0892860000
C 2.4223320000 -2.3543610000 -1.0474470000
H 2.8091280000 -3.3051770000 -1.4261170000
H 2.5084420000 -1.6150100000 -1.8465760000
H 3.0614110000 -2.0421910000 -0.2165890000
C -2.2087700000 2.9613810000 -1.0840960000
H -3.1123700000 2.3506730000 -1.0611300000
H -2.4897330000 4.0029460000 -0.8967390000
H -1.7693360000 2.9035910000 -2.0855990000
C 0.0165750000 3.4566750000 -0.0569810000
H 0.7855660000 3.1760330000 0.6695820000
H 0.4735600000 3.4871180000 -1.0508330000
H -0.3159080000 4.4713500000 0.1818000000
C -1.8306210000 2.5992770000 1.3904100000
H -2.1121810000 3.6366550000 1.5981000000
H -2.7272340000 1.9820200000 1.4664020000
H -1.1189830000 2.2827020000 2.1608250000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.396355 (Hartree/Particle)
Thermal correction to Energy= 0.420528
Thermal correction to Enthalpy= 0.421472
Thermal correction to Gibbs (Free) Energy= 0.341706
Sum of electronic and zero-point Energies= -1137.525177
Sum of electronic and thermal Energies= -1137.501005
Sum of electronic and thermal Enthalpies= -1137.500061
Sum of electronic and thermal (Free) Energies= -1137.579827

cc/s PT

C 1.7740470000 1.2367120000 0.3489130000
C 0.4847240000 0.8617630000 0.5141030000
C -0.1180200000 -0.4501410000 0.4567960000
C -1.4639250000 -0.2974060000 -0.0134140000
C -1.7895060000 1.0468390000 0.0805310000
C -0.6661210000 1.8808040000 0.5626050000
C 0.3583910000 -1.7600130000 1.0490600000
C 2.8640920000 0.4405090000 -0.2115010000
O -2.2249600000 -1.2948140000 -0.3457670000
C 1.7304480000 -1.7121020000 1.7358610000
C 0.3474420000 -2.8821130000 -0.0130940000
C -0.6944300000 -2.0975600000 2.1485750000

C 4.1720950000 0.6006610000 0.2685610000
C 2.6294720000 -0.4491570000 -1.2687140000
C 3.6704650000 -1.2073560000 -1.7943050000
H 1.6319820000 -0.5272950000 -1.6902790000
C 4.9565290000 -1.0792830000 -1.2753560000
H 3.4775240000 -1.8929590000 -2.6129240000
C 5.2067350000 -0.1690520000 -0.2466860000
H 4.3664500000 1.3076340000 1.0701750000
H 5.7680480000 -1.6735410000 -1.6825110000
H 6.2111950000 -0.0583150000 0.1485050000
B -3.7148050000 -1.0617490000 -0.5962940000
F -4.2464620000 -0.5086150000 0.5798430000
F -4.2450830000 -2.2944850000 -0.8949900000
F -3.8328410000 -0.1436690000 -1.6498140000
H 2.0150480000 2.2812790000 0.5304470000
H -2.7870970000 1.4217550000 -0.1076900000
H -0.8531890000 2.0697620000 1.6339940000
C -0.4721880000 3.2535680000 -0.1338540000
C -1.7839540000 3.8230890000 -0.6856630000
H 0.2038290000 3.0985970000 -0.9836680000
C 0.1593050000 4.2681540000 0.8278450000
H -0.5500400000 4.5236210000 1.6238880000
H 0.4162430000 5.1920080000 0.3017830000
H 1.0674760000 3.8965410000 1.3119170000
H -2.2041760000 3.2000570000 -1.4796270000
H -1.6069930000 4.8179470000 -1.1046860000
H -2.5371680000 3.9268390000 0.1038820000
H -0.6959020000 -1.3330810000 2.9323470000
H -0.4143350000 -3.0508920000 2.6060340000
H -1.7000200000 -2.1931940000 1.7386280000
H 0.5891230000 -3.8269470000 0.4838320000
H 1.1080890000 -2.7017160000 -0.7774330000
H -0.6294210000 -2.9760980000 -0.4887080000
H 1.8310650000 -0.8421140000 2.3923210000
H 2.5572430000 -1.7110290000 1.0259890000
H 1.8345770000 -2.6081780000 2.3544740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.399753 (Hartree/Particle)
Thermal correction to Energy= 0.423758
Thermal correction to Enthalpy= 0.424702
Thermal correction to Gibbs (Free) Energy= 0.345130
Sum of electronic and zero-point Energies= -1137.564472
Sum of electronic and thermal Energies= -1137.540468
Sum of electronic and thermal Enthalpies= -1137.539524
Sum of electronic and thermal (Free) Energies= -1137.619096

c/d RT

C 2.1407300000 0.6424150000 1.0244310000
C 1.0372200000 -0.0574730000 0.9742690000
H 2.2408230000 1.3822850000 1.8178290000
C 3.2728190000 0.5071260000 0.0850870000
C -0.0272900000 -0.8289980000 0.8709670000
C 4.4276720000 1.2666660000 0.2962440000
C 3.2218020000 -0.3618800000 -1.0124790000
C -1.1016700000 -0.3594650000 -0.0317020000
C -0.1167840000 -2.2097420000 1.5535200000
C 5.5137540000 1.1587890000 -0.5684980000
H 4.4767400000 1.9448700000 1.1439270000
C 4.3058630000 -0.4679650000 -1.8745450000
H 2.3275620000 -0.9523040000 -1.1920150000
C -1.4180800000 1.0511220000 -0.2014630000
O -1.7291430000 -1.2448020000 -0.6624270000
C 0.9502620000 -2.3012420000 2.6529870000
C 0.1383030000 -3.3231960000 0.5196870000
C -1.5066080000 -2.3799260000 2.1920770000
C 5.4559980000 0.2913180000 -1.6557390000
H 6.4040900000 1.7538060000 -0.3918230000
H 4.2528450000 -1.1430560000 -2.7226280000
C -1.2341240000 1.9597050000 0.7696330000
H -1.9137920000 1.3092910000 -1.1301430000
B -3.0102890000 -1.0279820000 -1.6230220000
H 0.8187260000 -1.5171490000 3.4064040000
H 1.9615450000 -2.2159790000 2.2437250000
H 0.8701330000 -3.2701640000 3.1550480000
H 0.1072480000 -4.2963660000 1.0213750000
H 1.1288450000 -3.2080860000 0.0668820000
H -0.6122370000 -3.3204900000 -0.2718260000
H -1.7077470000 -1.5803210000 2.9136920000
H -1.5450610000 -3.3328660000 2.7292050000
H -2.3039390000 -2.3864000000 1.4459720000
H 6.3007900000 0.2069800000 -2.3316680000
C -1.6270000000 3.4053200000 0.7020720000
H -0.8119010000 1.6392350000 1.7210710000
F -3.9403310000 -0.3734560000 -0.8413860000
F -2.5574440000 -0.2625650000 -2.6802360000
F -3.3549780000 -2.3045900000 -1.9600430000
C -2.1689800000 3.8485740000 -0.6553560000
H -0.7077720000 3.9729190000 0.9143880000
C -2.6237010000 3.7093850000 1.8349530000
H -1.4523090000 3.6579810000 -1.4596300000
H -2.3802190000 4.9214030000 -0.6402470000
H -3.1016170000 3.3278140000 -0.8966990000
H -3.5583570000 3.1619180000 1.6774050000
H -2.8533000000 4.7784160000 1.8587760000
H -2.2228480000 3.4268910000 2.8136200000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.396665 (Hartree/Particle)
Thermal correction to Energy= 0.422236
Thermal correction to Enthalpy= 0.423180
Thermal correction to Gibbs (Free) Energy= 0.337900
Sum of electronic and zero-point Energies= -1137.556896
Sum of electronic and thermal Energies= -1137.531325
Sum of electronic and thermal Enthalpies= -1137.530381
Sum of electronic and thermal (Free) Energies= -1137.615661

c/d TS

C 1.8837640000 0.7260210000 0.8625300000
C 0.6554200000 0.2289910000 0.8231410000
H 2.0849750000 1.5660020000 1.5247680000
C 3.0002440000 0.2662970000 0.0230790000
C -0.2614160000 -0.7544440000 0.6401010000
C 4.3034030000 0.6653420000 0.3456570000
C 2.7980980000 -0.5573970000 -1.0926020000
C -1.4833970000 -0.2619560000 0.0369150000
C -0.0869630000 -2.1995960000 1.1046840000
C 5.3840210000 0.2278550000 -0.4133570000
H 4.4698330000 1.3128260000 1.2022970000
C 3.8785760000 -0.9904260000 -1.8510910000
H 1.7891910000 -0.8447870000 -1.3726060000
C -1.5168630000 1.1572260000 0.0006190000
O -2.3542020000 -1.0538510000 -0.4547330000
C 1.2356490000 -2.3835780000 1.8596450000
C -0.0912200000 -3.1169320000 -0.1366970000
C -1.2575260000 -2.5727330000 2.0347790000
C 5.1749040000 -0.6033400000 -1.5118010000
H 6.3895790000 0.5379040000 -0.1480160000
H 3.7081320000 -1.6252010000 -2.7145870000
C -0.6962290000 1.8339410000 0.8873990000
H -2.0661650000 1.6574050000 -0.7903760000
B -3.7267200000 -0.5223720000 -0.9796430000
H 1.2845420000 -1.7473970000 2.7491370000
H 2.1010400000 -2.1600800000 1.2286200000
H 1.3189520000 -3.4248190000 2.1852450000
H -0.0024450000 -4.1574440000 0.1923350000
H 0.7603900000 -2.8984770000 -0.7887700000
H -1.0141060000 -3.0138120000 -0.7099330000
H -1.2775610000 -1.9231040000 2.9164390000
H -1.1316390000 -3.6039820000 2.3797390000
H -2.2194380000 -2.4998120000 1.5235690000
H 6.0170260000 -0.9416190000 -2.1066880000
C -0.2465840000 3.2552410000 0.6580930000
H -0.6877670000 1.5218810000 1.9313820000
F -4.2678400000 0.2467510000 0.0472260000
F -3.4445970000 0.2614150000 -2.0982610000
F -4.4532800000 -1.6473400000 -1.2680400000
C 0.1643340000 3.5229710000 -0.7906410000
H 0.6252770000 3.4220040000 1.3037900000
C -1.3550200000 4.2144360000 1.1284730000
H 0.9220340000 2.8071790000 -1.1245920000
H 0.5783780000 4.5307150000 -0.8863350000
H -0.6920120000 3.4530090000 -1.4685300000
H -2.2549890000 4.0939000000 0.5177000000
H -1.0153590000 5.2501510000 1.0370720000
H -1.6283720000 4.0352720000 2.1725380000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.396247 (Hartree/Particle)
Thermal correction to Energy= 0.420698
Thermal correction to Enthalpy= 0.421643
Thermal correction to Gibbs (Free) Energy= 0.340931
Sum of electronic and zero-point Energies= -1137.534495
Sum of electronic and thermal Energies= -1137.510044
Sum of electronic and thermal Enthalpies= -1137.509100
Sum of electronic and thermal (Free) Energies= -1137.589812

c/d PT

C -1.7717270000 1.2152990000 -0.6633760000
C -0.4844440000 0.7976760000 -0.7187270000
C 0.1111950000 -0.4937710000 -0.4879650000
C 1.4742150000 -0.2849960000 -0.0837910000
C 1.8038120000 1.0304340000 -0.3690300000
C 0.6602210000 1.8034840000 -0.8937170000
C -0.3879530000 -1.8782780000 -0.8481350000
C -2.8991930000 0.5503260000 -0.0171450000
O 2.2348780000 -1.2297920000 0.3771250000
C -1.7664100000 -1.9288170000 -1.5222020000
C -0.3847890000 -2.7924190000 0.3984180000
C 0.6433540000 -2.4269780000 -1.8790640000
C -4.1906820000 0.6634510000 -0.5517920000
C -2.7142040000 -0.1575770000 1.1787890000
C -3.7888110000 -0.7887520000 1.7956600000
H -1.7277560000 -0.1920410000 1.6311590000
C -5.0588880000 -0.7144330000 1.2284450000
H -3.6349330000 -1.3332480000 2.7215040000
C -5.2589110000 0.0173170000 0.0564230000
H -4.3460350000 1.2322530000 -1.4641480000
H -5.8969680000 -1.2104260000 1.7071010000
H -6.2507550000 0.0868550000 -0.3780080000
B 3.7169720000 -0.9537620000 0.6308340000
F 4.2778000000 -0.5518760000 -0.5912700000
F 4.2454170000 -2.1327280000 1.1009690000
F 3.8004860000 0.0938580000 1.5604670000
H -1.9730200000 2.2240600000 -1.0214760000
H 2.8006050000 1.4310160000 -0.2327010000
H 0.7922040000 1.9283990000 -1.9812240000
C 0.5064280000 3.2058310000 -0.2618160000
C 0.3758080000 3.1315710000 1.2619380000
H -0.4098370000 3.6499970000 -0.6707730000
C 1.6679270000 4.1157170000 -0.6741040000
H 2.6191070000 3.7688070000 -0.2577520000
H 1.5014640000 5.1309940000 -0.3028350000
H 1.7728240000 4.1685330000 -1.7627170000
H -0.4577690000 2.4913030000 1.5681500000
H 0.2025240000 4.1275720000 1.6793960000
H 1.2908530000 2.7347670000 1.7146550000
H 0.6492450000 -1.8122190000 -2.7850220000
H 0.3390830000 -3.4396370000 -2.1592040000
H 1.6521830000 -2.4709040000 -1.4690820000
H -0.6499350000 -3.8060500000 0.0816880000
H -1.1318410000 -2.4624820000 1.1256070000
H 0.5965690000 -2.8193830000 0.8736930000
H -1.8609720000 -1.1855950000 -2.3201590000
H -2.5868130000 -1.7921500000 -0.8186680000
H -1.8889330000 -2.9170800000 -1.9746990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.399303 (Hartree/Particle)
Thermal correction to Energy= 0.423358
Thermal correction to Enthalpy= 0.424302
Thermal correction to Gibbs (Free) Energy= 0.345420
Sum of electronic and zero-point Energies= -1137.563154
Sum of electronic and thermal Energies= -1137.539100
Sum of electronic and thermal Enthalpies= -1137.538156
Sum of electronic and thermal (Free) Energies= -1137.617038

cc/d RT

C -1.6599820000 -1.1041130000 -1.4017610000
C -0.4924650000 -1.1927890000 -0.8189970000
C -2.9198260000 -0.7972560000 -0.6953900000
H -1.7028830000 -1.2221630000 -2.4836180000
C 0.6914860000 -1.2707630000 -0.2456560000
C -4.0010800000 -0.2779430000 -1.4145690000
C -3.0513650000 -0.9804200000 0.6870250000
C 1.4872220000 -0.0203830000 -0.2032220000
C 1.2772110000 -2.5963060000 0.2805910000
C -5.1788520000 0.0768330000 -0.7631060000
H -3.9124690000 -0.1366830000 -2.4881290000
C -4.2286280000 -0.6273150000 1.3370420000
H -2.2287280000 -1.4112040000 1.2514070000
C 0.8734970000 1.2935530000 -0.0785080000
O 2.7320960000 -0.1492860000 -0.2932460000
C 0.1533950000 -3.6353120000 0.3992400000
C 1.8892050000 -2.3660630000 1.6741090000
C 2.3462230000 -3.1281400000 -0.6923740000
C -5.2948900000 -0.0920070000 0.6148080000
H -6.0063570000 0.4871140000 -1.3329650000
H -4.3169110000 -0.7757770000 2.4086120000
C -0.3071360000 1.4981720000 0.5286640000
H 1.4798150000 2.1217980000 -0.4265870000
B 3.8428440000 1.0177170000 -0.1624940000
H -0.3069910000 -3.8479880000 -0.5702650000
H -0.6337430000 -3.3024140000 1.0844340000
H 0.5647240000 -4.5709820000 0.7897210000
H 2.2437190000 -3.3200970000 2.0768540000
H 1.1433920000 -1.9648970000 2.3695990000
H 2.7397650000 -1.6820880000 1.6415670000
H 1.9169830000 -3.2889780000 -1.6867700000
H 2.7225890000 -4.0891050000 -0.3254920000
H 3.1881700000 -2.4407080000 -0.7824570000
H -6.2133770000 0.1835510000 1.1226640000
H -0.8509230000 0.6486560000 0.9378060000
C -0.9778680000 2.8248630000 0.7215900000
F 5.0171550000 0.3260800000 -0.2330110000
F 3.6017010000 1.6084030000 1.0608730000
F 3.6177250000 1.8674400000 -1.2280200000
C -0.1796710000 4.0174410000 0.1994450000
H -1.1100680000 2.9400850000 1.8078240000
C -2.3851000000 2.7636580000 0.0978360000
H 0.8061430000 4.0836510000 0.6686240000
H -0.7166970000 4.9464340000 0.4104180000
H -0.0391110000 3.9531510000 -0.8851390000
H -2.3183820000 2.6254170000 -0.9863760000
H -2.9202670000 3.6979880000 0.2904500000
H -2.9768700000 1.9393890000 0.5070800000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.397090 (Hartree/Particle)
Thermal correction to Energy= 0.422405
Thermal correction to Enthalpy= 0.423349
Thermal correction to Gibbs (Free) Energy= 0.340582
Sum of electronic and zero-point Energies= -1137.561047
Sum of electronic and thermal Energies= -1137.535732
Sum of electronic and thermal Enthalpies= -1137.534788
Sum of electronic and thermal (Free) Energies= -1137.617555

cc/d TS

C 1.6210320000 0.9145900000 -0.9528930000
C 0.4126050000 0.6133000000 -0.4723640000
C 2.8990190000 0.6404500000 -0.2930080000
H 1.6592750000 1.3904560000 -1.9329470000
C -0.8725610000 1.0107880000 -0.2688180000
C 4.0425950000 0.3661450000 -1.0551400000
C 3.0058410000 0.6771960000 1.1045880000
C -1.7750510000 -0.1023180000 -0.0858030000
C -1.3218300000 2.4646900000 -0.1285350000
C 5.2528150000 0.0852010000 -0.4321510000
H 3.9735090000 0.3536170000 -2.1394160000
C 4.2190960000 0.4031710000 1.7262320000
H 2.1391650000 0.9480800000 1.7008590000
C -1.0752640000 -1.3295160000 -0.0257350000
O -3.0428460000 0.0513810000 -0.0582780000
C -0.1420920000 3.4402390000 -0.2281080000
C -2.0095940000 2.6543930000 1.2374560000
C -2.3163810000 2.7675240000 -1.2700570000
C 5.3417660000 0.0960830000 0.9601340000
H 6.1285660000 -0.1417460000 -1.0312770000
H 4.2900110000 0.4352430000 2.8085070000
C 0.2912380000 -1.2913500000 0.2411170000
H -1.5753710000 -2.2437980000 -0.3294410000
B -3.9955350000 -1.1315740000 0.2939690000
H 0.3509600000 3.3875020000 -1.2036680000
H 0.6088950000 3.2552880000 0.5465820000
H -0.5130640000 4.4615280000 -0.1002290000

H -2.3349590000 3.6948150000 1.3381320000
H -1.3145740000 2.4380350000 2.0561390000
H -2.8856570000 2.0123280000 1.3428070000
H -1.8407530000 2.6366580000 -2.2478490000
H -2.6450220000 3.8088620000 -1.1895790000
H -3.1950100000 2.1228730000 -1.2176350000
H 6.2880870000 -0.1199420000 1.4451900000
H 0.6449920000 -0.7770910000 1.1368980000
C 1.1387740000 -2.4630510000 -0.2347980000
F -5.2402920000 -0.5656260000 0.3916630000
F -3.5301460000 -1.6683980000 1.4925010000
F -3.8852620000 -2.0561730000 -0.7448420000
C 1.4113150000 -2.4139500000 -1.7453230000
H 0.4895970000 -3.3334030000 -0.0635810000
C 2.4192780000 -2.6928650000 0.5700100000
H 0.4935430000 -2.2233280000 -2.3094810000
H 1.8256930000 -3.3689510000 -2.0808450000
H 2.1351500000 -1.6304530000 -1.9861260000
H 3.1842880000 -1.9472970000 0.3436720000
H 2.8339310000 -3.6759140000 0.3280390000
H 2.2248800000 -2.6690980000 1.6469170000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.396222 (Hartree/Particle)
Thermal correction to Energy= 0.420415
Thermal correction to Enthalpy= 0.421359
Thermal correction to Gibbs (Free) Energy= 0.342466
Sum of electronic and zero-point Energies= -1137.529302
Sum of electronic and thermal Energies= -1137.505108
Sum of electronic and thermal Enthalpies= -1137.504164
Sum of electronic and thermal (Free) Energies= -1137.583058

cc/d PT

C -1.7508680000 0.9874680000 -0.2478120000
C -0.5810510000 0.3167620000 -0.1123380000
C 0.7378860000 0.9180180000 -0.1177070000
C 1.6892750000 -0.1082510000 -0.4296250000
C 1.0258230000 -1.3248210000 -0.4309520000
C -0.3974720000 -1.1904090000 -0.0811840000
C 1.1911150000 2.3288780000 0.1784890000
O 2.9588080000 0.1121960000 -0.6114860000
C 0.0972600000 3.3218920000 0.5961740000
C 1.9123740000 2.8892100000 -1.0713380000
C 2.1935400000 2.2228710000 1.3615100000
H 1.5277110000 -2.2748120000 -0.5743420000
C -3.0896760000 0.4223500000 -0.4623720000
H -1.7260960000 2.0687190000 -0.2113600000
C -4.1625820000 0.9550290000 0.2676380000
C -5.4429930000 0.4354990000 0.1246960000
C -5.6797160000 -0.5964960000 -0.7832130000
C -4.6321680000 -1.0956250000 -1.5531560000
C -3.3446710000 -0.5925360000 -1.3935790000
H -3.9815250000 1.7629880000 0.9713430000
H -6.2587810000 0.8401240000 0.7147270000
H -6.6813430000 -0.9964180000 -0.9027980000
H -4.8170460000 -1.8751440000 -2.2850550000
H -2.5439170000 -0.9612280000 -2.0250880000
B 3.9364290000 -1.0545050000 -0.5189430000
F 5.1945280000 -0.5049740000 -0.5948460000
F 3.6609480000 -1.9420490000 -1.5681490000
F 3.6936060000 -1.6896170000 0.7146010000
H 1.6892910000 1.8618090000 2.2636000000
H 2.5867360000 3.2229910000 1.5679000000
H 3.0296240000 1.5631150000 1.1312130000
H 2.2693840000 3.8983790000 -0.8426490000
H 1.2221500000 2.9565670000 -1.9187080000
H 2.7652270000 2.2714190000 -1.3530780000
H -0.5135680000 2.9469840000 1.4235110000
H -0.5505200000 3.6093970000 -0.2373600000
H 0.5851690000 4.2380690000 0.9409000000
H -1.0305000000 -1.7215560000 -0.7982540000
C -0.6597690000 -1.8462130000 1.3265460000
C 0.1806980000 -1.2106660000 2.4356430000
H -0.3330800000 -2.8869880000 1.2087980000
C -2.1419890000 -1.8611790000 1.6991280000
H 1.2543830000 -1.3017690000 2.2505810000
H -0.0395810000 -1.7004770000 3.3884320000
H -0.0584740000 -0.1465760000 2.5525700000
H -2.5055190000 -0.8540590000 1.9248760000
H -2.2881630000 -2.4751060000 2.5929830000
H -2.7660130000 -2.2723920000 0.9001370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.399628 (Hartree/Particle)
Thermal correction to Energy= 0.423580
Thermal correction to Enthalpy= 0.424524
Thermal correction to Gibbs (Free) Energy= 0.345171
Sum of electronic and zero-point Energies= -1137.566694
Sum of electronic and thermal Energies= -1137.542742
Sum of electronic and thermal Enthalpies= -1137.541798
Sum of electronic and thermal (Free) Energies= -1137.621150

c/u RT

C -2.1102690000 0.2123080000 -1.0271840000
C -0.9189540000 -0.3240040000 -0.9721800000
H -2.3431020000 0.8525110000 -1.8774000000
C -3.1724010000 0.0218520000 -0.0186470000
C 0.2505580000 -0.9222820000 -0.8530540000
C -4.4234600000 0.6108680000 -0.2263190000
C -2.9599750000 -0.7317760000 1.1429480000
C 1.2780490000 -0.2157470000 -0.0559240000
C 0.5144320000 -2.3382120000 -1.4057190000
C -5.4455720000 0.4484840000 0.7054100000
H -4.5979040000 1.1984910000 -1.1236890000
C -3.9804760000 -0.8926990000 2.0714590000
H -1.9903100000 -1.1890870000 1.3192850000
C 1.3691950000 1.2366990000 -0.0155120000
O 2.0630890000 -0.9351150000 0.6082890000
C -0.5713610000 -2.6920290000 -2.4312210000
C 0.4674890000 -3.3649600000 -0.2578900000
C 1.8872470000 -2.3743240000 -2.1003030000
C -5.2271070000 -0.3037380000 1.8562190000
H -6.4118820000 0.9108010000 0.5309310000
H -3.8025280000 -1.4771850000 2.9684110000
C 0.9797210000 2.0177940000 -1.0353200000
H 1.8557210000 1.6491450000 0.8608030000
B 3.3272580000 -0.4393480000 1.4844500000
H -0.5865990000 -1.9785640000 -3.2621690000
H -1.5668980000 -2.7093700000 -1.9772020000
H -0.3707430000 -3.6860950000 -2.8421340000
H 0.6212960000 -4.3699600000 -0.6652940000
H -0.5102980000 -3.3465620000 0.2351690000
H 1.2406850000 -3.1743170000 0.4875930000
H 1.9401010000 -1.6321910000 -2.9046230000
H 2.0426330000 -3.3620740000 -2.5455770000
H 2.7060330000 -2.1917050000 -1.4013010000
H -6.0219970000 -0.4304910000 2.5840370000
C 1.0532260000 3.5146810000 -1.0745010000
H 0.5723890000 1.5517200000 -1.9313390000
F 4.1125730000 0.2823680000 0.6095100000
F 2.7951260000 0.3340970000 2.4982020000
F 3.8821730000 -1.6129220000 1.9051140000
C -0.3637320000 4.0642960000 -1.3240430000
H 1.6621020000 3.7687430000 -1.9546130000
C 1.6926110000 4.1477040000 0.1594150000
H -0.8062130000 3.6426350000 -2.2325800000
H -0.3327080000 5.1516240000 -1.4373420000
H -1.0210550000 3.8266390000 -0.4811030000
H 1.1050250000 3.9379760000 1.0598020000
H 1.7412610000 5.2335220000 0.0391700000
H 2.7098280000 3.7800510000 0.3213790000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.396561 (Hartree/Particle)
Thermal correction to Energy= 0.422130
Thermal correction to Enthalpy= 0.423075
Thermal correction to Gibbs (Free) Energy= 0.337887
Sum of electronic and zero-point Energies= -1137.557350
Sum of electronic and thermal Energies= -1137.531781
Sum of electronic and thermal Enthalpies= -1137.530837
Sum of electronic and thermal (Free) Energies= -1137.616024

c/u TS

C 1.8679580000 0.6253960000 0.7686560000
C 0.5878810000 0.2727270000 0.7590120000
H 2.1737200000 1.4612790000 1.3919630000
C 2.9119210000 0.0050780000 -0.0586930000

C -0.4074920000 -0.6429680000 0.6410590000
C 4.2566050000 0.2547690000 0.2439660000
C 2.6017360000 -0.8257850000 -1.1438920000
C -1.5995840000 -0.0868830000 0.0359580000
C -0.3429270000 -2.0702050000 1.1841660000
C 5.2697730000 -0.3381730000 -0.5022390000
H 4.5071960000 0.9071720000 1.0760870000
C 3.6153870000 -1.4142250000 -1.8897310000
H 1.5630380000 -0.9963920000 -1.4099780000
C -1.5258510000 1.3242380000 -0.0680250000
O -2.5433060000 -0.8322980000 -0.3927030000
C 0.9720230000 -2.3258870000 1.9315480000
C -0.4462340000 -3.0508880000 -0.0035160000
C -1.5232140000 -2.2921540000 2.1502170000
C 4.9518250000 -1.1765850000 -1.5687320000
H 6.3077280000 -0.1437840000 -0.2522610000
H 3.3623510000 -2.0532850000 -2.7294650000
C -0.6086300000 1.9826240000 0.7400360000
H -2.0807810000 1.8363840000 -0.8478630000
B -3.8833150000 -0.2262890000 -0.9147950000
H 1.0926760000 -1.6459490000 2.7809050000
H 1.8422970000 -2.2185670000 1.2775590000
H 0.9686500000 -3.3496080000 2.3177100000
H -0.4398270000 -4.0753240000 0.3828940000
H 0.4094580000 -2.9420690000 -0.6773710000
H -1.3671460000 -2.9016200000 -0.5696110000
H -1.4729120000 -1.5952110000 2.9937250000
H -1.4757110000 -3.3095530000 2.5513950000
H -2.4853400000 -2.1679830000 1.6496290000
H 5.7417070000 -1.6361950000 -2.1538450000
C -0.1044240000 3.3613890000 0.3659860000
H -0.5793300000 1.7450200000 1.8036420000
F -4.3421360000 0.6309780000 0.0823600000
F -3.5731170000 0.4786030000 -2.0780750000
F -4.6985540000 -1.3063420000 -1.1309560000
C 0.6958300000 4.0255550000 1.4885410000
H -1.0204540000 3.9534640000 0.2215240000
C 0.6563480000 3.3662320000 -0.9669860000
H 0.1425520000 4.0214430000 2.4328490000
H 0.9150750000 5.0660510000 1.2339130000
H 1.6554310000 3.5241610000 1.6519610000
H 1.6011500000 2.8206810000 -0.8811410000
H 0.8825640000 4.3929210000 -1.2681930000
H 0.0696140000 2.9021100000 -1.7643710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395939 (Hartree/Particle)
Thermal correction to Energy= 0.420456
Thermal correction to Enthalpy= 0.421400
Thermal correction to Gibbs (Free) Energy= 0.340626
Sum of electronic and zero-point Energies= -1137.532912
Sum of electronic and thermal Energies= -1137.508396
Sum of electronic and thermal Enthalpies= -1137.507451
Sum of electronic and thermal (Free) Energies= -1137.588226

c/u PT

C -1.7976590000 1.0381310000 -0.6557010000
C -0.4687680000 0.7692400000 -0.6982310000
C 0.2516280000 -0.4596670000 -0.4902320000
C 1.5975710000 -0.1291860000 -0.1071490000
C 1.7944200000 1.2117720000 -0.3886660000
C 0.5691500000 1.8886690000 -0.8600840000
C -0.1154230000 -1.8828180000 -0.8644800000
C -2.8384850000 0.2629020000 0.0087340000
O 2.4507060000 -1.0036280000 0.3294620000
C -1.4907790000 -2.0641500000 -1.5225870000
C -0.0066260000 -2.8059000000 0.3708740000
C 0.9498310000 -2.3169950000 -1.9150610000
C -4.1427530000 0.2387580000 -0.5072740000
C -2.5636470000 -0.4156450000 1.2048610000
C -3.5573610000 -1.1536020000 1.8383520000
H -1.5732620000 -0.3422890000 1.6437680000
C -4.8359340000 -1.2149750000 1.2888730000
H -3.3349220000 -1.6747010000 2.7636990000
C -5.1285810000 -0.5128390000 0.1178880000
H -4.3692230000 0.7844910000 -1.4188710000
H -5.6107810000 -1.7937020000 1.7810240000
H -6.1284670000 -0.5493300000 -0.3018160000
B 3.8993080000 -0.5885270000 0.5890640000
F 4.4152800000 -0.1034990000 -0.6223870000
F 4.5424310000 -1.7216160000 1.0292210000
F 3.8802600000 0.4372510000 1.5453280000
H -2.1139750000 2.0023870000 -1.0447750000
H 2.7471230000 1.7142870000 -0.2696270000
H 0.6581840000 2.0740280000 -1.9427550000
C 0.3767550000 3.2514250000 -0.1435930000
C -0.6318230000 4.1884340000 -0.8162360000
H 1.3580200000 3.7367550000 -0.2323430000
C 0.0817400000 3.0856380000 1.3499890000
H -0.9059810000 2.6404180000 1.5125950000
H 0.0906570000 4.0594090000 1.8480970000
H 0.8288380000 2.4540150000 1.8405820000
H -0.5106250000 4.2064340000 -1.9045300000
H -0.4904280000 5.2094180000 -0.4495380000
H -1.6669230000 3.9149980000 -0.5875860000
H 0.8820120000 -1.6951730000 -2.8136760000
H 0.7428980000 -3.3517870000 -2.2029650000
H 1.9638810000 -2.2658250000 -1.5192530000
H -0.1770140000 -3.8369870000 0.0453860000
H -0.7719910000 -2.5574130000 1.1113570000
H 0.9791600000 -2.7432160000 0.8333370000
H -1.6734200000 -1.3204860000 -2.3047140000
H -2.3112740000 -2.0269770000 -0.8069210000
H -1.5159560000 -3.0514510000 -1.9926240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.399257 (Hartree/Particle)
Thermal correction to Energy= 0.423314
Thermal correction to Enthalpy= 0.424259
Thermal correction to Gibbs (Free) Energy= 0.344784
Sum of electronic and zero-point Energies= -1137.560329
Sum of electronic and thermal Energies= -1137.536271
Sum of electronic and thermal Enthalpies= -1137.535327
Sum of electronic and thermal (Free) Energies= -1137.614802

cc/u RT

C -1.6736490000 -1.2637040000 -1.4237460000
C -0.5172810000 -1.3121570000 -0.8141930000
C -2.9359600000 -0.8488740000 -0.7782930000
H -1.7031090000 -1.4960650000 -2.4873360000
C 0.6553790000 -1.3311750000 -0.2130480000
C -3.9955850000 -0.3970100000 -1.5721820000
C -3.0920310000 -0.8626790000 0.6139770000
C 1.4484290000 -0.0790860000 -0.2809560000
C 1.2264920000 -2.5910370000 0.4661240000
C -5.1754180000 0.0548390000 -0.9874840000
H -3.8895390000 -0.3890680000 -2.6534290000
C -4.2699370000 -0.4095110000 1.1971780000
H -2.2900360000 -1.2449610000 1.2399020000
C 0.8199590000 1.2335050000 -0.2975760000
O 2.6953570000 -0.2079400000 -0.3335210000
C 0.0988650000 -3.6134120000 0.6653400000
C 1.8023390000 -2.2119660000 1.8423200000
C 2.3201910000 -3.2207370000 -0.4167400000
C -5.3144120000 0.0553010000 0.3985430000
H -5.9866680000 0.4074690000 -1.6163000000
H -4.3771960000 -0.4281380000 2.2771930000
C -0.3808180000 1.4673520000 0.2573180000
H 1.4193550000 2.0350430000 -0.7139790000
B 3.7940330000 0.9763800000 -0.2890520000
H -0.3355160000 -3.9290800000 -0.2880170000
H -0.7060930000 -3.2100830000 1.2893170000
H 0.4983440000 -4.5013390000 1.1645020000
H 2.1472830000 -3.1163460000 2.3533510000
H 1.0386800000 -1.7415470000 2.4719620000
H 2.6527820000 -1.5321870000 1.7585110000
H 1.9167540000 -3.4880480000 -1.3989250000
H 2.6871720000 -4.1359260000 0.0602260000
H 3.1642080000 -2.5445980000 -0.5584290000
H -6.2344670000 0.4063840000 0.8543930000
H -0.9069620000 0.6498250000 0.7451030000
C -1.0922630000 2.7834260000 0.3184490000
F 4.9752660000 0.2931700000 -0.2735920000
F 3.5235930000 1.6735410000 0.8706930000
F 3.5835060000 1.7237510000 -1.4315790000
C -1.4503330000 3.1004990000 1.7803150000
H -2.0406300000 2.6174280000 -0.2171230000
C -0.3457720000 3.9367540000 -0.3479330000

H -2.0246020000 2.2871640000 2.2355910000
H -2.0536920000 4.0111230000 1.8327570000
H -0.5433780000 3.2567320000 2.3732480000
H 0.6053270000 4.1340610000 0.1580400000
H -0.9465840000 4.8492340000 -0.3002920000
H -0.1349090000 3.7284210000 -1.4010240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.396782 (Hartree/Particle)
Thermal correction to Energy= 0.422270
Thermal correction to Enthalpy= 0.423214
Thermal correction to Gibbs (Free) Energy= 0.339030
Sum of electronic and zero-point Energies= -1137.559513
Sum of electronic and thermal Energies= -1137.534025
Sum of electronic and thermal Enthalpies= -1137.533081
Sum of electronic and thermal (Free) Energies= -1137.617265

cc/u TS

C 1.6651590000 1.0794990000 -0.9167060000
C 0.4681260000 0.8096450000 -0.4001920000
C 2.9597270000 0.7165730000 -0.3303260000
H 1.6796420000 1.5704130000 -1.8901510000
C -0.8332710000 1.1405690000 -0.1906450000
C 4.0343830000 0.3843250000 -1.1654570000
C 3.1444570000 0.6858270000 1.0591310000
C -1.6905890000 -0.0205090000 -0.0894910000
C -1.3442630000 2.5662500000 0.0065430000
C 5.2526960000 -0.0100690000 -0.6235920000
H 3.9035900000 0.4156070000 -2.2435350000
C 4.3640900000 0.2920660000 1.5994450000
H 2.3346590000 0.9952850000 1.7138130000
C -0.9380250000 -1.2208850000 -0.0526330000
O -2.9630070000 0.0774650000 -0.1176140000
C -0.1930390000 3.5801870000 0.0109310000
C -2.0976570000 2.6578920000 1.3473200000
C -2.2989540000 2.8945770000 -1.1612990000
C 5.4180990000 -0.0643810000 0.7598960000
H 6.0741450000 -0.2769760000 -1.2805390000
H 4.4954630000 0.2732440000 2.6765040000
C 0.3966630000 -1.1264500000 0.3145400000
H -1.3739220000 -2.1352700000 -0.4421490000
B -3.8744550000 -1.1646090000 0.1323660000
H 0.3454320000 3.5914130000 -0.9416910000
H 0.5283880000 3.3736940000 0.8081450000
H -0.5999950000 4.5823730000 0.1751580000
H -2.4663540000 3.6791090000 1.4873720000
H -1.4322250000 2.4221330000 2.1849330000
H -2.9524610000 1.9799190000 1.3775140000
H -1.7768920000 2.8344910000 -2.1221340000
H -2.6713410000 3.9172120000 -1.0409360000
H -3.1531910000 2.2158730000 -1.1824640000
H 6.3696730000 -0.3706860000 1.1819870000
H 0.6500340000 -0.5928220000 1.2315690000
C 1.4039930000 -2.1748390000 -0.0923210000
F -5.1470600000 -0.6609090000 0.2005430000
F -3.4359550000 -1.7405100000 1.3226430000
F -3.6740660000 -2.0278530000 -0.9448420000
C 1.2431870000 -3.4000230000 0.8253850000
H 2.3982720000 -1.7561330000 0.0930430000
C 1.3055460000 -2.5511880000 -1.5712660000
H 1.3434160000 -3.1273470000 1.8801870000
H 2.0116590000 -4.1423280000 0.5910030000
H 0.2627380000 -3.8668550000 0.6880050000
H 0.3552040000 -3.0428650000 -1.8021980000
H 2.1099060000 -3.2427380000 -1.8378380000
H 1.3922580000 -1.6643790000 -2.2071990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395901 (Hartree/Particle)
Thermal correction to Energy= 0.420373
Thermal correction to Enthalpy= 0.421317
Thermal correction to Gibbs (Free) Energy= 0.340884
Sum of electronic and zero-point Energies= -1137.533635
Sum of electronic and thermal Energies= -1137.509163
Sum of electronic and thermal Enthalpies= -1137.508219
Sum of electronic and thermal (Free) Energies= -1137.588652

cc/u PT

C -1.7750880000 1.1129130000 -0.1247920000
C -0.5860230000 0.4634910000 -0.2276680000
C 0.7331320000 1.0471280000 -0.1333170000
C 1.6996900000 0.0009370000 -0.3148780000
C 1.0244260000 -1.1939610000 -0.5026560000
C -0.4330910000 -1.0373420000 -0.4001050000
C 1.1903960000 2.4705210000 0.1050510000
O 2.9860370000 0.1901690000 -0.2859680000
C 0.0948370000 3.5305510000 0.2815030000
C 2.0621500000 2.8947150000 -1.1047180000
C 2.0483380000 2.4627710000 1.3980980000
H 1.5296340000 -2.1386630000 -0.6601020000
C -3.1209390000 0.5478390000 -0.2564440000
H -1.7655770000 2.1640540000 0.1263470000
C -4.1140170000 1.0143620000 0.6202060000
C -5.4033700000 0.4990260000 0.5726810000
C -5.7333470000 -0.4645180000 -0.3792460000
C -4.7697340000 -0.9025660000 -1.2855340000
C -3.4735970000 -0.4034540000 -1.2255360000
H -3.8615550000 1.7712480000 1.3577460000
H -6.1532050000 0.8549770000 1.2714140000
H -6.7426170000 -0.8603910000 -0.4253560000
H -5.0295720000 -1.6303910000 -2.0471670000
H -2.7447960000 -0.7252680000 -1.9601330000
B 3.9230080000 -1.0130490000 -0.2411830000
F 5.1909500000 -0.5009840000 -0.0948600000
F 3.7576540000 -1.7340260000 -1.4325560000
F 3.5258420000 -1.8062050000 0.8506630000
H 1.4421550000 2.1690980000 2.2614660000
H 2.4194600000 3.4775340000 1.5724750000
H 2.9011750000 1.7894170000 1.3153000000
H 2.4392930000 3.9057870000 -0.9220600000
H 1.4646400000 2.9157560000 -2.0220580000
H 2.9122750000 2.2276600000 -1.2456450000
H -0.5249550000 3.3489720000 1.1652350000
H -0.5405520000 3.6299300000 -0.6039510000
H 0.5838340000 4.4972460000 0.4325530000
H -0.8989570000 -1.3807610000 -1.3325860000
C -1.0400750000 -1.8841520000 0.7644130000
C -0.9612810000 -3.3768750000 0.4395770000
H -2.0990500000 -1.6111550000 0.8245660000
C -0.3794230000 -1.5687290000 2.1083310000
H -1.4410160000 -3.6052600000 -0.5183110000
H -1.4702260000 -3.9569000000 1.2149340000
H 0.0751100000 -3.7273190000 0.3968480000
H 0.6705950000 -1.8788290000 2.1230730000
H -0.8993770000 -2.0990180000 2.9114050000
H -0.4179720000 -0.4988470000 2.3386340000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.399627 (Hartree/Particle)
Thermal correction to Energy= 0.423751
Thermal correction to Enthalpy= 0.424695
Thermal correction to Gibbs (Free) Energy= 0.344195
Sum of electronic and zero-point Energies= -1137.570007
Sum of electronic and thermal Energies= -1137.545883
Sum of electronic and thermal Enthalpies= -1137.544939
Sum of electronic and thermal (Free) Energies= -1137.625439

6d

cRT

C -1.7609170000 -1.4781010000 0.8617370000
C -1.2321050000 -0.2838960000 0.9373530000
C -0.7724160000 0.9505250000 0.9612610000
C 0.3128980000 1.2736250000 0.0050270000
C 1.3933240000 0.3534190000 -0.2873460000
C 1.7699120000 -0.6216200000 0.5653680000
H 1.9345180000 0.5520750000 -1.2045080000
C -1.3934500000 2.0546030000 1.8417730000
H -1.3798590000 -2.2509320000 1.5285350000
C -2.8454490000 -1.8657610000 -0.0633530000
O 0.2412280000 2.3962500000 -0.5561220000
C -2.2058240000 1.4029770000 2.9690780000
C -2.3318880000 2.9346700000 0.9946320000
C -0.2734520000 2.9090470000 2.4607120000
C -3.3661890000 -3.1617720000 0.0012960000
C -3.3678260000 -0.9694610000 -1.0047260000
C -4.3910190000 -1.3641650000 -1.8572070000

H -2.9666700000 0.0381220000 -1.0705630000
C -4.9076430000 -2.6584150000 -1.7846720000
H -4.7852700000 -0.6608800000 -2.5836980000
C -4.3922020000 -3.5559340000 -0.8537310000
H -2.9659950000 -3.8656270000 0.7261290000
H -5.7063300000 -2.9641120000 -2.4527740000
H -4.7870270000 -4.5650370000 -0.7919450000
B 1.3307250000 3.0525380000 -1.5441710000
F 0.8123280000 4.2895710000 -1.7955930000
F 1.3834120000 2.2230320000 -2.6500590000
F 2.5099920000 3.0626150000 -0.8263110000
H 0.3006950000 3.4456990000 1.7021640000
H 0.4147250000 2.2906010000 3.0477130000
H -0.7124270000 3.6522600000 3.1336950000
H -3.1345360000 2.3310860000 0.5578860000
H -1.7957620000 3.4397990000 0.1900270000
H -2.7907510000 3.6957330000 1.6350190000
H -3.0335340000 0.8043460000 2.5768450000
H -2.6275700000 2.1833670000 3.6098150000
H -1.5793870000 0.7549320000 3.5914890000
C 2.8695740000 -1.5636510000 0.3732710000
H 1.2319230000 -0.7260820000 1.5047210000
C 3.7101730000 -1.5373860000 -0.7512460000
C 3.0867820000 -2.5398850000 1.3565680000
C 4.7316500000 -2.4676070000 -0.8839210000
C 4.1089920000 -3.4726610000 1.2217340000
C 4.9328640000 -3.4376230000 0.0995190000
H 2.4457480000 -2.5648810000 2.2339000000
H 3.5733370000 -0.7852650000 -1.5209060000
H 4.2638440000 -4.2226050000 1.9903990000
H 5.3767790000 -2.4359330000 -1.7556460000
H 5.7337780000 -4.1618820000 -0.0095730000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.393359 (Hartree/Particle)
Thermal correction to Energy= 0.419397
Thermal correction to Enthalpy= 0.420341
Thermal correction to Gibbs (Free) Energy= 0.332788
Sum of electronic and zero-point Energies= -1250.628880
Sum of electronic and thermal Energies= -1250.602843
Sum of electronic and thermal Enthalpies= -1250.601898
Sum of electronic and thermal (Free) Energies= -1250.689452

cTS

C 1.7537450000 -0.3669140000 0.7307760000
C 0.4282860000 -0.3818370000 0.7467470000
C 2.5968990000 -1.2578850000 -0.0780640000
H 2.2684440000 0.3998330000 1.3080370000
C -0.7930280000 -0.9675780000 0.6349550000
C 3.9704800000 -1.3187460000 0.1891900000
C 2.0696580000 -2.0466770000 -1.1095950000
C -1.7713770000 -0.0859460000 0.0318370000
C -1.1477410000 -2.3478810000 1.1854800000
C 4.7941910000 -2.1713080000 -0.5385370000
H 4.3909530000 -0.7005090000 0.9775430000
C 2.8946630000 -2.8947750000 -1.8375490000
H 1.0128410000 -1.9806640000 -1.3493410000
C -1.2994000000 1.2480210000 -0.0482630000
O -2.8865120000 -0.5268830000 -0.4089990000
C 0.0406600000 -2.9702960000 1.9293400000
C -1.5411340000 -3.2625850000 0.0059400000
C -2.3367350000 -2.2084670000 2.1562230000
C 4.2581850000 -2.9636410000 -1.5515440000
H 5.8555590000 -2.2146840000 -0.3164980000
H 2.4745310000 -3.4978610000 -2.6359380000
C -0.2322710000 1.5869470000 0.7819680000
H -1.6937930000 1.9248040000 -0.7983320000
B -3.9950520000 0.4388200000 -0.9282620000
H 0.3556190000 -2.3518360000 2.7758660000
H 0.9026240000 -3.1181470000 1.2720130000
H -0.2549940000 -3.9490950000 2.3188170000
H -1.8334510000 -4.2410400000 0.4009100000
H -0.6957410000 -3.4151980000 -0.6723050000
H -2.3804700000 -2.8527420000 -0.5581170000
H -2.0804380000 -1.5528170000 2.9954100000
H -2.5888190000 -3.1927930000 2.5634580000
H -3.2218480000 -1.8093710000 1.6570000000
H 4.9008930000 -3.6258750000 -2.1224650000
H -0.2952900000 1.3367310000 1.8402510000
C 0.7133560000 2.6680360000 0.4716400000
F -4.2086180000 1.3734350000 0.0817240000
F -5.0781040000 -0.3652400000 -1.1723330000
F -3.4853730000 1.0479310000 -2.0758500000
C 1.0042180000 3.0146780000 -0.8542600000
C 1.3674930000 3.3375080000 1.5128110000
C 1.9127800000 4.0288730000 -1.1294730000
H 0.5270380000 2.4769500000 -1.6684740000
C 2.2776450000 4.3528600000 1.2369930000
H 1.1495700000 3.0697540000 2.5436670000
C 2.5491960000 4.6999890000 -0.0848280000
H 2.1318510000 4.2924100000 -2.1588490000
H 2.7720320000 4.8734510000 2.0505550000
H 3.2604810000 5.4902780000 -0.3024970000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392815 (Hartree/Particle)
Thermal correction to Energy= 0.417656
Thermal correction to Enthalpy= 0.418600
Thermal correction to Gibbs (Free) Energy= 0.336048
Sum of electronic and zero-point Energies= -1250.607607
Sum of electronic and thermal Energies= -1250.582766
Sum of electronic and thermal Enthalpies= -1250.581821
Sum of electronic and thermal (Free) Energies= -1250.664373

cPT

C -1.8140310000 0.4059950000 -0.6747550000
C -0.4816840000 0.1852390000 -0.7655600000
C 0.3310030000 -0.9708640000 -0.5031170000
C 1.6406960000 -0.5152780000 -0.1158420000
C 1.7378470000 0.8290190000 -0.4417520000
C 0.4830440000 1.3603040000 -1.0143090000
C 0.0714970000 -2.4295790000 -0.8132890000
C -2.8072090000 -0.4121120000 0.0142030000
O 2.5481800000 -1.3024200000 0.3707180000
C -1.2856740000 -2.7265000000 -1.4661470000
C 0.2380810000 -3.2899150000 0.4602940000
C 1.1731920000 -2.8294730000 -1.8395280000
C -4.1114020000 -0.5135700000 -0.4908780000
C -2.4873090000 -1.0591590000 1.2158940000
C -3.4353970000 -1.8396510000 1.8681320000
H -1.4990150000 -0.9278470000 1.6456560000
C -4.7131810000 -1.9771760000 1.3305860000
H -3.1780680000 -2.3349370000 2.7986430000
C -5.0510390000 -1.3084480000 0.1527460000
H -4.3743440000 0.0082300000 -1.4065440000
H -5.4520870000 -2.5896790000 1.8369300000
H -6.0506180000 -1.4036150000 -0.2584980000
B 3.9615650000 -0.7707500000 0.6247350000
F 4.4495650000 -0.2968450000 -0.6016400000
F 4.6804210000 -1.8364100000 1.1126110000
F 3.8549970000 0.2850940000 1.5399980000
H -2.1689110000 1.3701250000 -1.0384340000
H 2.6375510000 1.4193470000 -0.3173870000
H 0.5977210000 1.4260450000 -2.1075840000
C 0.0668680000 2.7124200000 -0.4828290000
C 0.1511840000 2.9833040000 0.8861000000
C -0.4260260000 3.6940800000 -1.3425570000
H 1.0728360000 -2.2489940000 -2.7624180000
H 1.0388270000 -3.8861030000 -2.0884890000
H 2.1774310000 -2.6940990000 -1.4380010000
H 0.1489870000 -4.3431650000 0.1762640000
H -0.5507340000 -3.0703590000 1.1849180000
H 1.2121320000 -3.1337120000 0.9256280000
H -1.5005630000 -2.0424970000 -2.2932530000
H -2.1129200000 -2.6880570000 -0.7581570000
H -1.2542310000 -3.7406320000 -1.8747890000
C -0.2561620000 4.2155040000 1.3851780000
C -0.7535790000 5.1908700000 0.5209370000
C -0.8368500000 4.9293570000 -0.8437250000
H -0.4838670000 3.4962960000 -2.4102690000
H -1.0689600000 6.1532360000 0.9109570000
H -1.2145330000 5.6872740000 -1.5226270000
H 0.5431910000 2.2263900000 1.5617760000
H -0.1811360000 4.4171100000 2.4488310000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395349 (Hartree/Particle)
Thermal correction to Energy= 0.419969

Thermal correction to Enthalpy= 0.420913
Thermal correction to Gibbs (Free) Energy= 0.338970
Sum of electronic and zero-point Energies= -1250.632587
Sum of electronic and thermal Energies= -1250.607967
Sum of electronic and thermal Enthalpies= -1250.607022
Sum of electronic and thermal (Free) Energies= -1250.688966

cRTccRT TS

C -1.6190020000 -1.6549210000 -1.2281360000
C -0.3665550000 -1.5635620000 -0.8641790000
C 0.8949550000 -1.5484170000 -0.4827560000
C 1.5508420000 -0.2590400000 -0.1455210000
C 0.9102180000 1.0446300000 -0.0185170000
C -0.2615120000 1.4536480000 -0.5412540000
H 1.5121440000 1.7466410000 0.5464640000
C 1.6782070000 -2.8813330000 -0.3599060000
H -1.8414450000 -1.6160370000 -2.2945280000
C -2.7626450000 -1.7619010000 -0.3010670000
O 2.7771700000 -0.3461600000 0.1168450000
C 0.7439130000 -4.0551360000 -0.6913750000
C 2.1808820000 -3.0663880000 1.0850990000
C 2.8549890000 -2.9049600000 -1.3540310000
C -4.0512800000 -1.9260630000 -0.8193290000
C -2.5913290000 -1.6874260000 1.0875240000
C -3.6873420000 -1.7835470000 1.9356200000
H -1.5957150000 -1.5486350000 1.5002590000
C -4.9695990000 -1.9516650000 1.4115170000
H -3.5423570000 -1.7228740000 3.0094240000
C -5.1485880000 -2.0221160000 0.0325620000
H -4.1942160000 -1.9832610000 -1.8950880000
H -5.8240270000 -2.0248730000 2.0764940000
H -6.1428780000 -2.1522510000 -0.3825810000
B 3.8297960000 0.8162300000 0.4995280000
F 5.0114120000 0.1356940000 0.5623230000
F 3.4001610000 1.3191960000 1.7130690000
F 3.7557710000 1.7395400000 -0.5221470000
H 3.6023390000 -2.1451150000 -1.1252900000
H 2.4993440000 -2.7540370000 -2.3789260000
H 3.3414650000 -3.8850510000 -1.3086110000
H 1.3456070000 -3.0364980000 1.7934030000
H 2.9118270000 -2.3092140000 1.3693710000
H 2.6598380000 -4.0468840000 1.1742180000
H -0.1184510000 -4.0935940000 -0.0175030000
H 1.2979220000 -4.9921580000 -0.5832520000
H 0.3716830000 -4.0017980000 -1.7192900000
C -0.8136960000 2.8012770000 -0.3963050000
H -0.8723610000 0.7663110000 -1.1136920000
C -0.0399530000 3.9010370000 0.0060360000
C -2.1757180000 2.9931750000 -0.6705300000
C -0.6244910000 5.1528500000 0.1473320000
C -2.7604200000 4.2456630000 -0.5206260000
C -1.9847960000 5.3276120000 -0.1099300000
H -2.7801800000 2.1476370000 -0.9887210000
H 1.0241690000 3.7851230000 0.1853830000
H -3.8175810000 4.3781040000 -0.7263930000
H -0.0159310000 5.9978460000 0.4521740000
H -2.4361110000 6.3083860000 0.0017160000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.393171 (Hartree/Particle)
Thermal correction to Energy= 0.418463
Thermal correction to Enthalpy= 0.419407
Thermal correction to Gibbs (Free) Energy= 0.334251
Sum of electronic and zero-point Energies= -1250.624024
Sum of electronic and thermal Energies= -1250.598732
Sum of electronic and thermal Enthalpies= -1250.597788
Sum of electronic and thermal (Free) Energies= -1250.682944

ccRT

C -0.8041660000 -2.0086900000 -1.4428540000
C 0.3099340000 -1.6980710000 -0.8319310000
C 1.4238020000 -1.3499370000 -0.2199460000
C 1.7677360000 0.0946100000 -0.2382600000
C 0.7623950000 1.1391380000 -0.2354810000
C -0.4859390000 0.9625330000 0.2431190000
H 1.0995680000 2.1015190000 -0.6027410000
C 2.3822880000 -2.3770260000 0.4156170000
H -0.7730760000 -2.1914640000 -2.5158720000
C -2.1211590000 -2.0577150000 -0.7725950000
O 2.9929090000 0.3721280000 -0.2800140000
C 1.6546640000 -3.7192620000 0.5755500000
C 2.8169540000 -1.8802490000 1.8061370000
C 3.6123680000 -2.5843580000 -0.4881400000
C -3.2823610000 -1.8314210000 -1.5191940000
C -2.2354300000 -2.2872560000 0.6045120000
C -3.4816040000 -2.2721020000 1.2225460000
H -1.3423820000 -2.4879200000 1.1897100000
C -4.6324090000 -2.0298340000 0.4731040000
H -3.5546740000 -2.4541490000 2.2900230000
C -4.5285810000 -1.8120310000 -0.8993410000
H -3.2062710000 -1.6523160000 -2.5878590000
H -5.6045900000 -2.0191020000 0.9552640000
H -5.4196940000 -1.6253450000 -1.4900240000
B 3.6542250000 1.8380620000 -0.1858950000
F 4.9923830000 1.5696690000 -0.1665930000
F 3.1650380000 2.3822780000 0.9848950000
F 3.2267990000 2.5166400000 -1.3125100000
H 4.1884630000 -1.6656690000 -0.6041770000
H 3.3077410000 -2.9347890000 -1.4797920000
H 4.2625120000 -3.3456840000 -0.0438030000
H 1.9480160000 -1.7050700000 2.4503590000
H 3.4005980000 -0.9592460000 1.7494160000
H 3.4407270000 -2.6419220000 2.2845230000
H 0.7756820000 -3.6273090000 1.2225520000
H 2.3323470000 -4.4462610000 1.0330910000
H 1.3283850000 -4.1223160000 -0.3879320000
C -1.5485270000 1.9647150000 0.2687770000
H -0.7629920000 -0.0039950000 0.6546990000
C -1.3122220000 3.3313600000 0.0528060000
C -2.8612260000 1.5282190000 0.5015890000
C -2.3686190000 4.2323880000 0.0591490000
C -3.9180230000 2.4315950000 0.4963610000
C -3.6730540000 3.7849660000 0.2755400000
H -3.0524420000 0.4719040000 0.6707110000
H -0.3006640000 3.6941900000 -0.0984440000
H -4.9299280000 2.0789650000 0.6675650000
H -2.1755080000 5.2881350000 -0.1002380000
H -4.4951300000 4.4937870000 0.2780320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.393875 (Hartree/Particle)
Thermal correction to Energy= 0.419620
Thermal correction to Enthalpy= 0.420564
Thermal correction to Gibbs (Free) Energy= 0.335714
Sum of electronic and zero-point Energies= -1250.633097
Sum of electronic and thermal Energies= -1250.607352
Sum of electronic and thermal Enthalpies= -1250.606408
Sum of electronic and thermal (Free) Energies= -1250.691258

ccTS

C -1.0458400000 -1.5005170000 -0.9782230000
C 0.0827010000 -1.0536500000 -0.4315550000
C -2.3703630000 -1.4666720000 -0.3460760000
H -0.9883840000 -1.8640520000 -2.0043930000
C 1.4316190000 -1.1271120000 -0.2696300000
C -3.5008030000 -1.1338080000 -1.1026430000
C -2.5231030000 -1.7617690000 1.0145640000
C 2.0332500000 0.1672320000 -0.0290340000
C 2.2321050000 -2.4270300000 -0.2522330000
C -4.7511190000 -1.0592870000 -0.5012980000
H -3.3899090000 -0.9041820000 -2.1584020000
C -3.7783490000 -1.7007610000 1.6118990000
H -1.6562610000 -2.0642060000 1.5958780000
C 1.0522470000 1.1668570000 0.1707000000
O 3.2983940000 0.3378670000 -0.0795310000
C 1.3164190000 -3.6527970000 -0.3638340000
C 3.0328250000 -2.5172290000 1.0609990000
C 3.1944040000 -2.4072010000 -1.4595720000
C -4.8924200000 -1.3403950000 0.8574900000
H -5.6175150000 -0.7799720000 -1.0918990000
H -3.8870330000 -1.9399830000 2.6650260000
C -0.2316680000 0.7319960000 0.5077940000
H 1.2724020000 2.2046240000 -0.0551660000
B 3.9502990000 1.6992020000 0.3112790000
H 0.7598910000 -3.6633300000 -1.3059790000
H 0.5952460000 -3.6983750000 0.4586490000
H 1.9272870000 -4.5597060000 -0.3277000000

H 3.6084420000 -3.4483360000 1.0710980000
H 2.3615560000 -2.5267940000 1.9266020000
H 3.7298750000 -1.6842100000 1.1673570000
H 2.6391610000 -2.3452770000 -2.4015120000
H 3.7739660000 -3.3361370000 -1.4680240000
H 3.8883110000 -1.5669330000 -1.4043330000
H -5.8711810000 -1.2893240000 1.3236590000
H -0.3556960000 0.0748000000 1.3694680000
C -1.4228540000 1.5243150000 0.1610020000
F 5.3008400000 1.4636630000 0.2859600000
F 3.4629560000 2.0211240000 1.5755720000
F 3.5306440000 2.6289960000 -0.6403540000
C -1.4967140000 2.1796900000 -1.0739860000
C -2.5052260000 1.6018300000 1.0431550000
C -2.6317210000 2.9052070000 -1.4159320000
H -0.6675010000 2.1005030000 -1.7719140000
C -3.6387910000 2.3308960000 0.7037390000
H -2.4586470000 1.0850110000 1.9967010000
C -3.7041070000 2.9807950000 -0.5271840000
H -2.6831820000 3.4082180000 -2.3760400000
H -4.4725670000 2.3867220000 1.3957350000
H -4.5918400000 3.5444030000 -0.7964110000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392709 (Hartree/Particle)
Thermal correction to Energy= 0.417375
Thermal correction to Enthalpy= 0.418319
Thermal correction to Gibbs (Free) Energy= 0.337291
Sum of electronic and zero-point Energies= -1250.607068
Sum of electronic and thermal Energies= -1250.582401
Sum of electronic and thermal Enthalpies= -1250.581457
Sum of electronic and thermal (Free) Energies= -1250.662485

ccPT

C 1.2108700000 -1.6440580000 0.0094100000
C 0.1349740000 -0.8538140000 -0.2587120000
C -1.2445540000 -1.1567380000 0.0167270000
C -2.0232920000 0.0399150000 -0.1649610000
C -1.1841770000 1.0420650000 -0.6211760000
C 0.2131580000 0.5823120000 -0.7646440000
C -1.9227030000 -2.4634910000 0.3699000000
O -3.3008500000 0.1027980000 0.0583160000
C -1.0183860000 -3.6996110000 0.4787680000
C -2.9625760000 -2.7478050000 -0.7467180000
C -2.6453160000 -2.2770980000 1.7279540000
H -1.5066730000 2.0530750000 -0.8374340000
C 2.6182900000 -1.3753920000 -0.2612430000
H 1.0367350000 -2.5591590000 0.5586820000
C 3.5644290000 -1.8535580000 0.6616660000
C 4.9186760000 -1.6077590000 0.4823550000
C 5.3552480000 -0.9132140000 -0.6454680000
C 4.4325580000 -0.4715780000 -1.5910610000
C 3.0750260000 -0.6960600000 -1.4005000000
H 3.2258080000 -2.4016660000 1.5365720000
H 5.6349750000 -1.9638600000 1.2152010000
H 6.4144110000 -0.7291970000 -0.7935390000
H 4.7713670000 0.0486990000 -2.4808000000
H 2.3703830000 -0.3748400000 -2.1583390000
B -4.0760420000 1.3771450000 -0.2781360000
F -5.3907860000 1.1041450000 0.0225570000
F -3.8706240000 1.6401080000 -1.6411100000
F -3.5415770000 2.4160780000 0.4949480000
H -1.9236660000 -2.0659790000 2.5242400000
H -3.1604950000 -3.2102940000 1.9763050000
H -3.3791270000 -1.4724650000 1.6883700000
H -3.5054270000 -3.6619380000 -0.4872390000
H -2.4623760000 -2.9108660000 -1.7069290000
H -3.6822750000 -1.9362100000 -0.8502230000
H -0.3578570000 -3.6612410000 1.3504690000
H -0.4248670000 -3.8687360000 -0.4248250000
H -1.6600400000 -4.5750340000 0.6139420000
H 0.4646790000 0.5769710000 -1.8348900000
C 1.1768820000 1.5053150000 -0.0370200000
C 1.1880280000 1.5472930000 1.3588400000
C 2.0225530000 2.3535080000 -0.7495350000
C 2.0492950000 2.4076970000 2.0300690000
C 2.9019110000 3.2451090000 1.3114190000
C 2.8833110000 3.2202540000 -0.0799310000
H 0.5187950000 0.9023410000 1.9227390000
H 2.0499490000 2.4309830000 3.1150410000
H 3.5724750000 3.9183900000 1.8355500000
H 2.0135050000 2.3360000000 -1.8364780000
H 3.5383850000 3.8741830000 -0.6466430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395860 (Hartree/Particle)
Thermal correction to Energy= 0.420474
Thermal correction to Enthalpy= 0.421418
Thermal correction to Gibbs (Free) Energy= 0.338719
Sum of electronic and zero-point Energies= -1250.637641
Sum of electronic and thermal Energies= -1250.613027
Sum of electronic and thermal Enthalpies= -1250.612083
Sum of electronic and thermal (Free) Energies= -1250.694782

RωB97X-D/6-31+G(d,p)/SCRF=(PCM, CH_2Cl_2, ε = 8.93)

6d

cRT

C -1.7320160000 -1.4182050000 0.8807080000
C -1.2132570000 -0.2192940000 0.9180870000
C -0.7619010000 1.0219000000 0.9147600000
C 0.3532880000 1.3097150000 -0.0037160000
C 1.3976700000 0.3585150000 -0.2814170000
C 1.7301900000 -0.6287030000 0.5842030000
H 1.9596770000 0.5228710000 -1.1927170000
C -1.4235970000 2.1425720000 1.7446300000
H -1.3498440000 -2.1580930000 1.5831380000
C -2.7988700000 -1.8523840000 -0.0444910000
O 0.3355840000 2.4523200000 -0.5615170000
C -2.2959920000 1.5112010000 2.8384400000
C -2.3160230000 3.0127040000 0.8398680000
C -0.3349860000 3.0007530000 2.4122810000
C -3.2608890000 -3.1711960000 0.0229820000
C -3.3617880000 -0.9798630000 -0.9859310000
C -4.3667960000 -1.4209700000 -1.8387170000
H -3.0103550000 0.0462410000 -1.0499790000
C -4.8241040000 -2.7382330000 -1.7651800000
H -4.7948340000 -0.7360410000 -2.5636660000
C -4.2685640000 -3.6114120000 -0.8327150000
H -2.8293740000 -3.8550840000 0.7484230000
H -5.6089720000 -3.0798950000 -2.4322800000
H -4.6179500000 -4.6370060000 -0.7697100000
B 1.4194210000 3.0725520000 -1.4731410000
F 0.9656490000 4.3550500000 -1.7201970000
F 1.4942330000 2.3106020000 -2.6364440000
F 2.6209750000 3.0639170000 -0.7736830000
H 0.2829810000 3.5231400000 1.6783240000
H 0.3153320000 2.3859690000 3.0437420000
H -0.8073760000 3.7557170000 3.0484350000
H -3.0942160000 2.4045560000 0.3672850000
H -1.7384510000 3.5090310000 0.0585520000
H -2.8065820000 3.7806360000 1.4473800000
H -3.1089590000 0.9157040000 2.4120840000
H -2.7408070000 2.3040570000 3.4472070000
H -1.7057550000 0.8656950000 3.4972080000
C 2.7713670000 -1.6298910000 0.3960520000
H 1.2054230000 -0.6828020000 1.5346530000
C 3.5116300000 -1.7492800000 -0.7931130000
C 3.0314690000 -2.5195180000 1.4508920000
C 4.4854020000 -2.7304750000 -0.9152760000
C 4.0081460000 -3.5015890000 1.3265490000
C 4.7361850000 -3.6073930000 0.1430740000
H 2.4631720000 -2.4361640000 2.3729420000
H 3.3272880000 -1.0797160000 -1.6264120000
H 4.2004660000 -4.1818170000 2.1493260000
H 5.0513470000 -2.8154520000 -1.8367950000
H 5.4988990000 -4.3726900000 0.0418040000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392897 (Hartree/Particle)
Thermal correction to Energy= 0.418816
Thermal correction to Enthalpy= 0.419760
Thermal correction to Gibbs (Free) Energy= 0.332715
Sum of electronic and zero-point Energies= -1250.648295
Sum of electronic and thermal Energies= -1250.622376
Sum of electronic and thermal Enthalpies= -1250.621431
Sum of electronic and thermal (Free) Energies= -1250.708477

cTS

C 1.7485990000 -0.4266310000 0.7362580000
C 0.4254280000 -0.4243750000 0.7327750000
C 2.5914150000 -1.3149540000 -0.0752330000
H 2.2627430000 0.3161880000 1.3442540000
C -0.8191740000 -0.9510780000 0.6174370000
C 3.9643440000 -1.3762070000 0.1983120000
C 2.0641380000 -2.1025300000 -1.1084800000
C -1.7544620000 -0.0300470000 0.0136230000
C -1.2228940000 -2.3178220000 1.1745880000
C 4.7890200000 -2.2294740000 -0.5288350000
H 4.3825430000 -0.7594160000 0.9885820000
C 2.8904850000 -2.9511050000 -1.8350240000
H 1.0082550000 -2.0364090000 -1.3524120000
C -1.2626440000 1.2859520000 -0.0574720000
O -2.8926350000 -0.4475510000 -0.4420620000
C -0.0558370000 -2.9696610000 1.9277990000
C -1.6333210000 -3.2315780000 0.0010200000
C -2.4075350000 -2.1377650000 2.1428740000
C 4.2540310000 -3.0203780000 -1.5445570000
H 5.8496520000 -2.2741960000 -0.3042290000
H 2.4723330000 -3.5543030000 -2.6341960000
C -0.1816910000 1.6049360000 0.7671410000
H -1.6470750000 1.9835800000 -0.7929930000
B -3.9898670000 0.4777700000 -0.9019030000
H 0.2730590000 -2.3539500000 2.7705380000
H 0.8028830000 -3.1464860000 1.2732080000
H -0.3820580000 -3.9369770000 2.3210500000
H -1.9425950000 -4.2021540000 0.4019460000
H -0.7925480000 -3.4009100000 -0.6785440000
H -2.4654970000 -2.8110790000 -0.5656920000
H -2.1329270000 -1.4811590000 2.9748630000
H -2.6870470000 -3.1115160000 2.5571000000
H -3.2812150000 -1.7187370000 1.6393360000
H 4.8976920000 -3.6826470000 -2.1143460000
H -0.2316920000 1.3253580000 1.8189320000
C 0.7850250000 2.6609310000 0.4618800000
F -4.2721670000 1.3952800000 0.1185780000
F -5.0834670000 -0.3389180000 -1.1688620000
F -3.5675140000 1.1532530000 -2.0574780000
C 1.0617820000 3.0330260000 -0.8618870000
C 1.4745300000 3.2848450000 1.5106690000
C 1.9932890000 4.0289450000 -1.1267340000
H 0.5602360000 2.5284740000 -1.6823670000
C 2.4064170000 4.2825440000 1.2436710000
H 1.2695680000 2.9927690000 2.5369550000
C 2.6644550000 4.6555830000 -0.0747280000
H 2.2049320000 4.3120340000 -2.1523340000
H 2.9307060000 4.7669740000 2.0604920000
H 3.3944040000 5.4306470000 -0.2848600000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392649 (Hartree/Particle)
Thermal correction to Energy= 0.417400
Thermal correction to Enthalpy= 0.418344
Thermal correction to Gibbs (Free) Energy= 0.336250
Sum of electronic and zero-point Energies= -1250.632154
Sum of electronic and thermal Energies= -1250.607404
Sum of electronic and thermal Enthalpies= -1250.606460
Sum of electronic and thermal (Free) Energies= -1250.688554

cPT

C -1.8357030000 0.2341930000 -0.7538900000
C -0.4784460000 0.1389200000 -0.7746890000
C 0.4194040000 -0.9306120000 -0.4791810000
C 1.6907980000 -0.3456670000 -0.1162250000
C 1.6663220000 0.9938010000 -0.4246890000
C 0.3682870000 1.4015370000 -1.0039590000
C 0.2814520000 -2.4139480000 -0.7582600000
C -2.7712570000 -0.6208030000 -0.0472500000
O 2.6790630000 -1.0617280000 0.3735620000
C -1.0472790000 -2.8401950000 -1.3986750000
C 0.5177190000 -3.2334070000 0.5304310000
C 1.4023550000 -2.7428500000 -1.7882010000
C -4.0643950000 -0.8169900000 -0.5596350000
C -2.4174160000 -1.2129080000 1.1760290000
C -3.3184400000 -2.0353350000 1.8420500000
H -1.4476750000 -0.9982970000 1.6139450000
C -4.5790650000 -2.2714180000 1.2956910000
H -3.0400180000 -2.4858730000 2.7887080000
C -4.9523320000 -1.6579810000 0.0970090000
H -4.3525410000 -0.3354530000 -1.4891220000
H -5.2807210000 -2.9174480000 1.8130470000
H -5.9397630000 -1.8309240000 -0.3173320000
B 4.0320070000 -0.4906930000 0.5924680000
F 4.5432070000 0.0060840000 -0.6233990000
F 4.8256860000 -1.5346300000 1.0725700000
F 3.9676030000 0.5568270000 1.5333090000
H -2.2626590000 1.1291100000 -1.2059850000
H 2.4927140000 1.6791760000 -0.2867140000
H 0.4865050000 1.4849500000 -2.0953350000
C -0.1847190000 2.7022250000 -0.4647910000
C -0.2566850000 2.9130430000 0.9161620000
C -0.6434790000 3.6941820000 -1.3311790000
H 1.2485140000 -2.1860340000 -2.7177500000
H 1.3491150000 -3.8105050000 -2.0186080000
H 2.3963110000 -2.5236860000 -1.3992970000
H 0.5043750000 -4.2955000000 0.2675930000
H -0.2792180000 -3.0554280000 1.2571780000
H 1.4792000000 -2.9986080000 0.9879920000
H -1.3255700000 -2.1911320000 -2.2344580000
H -1.8702610000 -2.8653220000 -0.6855900000
H -0.9255770000 -3.8539860000 -1.7900590000
C -0.7810290000 4.0982160000 1.4209640000
C -1.2394350000 5.0873980000 0.5489870000
C -1.1697350000 4.8838820000 -0.8267660000
H -0.5900910000 3.5392190000 -2.4055340000
H -1.6475180000 6.0127450000 0.9427830000
H -1.5220710000 5.6497520000 -1.5102970000
H 0.0959600000 2.1424620000 1.5979450000
H -0.8315470000 4.2518400000 2.4941300000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.394969 (Hartree/Particle)
Thermal correction to Energy= 0.419560
Thermal correction to Enthalpy= 0.420504
Thermal correction to Gibbs (Free) Energy= 0.338948
Sum of electronic and zero-point Energies= -1250.660949
Sum of electronic and thermal Energies= -1250.636358
Sum of electronic and thermal Enthalpies= -1250.635414
Sum of electronic and thermal (Free) Energies= -1250.716971

ccRT

C -0.7996080000 -1.9456590000 -1.4514700000
C 0.3158050000 -1.6389160000 -0.8442490000
C 1.4422650000 -1.3051440000 -0.2398610000
C 1.7703670000 0.1330250000 -0.2197650000
C 0.7654770000 1.1661960000 -0.2078020000
C -0.4893760000 0.9646940000 0.2578100000
H 1.0872020000 2.1392160000 -0.5599110000
C 2.4085160000 -2.3551740000 0.3470780000
H -0.7733380000 -2.1051300000 -2.5283760000
C -2.1098230000 -2.0205460000 -0.7687790000
O 3.0081650000 0.4219960000 -0.2447580000
C 1.6829910000 -3.7035060000 0.4613470000
C 2.8530880000 -1.9156810000 1.7534330000
C 3.6297660000 -2.5306680000 -0.5747670000
C -3.2780790000 -1.7736460000 -1.4987040000
C -2.2077500000 -2.2935270000 0.6019550000
C -3.4485070000 -2.3007980000 1.2324500000
H -1.3100530000 -2.5082320000 1.1748170000
C -4.6070400000 -2.0364200000 0.5017950000
H -3.5102700000 -2.5148720000 2.2945330000
C -4.5180220000 -1.7754670000 -0.8648550000
H -3.2131180000 -1.5638460000 -2.5623380000
H -5.5740570000 -2.0397250000 0.9941750000
H -5.4154620000 -1.5712730000 -1.4398160000
B 3.6540380000 1.8207050000 -0.1162510000
F 5.0128810000 1.5670650000 -0.0800590000
F 3.1939190000 2.3977000000 1.0619060000
F 3.2908100000 2.5685850000 -1.2334530000
H 4.2099520000 -1.6106870000 -0.6579930000
H 3.3148740000 -2.8381120000 -1.5772450000
H 4.2795830000 -3.3122650000 -0.1671150000
H 1.9876360000 -1.7671240000 2.4081000000
H 3.4360890000 -0.9924680000 1.7302000000

H 3.4806350000 -2.6960980000 2.1950200000
H 0.8076140000 -3.6352420000 1.1152970000
H 2.3652090000 -4.4440670000 0.8891840000
H 1.3540280000 -4.0709100000 -0.5152420000
C -1.5824890000 1.9278740000 0.2620470000
H -0.7384590000 -0.0023200000 0.6856210000
C -1.4237000000 3.2741110000 -0.1089100000
C -2.8574010000 1.4673690000 0.6288500000
C -2.5160890000 4.1305370000 -0.1137670000
C -3.9514880000 2.3253160000 0.6136170000
C -3.7815730000 3.6580370000 0.2436300000
H -2.9897000000 0.4267040000 0.9119110000
H -0.4471030000 3.6587040000 -0.3834270000
H -4.9327230000 1.9545040000 0.8906330000
H -2.3842180000 5.1697470000 -0.3957480000
H -4.6323010000 4.3318150000 0.2349880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.393246 (Hartree/Particle)
Thermal correction to Energy= 0.418937
Thermal correction to Enthalpy= 0.419881
Thermal correction to Gibbs (Free) Energy= 0.335256
Sum of electronic and zero-point Energies= -1250.651681
Sum of electronic and thermal Energies= -1250.625990
Sum of electronic and thermal Enthalpies= -1250.625046
Sum of electronic and thermal (Free) Energies= -1250.709671

ccTS

C 1.0579730000 1.4894380000 -0.9996800000
C -0.0761640000 1.0648530000 -0.4532050000
C 2.3801840000 1.4676210000 -0.3659920000
H 1.0028020000 1.8226030000 -2.0364610000
C -1.4203620000 1.1195830000 -0.2711820000
C 3.5123680000 1.1618650000 -1.1327130000
C 2.5300580000 1.7503180000 0.9981540000
C -2.0049540000 -0.1811320000 -0.0392360000
C -2.2211760000 2.4216460000 -0.2308370000
C 4.7658350000 1.0996840000 -0.5350420000
H 3.4020870000 0.9497000000 -2.1921150000
C 3.7886460000 1.7036080000 1.5898540000
H 1.6615490000 2.0294090000 1.5881330000
C -1.0428070000 -1.1802310000 0.1745160000
O -3.2877790000 -0.3519900000 -0.1078970000
C -1.2980630000 3.6442210000 -0.3204440000
C -3.0169040000 2.4950710000 1.0857680000
C -3.1813020000 2.4329690000 -1.4390760000
C 4.9058700000 1.3684640000 0.8270810000
H 5.6352900000 0.8425620000 -1.1311100000
H 3.8964920000 1.9294460000 2.6457310000
C 0.2490940000 -0.7578730000 0.5081010000
H -1.2647900000 -2.2215950000 -0.0292200000
B -3.9717580000 -1.6358770000 0.2812040000
H -0.7408970000 3.6657100000 -1.2617120000
H -0.5796260000 3.6691880000 0.5049360000
H -1.9053320000 4.5527400000 -0.2697240000
H -3.5820180000 3.4319960000 1.1148510000
H -2.3419340000 2.4791990000 1.9478190000
H -3.7233840000 1.6680720000 1.1787080000
H -2.6240590000 2.3832150000 -2.3800640000
H -3.7521640000 3.3670890000 -1.4301760000
H -3.8836570000 1.5986160000 -1.4019900000
H 5.8863840000 1.3257700000 1.2902200000
H 0.3743860000 -0.0706850000 1.3460750000
C 1.4355470000 -1.5515210000 0.1737590000
F -5.3361110000 -1.3724660000 0.2119600000
F -3.5844660000 -1.9881190000 1.5811690000
F -3.6051610000 -2.6456720000 -0.6226030000
C 1.5045090000 -2.2471050000 -1.0412610000
C 2.5244380000 -1.5922730000 1.0531560000
C 2.6417710000 -2.9769940000 -1.3653140000
H 0.6746070000 -2.1911340000 -1.7401570000
C 3.6588750000 -2.3284780000 0.7315660000
H 2.4799750000 -1.0453110000 1.9894820000
C 3.7192610000 -3.0182780000 -0.4785600000
H 2.6938340000 -3.5068600000 -2.3106040000
H 4.4977480000 -2.3568880000 1.4188330000
H 4.6091920000 -3.5839530000 -0.7354980000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.392085 (Hartree/Particle)
Thermal correction to Energy= 0.416807
Thermal correction to Enthalpy= 0.417751
Thermal correction to Gibbs (Free) Energy= 0.336436
Sum of electronic and zero-point Energies= -1250.632549
Sum of electronic and thermal Energies= -1250.607827
Sum of electronic and thermal Enthalpies= -1250.606883
Sum of electronic and thermal (Free) Energies= -1250.688198

ccPT

C -1.2393620000 1.6176410000 -0.0094130000
C -0.1541720000 0.8275350000 -0.2775360000
C 1.2112700000 1.1527750000 -0.0031950000
C 2.0023850000 -0.0431280000 -0.1922150000
C 1.1876140000 -1.0522680000 -0.6385550000
C -0.2178730000 -0.6086530000 -0.7757890000
C 1.8687170000 2.4712280000 0.3487700000
O 3.2996080000 -0.0826730000 0.0355580000
C 0.9473090000 3.6952450000 0.4536930000
C 2.9027580000 2.7728600000 -0.7683920000
C 2.5877140000 2.3022750000 1.7108140000
H 1.5090430000 -2.0610930000 -0.8622280000
C -2.6414610000 1.3587770000 -0.2715740000
H -1.0625380000 2.5292330000 0.5433090000
C -3.5777200000 1.9522970000 0.5978210000
C -4.9367700000 1.7211860000 0.4394670000
C -5.3865480000 0.9272770000 -0.6165390000
C -4.4746400000 0.3715750000 -1.5138570000
C -3.1128070000 0.5796510000 -1.3431180000
H -3.2266520000 2.5788320000 1.4125540000
H -5.6459710000 2.1656560000 1.1292100000
H -6.4495500000 0.7544620000 -0.7493750000
H -4.8263680000 -0.2240040000 -2.3493000000
H -2.4201510000 0.1706880000 -2.0676800000
B 4.1123820000 -1.2904440000 -0.2417930000
F 5.4309820000 -0.9603900000 0.0827800000
F 4.0096000000 -1.6384850000 -1.6049810000
F 3.6635570000 -2.3699300000 0.5464200000
H 1.8643400000 2.0843680000 2.5026960000
H 3.0861690000 3.2451940000 1.9551450000
H 3.3347190000 1.5097390000 1.6817430000
H 3.4249680000 3.6990130000 -0.5107850000
H 2.3985220000 2.9220730000 -1.7281870000
H 3.6402120000 1.9775850000 -0.8708970000
H 0.2895000000 3.6516790000 1.3262140000
H 0.3525330000 3.8527630000 -0.4507490000
H 1.5792140000 4.5780820000 0.5846860000
H -0.4671030000 -0.6082320000 -1.8460670000
C -1.1663400000 -1.5447170000 -0.0432510000
C -1.2373200000 -1.5288160000 1.3519140000
C -1.9402280000 -2.4614170000 -0.7546220000
C -2.0858450000 -2.4033600000 2.0235070000
C -2.8655340000 -3.3113940000 1.3063600000
C -2.7874710000 -3.3417480000 -0.0839410000
H -0.6332900000 -0.8229030000 1.9162340000
H -2.1377560000 -2.3772460000 3.1072560000
H -3.5288300000 -3.9921120000 1.8302670000
H -1.8899730000 -2.4837740000 -1.8400760000
H -3.3891050000 -4.0460790000 -0.6495230000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.395902 (Hartree/Particle)
Thermal correction to Energy= 0.420400
Thermal correction to Enthalpy= 0.421344
Thermal correction to Gibbs (Free) Energy= 0.339506
Sum of electronic and zero-point Energies= -1250.667711
Sum of electronic and thermal Energies= -1250.643213
Sum of electronic and thermal Enthalpies= -1250.642269
Sum of electronic and thermal (Free) Energies= -1250.724106

APPENDIX 2 CARTESIAN COORDINATES, ENERGIES AND GEOMETRICAL PARAMETERS FOR COMPOUNDS **7-10** STUDIED IN CHAPTER 4

TABLE A2.1 Conformational analysis of silyl enol ethers and oxyallyl cation precursors of systems **7-10** at the B3LYP/6-31G(d) level of theory.

TABLES A2.2-A2.5 Energies and geometrical parameters of systems **7-10** at the B3LYP/6-31G(d) level of theory.

Cartesian coordinates for systems **7-10**

TABLE A2.1 Conformational analysis of silyl enol ethers (or enolates) and oxyallyl cation precursors of systems **7-10** at the B3LYP/6-31G(d) level of theory.

Structure / Entry Number	Energies							Geometrical Parameters	
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	D(R',O',C_2',C_1') (degrees)	D(C_3,C_2,O,B) (degrees)
Oxyallyl Cation (OAC)									
RT	-593.869342	0.111363	-593.757979	0.0	0.075766	-593.793575	0.0		0.0
TS	-593.861031	0.111020	-593.750011	20.9	0.076811	-593.784219	24.6		± 87.0
Enols (ENL, R' = OH)									
7a									
RT (*anti*)	-153.802228	0.056240	-153.745988	7.8	0.031553	-153.770675	7.1	180.0	
TS (*anti* ↔ *syn*)	-153.796260	0.055362	-153.740898	21.2	0.031004	-153.765256	21.4	± 87.0	
RT (*syn*)	-153.805672	0.056717	-153.748955	0.0	0.032275	-153.773398	0.0	0.0	
8a									
RT (*anti*)	-193.124936	0.084562	-193.040374	8.3	0.057462	-193.067473	7.5	180.0	
TS (*anti* ↔ *syn*)	-193.119138	0.083768	-193.035370	21.4	0.057132	-193.062006	21.8	± 87.6	
RT (*syn*)	-193.128534	0.085011	-193.043523	0.0	0.058206	-193.070328	0.0	0.0	
9a									
RT (*anti*)	-232.442944	0.112798	-232.330146	4.4	0.082711	-232.360234	4.2	180.0	
TS (*anti* ↔ *syn*)	-232.438257	0.112175	-232.326082	15.1	0.083246	-232.355012	17.9	± 86.5	
RT (*syn*)	-232.444984	0.113148	-232.331836	0.0	0.083161	-232.361822	0.0	0.0	
10a									
RT (*anti*)	-232.440227	0.112636	-232.327591	7.0	0.082079	-232.358148	3.9	180.0	
TS (*anti* ↔ *syn*)	-232.435767	0.112132	-232.323635	17.4	0.083099	-232.352669	18.3	± 85.7	
RT (*syn*)	-232.443584	0.113314	-232.330270	0.0	0.083960	-232.359623	0.0	0.0	
Silyl Enol Ethers (SEE, R' = TMS)									
7b									
RT (*gauche*)	-562.524023	0.158694	-562.365329	0.2	0.121148	-562.402875	0.0	± 169.4	
TS (*gauche* ↔ *anti* ↔ *gauche*)	-562.524020	0.158628	-562.365392	0.0	0.123131	-562.400889	5.2	180.0	
RT (*syn*)	-562.523756	0.159081	-562.364675	1.9	0.122687	-562.401070	4.7	0.0	
TS (*syn* ↔ *gauche* ↔ *gauche*)	-562.522426	0.158764	-562.363662	4.5	0.123493	-562.398933	10.3	± 73.0	
8b									
RT (*syn*)	-601.846022	0.187184	-601.658838	0.0	0.148482	-601.697540	0.0	0.0	
TS (*syn* ↔ *anti* ↔ *syn*)	-601.842862	0.187189	-601.655673	8.3	0.150698	-601.692164	14.1	180.0	
9b									
RT (*gauche*)	-641.161521	0.215435	-640.946086	0.0	0.174371	-640.987150	0.0	± 130.3	
TS (*gauche* ↔ *anti* ↔ *gauche*)	-641.160988	0.215448	-640.945540	1.4	0.176770	-640.984218	7.7	180.0	
TS (*gauche* ↔ *syn* ↔ *gauche*)	-641.156798	0.215376	-640.941422	12.2	0.176107	-640.980691	17.0	0.0	
10b									
RT (*gauche*)	-641.160366	0.215451	-640.944915	0.7	0.174444	-640.985921	3.1	± 74.3	
TS (*gauche* ↔ *anti* ↔ *gauche*)	-641.158099	0.215412	-640.942687	6.6	0.176698	-640.981401	14.9	180.0	
RT (*syn*)	-641.160549	0.215367	-640.945182	0.0	0.173457	-640.987092	0.0	0.0	
TS (*syn* ↔ *gauche* ↔ *gauche*)	-641.160311	0.215376	-640.944935	0.6	0.176537	-640.983774	8.7	± 59.0	

[a] Energies relative to that of the lowest lying conformation for each respective system.

TABLE A2.2 Energies and geometrical parameters of system **7** at the B3LYP/6-31G(d) level of theory.

Structure / Entry Number (Type)	Energies							Geometrical Parameters			
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(C_3,C_1') (Å)	D(C_2',C_1',C_1,C_2) (degrees)	D(R',O',C_2',C_1') (degrees)	D(C_3,C_2,O,B) (degrees)
7a, R^{i} = OH											
RC 1 (5)	-747.698960	0.171001	-747.527959	-31.7	0.129987	-747.568973	-25.7	4.653	52.9	-178.5	-129.0
2 (5)	-747.685985	0.170106	-747.515879	0.0	0.126809	-747.559177	0.0	3.229	-62.5	-8.2	-163.5
3 (6)	-747.684985	0.170008	-747.514977	2.4	0.126503	-747.558482	1.8	3.150	-66.8	-8.2	-22.4
4 (6)	-747.685018	0.170131	-747.514887	2.6	0.126091	-747.558927	0.7	3.006	-81.1	-8.1	-177.1
5 (4)	-747.681305	0.169015	-747.512290	9.4	0.123529	-747.557775	3.7	3.907	-139.3	-161.3	-175.0
6 (3)	-747.681497	0.170198	-747.511299	12.0	0.127570	-747.553927	11.4	2.865	-65.2	170.3	170.0
7 (4)	-747.678366	0.169219	-747.509147	17.7	0.123515	-747.554850	13.8	3.205	152.9	-166.3	-22.4
8 (3)	-747.677652	0.169571	-747.508081	20.5	0.125777	-747.551875	19.2	3.025	-76.6	-76.6	10.1
TS 1 (5)	-747.690471	0.171384	-747.519087	-8.4	0.131136	-747.559336	-0.4	2.545	30.4	155.3	153.8
2 (5)	-747.684337	0.171145	-747.513192	7.1	0.130179	-747.554158	13.2	2.472	-0.3	-7.4	166.6
4 (6)	-747.681995	0.171941	-747.510054	15.3	0.130949	-747.551046	21.3	2.152	-82.0	-9.0	-178.6
6 (3)	-747.681058	0.171309	-747.509749	16.1	0.130966	-747.550093	23.9	2.369	-64.8	-179.7	171.8
3 (6)	-747.681094	0.171856	-747.509238	17.4	0.131208	-747.549885	24.4	2.177	-72.8	-9.0	-44.3
5 (4)	-747.678688	0.171164	-747.507524	21.9	0.129753	-747.548935	26.9	2.355	-179.1	177.5	167.7
8 (3)	-747.675334	0.171251	-747.504083	31.0	0.130639	-747.544696	38.0	2.235	-65.5	-175.9	-3.7
7 (4)	-747.675342	0.171515	-747.503827	31.6	0.130213	-747.545128	36.9	2.179	160.2	176.4	-42.9
RC → TS 6 (3)				4.1			10.1	-0.496	0.4	-26.2	1.8
2 (5)				7.1			13.2	-0.757	62.2	0.8	-29.9
8 (3)				10.5			18.8	-0.790	11.1	-0.9	-13.8
5 (4)				12.5			23.2	-0.854	-0.9	10.0	-1.5
4 (6)				12.7			20.7	-0.973	-6.0	-0.8	-21.9
7 (4)				14.0			25.5	-1.552	-39.8	-21.2	-17.3
3 (6)				15.1			22.6	-2.108	-22.5	-99.3	-77.2
1 (5)				23.3			25.3	-1.026	7.3	-17.3	-20.5
ENL (*anti*) + OAC				31.3			-13.3			(ENL *anti*) 180.0	(OAC) 0.0
ENL (*syn*) + OAC				23.5			-20.5			(ENL *syn*) 0.0	
PC 1 (5)	-747.748609	0.177282	-747.571327	-145.6	0.138667	-747.609942	-133.3	1.539	35.4	178.3	56.2
2 (5)	-747.741042	0.176412	-747.564630	-128.0	0.136126	-747.604915	-120.1	1.534	34.8	50.0	64.9
3 (6)	-747.737023	0.177118	-747.559905	-115.6	0.136562	-747.600461	-108.8	1.542	-55.9	-50.3	-56.2
4 (6)	-747.691259	0.173592	-747.517667	-4.7	0.134258	-747.557002	5.7	1.580	-58.4	2.3	-167.0
6 (3)	-747.689988	0.173920	-747.516068	-0.5	0.135039	-747.554950	11.1	1.650	-56.0	-174.3	-178.3
5 (4)	-747.685674	0.173904	-747.511770	10.8	0.133545	-747.552129	18.5	1.671	179.2	173.9	166.1
8 (3)	-747.684643	0.173595	-747.511048	12.7	0.134392	-747.550251	23.4	1.640	-54.3	-173.7	-9.5
7 (4)	-747.679988	0.173484	-747.506504	24.6	0.132392	-747.547597	30.4	1.681	169.4	173.0	-46.9
7b, R^{i} = TMS											
RC 24 (3)	-1156.410181	0.272875	-1156.137306	0.0	0.228471	-1156.196741	0.0	2.930	-83.9	90.7	-25.0
25 (3)	-1156.408868	0.273007	-1156.135861	3.8	0.221141	-1156.187727	23.7	2.780	-75.1	76.5	8.4
26 (6)	-1156.402856	0.272075	-1156.130781	17.1	0.216413	-1156.186443	27.0	3.016	-66.0	-29.7	-21.0
TS 24 (3)	-1156.408491	0.273781	-1156.134710	6.8	0.224017	-1156.184475	32.2	2.308	-75.5	113.6	-35.1
25 (3)	-1156.408255	0.274021	-1156.134234	8.1	0.224641	-1156.183615	34.5	2.344	-71.5	64.6	10.5
26 (6)	-1156.400496	0.273544	-1156.126952	27.2	0.221882	-1156.178614	47.5	2.261	-76.2	-27.3	-43.3
RC → TS 25 (3)				4.3			10.8	-0.622	8.4	22.9	10.1
24 (3)				6.8			32.2	-0.436	3.6	-11.9	2.1
26 (6)				10.1			20.6	-0.755	10.2	2.4	-22.3
SEE (*gauche*) + OAC				36.8			0.8			(SEE *gauche*) ± 169.4	(OAC) 0.0
SEE (*syn*) + OAC				38.5			5.5			(SEE *syn*) 0.0	
PC 26 (6)	-1156.460159	0.279068	-1156.181091	-115.0	0.227379	-1156.232780	-94.6	1.542	-53.9	-168.2	-57.1
24 (3)	-1156.425212	0.276531	-1156.148681	-29.9	0.221647	-1156.188534	21.5	1.620	-56.5	171.6	-24.3
25 (3)	-1156.421250	0.276921	-1156.144329	-18.4	0.228261	-1156.192989	9.9	1.628	-68.8	25.9	9.5

[a] Energies relative to that of the second lowest lying reactant complex according to zero point-corrected electronic energies, E+ZPE.

TABLE A2.3 Energies and geometrical parameters of system **8** at the B3LYP/6-31G(d) level of theory.

Structure / Entry Number (Type)	Energies							Geometrical Parameters			
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(C_1,C_1') (Å)	D(C_2',C_1',C_1,C_2) (degrees)	D(R',O',C_2',C_1') (degrees)	D(C_3,C_2,O,B) (degrees)
8a, R^{i} = OH											
RC 9 (6)	-787.010495	0.198891	-786.811604	0.0	0.155240	-786.855255	0.0	2.745	-93.3	-7.4	-35.7
10 (2)	-787.008942	0.198608	-786.810334	3.3	0.154255	-786.854687	1.5	2.816	106.4	5.7	-28.0
11 (3)	-787.000580	0.197788	-786.802792	23.1	0.151813	-786.848767	17.0	2.896	-78.1	169.0	7.6
TS 9 (6)	-787.009984	0.199414	-786.810570	2.7	0.156763	-786.853222	5.3	2.386	-86.9	-8.2	-41.3
10 (2)	-787.008637	0.199266	-786.809371	5.9	0.156709	-786.851928	8.7	2.434	105.8	6.9	-33.7
11 (3)	-786.999585	0.198982	-786.800603	28.9	0.155793	-786.843792	30.1	2.322	-70.5	-177.4	-3.6
RC → TS 10 (2)				2.5			7.2	-0.359	-0.6	-0.8	-5.6
9 (6)				2.7			5.3	-0.382	64.5	1.2	-5.7
11 (3)				5.7			13.1	-0.574	7.6	7.6	-11.2
ENL (*anti*) + OAC				34.8			-15.2			(ENL *anti*) 180.0	(OAC) 0.0
ENL (*syn*) + OAC				26.5			-22.7			(ENL *syn*) 0.0	
PC 10 (2)	-787.061668	0.203694	-786.857974	-121.7	0.161508	-786.900159	-117.9	1.534	35.0	-50.9	0.7
9 (6)	-787.028245	0.202555	-786.825690	-37.0	0.162235	-786.866011	-28.2	1.616	-73.3	-2.5	-60.2
11 (3)	-787.011959	0.201840	-786.810119	3.9	0.159942	-786.852017	8.5	1.626	-59.5	-174.9	-12.2
8b, R^{i} = TMS											
RC 27 (3)	-1195.732150	0.301284	-1195.430866	0.0	0.248813	-1195.483337	0.0	2.797	-91.1	83.8	-30.6
28 (6)	-1195.728082	0.300820	-1195.427262	9.5	0.245756	-1195.482325	2.7	2.688	-95.1	-33.4	-35.3
29 (2)	-1195.726600	0.300613	-1195.425987	12.8	0.245357	-1195.481243	5.5	2.760	108.8	26.5	-28.4
TS 27 (3)	-1195.731858	0.301800	-1195.430058	2.1	0.250743	-1195.481115	5.8	2.411	-90.8	82.9	-38.2
28 (6)	-1195.727912	0.301336	-1195.426576	11.3	0.248151	-1195.479761	9.4	2.405	-92.8	-30.5	-38.7
29 (2)	-1195.726437	0.301053	-1195.425384	14.4	0.247513	-1195.478924	11.6	2.468	108.2	29.8	-32.9
RC → TS 29 (2)				1.6			6.1	-0.386	0.3	-0.9	-7.6
28 (6)				1.8			6.7	-0.283	2.3	2.9	-3.4
27 (3)				2.1			5.8	-0.292	-0.6	3.3	-4.5
SEE (*syn*) + OAC				36.9			-20.4			(SEE *syn*) 0.0	(OAC) 0.0
PC 29 (2)	-1195.784613	0.306781	-1195.477832	-123.3	0.257471	-1195.527142	-115.0	1.532	38.5	-162.6	-6.1
28 (6)	-1195.749073	0.304431	-1195.444642	-36.2	0.253007	-1195.496066	-33.4	1.602	-75.7	-12.1	-59.5
27 (3)	-1195.750365	0.304820	-1195.445545	-38.5	0.253564	-1195.496801	-35.3	1.603	-69.8	160.5	-39.7

[a] Energies relative to that of the lowest lying reactant complex according to zero point-corrected electronic energies, E+ZPE.

TABLE A2.4 Energies and geometrical parameters of system **9** at the B3LYP/6-31G(d) level of theory.

Structure / Entry Number (Type)	Energies							Geometrical Parameters			
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(C_1,C_1') (Å)	D(C_2',C_1',C_1,C_2) (degrees)	D(R',O',C_2',C_1') (degrees)	D(C_3,C_2,O,B) (degrees)
9a, R^{i} = OH											
RC 12 (1)	-826.328357	0.227067	-826.101290	0.0	0.181420	-826.146937	0.0	2.856	-169.7	8.7	-6.6
13 (6)	-826.328468	0.227340	-826.101128	0.4	0.182169	-826.146299	1.7	2.780	-97.6	-6.5	-34.6
14 (6)	-826.327982	0.227275	-826.100707	1.5	0.181935	-826.146048	2.3	2.702	-89.5	-172.9	-36.3
15 (2)	-826.326407	0.227105	-826.099302	5.2	0.180973	-826.145434	3.9	2.776	102.2	178.5	-34.4
16 (1)	-826.325772	0.226667	-826.099105	5.7	0.180761	-826.145011	5.1	2.897	-174.8	171.5	-5.7
17 (2)	-826.324995	0.226948	-826.098047	8.5	0.180469	-826.144526	6.3	2.799	111.5	6.2	-37.3
18 (3)	-826.322209	0.225756	-826.096453	12.7	0.177777	-826.144433	6.6	4.109	-93.5	157.5	-167.9
19 (3)	-826.320537	0.225495	-826.095042	16.4	0.175815	-826.144722	5.8	4.912	-82.9	148.8	-8.7
20 (4)	-826.319807	0.226049	-826.093758	19.8	0.178348	-826.141459	14.4	3.255	160.6	-161.6	-14.7
TS 14 (6)	-826.327577	0.227774	-826.099803	3.9	0.183835	-826.143741	8.4	2.389	-81.7	179.6	-41.3
13 (6)	-826.327231	0.227886	-826.099345	5.1	0.184189	-826.143042	10.2	2.367	-86.5	-7.3	-41.9
12 (1)	-826.326821	0.228397	-826.098424	7.5	0.184715	-826.142107	12.7	2.243	-176.6	8.1	-16.9
15 (2)	-826.325649	0.228397	-826.097252	10.6	0.184598	-826.141051	15.5	2.326	100.1	-177.4	-38.2
17 (2)	-826.324115	0.228266	-826.095849	14.3	0.184430	-826.139685	19.0	2.329	108.5	5.9	-41.5
16 (1)	-826.323383	0.228306	-826.095077	16.3	0.184383	-826.139000	20.8	2.182	177.2	-175.4	-18.4
19 (3)	-826.314668	0.228075	-826.086593	38.6	0.184184	-826.130483	43.2	2.287	-67.1	-172.7	-27.7
20 (4)	-826.315043	0.228509	-826.086534	38.7	0.184404	-826.130639	42.8	2.138	159.2	174.2	-17.6
18 (3)	-826.313439	0.228495	-826.084944	42.9	0.184976	-826.128463	48.5	2.175	-76.6	-174.6	134.7
RC → TS 14 (6)				2.4			6.1	-0.313	7.8	-7.5	-5.0
13 (6)				4.7			12.7	-0.470	-3.0	-0.3	-4.2
15 (2)				5.4			11.5	-0.450	-2.1	4.1	-3.8
17 (2)				5.8			8.6	-0.413	11.1	-0.8	-7.3
12 (1)				7.5			12.7	-0.613	-6.9	-0.6	-9.4
16 (1)				10.6			15.8	-0.715	-8.0	13.1	-12.7
20 (4)				19.0			28.4	-1.117	-1.4	-24.2	-2.9
19 (3)				22.2			37.4	-2.679	15.8	38.5	-19.0
18 (3)				30.2			41.9	-1.934	16.4	27.9	-57.4
ENL (*anti*) + OAC				34.6			-18.0			(ENL *anti*) 180.0	(OAC) 0.0
ENL (*syn*) + OAC				30.1			-22.2			(ENL *syn*) 0.0	
PC 15 (2)	-826.385274	0.232834	-826.152440	-134.3	0.191708	-826.193566	-122.4	1.540	37.9	-168.1	33.7
17 (2)	-826.376822	0.231696	-826.145126	-115.1	0.187768	-826.189054	-110.6	1.537	35.7	-52.9	1.1
13 (6)	-826.343381	0.230756	-826.112625	-29.8	0.188925	-826.154457	-19.7	1.625	-74.0	-2.7	-59.8
14 (6)	-826.342632	0.230675	-826.111957	-28.0	0.188812	-826.153821	-18.1	1.631	-71.9	177.8	-55.7
12 (1)	-826.335102	0.230523	-826.104579	-8.6	0.186249	-826.148852	-5.0	1.649	174.0	6.1	-29.4
16 (1)	-826.329034	0.230274	-826.098760	6.6	0.186077	-826.142956	10.5	1.670	170.8	-174.4	-29.0
19 (3)	-826.325362	0.230518	-826.094844	16.9	0.188188	-826.137175	25.6	1.631	-58.9	-175.8	-31.9
18 (3)	-826.322847	0.230374	-826.092473	23.1	0.188190	-826.134657	32.2	1.623	-54.2	-177.1	168.9
20 (4)	-826.320212	0.230364	-826.089848	30.0	0.186391	-826.133821	34.4	1.664	-174.6	174.3	-33.5
9b, R^{i} = TMS											
RC 30 (6)	-1235.045917	0.329281	-1234.716636	0.0	0.272900	-1234.773016	2.5	2.747	-93.2	-134.6	-34.3
31 (1)	-1235.044699	0.32863	-1234.716069	1.5	0.270736	-1234.773963	0.0	2.932	-173.2	113.2	-5.2
32 (2)	-1235.043997	0.329266	-1234.714731	5.0	0.272129	-1234.771868	5.5	2.731	108.2	159.7	-36.3
TS 30 (6)	-1235.045474	0.32963	-1234.715844	2.1	0.274842	-1234.770632	8.7	2.411	-85.6	-159.1	-37.8
32 (2)	-1235.043796	0.329938	-1234.713858	7.3	0.274904	-1234.768892	13.3	2.439	106.4	171.9	-38.7
31 (1)	-1235.042850	0.33002	-1234.71283	10.0	0.274573	-1234.768277	14.9	2.272	178.6	160.4	-16.4
RC → TS 30 (6)				2.1			6.3	-0.336	7.6	-24.5	-3.5
32 (2)				2.3			7.8	-0.292	-1.8	12.2	-2.4
31 (1)				8.5			14.9	-0.660	-8.2	47.2	-11.2
SEE (*gauche*) + OAC				33.0			-17.8			(SEE *gauche*) ± 130.3	(OAC) 0.0
PC 32 (2)	-1235.099567	0.334779	-1234.764788	-126.4	0.283615	-1234.815952	-110.2	1.554	39.0	-161.5	-6.3
30 (6)	-1235.064378	0.332495	-1234.731883	-40.0	0.279754	-1234.784625	-28.0	1.619	-72.6	-179.9	-57.9
31 (1)	-1235.052388	0.332281	-1234.720107	-9.1	0.277119	-1234.775268	-3.4	1.646	170.8	-175.4	-29.8

[a] Energies relative to that of the lowest lying reactant complex according to zero point-corrected electronic energies, E+ZPE.

TABLE A2.5 Energies and geometrical parameters of system **10** at the B3LYP/6-31G(d) level of theory.

Structure / Entry Number (Type)	Energies							Geometrical Parameters			
	E (Ha)	ZPE (Ha)	E+ZPE (Ha)	Δ(E+ZPE) [a] (kJ mol^{-1})	G_{corr} (Ha)	E+G_{corr} (Ha)	Δ(E+G_{corr}) [a] (kJ mol^{-1})	R(C_3,C_1) (Å)	D(C_2',C_1',C_1,C_2) (degrees)	D(R',O',C_2',C_1') (degrees)	D(C_3,C_2,O,B) (degrees)
10a, R' = OH											
RC 21 (6)	-826.327716	0.227121	-826.100595	0.0	0.182262	-826.145454	0.0	2.979	-82.7	-9.4	-22.6
22 (1)	-826.322095	0.226046	-826.096049	11.9	0.178708	-826.143387	5.4	3.053	162.8	174.9	-12.3
23 (4)	-826.321675	0.226462	-826.095213	14.1	0.179844	-826.141832	9.5	2.826	-175.6	-172.6	-9.2
TS 21 (6)	-826.324923	0.228184	-826.096739	10.1	0.185469	-826.139454	15.8	2.311	-64.5	-11.0	-32.6
23 (4)	-826.320010	0.227996	-826.092014	22.5	0.183927	-826.136084	24.6	2.214	176.9	174.5	-16.7
22 (1)	-826.317242	0.228417	-826.088825	30.9	0.184375	-826.132867	33.0	2.119	158.8	-170.5	-16.3
RC → TS 23 (4)				8.4			15.1	-0.612	-7.5	-12.9	-10.0
21 (6)				10.1			15.8	-0.668	18.2	-1.6	-4.0
22 (1)				19.0			27.6	-0.934	-4.0	14.6	-7.5
ENL (*anti*) + OAC				39.4			-16.5			(ENL *anti*) 180.0	(OAC) 0.0
ENL (*syn*) + OAC				32.4			-20.3			(ENL *syn*) 0.0	
PC 21 (6)	-826.339239	0.230878	-826.108361	-20.4	0.188888	-826.141163	-12.9	1.612	-59.5	-1.5	-39.0
23 (4)	-826.326787	0.230116	-826.096671	10.3	0.185623	0.185623	11.3	1.660	170.9	173.8	-28.4
22 (1)	-826.321787	0.230295	-826.091492	23.9	0.186257	-826.135530	26.1	1.669	174.1	-172.7	-29.8
10b, R' = TMS											
RC 33 (3)	-1235.048560	0.329579	-1234.718981	0.0	0.275506	-1234.773055	0.0	2.832	-94.0	83.8	-28.2
TS 33 (3)	-1235.047213	0.330365	-1234.716848	5.6	0.277726	-1234.769487	9.4	2.778	-92.0	87.4	-39.8
RC → TS 33 (3)				5.6			9.4	-0.555	2.0	3.6	-11.6
SEE (*gauche*) + OAC										(SEE *gauche*) ± 74.3	(OAC) 0.0
SEE (*syn*) + OAC				41.5			-20.0			(SEE *syn*) 0.0	
PC 33 (3)	-1235.063013	0.333051	-1234.729962	-28.8	0.281030	-1234.769487	-23.4	1.615	-70.7	159.7	-38.6

[a] Energies relative to that of the lowest lying reactant complex according to zero point-corrected electronic energies, E+ZPE.

Cartesian coordinates for systems **7-10**

RB3LYP/6-31G(d)

OAC RT

C -1.8064280000 1.2340940000 0.0000000000
C -0.6068350000 0.4994050000 0.0000010000
C -0.9989030000 -0.8684690000 0.0000010000
C -2.4616830000 -1.0437260000 0.0000000000
O 0.5789520000 1.0015490000 0.0000010000
H -0.2867160000 -1.6845000000 0.0000030000
B 1.7694530000 -0.0166820000 0.0000000000
F 1.5965200000 -0.7980100000 1.1426300000
F 2.9046040000 0.7321220000 -0.0000010000
F 1.5965180000 -0.7980090000 -1.1426300000
H -2.7880690000 -1.6297070000 -0.8731880000
H -2.7880710000 -1.6297070000 0.8731880000
H -1.8273520000 2.3205490000 0.0000000000
C -3.0193370000 0.3905580000 -0.0000010000
H -3.6541670000 0.5991430000 0.8745680000
H -3.6541660000 0.5991430000 -0.8745690000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.111363 (Hartree/Particle)
Thermal correction to Energy= 0.120690
Thermal correction to Enthalpy= 0.121634
Thermal correction to Gibbs (Free) Energy= 0.075766
Sum of electronic and zero-point Energies= -593.757979
Sum of electronic and thermal Energies= -593.748652
Sum of electronic and thermal Enthalpies= -593.747708
Sum of electronic and thermal (Free) Energies= -593.793575

OAC TS

C 1.3172140000 1.1239400000 -0.2774660000
C 0.5456420000 -0.0000100000 -0.6276300000
C 1.3172140000 -1.1239490000 -0.2774280000
C 2.6550870000 -0.7714940000 0.2385930000
O -0.6688990000 -0.0000180000 -1.0809790000
H 0.9422420000 -2.1388060000 -0.3672160000
B -1.6936090000 0.0000020000 0.1123980000
F -1.3943640000 -1.1471820000 0.8488790000
F -2.9366060000 -0.0000070000 -0.4401320000
F -1.3943640000 1.1472100000 0.8488420000
H 2.8048100000 -1.1886630000 1.2454790000
H 3.4558320000 -1.2066370000 -0.3783230000
H 0.9422430000 2.1387940000 -0.3672880000
C 2.6550870000 0.7715020000 0.2385670000
H 3.4558330000 1.2066240000 -0.3783630000
H 2.8048100000 1.1887040000 1.2454390000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.111020 (Hartree/Particle)
Thermal correction to Energy= 0.119539
Thermal correction to Enthalpy= 0.120483
Thermal correction to Gibbs (Free) Energy= 0.076811
Sum of electronic and zero-point Energies= -593.750011
Sum of electronic and thermal Energies= -593.741492
Sum of electronic and thermal Enthalpies= -593.740548
Sum of electronic and thermal (Free) Energies= -593.784219

7a

ENL RT (*anti*)

C 1.2284530000 -0.1787840000 0.0000000000
H 2.1304830000 0.4213440000 0.0000000000
C 0.0353210000 0.4124960000 0.0000000000
O -1.1361410000 -0.2976340000 0.0000000000
H -1.8803840000 0.3196450000 0.0000000000
H 1.3249040000 -1.2596340000 0.0000000000
H -0.0685190000 1.4974510000 0.0000000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.056240 (Hartree/Particle)
Thermal correction to Energy= 0.060117
Thermal correction to Enthalpy= 0.061061
Thermal correction to Gibbs (Free) Energy= 0.031553
Sum of electronic and zero-point Energies= -153.745988
Sum of electronic and thermal Energies= -153.742111
Sum of electronic and thermal Enthalpies= -153.741166
Sum of electronic and thermal (Free) Energies= -153.770675

ENL TS (*anti* ↔ *syn*)

C -1.2070630000 -0.2178240000 0.0045800000
H -2.1463740000 0.3233390000 0.0557650000
C -0.0509860000 0.4393450000 0.0090470000
O 1.1818140000 -0.1788210000 -0.1118650000
H 1.4882300000 -0.4497230000 0.7670210000
H -1.2432540000 -1.3015680000 -0.0578590000
H -0.0048230000 1.5293980000 0.0482320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.055362 (Hartree/Particle)
Thermal correction to Energy= 0.058726
Thermal correction to Enthalpy= 0.059670
Thermal correction to Gibbs (Free) Energy= 0.031004
Sum of electronic and zero-point Energies= -153.740898
Sum of electronic and thermal Energies= -153.737534
Sum of electronic and thermal Enthalpies= -153.736590
Sum of electronic and thermal (Free) Energies= -153.765256

ENL RT (*syn*)

C 1.2042400000 -0.2037350000 0.0000000000
H 2.1328610000 0.3544440000 -0.0000010000
C 0.0351260000 0.4391000000 0.0000000000
O -1.2102520000 -0.1147480000 0.0000000000
H -1.1200180000 -1.0821160000 -0.0000010000
H 1.2718910000 -1.2895430000 0.0000010000
H -0.0389160000 1.5230100000 0.0000010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.056717 (Hartree/Particle)
Thermal correction to Energy= 0.060326
Thermal correction to Enthalpy= 0.061270
Thermal correction to Gibbs (Free) Energy= 0.032275
Sum of electronic and zero-point Energies= -153.748955
Sum of electronic and thermal Energies= -153.745347
Sum of electronic and thermal Enthalpies= -153.744403
Sum of electronic and thermal (Free) Energies= -153.773398

Entry 1

RC

C -2.9813180000 1.9353720000 -0.5462300000
C -1.6458940000 1.8505450000 -0.4577750000
H -3.4515210000 2.1150460000 -1.5057690000
O -1.0088860000 1.6287920000 0.7167480000
C -0.1752070000 -1.7749550000 -0.6530270000
C 0.1485610000 -1.0600850000 0.5023560000
C -1.0537930000 -0.8795330000 1.2244720000
C -2.2246340000 -1.3991610000 0.5029860000
O 1.3005970000 -0.5811230000 0.9006540000
H -1.0895810000 -0.4330290000 2.2114270000
B 2.1328830000 0.2340300000 -0.0752890000
F 2.1927180000 -0.4202250000 -1.2995930000
F 3.3443050000 0.4555700000 0.5000920000
F 1.4055140000 1.4683630000 -0.2510380000
H -2.8808680000 -2.0212660000 1.1244540000
H -2.8344690000 -0.5304060000 0.1799120000
H 0.5539460000 -2.0320950000 -1.4114380000
C -1.6182970000 -2.1124870000 -0.7240770000
H -2.0659930000 -1.8004810000 -1.6769960000
H -1.7705080000 -3.2012300000 -0.6665670000
H -3.6107630000 1.8990650000 0.3378360000
H -0.9957430000 1.9306970000 -1.3275320000
H -0.0319520000 1.6306550000 0.5345180000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171001 (Hartree/Particle)
Thermal correction to Energy= 0.184567
Thermal correction to Enthalpy= 0.185511
Thermal correction to Gibbs (Free) Energy= 0.129987
Sum of electronic and zero-point Energies= -747.527959
Sum of electronic and thermal Energies= -747.514393
Sum of electronic and thermal Enthalpies= -747.513449

Sum of electronic and thermal (Free) Energies= -747.568973

TS

C -1.5388670000 1.9163840000 -1.0011890000
C -0.5430310000 2.1357160000 -0.1083050000
H -1.3443460000 2.0358170000 -2.0603890000
O -0.7894400000 2.1136750000 1.2098100000
C -0.8419880000 -0.5273470000 -0.8623240000
C -0.3480900000 -0.6447980000 0.4773170000
C -1.3774180000 -1.1396660000 1.2560020000
C -2.6212120000 -1.3963840000 0.4782970000
O 0.8297920000 -0.2556680000 0.9066770000
H -1.2789590000 -1.3317800000 2.3196870000
B 2.0227720000 -0.3208130000 -0.0779450000
F 1.9211590000 -1.5273120000 -0.7571190000
F 3.1464080000 -0.1903030000 0.6869360000
F 1.8706770000 0.7486280000 -0.9886590000
H -3.0299240000 -2.3989130000 0.6602440000
H -3.4176830000 -0.6890880000 0.7575700000
H -0.1992440000 -0.2917460000 -1.6996000000
C -2.1734920000 -1.1821810000 -0.9862210000
H -2.8848160000 -0.6241670000 -1.6022620000
H -2.0275120000 -2.1515030000 -1.4884200000
H -2.5679500000 1.8145290000 -0.6708000000
H 0.4920250000 2.2309020000 -0.4199410000
H 0.0421280000 1.8965140000 1.6698570000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171384 (Hartree/Particle)
Thermal correction to Energy= 0.184348
Thermal correction to Enthalpy= 0.185292
Thermal correction to Gibbs (Free) Energy= 0.131136
Sum of electronic and zero-point Energies= -747.519087
Sum of electronic and thermal Energies= -747.506123
Sum of electronic and thermal Enthalpies= -747.505179
Sum of electronic and thermal (Free) Energies= -747.559336

PC

C -0.9926400000 1.9364230000 -0.1963930000
C 0.4888260000 1.5555610000 -0.1573090000
H -1.1573850000 2.7691970000 -0.8853480000
O 1.1930610000 2.2559560000 0.7737030000
C -1.6841950000 0.6226250000 -0.6014430000
C -0.8331340000 -0.3923490000 0.0951880000
C -1.4660570000 -1.4631790000 0.5589400000
C -2.9407600000 -1.3118950000 0.2129110000
O 0.4633900000 0.0770370000 0.2480540000
H -1.0266330000 -2.2982500000 1.0889820000
B 1.8455140000 -0.8248420000 -0.1409780000
F 1.7188000000 -1.9278460000 0.6283600000
F 2.8248290000 0.0692310000 0.2358380000
F 1.7487210000 -1.0070850000 -1.4830600000
H -3.2199740000 -1.9315450000 -0.6521250000
H -3.5925860000 -1.6181030000 1.0393130000
H -1.6027660000 0.4953870000 -1.6926140000
C -3.0882510000 0.2120060000 -0.1102020000
H -3.3246150000 0.7541050000 0.8132380000
H -3.8809490000 0.4193720000 -0.8348010000
H -1.2866110000 2.2478930000 0.8119480000
H 0.9670910000 1.5304250000 -1.1418640000
H 2.1113490000 1.9279380000 0.7437080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.177282 (Hartree/Particle)
Thermal correction to Energy= 0.189148
Thermal correction to Enthalpy= 0.190092
Thermal correction to Gibbs (Free) Energy= 0.138667
Sum of electronic and zero-point Energies= -747.571327
Sum of electronic and thermal Energies= -747.559461
Sum of electronic and thermal Enthalpies= -747.558517
Sum of electronic and thermal (Free) Energies= -747.609942

Entry 2

RC

C 0.7738340000 2.5669820000 0.5468340000
C 1.3290690000 1.9779770000 -0.5193520000
H -0.3051830000 2.5897670000 0.6270350000
O 2.6694910000 1.8450080000 -0.7633670000
C 0.6769790000 -0.6423080000 0.8862500000
C -0.0955930000 -1.3205180000 -0.1018980000
C 0.7639660000 -2.2703130000 -0.6720270000
C 2.1402460000 -2.2238410000 -0.1314510000
O -1.3434900000 -1.1751050000 -0.4131600000
H 0.4343280000 -2.9778560000 -1.4276220000
B -2.1227180000 0.1061610000 -0.0359770000
F -1.8884160000 0.3669620000 1.3218260000
F -3.4320240000 -0.1555310000 -0.3108740000
F -1.5883070000 1.1365380000 -0.8185500000
H 2.4067930000 -3.1684560000 0.3670280000
H 2.8863330000 -2.0920160000 -0.9285670000
H 0.2352510000 0.0488270000 1.5909010000
C 2.0937900000 -1.0555720000 0.8733970000
H 2.7225730000 -0.2153070000 0.5347170000
H 2.4534490000 -1.3213010000 1.8768570000
H 1.3688410000 3.0297220000 1.3328090000
H 0.7300210000 1.5281440000 -1.3026640000
H 3.1581530000 2.3622810000 -0.1005380000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170106 (Hartree/Particle)
Thermal correction to Energy= 0.184370
Thermal correction to Enthalpy= 0.185314
Thermal correction to Gibbs (Free) Energy= 0.126809
Sum of electronic and zero-point Energies= -747.515879
Sum of electronic and thermal Energies= -747.501616
Sum of electronic and thermal Enthalpies= -747.500672
Sum of electronic and thermal (Free) Energies= -747.559177

TS

C 1.0199320000 1.7802050000 1.2162990000
C 0.6629760000 2.1096600000 -0.0515740000
H 0.2636800000 1.8272440000 1.9890010000
O 1.4932720000 2.1733240000 -1.1004620000
C 0.7261750000 -0.6522210000 0.8885010000
C 0.2975350000 -0.7534880000 -0.4787730000
C 1.3820820000 -1.2074550000 -1.2150650000
C 2.5887700000 -1.4725060000 -0.3824370000
O -0.8604030000 -0.4096900000 -0.9610050000
H 1.3352240000 -1.3880190000 -2.2841950000
B -2.0740050000 -0.2163190000 -0.0225920000
F -2.0121950000 -1.2225560000 0.9441530000
F -3.1808550000 -0.2858700000 -0.8172110000
F -1.9311980000 1.0405020000 0.5947350000
H 2.9769240000 -2.4899100000 -0.5296420000
H 3.4236830000 -0.8018010000 -0.6390920000
H 0.0236640000 -0.5237160000 1.6990400000
C 2.0840630000 -1.2416420000 1.0605130000
H 2.7538520000 -0.6352080000 1.6795510000
H 1.9757710000 -2.1997890000 1.5920420000
H 2.0626620000 1.7151560000 1.5191200000
H -0.3734290000 2.2408460000 -0.3366650000
H 2.4140740000 2.0637170000 -0.8043340000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171145 (Hartree/Particle)
Thermal correction to Energy= 0.184219
Thermal correction to Enthalpy= 0.185163
Thermal correction to Gibbs (Free) Energy= 0.130179
Sum of electronic and zero-point Energies= -747.513192
Sum of electronic and thermal Energies= -747.500118
Sum of electronic and thermal Enthalpies= -747.499174
Sum of electronic and thermal (Free) Energies= -747.554158

PC

C 1.0556920000 1.9010980000 0.3176940000
C -0.4457920000 1.6076260000 0.1202000000
H 1.1964550000 2.6718950000 1.0802810000
O -1.1213360000 2.4177750000 -0.7534090000
C 1.6438210000 0.5254210000 0.6568150000
C 0.7857670000 -0.3592700000 -0.1936120000
C 1.3944580000 -1.4208910000 -0.7122620000
C 2.8450350000 -1.4001020000 -0.2532250000
O -0.4755000000 0.1827010000 -0.3751130000
H 0.9491110000 -2.1813250000 -1.3406910000

B -1.9373640000 -0.8556410000 0.1825520000
F -1.7027080000 -1.9627110000 -0.5413580000
F -2.9362870000 -0.0470170000 -0.1992670000
F -1.6670050000 -0.9097390000 1.5046930000
H 3.0225380000 -2.1174240000 0.5618980000
H 3.5402520000 -1.6662020000 -1.0582510000
H 1.4643050000 0.3091420000 1.7216110000
C 3.0557700000 0.0712780000 0.2334240000
H 3.4001410000 0.6835930000 -0.6091470000
H 3.7980910000 0.1541630000 1.0325650000
H 1.4718000000 2.2749920000 -0.6283190000
H -1.0129160000 1.6040890000 1.0513380000
H -0.6227640000 2.4657080000 -1.5866640000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.176412 (Hartree/Particle)
Thermal correction to Energy= 0.188854
Thermal correction to Enthalpy= 0.189799
Thermal correction to Gibbs (Free) Energy= 0.136126
Sum of electronic and zero-point Energies= -747.564630
Sum of electronic and thermal Energies= -747.552187
Sum of electronic and thermal Enthalpies= -747.551243
Sum of electronic and thermal (Free) Energies= -747.604915

Entry 3

RC

C -1.6599540000 -2.2578380000 0.8105750000
C -1.6505290000 -1.7150650000 -0.4151130000
O -2.7476670000 -1.3617970000 -1.1453770000
C -1.1463520000 0.8197290000 1.2428870000
C 0.1216590000 0.7872370000 0.6281290000
C 0.0613970000 1.6982150000 -0.4454570000
C -1.2730090000 2.3143130000 -0.5998620000
O 1.0988690000 0.0202670000 1.0003100000
H 0.9150970000 1.9074300000 -1.0797280000
B 2.1573520000 -0.3200550000 -0.0820300000
F 1.4172600000 -0.7994580000 -1.1801020000
F 2.9768070000 -1.2590720000 0.4687320000
F 2.8039850000 0.8639100000 -0.4288850000
H -1.2209190000 3.4108390000 -0.5226900000
H -1.6878560000 2.1108980000 -1.5984220000
H -1.3737290000 0.2741940000 2.1519920000
C -2.1085560000 1.6911920000 0.5360040000
H -2.9397180000 1.0855790000 0.1414670000
H -2.5645680000 2.4374760000 1.2015070000
H -0.7199300000 -2.5019590000 1.2908270000
H -2.5819520000 -2.5003050000 1.3365500000
H -0.7286980000 -1.4823450000 -0.9407900000
H -3.5445030000 -1.6844070000 -0.6906990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170008 (Hartree/Particle)
Thermal correction to Energy= 0.184415
Thermal correction to Enthalpy= 0.185360
Thermal correction to Gibbs (Free) Energy= 0.126503
Sum of electronic and zero-point Energies= -747.514977
Sum of electronic and thermal Energies= -747.500570
Sum of electronic and thermal Enthalpies= -747.499626
Sum of electronic and thermal (Free) Energies= -747.558482

TS

C -1.3006020000 -1.5266150000 0.9382450000
C -1.5540960000 -1.6574730000 -0.3997040000
O -2.7535140000 -1.8236640000 -0.9563770000
C -1.1426380000 0.6328540000 1.1639250000
C 0.1308830000 0.9165630000 0.5435750000
C -0.0909530000 1.7679370000 -0.5168560000
C -1.5398700000 2.0497490000 -0.7368870000
O 1.2322410000 0.3541990000 0.9784760000
H 0.7074380000 2.1540890000 -1.1374550000
B 2.1605600000 -0.2584550000 -0.0830600000
F 1.3741220000 -1.2369010000 -0.7456290000
F 3.2082090000 -0.8171860000 0.5949820000
F 2.5434120000 0.7315490000 -0.9810390000
H -1.7572800000 3.1239060000 -0.8104730000
H -1.8881610000 1.6100900000 -1.6849350000
H -1.1969080000 0.3917420000 2.2212940000
C -2.2351100000 1.4122050000 0.4913580000
H -3.1066330000 0.8010540000 0.2286400000
H -2.6009690000 2.1833550000 1.1828230000
H -0.2652840000 -1.6157380000 1.2516010000
H -2.0802030000 -1.7407830000 1.6678830000
H -0.7554090000 -1.5462540000 -1.1282230000
H -3.4265900000 -1.9819580000 -0.2694150000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171856 (Hartree/Particle)
Thermal correction to Energy= 0.184732
Thermal correction to Enthalpy= 0.185676
Thermal correction to Gibbs (Free) Energy= 0.131208
Sum of electronic and zero-point Energies= -747.509238
Sum of electronic and thermal Energies= -747.496362
Sum of electronic and thermal Enthalpies= -747.495417
Sum of electronic and thermal (Free) Energies= -747.549885

PC

C -1.2205690000 -1.1895270000 0.8771410000
C -0.8384820000 -1.8483240000 -0.4434140000
O -0.9000680000 -3.2295370000 -0.3953480000
C -1.3451890000 0.3479840000 0.8935240000
C -0.1215770000 1.1084200000 0.4312380000
C -0.3977550000 2.1618790000 -0.3386660000
C -1.8869960000 2.3002640000 -0.5409670000
O 1.0985070000 0.6999000000 0.9178600000
H 0.3340090000 2.8594170000 -0.7306130000
B 2.1689520000 0.4380740000 0.1261360000
F 0.4716900000 -1.4529920000 -0.7831210000
F 3.2194290000 -0.1493290000 0.6810700000
F 2.2387410000 0.8006940000 -1.1466640000
H -2.2806270000 3.1532450000 0.0319890000
H -2.1619080000 2.4797540000 -1.5876860000
H -1.5401110000 0.6178780000 1.9437230000
C -2.4527120000 0.9513260000 -0.0127510000
H -2.6435840000 0.2854450000 -0.8616790000
H -3.4017220000 1.0695950000 0.5191010000
H -0.4705200000 -1.4933340000 1.6208010000
H -2.1774680000 -1.6257240000 1.1886800000
H -1.4729720000 -1.5489600000 -1.2807060000
H -0.4064250000 -3.5280660000 0.3874120000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.177118 (Hartree/Particle)
Thermal correction to Energy= 0.189756
Thermal correction to Enthalpy= 0.190700
Thermal correction to Gibbs (Free) Energy= 0.136562
Sum of electronic and zero-point Energies= -747.559905
Sum of electronic and thermal Energies= -747.547267
Sum of electronic and thermal Enthalpies= -747.546323
Sum of electronic and thermal (Free) Energies= -747.600461

Entry 4

RC

C -0.9887890000 -2.2784640000 0.1526830000
C -1.9435790000 -1.7401180000 -0.6165460000
H 0.0414380000 -2.3025330000 -0.1849560000
O -3.2676070000 -1.6163600000 -0.3048750000
C -0.5777990000 0.6182620000 0.8434250000
C 0.2057350000 1.1682460000 -0.2164160000
C -0.5860890000 2.1696350000 -0.7946950000
C -1.9252550000 2.3010810000 -0.1778580000
O 1.4083550000 0.8792760000 -0.5944270000
H -0.2321090000 2.7958130000 -1.6087040000
B 2.2530670000 -0.2709530000 0.0080440000
F 1.9297670000 -0.3693080000 1.3688490000
F 3.5554480000 0.0796160000 -0.2019180000
F 1.8872860000 -1.4360960000 -0.6673320000
H -2.0900360000 3.3147550000 0.2170600000
H -2.7287700000 2.1396750000 -0.9123940000
H -0.1731460000 -0.0911980000 1.5514000000
C -1.9143880000 1.2411130000 0.9406860000
H -2.7117610000 0.4926480000 0.8142760000
H -2.0690980000 1.6767610000 1.9390380000
H -1.2182260000 -2.7071450000 1.1275230000
H -1.7408740000 -1.3132810000 -1.5940920000

H -3.4402760000 -2.1004880000 0.5209740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170131 (Hartree/Particle)
Thermal correction to Energy= 0.184471
Thermal correction to Enthalpy= 0.185415
Thermal correction to Gibbs (Free) Energy= 0.126091
Sum of electronic and zero-point Energies= -747.514887
Sum of electronic and thermal Energies= -747.500547
Sum of electronic and thermal Enthalpies= -747.499603
Sum of electronic and thermal (Free) Energies= -747.558927

TS

C -0.9131240000 -1.6313720000 0.1813020000
C -1.9978810000 -1.5170990000 -0.6420190000
H 0.0887130000 -1.6872340000 -0.2455340000
O -3.2718610000 -1.7308380000 -0.3018170000
C -0.5946160000 0.3997750000 0.8181100000
C 0.1558440000 1.0729030000 -0.2366120000
C -0.6728040000 2.0295940000 -0.7869270000
C -2.0492790000 2.0135490000 -0.2122490000
O 1.3859120000 0.8415940000 -0.6005820000
H -0.3459370000 2.7212650000 -1.5562760000
B 2.2863940000 -0.2392510000 -0.0056300000
F 2.0159420000 -0.3492080000 1.3688880000
F 3.5720430000 0.1397000000 -0.2618430000
F 1.9494630000 -1.4502920000 -0.6450310000
H -2.4221270000 3.0134260000 0.0445100000
H -2.7796350000 1.5960500000 -0.9271770000
H -0.0489740000 -0.0588920000 1.6330500000
C -1.9004090000 1.1089710000 1.0305700000
H -2.7530080000 0.4430000000 1.2027450000
H -1.8023570000 1.7248930000 1.9356330000
H -1.0474880000 -2.0870700000 1.1620430000
H -1.9197600000 -1.1540180000 -1.6630620000
H -3.3172270000 -2.1209410000 0.5902340000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171941 (Hartree/Particle)
Thermal correction to Energy= 0.184774
Thermal correction to Enthalpy= 0.185719
Thermal correction to Gibbs (Free) Energy= 0.130949
Sum of electronic and zero-point Energies= -747.510054
Sum of electronic and thermal Energies= -747.497221
Sum of electronic and thermal Enthalpies= -747.496276
Sum of electronic and thermal (Free) Energies= -747.551046

PC

C -0.9189610000 -1.0829520000 0.6753150000
C -1.7740010000 -1.3695210000 -0.4353220000
H 0.0990430000 -1.4652660000 0.3516990000
O -2.5659780000 -2.3980350000 -0.5291290000
C -0.6183120000 0.4500650000 0.9132960000
C 0.0284170000 1.0556290000 -0.3307130000
C -0.9046840000 1.7640060000 -1.0305730000
C -2.2396030000 1.7438680000 -0.3480210000
O 1.2800390000 0.8699300000 -0.6771260000
H -0.7051430000 2.2590410000 -1.9743140000
B 2.1930140000 -0.1378020000 -0.0324330000
F 2.1842860000 0.0163700000 1.3538880000
F 3.4275980000 0.0059360000 -0.5893840000
F 1.6492770000 -1.4443130000 -0.3349460000
H -2.7751600000 2.7008620000 -0.3725750000
H -2.9387320000 1.0133600000 -0.8177330000
H 0.0587380000 0.4714550000 1.7663710000
C -1.8921070000 1.2958600000 1.0873430000
H -2.7064600000 0.7593210000 1.5903740000
H -1.6475260000 2.1736450000 1.6943990000
H -1.2194580000 -1.6240130000 1.5831430000
H -1.7442300000 -0.7721240000 -1.3444460000
H -2.5335690000 -2.9460940000 0.2813110000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173592 (Hartree/Particle)
Thermal correction to Energy= 0.185937
Thermal correction to Enthalpy= 0.186881
Thermal correction to Gibbs (Free) Energy= 0.134258
Sum of electronic and zero-point Energies= -747.517667
Sum of electronic and thermal Energies= -747.505323
Sum of electronic and thermal Enthalpies= -747.504379
Sum of electronic and thermal (Free) Energies= -747.557002

Entry 5

RC

C -1.9829220000 -2.0772760000 -0.9094170000
C -3.1353370000 -1.6924760000 -0.3692770000
H -2.0005010000 -2.6160870000 -1.8505050000
O -3.1979600000 -0.9491570000 0.7966540000
C -0.1272890000 0.9049770000 0.8025210000
C 0.6271930000 1.1052560000 -0.3869290000
C -0.0417320000 2.1178550000 -1.0918790000
C -1.2664580000 2.5959190000 -0.4156420000
O 1.7045040000 0.5051630000 -0.7726200000
H 0.3080280000 2.4965110000 -2.0483650000
B 2.2095730000 -0.6696860000 0.1087630000
F 2.4746810000 -0.1368890000 1.3690090000
F 3.3004440000 -1.1822540000 -0.5228650000
F 1.1355500000 -1.5717340000 0.1965320000
H -1.2072670000 3.6709900000 -0.1869010000
H -2.1490430000 2.4833660000 -1.0632980000
H 0.1648410000 0.2033420000 1.5742660000
C -1.3392990000 1.7327200000 0.8552860000
H -2.2194790000 1.0658650000 0.8718510000
H -1.3937910000 2.3185420000 1.7848440000
H -1.0161740000 -1.8903460000 -0.4517720000
H -4.0999650000 -1.9078520000 -0.8278320000
H -4.0878790000 -1.0279230000 1.1695680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169015 (Hartree/Particle)
Thermal correction to Energy= 0.183947
Thermal correction to Enthalpy= 0.184891
Thermal correction to Gibbs (Free) Energy= 0.123529
Sum of electronic and zero-point Energies= -747.512290
Sum of electronic and thermal Energies= -747.497358
Sum of electronic and thermal Enthalpies= -747.496414
Sum of electronic and thermal (Free) Energies= -747.557775

TS

C -1.2854480000 -1.1422150000 -1.1315340000
C -2.1786840000 -1.9057590000 -0.4560630000
H -1.6631370000 -0.4706170000 -1.8942720000
O -1.7760700000 -2.8276450000 0.4374310000
C -0.7911670000 0.4249570000 0.5559410000
C 0.1399210000 1.2315670000 -0.1985110000
C -0.5189380000 2.4110510000 -0.5215990000
C -1.9299260000 2.4499190000 -0.0526220000
O 1.3569040000 0.9365000000 -0.5405300000
H -0.0317160000 3.2296610000 -1.0419910000
B 2.1197420000 -0.2543420000 0.0752880000
F 1.7388200000 -0.3461460000 1.4194200000
F 3.4468580000 0.0221330000 -0.0898570000
F 1.7199450000 -1.4060420000 -0.6186430000
H -2.1778390000 3.3870880000 0.4629730000
H -2.6393870000 2.3724890000 -0.8926250000
H -0.4633190000 -0.4222510000 1.1428680000
C -2.0192970000 1.2145020000 0.8710680000
H -2.9493800000 0.6465310000 0.7793060000
H -1.9523090000 1.5307070000 1.9233860000
H -0.2223730000 -1.3743820000 -1.1174500000
H -3.2558290000 -1.7783710000 -0.5680950000
H -2.5394700000 -3.2536490000 0.8558960000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171164 (Hartree/Particle)
Thermal correction to Energy= 0.184325
Thermal correction to Enthalpy= 0.185270
Thermal correction to Gibbs (Free) Energy= 0.129753
Sum of electronic and zero-point Energies= -747.507524
Sum of electronic and thermal Energies= -747.494363
Sum of electronic and thermal Enthalpies= -747.493419
Sum of electronic and thermal (Free) Energies= -747.548935

PC

C 1.0845450000 0.9232920000 -0.9105330000
C 1.8657610000 2.0226480000 -0.4699060000
H 1.5567930000 0.4038330000 -1.7448010000
O 1.3437140000 2.8928300000 0.3621850000
C 0.9133230000 -0.1439020000 0.3643290000
C 0.0230180000 -1.2436760000 -0.1473490000
C 0.7710150000 -2.3751810000 -0.3440090000
C 2.2224950000 -2.1753070000 -0.0370840000
O -1.2400960000 -1.1002990000 -0.4345950000
H 0.3395010000 -3.3212190000 -0.6527690000
B -2.1098180000 0.0551990000 0.0706660000
F -1.7505680000 0.3390370000 1.3905350000
F -3.4065660000 -0.3548750000 -0.0586240000
F -1.8328110000 1.1771690000 -0.7484060000
H 2.6606890000 -3.0034260000 0.5348200000
H 2.8324620000 -2.0869340000 -0.9526130000
H 0.4404420000 0.4549230000 1.1410100000
C 2.2151820000 -0.8510650000 0.7681600000
H 3.1162840000 -0.2454850000 0.6137530000
H 2.1586550000 -1.0830120000 1.8373710000
H 0.0334180000 1.1872340000 -1.1033440000
H 2.9237150000 2.1376670000 -0.7096230000
H 1.9956580000 3.5473360000 0.6689520000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173904 (Hartree/Particle)
Thermal correction to Energy= 0.186747
Thermal correction to Enthalpy= 0.187691
Thermal correction to Gibbs (Free) Energy= 0.133545
Sum of electronic and zero-point Energies= -747.511770
Sum of electronic and thermal Energies= -747.498927
Sum of electronic and thermal Enthalpies= -747.497983
Sum of electronic and thermal (Free) Energies= -747.552129

Entry 6

RC

C 1.2137490000 1.9143160000 1.0293070000
C 2.2519970000 1.7843550000 0.1918270000
H 1.4108540000 2.0997220000 2.0799520000
O 2.0720800000 1.5264120000 -1.1365020000
C 0.3716810000 -0.8220810000 0.9207080000
C 0.0318240000 -0.7187430000 -0.4555110000
C 1.1146340000 -1.2544980000 -1.1632720000
C 2.1862720000 -1.7807140000 -0.2850700000
O -1.0295220000 -0.2024970000 -0.9877610000
H 1.1438790000 -1.2966880000 -2.2475900000
B -2.2249390000 0.1259110000 -0.0617480000
F -2.4302860000 -1.0021360000 0.7351650000
F -3.2730230000 0.4238500000 -0.8806730000
F -1.8298770000 1.2057800000 0.7457260000
H 2.4484320000 -2.8198270000 -0.5281000000
H 3.1153530000 -1.2021820000 -0.4039880000
H -0.2700100000 -0.4654500000 1.7158770000
C 1.6111470000 -1.6017380000 1.1359070000
H 2.2995880000 -1.1105350000 1.8327230000
H 1.3612930000 -2.5728850000 1.5921590000
H 0.1824910000 1.9192400000 0.6908450000
H 3.2873440000 1.8370890000 0.5292270000
H 2.9158590000 1.6178190000 -1.6035990000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.170198 (Hartree/Particle)
Thermal correction to Energy= 0.184486
Thermal correction to Enthalpy= 0.185430
Thermal correction to Gibbs (Free) Energy= 0.127570
Sum of electronic and zero-point Energies= -747.511299
Sum of electronic and thermal Energies= -747.497012
Sum of electronic and thermal Enthalpies= -747.496067
Sum of electronic and thermal (Free) Energies= -747.553927

TS

C -1.0209240000 -1.6661920000 1.0533220000
C -2.0548790000 -1.7431090000 0.1805720000
H -1.2390500000 -1.7428600000 2.1132690000
O -1.8330810000 -1.6977150000 -1.1456040000
C -0.5354700000 0.6489670000 0.9170960000
C -0.1042820000 0.7391200000 -0.4530910000
C -1.1703630000 1.2695370000 -1.1726070000
C -2.3520110000 1.5734810000 -0.3211860000
O 1.0319860000 0.3642050000 -0.9553320000
H -1.1226920000 1.4671590000 -2.2385800000
B 2.2112550000 -0.0346410000 -0.0480450000
F 2.2429490000 0.8708230000 1.0189310000
F 3.3273600000 0.0127380000 -0.8320620000
F 1.9452830000 -1.3273480000 0.4358400000
H -2.7711250000 2.5702760000 -0.5088570000
H -3.1762500000 0.8617930000 -0.5053360000
H 0.1552470000 0.4292760000 1.7203160000
C -1.8119140000 1.3932120000 1.1143440000
H -2.5078240000 0.9049200000 1.8035230000
H -1.5724710000 2.3727850000 1.5555330000
H 0.0094460000 -1.7893620000 0.7267770000
H -3.0962450000 -1.7702120000 0.5012220000
H -2.6678340000 -1.7585020000 -1.6352210000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171309 (Hartree/Particle)
Thermal correction to Energy= 0.184211
Thermal correction to Enthalpy= 0.185156
Thermal correction to Gibbs (Free) Energy= 0.130966
Sum of electronic and zero-point Energies= -747.509749
Sum of electronic and thermal Energies= -747.496847
Sum of electronic and thermal Enthalpies= -747.495903
Sum of electronic and thermal (Free) Energies= -747.550093

PC

C 0.9426760000 1.1218370000 1.1619300000
C 1.8685110000 1.6730760000 0.2138320000
H 1.3003250000 1.2491750000 2.1849140000
O 1.4507150000 1.7618770000 -1.0245940000
C 0.6599300000 -0.4847040000 0.9155800000
C 0.1762090000 -0.7290490000 -0.4925110000
C 1.2513420000 -1.1363830000 -1.2592490000
C 2.4889650000 -1.2067050000 -0.4374950000
O -1.0273660000 -0.5190260000 -0.9243640000
H 1.1898580000 -1.3663250000 -2.3166790000
B -2.1763980000 -0.0281220000 -0.0269000000
F -2.2150480000 -0.8290690000 1.1144570000
F -3.3082800000 -0.1106600000 -0.7850460000
F -1.8739150000 1.3048720000 0.3321700000
H 3.1921510000 -1.9997810000 -0.7145110000
H 3.0776960000 -0.2510020000 -0.5064500000
H -0.0994050000 -0.7047680000 1.6645420000
C 1.9555810000 -1.2940940000 1.0031670000
H 2.6573380000 -0.9163930000 1.7565880000
H 1.7178790000 -2.3338400000 1.2516760000
H -0.0640800000 1.5408840000 1.0168150000
H 2.8913980000 1.9697580000 0.4399140000
H 2.1479490000 2.0599420000 -1.6364010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173920 (Hartree/Particle)
Thermal correction to Energy= 0.186217
Thermal correction to Enthalpy= 0.187161
Thermal correction to Gibbs (Free) Energy= 0.135039
Sum of electronic and zero-point Energies= -747.516068
Sum of electronic and thermal Energies= -747.503771
Sum of electronic and thermal Enthalpies= -747.502827
Sum of electronic and thermal (Free) Energies= -747.554950

Entry 7

RC

C 1.8973440000 -1.3693340000 1.2244170000
C 3.0123050000 -1.4606870000 0.4967660000
H 1.9807930000 -1.2047580000 2.2931550000
O 2.9898720000 -1.6182240000 -0.8680180000
C 1.1258610000 1.0274910000 -0.7582290000
C -0.2271460000 0.7322550000 -0.4928550000
C -0.7256960000 1.8261900000 0.2506030000
C 0.2873640000 2.8764430000 0.4758930000
O -0.8218640000 -0.3587030000 -0.8522060000
H -1.7471850000 1.8638450000 0.6117690000
B -2.0677960000 -0.8120040000 -0.0332220000
F -2.5084590000 -1.9595960000 -0.6221640000

F -3.0001000000 0.2296830000 -0.0839530000
F -1.5967740000 -0.9838280000 1.2682320000
H -0.0554060000 3.8543690000 0.1059890000
H 0.4658220000 3.0220520000 1.5526830000
H 1.7836100000 0.3402610000 -1.2838820000
C 1.5406000000 2.3514290000 -0.2505570000
H 2.4143610000 2.2619170000 0.4101060000
H 1.8595290000 3.0125550000 -1.0711660000
H 0.9031820000 -1.4963510000 0.8086330000
H 4.0044340000 -1.3795830000 0.9413180000
H 3.8699800000 -1.8779240000 -1.1759730000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169219 (Hartree/Particle)
Thermal correction to Energy= 0.184111
Thermal correction to Enthalpy= 0.185055
Thermal correction to Gibbs (Free) Energy= 0.123515
Sum of electronic and zero-point Energies= -747.509147
Sum of electronic and thermal Energies= -747.494255
Sum of electronic and thermal Enthalpies= -747.493311
Sum of electronic and thermal (Free) Energies= -747.554850

TS

C 1.5422210000 -0.8388940000 0.8873630000
C 2.7441770000 -1.3588620000 0.5066720000
H 1.5402960000 -0.1636480000 1.7361660000
O 2.8191970000 -2.3062300000 -0.4378240000
C 1.2358310000 0.6062180000 -0.7148410000
C -0.1923870000 0.7433060000 -0.5433360000
C -0.4252810000 1.9591320000 0.0786720000
C 0.8314220000 2.6981970000 0.3894040000
O -1.0115580000 -0.1955670000 -0.9229030000
H -1.4208880000 2.3205640000 0.3011350000
B -2.1715550000 -0.5997680000 0.0131770000
F -2.9380840000 -1.4860160000 -0.6931250000
F -2.8648890000 0.5512840000 0.3855510000
F -1.5517760000 -1.1846780000 1.1306280000
H 0.7934350000 3.7483660000 0.0707900000
H 1.0222980000 2.7230530000 1.4744820000
H 1.6297200000 -0.0752730000 -1.4621040000
C 1.9207840000 1.8937120000 -0.3609470000
H 2.8489260000 1.7612600000 0.2039020000
H 2.1953160000 2.4082640000 -1.2931080000
H 0.6059650000 -1.3470630000 0.6655190000
H 3.6904080000 -0.9763920000 0.8898080000
H 3.7433290000 -2.5280730000 -0.6320680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171515 (Hartree/Particle)
Thermal correction to Energy= 0.184577
Thermal correction to Enthalpy= 0.185521
Thermal correction to Gibbs (Free) Energy= 0.130213
Sum of electronic and zero-point Energies= -747.503827
Sum of electronic and thermal Energies= -747.490765
Sum of electronic and thermal Enthalpies= -747.489821
Sum of electronic and thermal (Free) Energies= -747.545128

PC

C 1.4077620000 -0.7483330000 0.6450470000
C 2.7028650000 -1.3132750000 0.5524560000
H 1.2416030000 -0.2507670000 1.5999300000
O 2.9722530000 -2.1673540000 -0.4128770000
C 1.2695200000 0.4024670000 -0.5722830000
C -0.1943590000 0.7229620000 -0.5417110000
C -0.3778100000 1.9748160000 -0.0200430000
C 0.9118580000 2.6294310000 0.3671740000
O -1.0367980000 -0.2005980000 -0.9105650000
H -1.3532160000 2.4317390000 0.0833010000
B -2.2160660000 -0.5636490000 0.0291210000
F -2.9956240000 -1.4454240000 -0.6717570000
F -2.8819060000 0.6030620000 0.3805320000
F -1.6072120000 -1.1538990000 1.1502220000
H 0.9852000000 3.6710840000 0.0280450000
H 1.0320920000 2.6634290000 1.4627950000
H 1.5844160000 -0.1313490000 -1.4722530000
C 1.9884050000 1.7277760000 -0.2956780000
H 2.8955460000 1.6242290000 0.3099770000
H 2.2906200000 2.1652570000 -1.2538010000
H 0.5807780000 -1.4286000000 0.4070190000
H 3.5366960000 -0.9890760000 1.1757030000
H 3.9161870000 -2.4028020000 -0.4395260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173484 (Hartree/Particle)
Thermal correction to Energy= 0.186513
Thermal correction to Enthalpy= 0.187457
Thermal correction to Gibbs (Free) Energy= 0.132392
Sum of electronic and zero-point Energies= -747.506504
Sum of electronic and thermal Energies= -747.493475
Sum of electronic and thermal Enthalpies= -747.492531
Sum of electronic and thermal (Free) Energies= -747.547597

Entry 8

RC

C -1.8537560000 1.9986090000 -1.0112100000
C -2.2615280000 1.8479550000 0.2544650000
H -2.5742750000 2.2599290000 -1.7779920000
O -1.3930580000 1.4900230000 1.2441610000
C -1.1992990000 -0.9434460000 -1.2733370000
C -0.0551240000 -0.6291050000 -0.5205200000
C -0.2822820000 -1.1537640000 0.7731740000
C -1.5472490000 -1.9125020000 0.8672540000
O 0.9526600000 0.0568990000 -0.9542510000
H 0.4134620000 -1.0164840000 1.5911560000
B 2.1988320000 0.1605690000 -0.0164610000
F 1.7802020000 0.8279400000 1.1332490000
F 3.1450400000 0.8336130000 -0.7324150000
F 2.5479880000 -1.1541930000 0.2926420000
H -1.3580920000 -2.9625460000 1.1377710000
H -2.1898140000 -1.5167530000 1.6663340000
H -1.3155940000 -0.6615660000 -2.3148510000
C -2.1820420000 -1.7668380000 -0.5308740000
H -3.1683020000 -1.2850200000 -0.4930880000
H -2.3425380000 -2.7350600000 -1.0283760000
H -0.8031270000 1.9308620000 -1.2744960000
H -3.3049090000 1.9610760000 0.5501620000
H -1.7991760000 1.6356720000 2.1114000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.169571 (Hartree/Particle)
Thermal correction to Energy= 0.184192
Thermal correction to Enthalpy= 0.185136
Thermal correction to Gibbs (Free) Energy= 0.125777
Sum of electronic and zero-point Energies= -747.508081
Sum of electronic and thermal Energies= -747.493460
Sum of electronic and thermal Enthalpies= -747.492516
Sum of electronic and thermal (Free) Energies= -747.551875

TS

C -1.8598580000 1.5840440000 -1.0172560000
C -2.0371130000 1.7210100000 0.3290130000
H -2.7234540000 1.6718990000 -1.6669130000
O -0.9702960000 1.7017960000 1.1245310000
C -1.3794900000 -0.5924220000 -1.1767920000
C -0.1278320000 -0.6106850000 -0.4737020000
C -0.3551620000 -1.2222130000 0.7579820000
C -1.7761990000 -1.6316550000 0.9340510000
O 0.9404100000 -0.0590000000 -0.9612190000
H 0.4296880000 -1.4058260000 1.4800740000
B 2.2032310000 0.0433000000 -0.0509530000
F 1.8394740000 0.8064050000 1.0560630000
F 3.1610890000 0.6339000000 -0.8295310000
F 2.5223350000 -1.2566220000 0.3376700000
H -1.8828440000 -2.6607620000 1.3008330000
H -2.2844890000 -0.9980560000 1.6829590000
H -1.4200480000 -0.4316790000 -2.2495150000
C -2.3992160000 -1.4258600000 -0.4647210000
H -3.4009600000 -0.9836540000 -0.4504450000
H -2.4917000000 -2.3892910000 -0.9862800000
H -0.8733510000 1.7683520000 -1.4341090000
H -3.0209210000 1.7404680000 0.7975350000
H -1.2058550000 1.7432270000 2.0648530000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.171251 (Hartree/Particle)

Thermal correction to Energy= 0.184237
Thermal correction to Enthalpy= 0.185181
Thermal correction to Gibbs (Free) Energy= 0.130639
Sum of electronic and zero-point Energies= -747.504083
Sum of electronic and thermal Energies= -747.491097
Sum of electronic and thermal Enthalpies= -747.490153
Sum of electronic and thermal (Free) Energies= -747.544696

PC

C 1.8955940000 1.1582540000 1.0433330000
C 1.9475380000 1.6306700000 -0.3244870000
H 2.8453090000 1.3025900000 1.5610980000
O 0.7847090000 1.6699330000 -0.9129720000
C 1.4599240000 -0.4198100000 1.1438770000
C 0.1608030000 -0.6114580000 0.4096760000
C 0.4335200000 -1.1259560000 -0.8486110000
C 1.8985360000 -1.2845360000 -1.0260770000
O -0.9374350000 -0.1917670000 0.9437020000
H -0.3223290000 -1.3508210000 -1.5878990000
B -2.2191490000 -0.0079500000 0.0579790000
F -1.9205130000 0.9998810000 -0.8568720000
F -3.2060000000 0.3406090000 0.9397260000
F -2.4505920000 -1.2156630000 -0.5881720000
H 2.2132530000 -2.1136750000 -1.6684930000
H 2.3376740000 -0.3588820000 -1.4972300000
H 1.3778020000 -0.5827810000 2.2210490000
C 2.4476270000 -1.3297300000 0.4109850000
H 3.4910990000 -1.0026020000 0.4935460000
H 2.3775100000 -2.3470680000 0.8096380000
H 1.0757380000 1.6652970000 1.5685500000
H 2.8492520000 1.8815550000 -0.8788070000
H 0.8049260000 1.8927710000 -1.8615020000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.173595 (Hartree/Particle)
Thermal correction to Energy= 0.185985
Thermal correction to Enthalpy= 0.186929
Thermal correction to Gibbs (Free) Energy= 0.134392
Sum of electronic and zero-point Energies= -747.511048
Sum of electronic and thermal Energies= -747.498658
Sum of electronic and thermal Enthalpies= -747.497714
Sum of electronic and thermal (Free) Energies= -747.550251

7b

SEE RT (*gauche*)

C 3.1973800000 0.2602400000 -0.0045080000
H 4.0546700000 -0.3993850000 0.0661690000
C 1.9672100000 -0.2495950000 -0.0574010000
O 0.8492800000 0.5219080000 -0.1676570000
Si -0.7549660000 0.0118560000 0.0051170000
C -1.7726220000 1.5155430000 -0.4712900000
H -2.8468490000 1.3125700000 -0.3830960000
H -1.5386150000 2.3688800000 0.1751240000
H -1.5712620000 1.8159520000 -1.5056740000
C -1.0915170000 -1.4393900000 -1.1530550000
H -0.4738700000 -2.3138110000 -0.9157690000
H -2.1402300000 -1.7542910000 -1.0826300000
H -0.8951220000 -1.1669430000 -2.1964880000
C -1.0648810000 -0.4904320000 1.7957110000
H -0.8669510000 0.3444120000 2.4778540000
H -2.1056970000 -0.8044430000 1.9439910000
H -0.4227120000 -1.3255850000 2.1002100000
H 3.3686580000 1.3314010000 -0.0358470000
H 1.7998430000 -1.3281940000 -0.0309740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.158694 (Hartree/Particle)
Thermal correction to Energy= 0.170038
Thermal correction to Enthalpy= 0.170982
Thermal correction to Gibbs (Free) Energy= 0.121148
Sum of electronic and zero-point Energies= -562.365329
Sum of electronic and thermal Energies= -562.353985
Sum of electronic and thermal Enthalpies= -562.353041
Sum of electronic and thermal (Free) Energies= -562.402875

SEE TS (*gauche*↔ *anti* ↔ *gauche*)

C 3.2017970000 0.2591040000 0.0000000000
H 4.0562730000 -0.4078660000 -0.0000020000
C 1.9663940000 -0.2407580000 0.0000030000
O 0.8508570000 0.5418850000 0.0000060000
Si -0.7561970000 0.0110190000 0.0000000000
C -1.7652690000 1.5938020000 0.0000150000
H -2.8408950000 1.3794170000 0.0000090000
H -1.5441330000 2.2010950000 0.8849100000
H -1.5441280000 2.2011150000 -0.8848660000
C -1.0833370000 -1.0141400000 -1.5490040000
H -0.4529090000 -1.9105170000 -1.5894520000
H -2.1281060000 -1.3473710000 -1.5848510000
H -0.8876540000 -0.4305430000 -2.4559830000
C -1.0833390000 -1.0141700000 1.5489830000
H -0.8876520000 -0.4305920000 2.4559740000
H -2.1281100000 -1.3473960000 1.5848250000
H -0.4529170000 -1.9105510000 1.5894120000
H 3.3795960000 1.3296620000 0.0000000000
H 1.7930650000 -1.3188300000 0.0000030000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.158628 (Hartree/Particle)
Thermal correction to Energy= 0.169085
Thermal correction to Enthalpy= 0.170029
Thermal correction to Gibbs (Free) Energy= 0.123131
Sum of electronic and zero-point Energies= -562.365392
Sum of electronic and thermal Energies= -562.354934
Sum of electronic and thermal Enthalpies= -562.353990
Sum of electronic and thermal (Free) Energies= -562.400889

SEE TS (*gauche* ↔ *syn* ↔ *gauche*)

C -2.7848280000 0.3472970000 -0.0386200000
H -3.7847610000 0.1436400000 0.3292280000
C -1.9497250000 -0.6637650000 -0.2818880000
O -0.6844230000 -0.5471210000 -0.7827830000
Si 0.6884940000 0.0272020000 0.0207040000
C 2.0849240000 -0.2626920000 -1.2022590000
H 3.0455400000 0.0751830000 -0.7946990000
H 2.1802230000 -1.3261950000 -1.4486250000
H 1.9084530000 0.2811470000 -2.1372500000
C 0.5158560000 1.8615210000 0.4214570000
H -0.3184080000 2.0490460000 1.1067780000
H 1.4282850000 2.2401940000 0.8995330000
H 0.3456440000 2.4531500000 -0.4856440000
C 0.9371400000 -0.9637510000 1.6057110000
H 1.0774410000 -2.0295570000 1.3907360000
H 1.8203240000 -0.6151110000 2.1552660000
H 0.0736840000 -0.8684060000 2.2746740000
H -2.5065810000 1.3818120000 -0.2126530000
H -2.2535820000 -1.7004300000 -0.1313400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.158764 (Hartree/Particle)
Thermal correction to Energy= 0.169148
Thermal correction to Enthalpy= 0.170092
Thermal correction to Gibbs (Free) Energy= 0.123493
Sum of electronic and zero-point Energies= -562.363662
Sum of electronic and thermal Energies= -562.353278
Sum of electronic and thermal Enthalpies= -562.352334
Sum of electronic and thermal (Free) Energies= -562.398933

Entry 24

RC

C -0.1235760000 0.9166960000 2.3137400000
C -0.8998610000 1.4492220000 1.3564140000
H 0.0378680000 1.4611460000 3.2389570000
O -1.1336030000 0.8567010000 0.1603990000
Si -2.4211470000 -0.2237960000 -0.2182480000
C -3.9764090000 0.8350540000 -0.3922550000
H -4.8365200000 0.2139890000 -0.6725550000
H -4.2329450000 1.3403240000 0.5469060000
H -3.8577140000 1.6031560000 -1.1657020000
C -2.6301410000 -1.4961180000 1.1425050000
H -1.7129260000 -2.0817470000 1.2480510000
H -2.8595800000 -1.0320760000 2.1084670000
H -3.4544510000 -2.1774790000 0.8964130000
C -1.9212040000 -0.9792820000 -1.8574430000

H -2.6668700000 -1.7148750000 -2.1834820000
H -1.8437510000 -0.2209470000 -2.6463460000
H -0.9568300000 -1.4897450000 -1.7664780000
C 2.1943200000 1.8052960000 0.6463060000
C 1.9934800000 0.6024030000 -0.0552360000
C 1.3521090000 0.9563510000 -1.2609830000
C 1.2008290000 2.4202110000 -1.4206930000
O 2.3447330000 -0.5596040000 0.4068290000
H 1.0470440000 0.2253050000 -1.9978950000
B 1.6755170000 -1.8799710000 0.0064860000
F 0.5099230000 -1.9745980000 0.7813980000
F 2.5747920000 -2.8694450000 0.2835320000
F 1.3384400000 -1.8248930000 -1.3577450000
H 1.6958350000 2.7734730000 -2.3374030000
H 0.1418930000 2.6899470000 -1.5270080000
H 2.6572630000 1.8404700000 1.6272790000
C 1.8216300000 3.0065560000 -0.1359850000
H 1.1297080000 3.6551130000 0.4159940000
H 2.7081990000 3.6250800000 -0.3446030000
H -1.3401210000 2.4444840000 1.4604960000
H 0.2978690000 -0.0773020000 2.2012240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.272875 (Hartree/Particle)
Thermal correction to Energy= 0.294536
Thermal correction to Enthalpy= 0.295480
Thermal correction to Gibbs (Free) Energy= 0.221647
Sum of electronic and zero-point Energies= -1156.137306
Sum of electronic and thermal Energies= -1156.115645
Sum of electronic and thermal Enthalpies= -1156.114701
Sum of electronic and thermal (Free) Energies= -1156.188534

TS

C 0.3026170000 1.2542360000 2.0662780000
C -0.6994120000 1.5729240000 1.1947480000
H 0.5256990000 1.9372150000 2.8797140000
O -1.0342580000 0.7794890000 0.1943840000
Si -2.4529100000 -0.1448460000 -0.1717090000
C -3.8688560000 1.0925560000 -0.3380460000
H -4.7973520000 0.5714630000 -0.6034890000
H -4.0587440000 1.6332170000 0.5972290000
H -3.6721040000 1.8319660000 -1.1233330000
C -2.7449820000 -1.3379210000 1.2418720000
H -1.8647680000 -1.9756530000 1.3623060000
H -2.9300970000 -0.8154260000 2.1880040000
H -3.6162580000 -1.9723290000 1.0366520000
C -2.0370430000 -0.9724690000 -1.7929660000
H -2.8101440000 -1.7029730000 -2.0610810000
H -1.9692580000 -0.2461940000 -2.6116320000
H -1.0791480000 -1.4970550000 -1.7120400000
C 2.1149130000 1.6504740000 0.6924890000
C 1.9931050000 0.4697700000 -0.1054260000
C 1.5051570000 0.8592490000 -1.3483870000
C 1.3398900000 2.3369720000 -1.4586730000
O 2.2846930000 -0.7069610000 0.3792790000
H 1.3069110000 0.1604570000 -2.1498630000
B 1.5018260000 -1.9715410000 0.0366200000
F 0.3493710000 -1.9437810000 0.8447840000
F 2.3146260000 -3.0319530000 0.3288150000
F 1.1303080000 -1.9366070000 -1.3187800000
H 1.8351670000 2.7446710000 -2.3502560000
H 0.2787630000 2.6112510000 -1.5502010000
H 2.6694300000 1.6518680000 1.6249560000
C 1.9465170000 2.8786520000 -0.1430350000
H 1.3480820000 3.6592370000 0.3366400000
H 2.9394060000 3.3168980000 -0.3232730000
H -1.1783390000 2.5573540000 1.2123190000
H 0.6407030000 0.2237730000 2.1323740000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.273781 (Hartree/Particle)
Thermal correction to Energy= 0.294291
Thermal correction to Enthalpy= 0.295235
Thermal correction to Gibbs (Free) Energy= 0.224017
Sum of electronic and zero-point Energies= -1156.134710
Sum of electronic and thermal Energies= -1156.114201
Sum of electronic and thermal Enthalpies= -1156.113257
Sum of electronic and thermal (Free) Energies= -1156.184475

PC

C 0.6679610000 -1.7381390000 -1.7930620000
C -0.6387830000 -1.6316110000 -1.1576710000
H 0.7375100000 -2.6346190000 -2.4133250000
O -0.9307180000 -0.5353320000 -0.5952000000
Si -2.3809060000 0.2038120000 0.1457690000
C -3.6162210000 -1.2096610000 0.3007020000
H -4.5362360000 -0.8333070000 0.7654260000
H -3.8997810000 -1.6357880000 -0.6689570000
H -3.2438500000 -2.0190120000 0.9399890000
C -2.8641960000 1.4906950000 -1.1164280000
H -2.0061120000 2.1508110000 -1.2752700000
H -3.1557960000 1.0462940000 -2.0746350000
H -3.7076710000 2.0889980000 -0.7508970000
C -1.8150370000 0.8831020000 1.7831530000
H -2.5928630000 1.5400510000 2.1933300000
H -1.6254350000 0.0893100000 2.5134240000
H -0.8979150000 1.4674130000 1.6528310000
C 1.8856940000 -1.7256530000 -0.7247350000
C 1.8036290000 -0.4743010000 0.1135560000
C 1.3574120000 -0.7901130000 1.3680080000
C 1.0730380000 -2.2576570000 1.4853830000
O 2.0763790000 0.6638050000 -0.4753360000
H 1.2039310000 -0.0688590000 2.1569940000
B 1.4749330000 2.0011740000 -0.0670500000
F 0.2069050000 2.0837620000 -0.6861120000
F 2.3244720000 2.9737170000 -0.5255690000
F 1.3026090000 2.0517620000 1.3252920000
H 1.3590840000 -2.6985980000 2.4481100000
H -0.0141260000 -2.4714270000 1.3740640000
H 2.7684610000 -1.7387320000 -1.3707370000
C 1.8382020000 -2.8715080000 0.2936820000
H 1.3834720000 -3.7898190000 -0.0972650000
H 2.8611320000 -3.1143770000 0.6004770000
H -1.3410490000 -2.4700970000 -1.0907730000
H 0.8439000000 -0.8293620000 -2.3820470000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.276531 (Hartree/Particle)
Thermal correction to Energy= 0.296630
Thermal correction to Enthalpy= 0.297575
Thermal correction to Gibbs (Free) Energy= 0.228471
Sum of electronic and zero-point Energies= -1156.148681
Sum of electronic and thermal Energies= -1156.128582
Sum of electronic and thermal Enthalpies= -1156.127637
Sum of electronic and thermal (Free) Energies= -1156.196741

Entry 25

RC

C 0.4934250000 1.5974810000 -2.0329260000
C 1.1101220000 1.8787970000 -0.8688110000
H 0.4141190000 2.3672730000 -2.7940750000
O 1.2636250000 1.0180610000 0.1539300000
Si 2.4025960000 -0.2828320000 0.2429470000
C 4.1055570000 0.5195240000 0.0946390000
H 4.8953840000 -0.2389770000 0.1619020000
H 4.2301720000 1.0354160000 -0.8650810000
H 4.2780420000 1.2488380000 0.8949320000
C 2.1277640000 -1.5115350000 -1.1457380000
H 1.1265100000 -1.9542810000 -1.1199090000
H 2.2802330000 -1.0525650000 -2.1296630000
H 2.8564260000 -2.3279820000 -1.0531030000
C 2.1333060000 -1.0134650000 1.9443530000
H 2.8921000000 -1.7775560000 2.1538760000
H 2.2048200000 -0.2499930000 2.7277910000
H 1.1497250000 -1.4881930000 1.9952530000
C -1.9766110000 1.8073960000 -0.7752130000
C -1.7861110000 0.5541040000 -0.1542350000
C -1.5953130000 0.8175900000 1.2143340000
C -1.6648460000 2.2615600000 1.5359560000
O -1.7571130000 -0.5621180000 -0.8166960000
H -1.4286670000 0.0377550000 1.9456170000
B -1.6685460000 -1.9478550000 -0.1451130000
F -0.8539820000 -1.8185490000 1.0015620000
F -1.0730420000 -2.7615580000 -1.0848000000
F -2.9426950000 -2.3325850000 0.2013570000
H -2.4047560000 2.4706340000 2.3216680000

H -0.7001170000 2.6099550000 1.9337880000
H -2.2150480000 1.9101160000 -1.8281550000
C -2.0095040000 2.9321200000 0.1903400000
H -1.3195380000 3.7390780000 -0.0849000000
H -3.0117100000 3.3873030000 0.2065020000
H 0.1378390000 0.5985560000 -2.2638200000
H 1.4694960000 2.8887980000 -0.6554630000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.273007 (Hartree/Particle)
Thermal correction to Energy= 0.294659
Thermal correction to Enthalpy= 0.295603
Thermal correction to Gibbs (Free) Energy= 0.221141
Sum of electronic and zero-point Energies= -1156.135861
Sum of electronic and thermal Energies= -1156.114209
Sum of electronic and thermal Enthalpies= -1156.113265
Sum of electronic and thermal (Free) Energies= -1156.187727

TS

C 0.4317120000 -1.7903580000 1.7916540000
C 1.1261250000 -1.9955670000 0.6359930000
H 0.3117390000 -2.6216680000 2.4787870000
O 1.4026540000 -1.0733940000 -0.2686330000
Si 2.3853430000 0.3711930000 -0.2011180000
C 4.1497020000 -0.2900990000 -0.1220680000
H 4.8689310000 0.5383440000 -0.1171370000
H 4.3235800000 -0.8789130000 0.7867010000
H 4.3796970000 -0.9244240000 -0.9857740000
C 1.9920410000 1.4051080000 1.3094610000
H 0.9747490000 1.8102550000 1.2916840000
H 2.1398980000 0.8489080000 2.2426150000
H 2.6848830000 2.2573110000 1.3326690000
C 2.0199720000 1.2277770000 -1.8184200000
H 2.6854880000 2.0905470000 -1.9464400000
H 2.1733920000 0.5580130000 -2.6723230000
H 0.9879630000 1.5907070000 -1.8270400000
C -1.7099570000 -1.8245450000 0.8395370000
C -1.6652980000 -0.5735550000 0.1503430000
C -1.6270080000 -0.8555230000 -1.2127530000
C -1.6330320000 -2.3178590000 -1.4936530000
O -1.6130780000 0.5507770000 0.8083950000
H -1.6118320000 -0.0893860000 -1.9760180000
B -1.7197060000 1.9340250000 0.1462200000
F -1.0831850000 1.8699880000 -1.1118360000
F -1.0429400000 2.7845250000 1.0014900000
F -3.0532560000 2.2412230000 0.0069860000
H -2.3925390000 -2.6005040000 -2.2347400000
H -0.6667660000 -2.6354530000 -1.9163460000
H -1.9986760000 -1.8877590000 1.8829640000
C -1.8850770000 -2.9617800000 -0.1121990000
H -1.2445840000 -3.8226820000 0.1059530000
H -2.9213630000 -3.3231470000 -0.0361020000
H 0.2220000000 -0.7886720000 2.1521640000
H 1.3898990000 -3.0105800000 0.3277150000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.274021 (Hartree/Particle)
Thermal correction to Energy= 0.294440
Thermal correction to Enthalpy= 0.295384
Thermal correction to Gibbs (Free) Energy= 0.224641
Sum of electronic and zero-point Energies= -1156.134234
Sum of electronic and thermal Energies= -1156.113816
Sum of electronic and thermal Enthalpies= -1156.112871
Sum of electronic and thermal (Free) Energies= -1156.183615

PC

C 0.1190060000 1.8786130000 -1.5251440000
C 1.0725570000 2.1377490000 -0.4613730000
H 0.1348390000 2.7130150000 -2.2330590000
O 1.7079470000 1.2783940000 0.2104230000
Si 2.3609080000 -0.4255600000 0.1593600000
C 4.1881250000 0.0071160000 0.2362470000
H 4.7808070000 -0.9152890000 0.2796000000
H 4.5179630000 0.5667880000 -0.6464270000
H 4.4266040000 0.5976570000 1.1272430000
C 1.9059400000 -1.2721570000 -1.4371070000
H 0.8699420000 -1.6269920000 -1.4398860000
H 2.0995820000 -0.6503200000 -2.3187940000
H 2.5524520000 -2.1565910000 -1.5262010000
C 1.7192890000 -1.1807770000 1.7302000000
H 2.2586930000 -2.1195330000 1.9135290000
H 1.8951310000 -0.5233330000 2.5888370000
H 0.6519460000 -1.4175690000 1.6603200000
C -1.3986330000 1.7915370000 -0.9429400000
C -1.5652200000 0.5548730000 -0.0999140000
C -1.7238010000 0.8924240000 1.2088180000
C -1.6512360000 2.3818570000 1.4042000000
O -1.4538620000 -0.5917790000 -0.7379940000
H -1.8524400000 0.1796710000 2.0107450000
B -1.6808880000 -1.9651110000 -0.1247000000
F -1.3281580000 -1.9293040000 1.2410490000
F -0.8125100000 -2.8068370000 -0.8234130000
F -3.0005460000 -2.3174080000 -0.2883240000
H -2.4053200000 2.7763270000 2.0971080000
H -0.6739550000 2.6912410000 1.8267250000
H -1.9759920000 1.7280860000 -1.8705410000
C -1.8321320000 2.9443540000 -0.0260220000
H -1.2955880000 3.8847400000 -0.2046800000
H -2.8937710000 3.1425210000 -0.2062130000
H 0.2915130000 0.9228230000 -2.0238430000
H 1.2042100000 3.1656260000 -0.1070240000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.276921 (Hartree/Particle)
Thermal correction to Energy= 0.297101
Thermal correction to Enthalpy= 0.298045
Thermal correction to Gibbs (Free) Energy= 0.228261
Sum of electronic and zero-point Energies= -1156.144329
Sum of electronic and thermal Energies= -1156.124149
Sum of electronic and thermal Enthalpies= -1156.123205
Sum of electronic and thermal (Free) Energies= -1156.192989

Entry 26

RC

C 0.6281700000 -1.0062300000 -1.4508280000
C 0.7213150000 -0.8055970000 -0.1247250000
O 1.7704640000 -0.2744870000 0.5493820000
Si 3.4393510000 -0.3029240000 0.2059360000
C 3.8448920000 0.9160350000 -1.1779730000
H 4.9313590000 0.9850390000 -1.3161830000
H 3.4117580000 0.6224520000 -2.1406380000
H 3.4833240000 1.9240430000 -0.9402940000
C 3.9526660000 -2.0529170000 -0.2532740000
H 3.7616920000 -2.7464170000 0.5735620000
H 3.4084170000 -2.4236910000 -1.1282190000
H 5.0244990000 -2.0940920000 -0.4829840000
C 4.2263410000 0.2577330000 1.8157140000
H 5.3193120000 0.2898840000 1.7302540000
H 3.8853110000 1.2598200000 2.1000860000
H 3.9738010000 -0.4248150000 2.6346940000
C -1.0657430000 1.4830330000 -1.2800600000
C -2.0747110000 0.8489320000 -0.5252550000
C -2.1899130000 1.5800480000 0.6718220000
C -1.2078040000 2.6818930000 0.7676700000
O -2.7103630000 -0.2167270000 -0.9047670000
H -2.9260780000 1.3428220000 1.4309400000
B -3.3584630000 -1.0746930000 0.2140140000
F -2.3233710000 -1.3289280000 1.1313480000
F -3.8299940000 -2.1992850000 -0.3958850000
F -4.3485950000 -0.3022060000 0.8180080000
H -1.7002710000 3.6523720000 0.9280990000
H -0.5469260000 2.5414860000 1.6365540000
H -0.8182760000 1.1942640000 -2.2950350000
C -0.4464210000 2.6244010000 -0.5720350000
H 0.6321270000 2.4543250000 -0.4383130000
H -0.5336800000 3.5557180000 -1.1504300000
H -0.2773430000 -1.4547590000 -1.8437470000
H 1.4307330000 -0.7765460000 -2.1454000000
H -0.1142630000 -1.0479970000 0.5293790000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.272075 (Hartree/Particle)
Thermal correction to Energy= 0.294341
Thermal correction to Enthalpy= 0.295285
Thermal correction to Gibbs (Free) Energy= 0.216413
Sum of electronic and zero-point Energies= -1156.130781

Sum of electronic and thermal Energies= -1156.108515
Sum of electronic and thermal Enthalpies= -1156.107570
Sum of electronic and thermal (Free) Energies= -1156.186443

TS

C -0.2793270000 -0.6948910000 1.0047160000
C -0.6633430000 -0.6303240000 -0.3060820000
O -1.8509830000 -0.2765310000 -0.7799760000
Si -3.4418270000 -0.3630680000 -0.1100800000
C -3.6488590000 0.9461220000 1.2276570000
H -4.6912980000 0.9616070000 1.5703200000
H -3.0212270000 0.7621040000 2.1064090000
H -3.4171790000 1.9486040000 0.8493240000
C -3.6962630000 -2.0999080000 0.5573170000
H -3.5751250000 -2.8471490000 -0.2349420000
H -2.9906990000 -2.3462890000 1.3578850000
H -4.7095820000 -2.2069600000 0.9634760000
C -4.5285420000 0.0060290000 -1.5901630000
H -5.5892930000 -0.0171580000 -1.3128240000
H -4.3137400000 0.9972920000 -2.0049030000
H -4.3736490000 -0.7302700000 -2.3863430000
C 0.8522450000 1.2556660000 1.1711960000
C 2.0806490000 0.9232300000 0.4979700000
C 2.1998740000 1.7545950000 -0.5982830000
C 1.0177470000 2.6460570000 -0.7757720000
O 2.8488200000 -0.0501570000 0.9202830000
H 3.0506380000 1.7253760000 -1.2669800000
B 3.3815820000 -1.0244840000 -0.1443170000
F 2.2302170000 -1.5789290000 -0.7519000000
F 4.1166360000 -1.9641130000 0.5259650000
F 4.1221740000 -0.3110060000 -1.0830670000
H 1.2970030000 3.7008610000 -0.9024740000
H 0.4540070000 2.3755060000 -1.6827900000
H 0.7173520000 1.0459200000 2.2270120000
C 0.1859330000 2.4218760000 0.5099440000
H -0.8802230000 2.2562540000 0.3197160000
H 0.2472190000 3.2935430000 1.1768320000
H 0.6630250000 -1.1894080000 1.2159610000
H -0.9949970000 -0.5753790000 1.8126160000
H 0.0808180000 -0.8198480000 -1.0780430000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.273544 (Hartree/Particle)
Thermal correction to Energy= 0.294366
Thermal correction to Enthalpy= 0.295310
Thermal correction to Gibbs (Free) Energy= 0.221882
Sum of electronic and zero-point Energies= -1156.126952
Sum of electronic and thermal Energies= -1156.106130
Sum of electronic and thermal Enthalpies= -1156.105186
Sum of electronic and thermal (Free) Energies= -1156.178614

PC

C -0.4177360000 1.1401880000 -1.3515120000
C 0.5205760000 0.7127190000 -0.2329350000
O 1.8213650000 0.7439350000 -0.6787730000
Si 3.1553840000 0.0764690000 0.1437240000
C 4.6246560000 1.0466460000 -0.5150980000
H 5.5662850000 0.6714580000 -0.0959370000
H 4.6907970000 0.9654460000 -1.6061420000
H 4.5460630000 2.1105570000 -0.2640900000
C 3.3105610000 -1.7484220000 -0.2832170000
H 2.4215760000 -2.3034630000 0.0337870000
H 3.4238800000 -1.8890940000 -1.3644850000
H 4.1848480000 -2.1967240000 0.2052150000
C 2.9410730000 0.3254940000 2.0007220000
H 3.8049330000 -0.0786180000 2.5428190000
H 2.8570390000 1.3871870000 2.2622750000
H 2.0483320000 -0.1883780000 2.3747400000
C -1.8934790000 1.3767600000 -0.9706270000
C -2.5813710000 0.2314270000 -0.2603650000
C -3.3537310000 0.6091180000 0.7596360000
C -3.3296000000 2.1088660000 0.9241950000
O -2.4213200000 -1.0301810000 -0.7849120000
H -3.9633270000 -0.0559930000 1.3613670000
B -2.0135400000 -2.0980880000 -0.0555660000
F 0.1981930000 -0.6154160000 0.1626290000
F -1.7098660000 -3.2136620000 -0.7033410000
F -1.9742840000 -2.1018440000 1.2704140000
H -4.2853510000 2.5506670000 0.6046460000
H -3.1794200000 2.4231240000 1.9647270000
H -2.4207120000 1.5556520000 -1.9210270000
C -2.1589140000 2.5582180000 0.0037250000
H -1.2688620000 2.7428060000 0.6156510000
H -2.3753060000 3.4890570000 -0.5293840000
H -0.3486590000 0.3739830000 -2.1319180000
H -0.0081620000 2.0637130000 -1.7770920000
H 0.3994160000 1.3006790000 0.6855550000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.279068 (Hartree/Particle)
Thermal correction to Energy= 0.299551
Thermal correction to Enthalpy= 0.300495
Thermal correction to Gibbs (Free) Energy= 0.227379
Sum of electronic and zero-point Energies= -1156.181091
Sum of electronic and thermal Energies= -1156.160608
Sum of electronic and thermal Enthalpies= -1156.159664
Sum of electronic and thermal (Free) Energies= -1156.232780

8a

ENL RT (*anti*)

C -1.2185480000 0.7895040000 0.0000000000
H -1.1407350000 1.8697650000 0.0000000000
C -0.1206680000 0.0289200000 0.0000000000
C 1.2887640000 0.5511660000 0.0000000000
H 1.8379990000 0.2016970000 0.8858200000
H 1.8380000000 0.2016970000 -0.8858200000
H 1.3071280000 1.6433360000 0.0000000000
O -0.2460500000 -1.3420830000 0.0000000000
H 0.6360350000 -1.7414250000 0.0000010000
H -2.2073170000 0.3440560000 0.0000010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.084562 (Hartree/Particle)
Thermal correction to Energy= 0.089658
Thermal correction to Enthalpy= 0.090602
Thermal correction to Gibbs (Free) Energy= 0.057462
Sum of electronic and zero-point Energies= -193.040374
Sum of electronic and thermal Energies= -193.035278
Sum of electronic and thermal Enthalpies= -193.034333
Sum of electronic and thermal (Free) Energies= -193.067473

ENL TS (*anti* ↔ *syn*)

C 0.9861890000 -1.0468670000 0.0085280000
H 0.6760670000 -2.0859290000 0.0460540000
C 0.0886060000 -0.0610030000 -0.0066100000
C -1.4033690000 -0.2351320000 0.0071600000
H -1.8469960000 0.2640420000 0.8793280000
H -1.8445110000 0.2315930000 -0.8820820000
H -1.6879960000 -1.2909500000 0.0292410000
O 0.4945040000 1.2699830000 -0.1097620000
H 0.6689530000 1.6139500000 0.7797030000
H 2.0498920000 -0.8345620000 -0.0286170000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.083768 (Hartree/Particle)
Thermal correction to Energy= 0.088304
Thermal correction to Enthalpy= 0.089249
Thermal correction to Gibbs (Free) Energy= 0.057132
Sum of electronic and zero-point Energies= -193.035370
Sum of electronic and thermal Energies= -193.030834
Sum of electronic and thermal Enthalpies= -193.029890
Sum of electronic and thermal (Free) Energies= -193.062006

ENL RT (*syn*)

C -0.9907900000 1.0339320000 0.0000000000
H -0.6809450000 2.0717880000 0.0000000000
C -0.0848330000 0.0490180000 0.0000000000
C 1.4026510000 0.2384500000 0.0000000000
H 1.8479960000 -0.2371390000 0.8821210000
H 1.8479960000 -0.2371400000 -0.8821200000
H 1.6638060000 1.2990410000 -0.0000010000
O -0.4015620000 -1.2857330000 0.0000000000
H -1.3684080000 -1.3740860000 -0.0000020000
H -2.0601220000 0.8349990000 0.0000000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.085011 (Hartree/Particle)
Thermal correction to Energy= 0.089839
Thermal correction to Enthalpy= 0.090783
Thermal correction to Gibbs (Free) Energy= 0.058206
Sum of electronic and zero-point Energies= -193.043523
Sum of electronic and thermal Energies= -193.038695
Sum of electronic and thermal Enthalpies= -193.037750
Sum of electronic and thermal (Free) Energies= -193.070328

Entry 9

RC

C 1.3478530000 -1.6262260000 -1.0480970000
C 2.0570350000 -1.4230420000 0.0842740000
O 3.3997090000 -1.1717580000 0.0937670000
C 1.4716180000 -1.4120600000 1.4591920000
H 1.8992460000 -2.2307310000 2.0509910000
H 1.7295380000 -0.4803250000 1.9787100000
H 0.3868250000 -1.5207290000 1.4161810000
C 0.8468230000 1.0676560000 -1.2087590000
C -0.3905910000 0.9968190000 -0.5182550000
C -0.2441390000 1.7713030000 0.6401740000
C 1.0961770000 2.4015010000 0.7464750000
O -1.4074570000 0.3218700000 -0.9651040000
H -1.0425950000 1.9005300000 1.3601010000
B -2.3586720000 -0.4076350000 0.0053280000
F -1.6252600000 -1.5078170000 0.4877920000
F -3.4432690000 -0.7831390000 -0.7342870000
F -2.6784290000 0.4591920000 1.0519880000
H 1.0138740000 3.4991050000 0.7542630000
H 1.6011090000 2.1416410000 1.6869780000
H 0.9715270000 0.6927500000 -2.2176570000
C 1.8492030000 1.9039610000 -0.5078190000
H 2.7467320000 1.3196480000 -0.2537190000
H 2.1986550000 2.7257950000 -1.1492750000
H 0.2857260000 -1.8322840000 -0.9881390000
H 1.8322660000 -1.6888550000 -2.0209170000
H 3.7511790000 -1.2828640000 -0.8060100000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198891 (Hartree/Particle)
Thermal correction to Energy= 0.214247
Thermal correction to Enthalpy= 0.215191
Thermal correction to Gibbs (Free) Energy= 0.155240
Sum of electronic and zero-point Energies= -786.811604
Sum of electronic and thermal Energies= -786.796249
Sum of electronic and thermal Enthalpies= -786.795304
Sum of electronic and thermal (Free) Energies= -786.855255

TS

C 1.2768480000 -1.3853070000 -1.1374590000
C 1.9173350000 -1.4483130000 0.0661380000
O 3.2634090000 -1.3620390000 0.1833340000
C 1.2201930000 -1.5098460000 1.3808610000
H 1.7147950000 -2.2340210000 2.0365770000
H 1.2757420000 -0.5298390000 1.8777340000
H 0.1665270000 -1.7578760000 1.2486470000
C 0.9222920000 0.9736320000 -1.1784490000
C -0.3181700000 1.0244100000 -0.4636360000
C -0.1011380000 1.7643560000 0.6920470000
C 1.2901230000 2.2939730000 0.7869830000
O -1.3909090000 0.4445650000 -0.9264830000
H -0.8816450000 1.9686890000 1.4134290000
B -2.3505470000 -0.3234090000 -0.0055050000
F -1.7176680000 -1.5627910000 0.2392210000
F -3.5195010000 -0.4710210000 -0.6983780000
F -2.4998610000 0.3841270000 1.1865370000
H 1.2923500000 3.3940230000 0.8041030000
H 1.7967210000 1.9863330000 1.7116110000
H 0.9522840000 0.7500970000 -2.2385620000
C 1.9863200000 1.7643750000 -0.4923930000
H 2.8761600000 1.1629650000 -0.2636300000
H 2.3311430000 2.5790180000 -1.1440080000
H 0.2076960000 -1.5631780000 -1.1767910000
H 1.8404490000 -1.4317110000 -2.0674080000
H 3.6709710000 -1.3841820000 -0.6999550000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199414 (Hartree/Particle)
Thermal correction to Energy= 0.213838
Thermal correction to Enthalpy= 0.214783
Thermal correction to Gibbs (Free) Energy= 0.156763
Sum of electronic and zero-point Energies= -786.810570
Sum of electronic and thermal Energies= -786.796146
Sum of electronic and thermal Enthalpies= -786.795202
Sum of electronic and thermal (Free) Energies= -786.853222

PC

C 1.1385480000 -0.8631960000 -1.1868470000
C 1.5579090000 -1.4591040000 0.0798250000
O 2.7753000000 -1.9258860000 0.2292440000
C 0.7009620000 -1.5038310000 1.2522520000
H 1.1792830000 -1.9752650000 2.1107740000
H 0.3800390000 -0.4596520000 1.4725480000
H -0.2667380000 -1.9517920000 0.9797210000
C 1.0417430000 0.7495540000 -1.1432680000
C -0.1746990000 1.1527150000 -0.3466200000
C 0.1874910000 1.8116870000 0.7852950000
C 1.6783720000 1.9981640000 0.8859220000
O -1.3534990000 0.7823500000 -0.8039440000
H -0.5182270000 2.1698190000 1.5246760000
B -2.2542690000 -0.1611630000 -0.0352430000
F -1.7657380000 -1.4831240000 -0.3200940000
F -3.5289840000 -0.0032390000 -0.4997360000
F -2.1216000000 0.0681550000 1.3336260000
H 1.9644870000 3.0415510000 1.0725430000
H 2.1125000000 1.4212300000 1.7187710000
H 0.9144440000 0.9853270000 -2.2049420000
C 2.2140480000 1.5109350000 -0.4931570000
H 3.1314360000 0.9159730000 -0.4025870000
H 2.4661670000 2.3724120000 -1.1191690000
H 0.1112420000 -1.1832740000 -1.4051570000
H 1.8182530000 -1.1530830000 -1.9974430000
H 3.2847080000 -1.8468030000 -0.6004850000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.202555 (Hartree/Particle)
Thermal correction to Energy= 0.216134
Thermal correction to Enthalpy= 0.217078
Thermal correction to Gibbs (Free) Energy= 0.162235
Sum of electronic and zero-point Energies= -786.825690
Sum of electronic and thermal Energies= -786.812112
Sum of electronic and thermal Enthalpies= -786.811168
Sum of electronic and thermal (Free) Energies= -786.866011

Entry 10

RC

C 1.8274020000 0.0890970000 1.1404270000
C 2.6053750000 -0.5848200000 0.2614080000
H 0.8676630000 -0.3126470000 1.4415350000
O 3.8504420000 -0.1624060000 -0.1004900000
C 2.2319720000 -1.8501170000 -0.4448870000
H 2.3294210000 -1.7161420000 -1.5290230000
H 2.9304250000 -2.6460240000 -0.1579680000
H 1.2100990000 -2.1581590000 -0.2239330000
C 0.4254530000 1.5810600000 -0.7935300000
C -0.6995410000 0.7600000000 -0.5568480000
C -1.6520630000 1.5549220000 0.0961280000
C -1.1694020000 2.9310440000 0.3551140000
O -0.7566440000 -0.5004720000 -0.8652660000
H -2.6310970000 1.1822240000 0.3751900000
B -1.6352820000 -1.3961560000 0.0396030000
F -1.3168040000 -1.0304200000 1.3606250000
F -1.2595340000 -2.6824100000 -0.2541130000
F -2.9659200000 -1.1115790000 -0.2295550000
H -1.8556940000 3.6906890000 -0.0459920000
H -1.1137510000 3.1287740000 1.4368990000
H 1.2769540000 1.2670100000 -1.3848700000
C 0.2192420000 2.9718650000 -0.3191760000
H 1.0213400000 3.2973770000 0.3561070000
H 0.2422570000 3.6752180000 -1.1654710000
H 2.2058640000 0.9641770000 1.6674830000
H 4.0922380000 0.6126680000 0.4336400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.198608 (Hartree/Particle)
Thermal correction to Energy= 0.214160
Thermal correction to Enthalpy= 0.215104
Thermal correction to Gibbs (Free) Energy= 0.154255
Sum of electronic and zero-point Energies= -786.810334
Sum of electronic and thermal Energies= -786.794782
Sum of electronic and thermal Enthalpies= -786.793838
Sum of electronic and thermal (Free) Energies= -786.854687

TS

C 1.7018150000 -0.0768780000 1.0448380000
C 2.3501060000 -0.9909940000 0.2630920000
H 0.7125430000 -0.3097100000 1.4212370000
O 3.6343010000 -0.8272920000 -0.1312530000
C 1.7473840000 -2.2314630000 -0.3096020000
H 1.8510100000 -2.2229930000 -1.4013960000
H 2.3043250000 -3.1030370000 0.0568660000
H 0.6908470000 -2.3314380000 -0.0634730000
C 0.8127710000 1.3364630000 -0.7255500000
C -0.5207020000 0.8533940000 -0.5734650000
C -1.2673900000 1.8595420000 0.0249770000
C -0.4561330000 3.0641380000 0.3455110000
O -0.8628280000 -0.3643240000 -0.8936630000
H -2.3241450000 1.7538710000 0.2412450000
B -1.8748760000 -1.0643200000 0.0342470000
F -1.4370660000 -0.8059690000 1.3500500000
F -1.7838060000 -2.4004270000 -0.2796270000
F -3.1287240000 -0.5135800000 -0.1743590000
H -0.8991980000 3.9874450000 -0.0530070000
H -0.3874830000 3.2138270000 1.4341880000
H 1.5270500000 0.8787860000 -1.3990490000
C 0.9210600000 2.7612210000 -0.2900130000
H 1.7659000000 2.9430860000 0.3841490000
H 1.0992770000 3.3952160000 -1.1713600000
H 2.2582280000 0.7268430000 1.5245000000
H 4.0171390000 -0.0501250000 0.3108880000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.199266 (Hartree/Particle)
Thermal correction to Energy= 0.213766
Thermal correction to Enthalpy= 0.214710
Thermal correction to Gibbs (Free) Energy= 0.156709
Sum of electronic and zero-point Energies= -786.809371
Sum of electronic and thermal Energies= -786.794871
Sum of electronic and thermal Enthalpies= -786.793927
Sum of electronic and thermal (Free) Energies= -786.851928

PC

C 1.2524980000 -1.7555110000 0.4280290000
C -0.2232920000 -1.5638630000 -0.0192990000
H 1.3221230000 -1.6347940000 1.5150810000
O -0.5226410000 -2.1959280000 -1.2235200000
C -1.2699590000 -1.9927030000 0.9889400000
H -2.2674260000 -1.8354640000 0.5745760000
H -1.1427020000 -3.0576560000 1.2059150000
H -1.1687650000 -1.4196680000 1.9128600000
C 1.9835240000 -0.6057980000 -0.2764800000
C 0.9296500000 0.4618790000 -0.2171840000
C 1.3969910000 1.7005110000 -0.0650450000
C 2.9147570000 1.6330370000 0.0102870000
O -0.3312820000 -0.0815170000 -0.2233720000
H 0.8155000000 2.6102530000 0.0016660000
B -2.0845590000 1.0916790000 0.0231550000
F -2.0979800000 1.0804290000 1.3554060000
F -2.9034020000 0.2737120000 -0.6330760000
F -1.5985690000 2.1623680000 -0.6034380000
H 3.3876540000 1.9371300000 -0.9363820000
H 3.3231360000 2.2932170000 0.7850090000
H 2.1905120000 -0.8838060000 -1.3246630000
C 3.1982770000 0.1291240000 0.3234270000
H 3.2097990000 -0.0166190000 1.4104400000
H 4.1577380000 -0.2187010000 -0.0716520000
H 1.5921090000 -2.7613550000 0.1672460000
H 0.1393850000 -1.9400130000 -1.8868010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.203694 (Hartree/Particle)
Thermal correction to Energy= 0.217825
Thermal correction to Enthalpy= 0.218769
Thermal correction to Gibbs (Free) Energy= 0.161508
Sum of electronic and zero-point Energies= -786.857974
Sum of electronic and thermal Energies= -786.843842
Sum of electronic and thermal Enthalpies= -786.842898
Sum of electronic and thermal (Free) Energies= -786.900159

Entry 11

RC

C -1.8343400000 -1.3862570000 1.2448860000
C -2.3096680000 -1.2570880000 -0.0071150000
H -2.5194080000 -1.4244860000 2.0838860000
O -1.4163690000 -1.1909660000 -1.0392510000
C -3.7623080000 -1.1371230000 -0.3744580000
H -3.9645180000 -0.1949380000 -0.9026660000
H -4.0635580000 -1.9559350000 -1.0426990000
H -4.3998510000 -1.1785580000 0.5113870000
C -0.6475900000 1.2551050000 1.2726720000
C 0.4089330000 0.7322470000 0.5019370000
C 0.2718690000 1.2925950000 -0.7856870000
C -0.8345900000 2.2714980000 -0.8691550000
O 1.2736570000 -0.1301950000 0.9309560000
H 0.9272920000 1.0389510000 -1.6090980000
B 2.4412140000 -0.5137370000 -0.0328270000
F 1.8561750000 -1.0843450000 -1.1621940000
F 3.2334580000 -1.3735720000 0.6715730000
F 3.0664480000 0.6861460000 -0.3701850000
H -0.4591250000 3.2697630000 -1.1412810000
H -1.5481640000 2.0036480000 -1.6609590000
H -0.7802830000 1.0265800000 2.3245540000
C -1.4671180000 2.2487370000 0.5382520000
H -2.5289040000 1.9686320000 0.5176480000
H -1.4297810000 3.2303800000 1.0339910000
H -0.7765000000 -1.5452090000 1.4234810000
H -1.8774340000 -1.2731970000 -1.8884870000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.197788 (Hartree/Particle)
Thermal correction to Energy= 0.213780
Thermal correction to Enthalpy= 0.214725
Thermal correction to Gibbs (Free) Energy= 0.151813
Sum of electronic and zero-point Energies= -786.802792
Sum of electronic and thermal Energies= -786.786800
Sum of electronic and thermal Enthalpies= -786.785856
Sum of electronic and thermal (Free) Energies= -786.848767

TS

C -1.7090990000 -1.1048230000 1.3161480000
C -2.0850710000 -1.3043850000 0.0187200000
H -2.4726630000 -1.0169460000 2.0803170000
O -1.1027830000 -1.4910830000 -0.8748800000
C -3.4966450000 -1.2608730000 -0.4892450000
H -3.6152250000 -0.5041220000 -1.2760720000
H -3.7740550000 -2.2308700000 -0.9233870000
H -4.2013370000 -1.0377300000 0.3142960000
C -0.8739250000 1.0589790000 1.2065330000
C 0.3103310000 0.7677030000 0.4574860000
C 0.1745340000 1.3790060000 -0.7869380000
C -1.1040270000 2.1308490000 -0.9235630000
O 1.2555930000 0.0122370000 0.9286300000
H 0.9478720000 1.3527050000 -1.5436770000
B 2.4294520000 -0.3771590000 -0.0193560000
F 1.8655340000 -1.0484910000 -1.1022350000
F 3.2594440000 -1.1609030000 0.7359720000
F 3.0169220000 0.8150250000 -0.4397030000
H -0.9344710000 3.1793560000 -1.2071730000
H -1.7390470000 1.7144890000 -1.7204450000
H -0.9025550000 0.9643280000 2.2864840000
C -1.7589550000 2.0162990000 0.4734160000
H -2.8090050000 1.7041440000 0.4442360000
H -1.7477330000 2.9854330000 0.9927880000
H -0.6965560000 -1.3563810000 1.6164780000
H -1.4449290000 -1.5850490000 -1.7787010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.

Zero-point correction= 0.198982 (Hartree/Particle)
Thermal correction to Energy= 0.213672
Thermal correction to Enthalpy= 0.214616
Thermal correction to Gibbs (Free) Energy= 0.155793
Sum of electronic and zero-point Energies= -786.800603
Sum of electronic and thermal Energies= -786.785913
Sum of electronic and thermal Enthalpies= -786.784969
Sum of electronic and thermal (Free) Energies= -786.843792

PC

C 1.6340150000 -0.6028150000 -1.3244200000
C 1.9154950000 -1.2305820000 -0.0422440000
H 2.5160740000 -0.5865680000 -1.9675500000
O 0.8408450000 -1.4268620000 0.6628940000
C 3.2648630000 -1.6045710000 0.4688080000
H 3.2897580000 -1.6718710000 1.5618060000
H 3.5495920000 -2.5882180000 0.0647490000
H 4.0217390000 -0.8900750000 0.1334470000
C 1.0354320000 0.9008790000 -1.1655690000
C -0.2426930000 0.8340910000 -0.3716760000
C -0.0435920000 1.3710700000 0.8761720000
C 1.3718080000 1.8278440000 1.0531020000
O -1.2553180000 0.2093660000 -0.8996970000
H -0.8133710000 1.4318650000 1.6331810000
B -2.4207620000 -0.2907620000 -0.0018080000
F -1.8904940000 -1.2681700000 0.8457290000
F -3.3491490000 -0.7995350000 -0.8753080000
F -2.8918360000 0.7933050000 0.7317100000
H 1.4727100000 2.7878940000 1.5747550000
H 1.9559880000 1.1044070000 1.6609090000
H 0.8672520000 1.1881970000 -2.2075480000
C 1.9267140000 1.8800590000 -0.3891300000
H 2.9974410000 1.6509150000 -0.4568050000
H 1.7858440000 2.8853900000 -0.7993840000
H 0.8002610000 -1.1303360000 -1.8066430000
H 0.9873610000 -1.7740760000 1.5631290000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.201840 (Hartree/Particle)
Thermal correction to Energy= 0.216018
Thermal correction to Enthalpy= 0.216962
Thermal correction to Gibbs (Free) Energy= 0.159942
Sum of electronic and zero-point Energies= -786.810119
Sum of electronic and thermal Energies= -786.795941
Sum of electronic and thermal Enthalpies= -786.794997
Sum of electronic and thermal (Free) Energies= -786.852017

8b

SEE RT (*syn*)

C 1.9557180000 1.3450510000 0.0000000000
H 2.9566370000 1.7604830000 -0.0000020000
C 1.7829460000 0.0167480000 0.0000010000
C 2.9126260000 -0.9748910000 0.0000000000
H 2.8488790000 -1.6245120000 0.8815760000
H 2.8488770000 -1.6245140000 -0.8815730000
H 3.8838070000 -0.4736740000 -0.0000010000
O 0.5735610000 -0.6220280000 0.0000030000
Si -1.0171310000 -0.0424620000 0.0000000000
C -2.0527710000 -1.6113430000 0.0000010000
H -3.1247070000 -1.3785300000 0.0000000000
H -1.8431710000 -2.2229150000 -0.8848890000
H -1.8431730000 -2.2229130000 0.8848920000
C -1.3518280000 0.9673900000 1.5574740000
H -0.7212820000 1.8603210000 1.6217870000
H -2.3985980000 1.2953840000 1.5858860000
H -1.1679620000 0.3676950000 2.4566100000
C -1.3518230000 0.9673850000 -1.5574780000
H -1.1679560000 0.3676880000 -2.4566120000
H -2.3985920000 1.2953810000 -1.5858930000
H -0.7212760000 1.8603150000 -1.6217930000
H 1.1306490000 2.0484360000 0.0000010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.187184 (Hartree/Particle)
Thermal correction to Energy= 0.199750
Thermal correction to Enthalpy= 0.200695
Thermal correction to Gibbs (Free) Energy= 0.148482
Sum of electronic and zero-point Energies= -601.658838
Sum of electronic and thermal Energies= -601.646272
Sum of electronic and thermal Enthalpies= -601.645327
Sum of electronic and thermal (Free) Energies= -601.697540

SEE TS (*syn* ↔ *anti* ↔ *syn*)

C 2.8522330000 1.0962450000 -0.0002710000
H 3.8800330000 0.7529810000 -0.0002480000
C 1.8417080000 0.2202680000 -0.0000830000
C 2.0337850000 -1.2729860000 0.0001700000
H 1.5758440000 -1.7335410000 0.8846290000
H 1.5757790000 -1.7338490000 -0.8840960000
H 3.0974110000 -1.5244040000 0.0001740000
O 0.5554620000 0.6884280000 -0.0001150000
Si -0.9966320000 0.0376130000 0.0000210000
C -2.1049470000 1.5557900000 -0.0001960000
H -3.1652320000 1.2746840000 -0.0001240000
H -1.9221430000 2.1766170000 0.8841360000
H -1.9221870000 2.1763320000 -0.8847360000
C -1.3084310000 -0.9947770000 -1.5499710000
H -0.7328070000 -1.9271270000 -1.5608770000
H -2.3700340000 -1.2655940000 -1.6168800000
H -1.0537070000 -0.4326940000 -2.4560570000
C -1.3083630000 -0.9942890000 1.5503500000
H -1.0536000000 -0.4319210000 2.4562480000
H -2.3699630000 -1.2650860000 1.6173910000
H -0.7327380000 -1.9266350000 1.5615240000
H 2.6665850000 2.1647200000 -0.0004490000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.187189 (Hartree/Particle)
Thermal correction to Energy= 0.198776
Thermal correction to Enthalpy= 0.199720
Thermal correction to Gibbs (Free) Energy= 0.150698
Sum of electronic and zero-point Energies= -601.655673
Sum of electronic and thermal Energies= -601.644086
Sum of electronic and thermal Enthalpies= -601.643142
Sum of electronic and thermal (Free) Energies= -601.692164

Entry 27

RC

C 0.3609580000 0.9794430000 -2.0229240000
C 1.2734420000 1.2417060000 -1.0597340000
H 0.3165800000 1.6025420000 -2.9104190000
O 1.3495960000 0.4894600000 0.0646270000
Si 2.1589430000 -1.0040190000 0.3433780000
C 2.2198420000 2.4118260000 -1.0917590000
H 2.1070880000 3.0268400000 -0.1897390000
H 3.2595340000 2.0611880000 -1.0990650000
H 2.0595280000 3.0392440000 -1.9725890000
C 3.9433180000 -0.5697510000 0.7920780000
H 3.9886240000 0.1159620000 1.6463890000
H 4.5000820000 -1.4751020000 1.0656640000
H 4.4774390000 -0.1015390000 -0.0438010000
C 2.1144570000 -2.0755360000 -1.1951000000
H 1.0844580000 -2.3545060000 -1.4314430000
H 2.5489540000 -1.5689700000 -2.0647760000
H 2.6923410000 -2.9927450000 -1.0240170000
C 1.2739090000 -1.7613640000 1.8093700000
H 1.7287830000 -2.7248630000 2.0714970000
H 1.3418740000 -1.1169020000 2.6945310000
H 0.2172620000 -1.9359860000 1.5829070000
C -1.6196650000 2.1780970000 -0.4890150000
C -1.9194990000 0.9275370000 0.0985540000
C -1.4695050000 0.9934710000 1.4257170000
C -0.9170940000 2.3235720000 1.7804700000
O -2.4992440000 -0.0363290000 -0.5559660000
H -1.5516720000 0.1622600000 2.1136720000
B -2.2493920000 -1.5186730000 -0.2692350000
F -1.0437580000 -1.8378350000 -0.9183140000
F -3.3161320000 -2.2026330000 -0.7785240000
F -2.1001390000 -1.7015630000 1.1161010000
H -1.4477160000 2.7612650000 2.6388100000
H 0.1343030000 2.2425900000 2.0851490000
H -1.9081680000 2.4337580000 -1.5023910000
C -1.0878390000 3.1555830000 0.4913320000
H -0.1572410000 3.6254200000 0.1507550000

H -1.8035940000 3.9813570000 0.6262370000
H -0.2631960000 0.0935330000 -1.9750790000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.301284 (Hartree/Particle)
Thermal correction to Energy= 0.324235
Thermal correction to Enthalpy= 0.325179
Thermal correction to Gibbs (Free) Energy= 0.248813
Sum of electronic and zero-point Energies= -1195.430866
Sum of electronic and thermal Energies= -1195.407915
Sum of electronic and thermal Enthalpies= -1195.406971
Sum of electronic and thermal (Free) Energies= -1195.483337

TS

C 0.2199060000 1.1108890000 -1.8602490000
C 1.2291600000 1.3198540000 -0.9633010000
H 0.1417020000 1.7587620000 -2.7271110000
O 1.4015480000 0.5177050000 0.0912260000
Si 2.1843080000 -1.0097980000 0.3109130000
C 2.1517310000 2.5069310000 -1.0120820000
H 2.1308210000 3.0496830000 -0.0593340000
H 3.1862850000 2.1694440000 -1.1551080000
H 1.8951110000 3.1922600000 -1.8237790000
C 3.9683080000 -0.5919420000 0.7695930000
H 4.0153930000 0.0550440000 1.6533100000
H 4.5272280000 -1.5076720000 1.0008540000
H 4.4977870000 -0.0863250000 -0.0472130000
C 2.1311970000 -1.9921940000 -1.2847110000
H 1.1016000000 -2.2646050000 -1.5286920000
H 2.5606410000 -1.4366500000 -2.1269930000
H 2.7154750000 -2.9137910000 -1.1674460000
C 1.2944250000 -1.8105880000 1.7461500000
H 1.7249070000 -2.7986100000 1.9528260000
H 1.3952480000 -1.2116440000 2.6593900000
H 0.2299980000 -1.9420340000 1.5282490000
C -1.5514160000 2.0905480000 -0.5504790000
C -1.9366080000 0.8831950000 0.1075360000
C -1.5716700000 1.0040380000 1.4432680000
C -0.9781280000 2.3338780000 1.7595610000
O -2.5159370000 -0.0926200000 -0.5409560000
H -1.7401610000 0.2226830000 2.1725000000
B -2.2074180000 -1.5564860000 -0.2632800000
F -0.9759210000 -1.8178180000 -0.9053690000
F -3.2306710000 -2.2914050000 -0.7929410000
F -2.0575580000 -1.7508630000 1.1191660000
H -1.5095810000 2.8298980000 2.5840700000
H 0.0653280000 2.2380710000 2.0863890000
H -1.9099370000 2.3427810000 -1.5417950000
C -1.1028700000 3.1197450000 0.4328200000
H -0.1870130000 3.6411350000 0.1366680000
H -1.8793890000 3.8963080000 0.5058260000
H -0.3364180000 0.1788180000 -1.8574920000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.301800 (Hartree/Particle)
Thermal correction to Energy= 0.323799
Thermal correction to Enthalpy= 0.324743
Thermal correction to Gibbs (Free) Energy= 0.250743
Sum of electronic and zero-point Energies= -1195.430058
Sum of electronic and thermal Energies= -1195.408059
Sum of electronic and thermal Enthalpies= -1195.407115
Sum of electronic and thermal (Free) Energies= -1195.481115

PC

C -0.3189330000 1.6687460000 -1.6190240000
C 0.9858560000 1.3492050000 -1.0212870000
H -0.2112990000 2.4790030000 -2.3451370000
O 1.0728420000 0.2660310000 -0.3724200000
Si 2.1336660000 -0.9988570000 0.3049880000
C 2.1579670000 2.2707400000 -1.1711660000
H 2.9084400000 2.1161060000 -0.3952360000
H 2.6272310000 2.0836940000 -2.1486160000
H 1.8261260000 3.3128580000 -1.1754860000
C 3.8022650000 -0.2143800000 0.6997740000
H 3.7200420000 0.6132440000 1.4139080000
H 4.4335840000 -0.9787610000 1.1718740000
H 4.3384300000 0.1389320000 -0.1879480000
C 2.2354200000 -2.2346560000 -1.0908710000
H 1.2204360000 -2.5513740000 -1.3469630000
H 2.7194650000 -1.8189280000 -1.9821530000
H 2.8139630000 -3.1114790000 -0.7744980000
C 1.2492800000 -1.5748560000 1.8342140000
H 1.7543990000 -2.4658680000 2.2296340000
H 1.2574620000 -0.8106110000 2.6192030000
H 0.2094070000 -1.8323640000 1.6054350000
C -1.4522020000 2.0575700000 -0.5535170000
C -1.8319280000 0.8243330000 0.2288530000
C -1.4496240000 0.9408380000 1.5259930000
C -0.7762500000 2.2604080000 1.7950390000
O -2.4045470000 -0.1481680000 -0.4545690000
H -1.5966140000 0.1713580000 2.2714680000
B -2.0605050000 -1.6021520000 -0.2762810000
F -0.8315520000 -1.8136240000 -0.9613160000
F -3.0719500000 -2.3392810000 -0.8375860000
F -1.8748510000 -1.9038620000 1.0848120000
H -1.1445310000 2.7615050000 2.7002240000
H 0.3130350000 2.1474020000 1.9461120000
H -2.2726500000 2.3891170000 -1.1989580000
C -1.0831690000 3.0955730000 0.5227110000
H -0.2646270000 3.7663630000 0.2339720000
H -1.9570810000 3.7291430000 0.7062810000
H -0.7173020000 0.7622900000 -2.0931340000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.304820 (Hartree/Particle)
Thermal correction to Energy= 0.326641
Thermal correction to Enthalpy= 0.327585
Thermal correction to Gibbs (Free) Energy= 0.253564
Sum of electronic and zero-point Energies= -1195.445545
Sum of electronic and thermal Energies= -1195.423725
Sum of electronic and thermal Enthalpies= -1195.422781
Sum of electronic and thermal (Free) Energies= -1195.496801

Entry 28

RC

C -0.3898040000 -1.1024000000 0.5664060000
C -0.8894790000 -0.6174030000 -0.5960610000
O -2.1026860000 -0.0185630000 -0.7123480000
Si -3.5807520000 -0.2900180000 0.1041490000
C -0.1229500000 -0.6422510000 -1.8835020000
H -0.6537150000 -1.2614020000 -2.6180100000
H -0.0662980000 0.3670320000 -2.3113240000
H 0.8835740000 -1.0378050000 -1.7366300000
C -3.5277370000 0.4599210000 1.8344190000
H -4.5246170000 0.4172800000 2.2912320000
H -2.8408020000 -0.0667370000 2.5060330000
H -3.2291470000 1.5146910000 1.8049980000
C -3.9145880000 -2.1393020000 0.1652440000
H -4.0005310000 -2.5580440000 -0.8439320000
H -3.1182790000 -2.6832810000 0.6843160000
H -4.8553470000 -2.3435710000 0.6910310000
C -4.8317880000 0.6169000000 -0.9614440000
H -5.8417510000 0.5277660000 -0.5432910000
H -4.5955940000 1.6846330000 -1.0349260000
H -4.8528680000 0.2091970000 -1.9781510000
C 0.7750740000 1.2574140000 1.1161680000
C 2.0398930000 0.9051540000 0.5742840000
C 2.2858480000 1.7942340000 -0.4777190000
C 1.1970990000 2.7887970000 -0.6589250000
O 2.7572900000 -0.0722630000 1.0458650000
H 3.1901770000 1.7585930000 -1.0721140000
B 3.6173800000 -0.9389580000 0.1064170000
F 2.7016470000 -1.7137980000 -0.6298790000
F 4.4169730000 -1.6981200000 0.9135200000
F 4.3367200000 -0.0979810000 -0.7451340000
H 1.5726970000 3.8135290000 -0.5166560000
H 0.7854010000 2.7684450000 -1.6773150000
H 0.4086360000 0.8519950000 2.0513140000
C 0.1598090000 2.4154680000 0.4244730000
H -0.8194510000 2.1511930000 -0.0007520000
H -0.0309630000 3.2373780000 1.1296160000
H 0.5836690000 -1.5792230000 0.5691190000
H -0.9743310000 -1.1201050000 1.4805040000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.300820 (Hartree/Particle)

Thermal correction to Energy= 0.324131
Thermal correction to Enthalpy= 0.325075
Thermal correction to Gibbs (Free) Energy= 0.245756
Sum of electronic and zero-point Energies= -1195.427262
Sum of electronic and thermal Energies= -1195.403950
Sum of electronic and thermal Enthalpies= -1195.403006
Sum of electronic and thermal (Free) Energies= -1195.482325

TS

C -0.3295900000 -0.9271810000 0.6125720000
C -0.8607390000 -0.6012300000 -0.6033320000
O -2.0983710000 -0.1006860000 -0.7711750000
Si -3.5610860000 -0.3075780000 0.1066460000
C -0.0775670000 -0.6966250000 -1.8747940000
H -0.5812700000 -1.3910030000 -2.5594890000
H -0.0556360000 0.2773650000 -2.3796910000
H 0.9398750000 -1.0449540000 -1.6896970000
C -3.5011470000 0.6640930000 1.7206450000
H -4.4887990000 0.6491460000 2.1987380000
H -2.7863370000 0.2524910000 2.4415880000
H -3.2402680000 1.7148270000 1.5476600000
C -3.8228730000 -2.1440200000 0.4084600000
H -3.8884830000 -2.6939080000 -0.5372420000
H -3.0121530000 -2.5877410000 0.9961160000
H -4.7590450000 -2.3114290000 0.9551100000
C -4.8485360000 0.4115920000 -1.0516210000
H -5.8509760000 0.3470310000 -0.6115330000
H -4.6470260000 1.4670230000 -1.2670810000
H -4.8659630000 -0.1266820000 -2.0056450000
C 0.7139830000 1.1868100000 1.0872680000
C 2.0147500000 0.9120970000 0.5556270000
C 2.2382120000 1.8118030000 -0.4784190000
C 1.1018830000 2.7549820000 -0.6805290000
O 2.7639480000 -0.0394210000 1.0428810000
H 3.1582280000 1.8324240000 -1.0482360000
B 3.6168650000 -0.9106740000 0.1106550000
F 2.6961700000 -1.7201190000 -0.5906510000
F 4.4413270000 -1.6461020000 0.9170500000
F 4.3084210000 -0.0871890000 -0.7775630000
H 1.4243330000 3.7997950000 -0.5604380000
H 0.6864530000 2.6919060000 -1.6957450000
H 0.4252750000 0.8568050000 2.0779270000
C 0.0815840000 2.3587720000 0.4151800000
H -0.9110930000 2.1241540000 0.0106130000
H -0.0717290000 3.1676410000 1.1435820000
H 0.6408080000 -1.4101120000 0.6503330000
H -0.9429440000 -0.9403260000 1.5072890000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.301336 (Hartree/Particle)
Thermal correction to Energy= 0.323677
Thermal correction to Enthalpy= 0.324621
Thermal correction to Gibbs (Free) Energy= 0.248151
Sum of electronic and zero-point Energies= -1195.426576
Sum of electronic and thermal Energies= -1195.404235
Sum of electronic and thermal Enthalpies= -1195.403291
Sum of electronic and thermal (Free) Energies= -1195.479761

PC

C 0.1684740000 -0.1738680000 -0.8474260000
C 0.6618760000 -0.3844280000 0.5233530000
O 1.9220560000 -0.3657300000 0.8149410000
Si 3.4514540000 -0.3846740000 -0.0675540000
C -0.2700000000 -0.6088480000 1.6289260000
H 0.2394280000 -0.7148210000 2.5868430000
H -1.0240160000 0.2035520000 1.6398100000
H -0.9071630000 -1.4731280000 1.3792920000
C 3.6133640000 1.1928650000 -1.0687390000
H 4.6183920000 1.2359460000 -1.5077940000
H 2.8929750000 1.2587770000 -1.8900290000
H 3.4937470000 2.0819870000 -0.4399090000
C 3.4567340000 -1.9454080000 -1.1063700000
H 3.2572510000 -2.8305690000 -0.4920800000
H 2.7203780000 -1.9235390000 -1.9162940000
H 4.4452170000 -2.0785550000 -1.5636090000
C 4.6752450000 -0.4508450000 1.3442610000
H 5.7033960000 -0.4760510000 0.9635570000
H 4.5818990000 0.4262910000 1.9940410000
H 4.5244520000 -1.3440190000 1.9601430000
C -0.6585240000 1.1816400000 -1.0626710000
C -2.0425190000 1.0331090000 -0.4736950000
C -2.2570270000 1.9396270000 0.5112250000
C -1.0849220000 2.8638210000 0.7080620000
O -2.7994810000 0.0631000000 -0.9523310000
H -3.1722740000 1.9955020000 1.0876390000
B -3.3037130000 -1.0722300000 -0.0920430000
F -2.2338800000 -2.0313870000 -0.0401190000
F -4.4033900000 -1.6112280000 -0.7038130000
F -3.5506810000 -0.6186720000 1.2021380000
H -1.3679010000 3.9234780000 0.6453150000
H -0.6209550000 2.7418040000 1.7000080000
H -0.7154070000 1.2367290000 -2.1557820000
C -0.1000990000 2.4823150000 -0.4400330000
H 0.9310760000 2.3825940000 -0.0825010000
H -0.0875810000 3.2698680000 -1.1999170000
H -0.5684600000 -0.9617370000 -1.0622210000
H 0.9891040000 -0.2147810000 -1.5666320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.304431 (Hartree/Particle)
Thermal correction to Energy= 0.326118
Thermal correction to Enthalpy= 0.327062
Thermal correction to Gibbs (Free) Energy= 0.253007
Sum of electronic and zero-point Energies= -1195.444642
Sum of electronic and thermal Energies= -1195.422954
Sum of electronic and thermal Enthalpies= -1195.422010
Sum of electronic and thermal (Free) Energies= -1195.496066

Entry 29

RC

C 0.4175130000 -0.2710150000 0.8626350000
C 1.0074280000 -1.0432440000 -0.0832020000
H -0.5626640000 -0.5374630000 1.2398820000
O 2.2551530000 -0.8207950000 -0.5704560000
Si 3.6314760000 -0.0664170000 0.0893240000
C 0.3458070000 -2.2170610000 -0.7421760000
H 0.3582900000 -2.0868750000 -1.8313710000
H 0.9205790000 -3.1270090000 -0.5269250000
H -0.6876000000 -2.3491450000 -0.4204580000
C 3.9628610000 -0.7610650000 1.8061600000
H 4.1614080000 -1.8379830000 1.7614520000
H 4.8400210000 -0.2796060000 2.2558190000
H 3.1147550000 -0.6083470000 2.4820980000
C 3.4006080000 1.8077640000 0.1424790000
H 3.0779510000 2.1942850000 -0.8317310000
H 2.6677120000 2.1228720000 0.8938890000
H 4.3508180000 2.2978850000 0.3894590000
C 4.9934200000 -0.5137970000 -1.1217950000
H 5.9538600000 -0.0833250000 -0.8133220000
H 5.1188550000 -1.6001360000 -1.1888680000
H 4.7682690000 -0.1421680000 -2.1279010000
C -0.8544600000 1.4039550000 -0.9248100000
C -2.0925360000 0.8190690000 -0.5705310000
C -2.7965350000 1.7744670000 0.1725770000
C -2.0252830000 3.0236480000 0.3766630000
O -2.4261130000 -0.4014690000 -0.8677540000
H -3.7960020000 1.5976340000 0.5532720000
B -3.3568240000 -1.1303030000 0.1280770000
F -2.8277690000 -0.8701620000 1.4059040000
F -3.2791670000 -2.4571040000 -0.2113670000
F -4.6276610000 -0.5838230000 0.0149090000
H -2.5854640000 3.9130550000 0.0543970000
H -1.8129630000 3.1818670000 1.4455410000
H -0.1523410000 0.9424000000 -1.6079770000
C -0.7372050000 2.8042010000 -0.4468860000
H 0.1845670000 2.9670440000 0.1260180000
H -0.6791450000 3.4951740000 -1.3018290000
H 0.9518940000 0.5375670000 1.3516090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.300613 (Hartree/Particle)
Thermal correction to Energy= 0.324037
Thermal correction to Enthalpy= 0.324981
Thermal correction to Gibbs (Free) Energy= 0.245357
Sum of electronic and zero-point Energies= -1195.425987
Sum of electronic and thermal Energies= -1195.402563

Sum of electronic and thermal Enthalpies= -1195.401619
Sum of electronic and thermal (Free) Energies= -1195.481243

TS

C 0.3397500000 -0.1435970000 0.8095730000
C 0.9381600000 -1.0134600000 -0.0588260000
H -0.6238060000 -0.4037210000 1.2322470000
O 2.1846190000 -0.8444480000 -0.5414940000
Si 3.5941880000 -0.1020010000 0.0829570000
C 0.2580600000 -2.2166610000 -0.6366250000
H 0.2742690000 -2.1574000000 -1.7320340000
H 0.8244610000 -3.1159170000 -0.3619340000
H -0.7772520000 -2.3138040000 -0.3105780000
C 3.8816320000 -0.7256430000 1.8334560000
H 4.0279910000 -1.8116670000 1.8451200000
H 4.7795290000 -0.2648720000 2.2633340000
H 3.0404690000 -0.4965520000 2.4966050000
C 3.4294770000 1.7766950000 0.0372150000
H 3.1066930000 2.1248790000 -0.9510210000
H 2.7214310000 2.1581700000 0.7814170000
H 4.4012340000 2.2419260000 0.2455290000
C 4.9322290000 -0.6711030000 -1.1010140000
H 5.9100870000 -0.2652370000 -0.8149230000
H 5.0119810000 -1.7636970000 -1.1098380000
H 4.7215360000 -0.3440120000 -2.1254850000
C -0.7371610000 1.3127630000 -0.8674320000
C -2.0474750000 0.8320260000 -0.5775670000
C -2.7166780000 1.8311300000 0.1187670000
C -1.8661280000 3.0249920000 0.3685660000
O -2.4352230000 -0.3748390000 -0.8853650000
H -3.7439560000 1.7269120000 0.4480090000
B -3.3662640000 -1.0827570000 0.1174580000
F -2.7972660000 -0.8723950000 1.3899190000
F -3.3403090000 -2.4090780000 -0.2430030000
F -4.6224410000 -0.4989620000 0.0485630000
H -2.3459210000 3.9583930000 0.0425930000
H -1.6722360000 3.1513580000 1.4451810000
H -0.0941570000 0.8537900000 -1.6077790000
C -0.5722130000 2.7279330000 -0.4242790000
H 0.3471700000 2.8936240000 0.1482390000
H -0.4930650000 3.3763820000 -1.3099240000
H 0.9032890000 0.6610000000 1.2711320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.301053 (Hartree/Particle)
Thermal correction to Energy= 0.323498
Thermal correction to Enthalpy= 0.324442
Thermal correction to Gibbs (Free) Energy= 0.247513
Sum of electronic and zero-point Energies= -1195.425384
Sum of electronic and thermal Energies= -1195.402939
Sum of electronic and thermal Enthalpies= -1195.401995
Sum of electronic and thermal (Free) Energies= -1195.478924

PC

C -0.9808280000 1.4402860000 1.5383010000
C 0.1010640000 0.4017700000 1.1645310000
H -1.6508190000 1.0162690000 2.2946880000
O 1.1427190000 1.0427630000 0.5554260000
Si 2.4804950000 0.6333250000 -0.4247080000
C 0.5074120000 -0.5237450000 2.2975270000
H 1.2616770000 -1.2407710000 1.9769290000
H 0.9229910000 0.0964560000 3.0984690000
H -0.3570550000 -1.0709520000 2.6778140000
C 3.3979640000 2.2737860000 -0.5159040000
H 3.7188170000 2.6079920000 0.4774320000
H 4.2934800000 2.1856790000 -1.1432560000
H 2.7663530000 3.0597840000 -0.9452120000
C 1.8901510000 0.1065470000 -2.1298780000
H 1.3393420000 -0.8376340000 -2.0973130000
H 1.2385070000 0.8662470000 -2.5769260000
H 2.7497850000 -0.0276970000 -2.7990360000
C 3.5729010000 -0.6800290000 0.3669650000
H 4.4971910000 -0.7845680000 -0.2160790000
H 3.8599140000 -0.4110710000 1.3901850000
H 3.0802990000 -1.6560640000 0.3865130000
C -1.7327760000 1.6638180000 0.2222330000
C -1.7576980000 0.2738570000 -0.3344080000
C -2.8615700000 -0.0531720000 -1.0013170000
C -3.7942220000 1.1483800000 -0.9861130000
O -0.6416890000 -0.4423500000 0.0790900000
H -3.0794260000 -0.9995090000 -1.4755620000
B -0.5462580000 -2.1666690000 -0.1160360000
F -1.2752720000 -2.6494900000 0.9188500000
F 0.8003290000 -2.3769590000 -0.0344780000
F -1.0775180000 -2.3341000000 -1.3515220000
H -3.7822440000 1.6836600000 -1.9477250000
H -4.8366330000 0.8604530000 -0.8049030000
H -1.1359330000 2.3249020000 -0.4227220000
C -3.2275050000 2.0387070000 0.1648270000
H -3.7118130000 1.7579790000 1.1080750000
H -3.4005470000 3.1072220000 0.0046370000
H -0.4949810000 2.3288130000 1.9477080000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.306781 (Hartree/Particle)
Thermal correction to Energy= 0.327922
Thermal correction to Enthalpy= 0.328866
Thermal correction to Gibbs (Free) Energy= 0.257471
Sum of electronic and zero-point Energies= -1195.477832
Sum of electronic and thermal Energies= -1195.456691
Sum of electronic and thermal Enthalpies= -1195.455747
Sum of electronic and thermal (Free) Energies= -1195.527142

9a

ENL RT (*anti*)

C 0.7159010000 -0.6922280000 0.0000000000
H 0.6567940000 -1.7776290000 -0.0000010000
C -0.4416810000 -0.0200920000 0.0000000000
C 2.0806120000 -0.0663360000 0.0000000000
H 2.6612740000 -0.3725240000 0.8812970000
H 2.6612730000 -0.3725220000 -0.8812990000
H 2.0165980000 1.0247170000 0.0000010000
C -1.8021760000 -0.6571530000 0.0000000000
H -2.3810240000 -0.3569800000 0.8856680000
H -2.3810240000 -0.3569800000 -0.8856680000
H -1.7287190000 -1.7473580000 0.0000010000
O -0.4341260000 1.3617500000 0.0000010000
H -1.3480980000 1.6801260000 -0.0000040000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.112798 (Hartree/Particle)
Thermal correction to Energy= 0.119601
Thermal correction to Enthalpy= 0.120545
Thermal correction to Gibbs (Free) Energy= 0.082711
Sum of electronic and zero-point Energies= -232.330146
Sum of electronic and thermal Energies= -232.323344
Sum of electronic and thermal Enthalpies= -232.322400
Sum of electronic and thermal (Free) Energies= -232.360234

ENL TS (*anti* ↔ *syn*)

C 0.6897240000 -0.7078140000 0.0222770000
H 0.6198070000 -1.7933720000 0.0632340000
C -0.4574030000 -0.0205060000 -0.0018710000
C 2.0647750000 -0.1076820000 -0.0094170000
H 2.6218280000 -0.3260910000 0.9126250000
H 2.6559210000 -0.5207580000 -0.8374260000
H 2.0149890000 0.9769800000 -0.1352170000
C -1.8321430000 -0.6256210000 0.0004070000
H -2.4116030000 -0.2846770000 0.8696130000
H -2.3875360000 -0.3102680000 -0.8917960000
H -1.7919870000 -1.7188620000 0.0198310000
O -0.4652340000 1.3740110000 -0.1064450000
H -0.3892590000 1.7547040000 0.7823250000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.112175 (Hartree/Particle)
Thermal correction to Energy= 0.118226
Thermal correction to Enthalpy= 0.119170
Thermal correction to Gibbs (Free) Energy= 0.083246
Sum of electronic and zero-point Energies= -232.326082
Sum of electronic and thermal Energies= -232.320032
Sum of electronic and thermal Enthalpies= -232.319088
Sum of electronic and thermal (Free) Energies= -232.355012

ENL RT (*syn*)

C 0.6867800000 -0.6891720000 0.0000000000
H 0.6098610000 -1.7729820000 0.0000010000
C -0.4668240000 -0.0034090000 0.0000000000
C 2.0794340000 -0.1205130000 0.0000000000
H 2.6470990000 -0.4464860000 0.8820360000
H 2.6471040000 -0.4465010000 -0.8820280000
H 2.1054180000 0.9774870000 -0.0000100000
C -1.8296030000 -0.6296210000 0.0000000000
H -2.3988190000 -0.3106830000 0.8818950000
H -2.3988180000 -0.3106840000 -0.8818960000
H -1.7618090000 -1.7201960000 0.0000000000
O -0.5731930000 1.3667190000 0.0000000000
H 0.3167810000 1.7525780000 0.0000010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.113148 (Hartree/Particle)
Thermal correction to Energy= 0.119710
Thermal correction to Enthalpy= 0.120654
Thermal correction to Gibbs (Free) Energy= 0.083161
Sum of electronic and zero-point Energies= -232.331836
Sum of electronic and thermal Energies= -232.325273
Sum of electronic and thermal Enthalpies= -232.324329
Sum of electronic and thermal (Free) Energies= -232.361822

Entry 12

RC

C 1.5667760000 -1.4188080000 0.2946950000
C 2.7687260000 -0.9054760000 -0.0576370000
H 1.0555940000 -2.0315350000 -0.4416160000
O 3.5373010000 -0.1317630000 0.7708560000
C 0.9143750000 -1.3108950000 1.6417980000
H 1.3121270000 -0.4926670000 2.2595660000
H -0.1653860000 -1.1538340000 1.5405700000
H 1.0461130000 -2.2403050000 2.2130690000
C 3.4355260000 -1.0964870000 -1.3852770000
H 3.6705240000 -0.1298440000 -1.8488890000
H 4.3875920000 -1.6249920000 -1.2566050000
H 2.8033350000 -1.6740710000 -2.0636770000
C 0.6661770000 0.9507190000 -1.0207580000
C -0.6308460000 0.6913080000 -0.5172530000
C -0.8947920000 1.6866480000 0.4366160000
C 0.2310990000 2.6382670000 0.5977500000
O -1.3589490000 -0.3123400000 -0.9029940000
H -1.8358050000 1.7600500000 0.9674670000
B -2.6772970000 -0.5906980000 -0.1408890000
F -2.3084660000 -0.8216750000 1.1956950000
F -3.2356130000 -1.6826990000 -0.7402540000
F -3.4563980000 0.5604910000 -0.2237370000
H -0.0815890000 3.6676870000 0.3664160000
H 0.5873050000 2.6719730000 1.6380220000
H 1.0731130000 0.4308250000 -1.8799070000
C 1.3009770000 2.1327660000 -0.3941700000
H 2.2495540000 1.8612410000 0.0952430000
H 1.5653960000 2.8871530000 -1.1493650000
H 3.1479790000 -0.1386720000 1.6613310000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227067 (Hartree/Particle)
Thermal correction to Energy= 0.244043
Thermal correction to Enthalpy= 0.244987
Thermal correction to Gibbs (Free) Energy= 0.181420
Sum of electronic and zero-point Energies= -826.101290
Sum of electronic and thermal Energies= -826.084314
Sum of electronic and thermal Enthalpies= -826.083370
Sum of electronic and thermal (Free) Energies= -826.146937

TS

C 1.4030270000 -1.0481800000 0.3275710000
C 2.7303870000 -0.9224750000 -0.0083120000
H 0.7905070000 -1.6869300000 -0.3023310000
O 3.6239100000 -0.3131500000 0.7949790000
C 0.8769640000 -0.7801910000 1.7155390000
H 1.2220410000 0.1777790000 2.1312300000
H -0.2166030000 -0.7630500000 1.7062840000
H 1.1879160000 -1.5779160000 2.4040120000
C 3.3399400000 -1.3599620000 -1.2993500000
H 3.7891400000 -0.5066620000 -1.8228680000
H 4.1472850000 -2.0753260000 -1.1035580000
H 2.5993040000 -1.8338970000 -1.9463060000
C 0.7694380000 0.6913100000 -0.9382360000
C -0.6171700000 0.6439930000 -0.5454130000
C -0.8927290000 1.7901350000 0.1791710000
C 0.2948860000 2.6796190000 0.3332210000
O -1.3612100000 -0.3835460000 -0.8517510000
H -1.8836810000 2.0272390000 0.5451180000
B -2.6776690000 -0.6157710000 -0.0792900000
F -2.3129500000 -0.8124780000 1.2642730000
F -3.2436490000 -1.7290890000 -0.6397200000
F -3.4613750000 0.5282760000 -0.2025610000
H 0.0982980000 3.6926940000 -0.0459300000
H 0.5748210000 2.8113150000 1.3889910000
H 1.0981700000 0.1788910000 -1.8356830000
C 1.3997690000 1.9790100000 -0.4971290000
H 2.3352090000 1.8315900000 0.0577170000
H 1.6704460000 2.5736530000 -1.3801090000
H 3.2085890000 -0.1168920000 1.6537480000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.228397 (Hartree/Particle)
Thermal correction to Energy= 0.244163
Thermal correction to Enthalpy= 0.245107
Thermal correction to Gibbs (Free) Energy= 0.184715
Sum of electronic and zero-point Energies= -826.098424
Sum of electronic and thermal Energies= -826.082658
Sum of electronic and thermal Enthalpies= -826.081714
Sum of electronic and thermal (Free) Energies= -826.142107

PC

C 1.2849590000 -0.6689660000 0.2235930000
C 2.6823520000 -0.9160740000 -0.0261080000
H 0.6641790000 -1.4661610000 -0.2101860000
O 3.6056590000 -0.5663440000 0.8407050000
C 0.9045380000 -0.4319360000 1.6877250000
H 1.2535060000 0.5379210000 2.0680680000
H -0.1864240000 -0.4504980000 1.7702390000
H 1.2936590000 -1.2319420000 2.3312040000
C 3.2268240000 -1.5012160000 -1.2780110000
H 4.0279110000 -0.8717450000 -1.6827290000
H 3.6736210000 -2.4781040000 -1.0478230000
H 2.4444000000 -1.6428950000 -2.0243170000
C 0.8534190000 0.5770230000 -0.7661560000
C -0.6382720000 0.6883570000 -0.5728360000
C -0.9630940000 1.9114730000 -0.0765350000
C 0.2351350000 2.7823390000 0.1590740000
O -1.3414970000 -0.3846010000 -0.8387690000
H -1.9847380000 2.2215560000 0.1002100000
B -2.6161580000 -0.6949430000 -0.0261210000
F -2.1894210000 -0.9090390000 1.2988810000
F -3.1389960000 -1.8327730000 -0.5876530000
F -3.4697230000 0.3973520000 -0.0974170000
H 0.1496350000 3.7589440000 -0.3378950000
H 0.3745590000 3.0072040000 1.2280510000
H 1.1017480000 0.2400950000 -1.7770420000
C 1.4266340000 1.9644910000 -0.4217560000
H 2.2744650000 1.9194190000 0.2729610000
H 1.8061430000 2.4385200000 -1.3325820000
H 3.1831140000 -0.2328460000 1.6587150000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.230523 (Hartree/Particle)
Thermal correction to Energy= 0.246234
Thermal correction to Enthalpy= 0.247178
Thermal correction to Gibbs (Free) Energy= 0.186249
Sum of electronic and zero-point Energies= -826.104579
Sum of electronic and thermal Energies= -826.088868
Sum of electronic and thermal Enthalpies= -826.087924
Sum of electronic and thermal (Free) Energies= -826.148852

Entry 13

RC

C 1.4532980000 -1.5723230000 -0.2060410000
C 2.0145770000 -0.8181190000 0.7724610000
O 3.3079080000 -0.3725170000 0.7561030000

C 1.2891980000 -0.3742580000 2.0017400000
H 1.7536410000 -0.8224770000 2.8889380000
H 1.3640970000 0.7139200000 2.1250850000
H 0.2383350000 -0.6646830000 1.9564240000
C 0.7181430000 0.9167440000 -1.2449000000
C -0.5898490000 0.8703100000 -0.6986400000
C -0.7159210000 1.9921110000 0.1305680000
C 0.4978200000 2.8488400000 0.1267050000
O -1.4340420000 -0.0785150000 -0.9810910000
H -1.6179250000 2.2069360000 0.6897800000
B -2.4326390000 -0.5910330000 0.0739480000
F -1.6603570000 -1.3268730000 0.9937670000
F -3.3297540000 -1.3720610000 -0.5982180000
F -3.0214300000 0.5064260000 0.7039720000
H 0.2691520000 3.8469700000 -0.2777590000
H 0.8835870000 3.0270980000 1.1394320000
H 1.0402320000 0.2603100000 -2.0443450000
C 1.4915180000 2.0927660000 -0.7842180000
H 2.4002710000 1.7782170000 -0.2467330000
H 1.8419260000 2.6978640000 -1.6327070000
C 2.1579320000 -2.1509750000 -1.4010740000
H 3.1024290000 -1.6478700000 -1.6527370000
H 2.3886080000 -3.2137700000 -1.2466090000
H 1.5197780000 -2.0994180000 -2.2911710000
H 0.4162910000 -1.8544770000 -0.0518860000
H 3.7754220000 -0.7632040000 -0.0008360000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227340 (Hartree/Particle)
Thermal correction to Energy= 0.244199
Thermal correction to Enthalpy= 0.245143
Thermal correction to Gibbs (Free) Energy= 0.182169
Sum of electronic and zero-point Energies= -826.101128
Sum of electronic and thermal Energies= -826.084269
Sum of electronic and thermal Enthalpies= -826.083325
Sum of electronic and thermal (Free) Energies= -826.146299

TS

C 1.3620680000 -1.3754020000 -0.4011330000
C 1.8139380000 -0.9174440000 0.8129120000
O 3.1158900000 -0.6392470000 1.0533250000
C 0.9242650000 -0.5937250000 1.9594950000
H 1.4282110000 -0.8126820000 2.9052630000
H 0.6752270000 0.4803510000 1.9518070000
H -0.0229730000 -1.1284750000 1.8794200000
C 0.8188380000 0.7908320000 -1.1844880000
C -0.5089240000 0.9186500000 -0.6576460000
C -0.5180420000 2.0103260000 0.1993430000
C 0.7887230000 2.7332830000 0.2256960000
O -1.4521850000 0.0848970000 -1.0047900000
H -1.4019170000 2.3300110000 0.7359060000
B -2.4511620000 -0.4845570000 0.0103340000
F -1.7625090000 -1.5331670000 0.6629690000
F -3.5195410000 -0.9450860000 -0.7088610000
F -2.7887850000 0.5106120000 0.9261220000
H 0.6772480000 3.7577750000 -0.1597560000
H 1.1942600000 2.8436200000 1.2400470000
H 1.0039390000 0.2653500000 -2.1140950000
C 1.7036270000 1.8978320000 -0.7079390000
H 2.5973580000 1.5285000000 -0.1868590000
H 2.0716090000 2.4833720000 -1.5611870000
C 2.2646680000 -1.8831940000 -1.4987430000
H 3.1665270000 -1.2718800000 -1.6492320000
H 2.5910320000 -2.9123120000 -1.2975500000
H 1.7340610000 -1.9033240000 -2.4555840000
H 0.3142820000 -1.6611100000 -0.4324940000
H 3.6598540000 -0.9197910000 0.2973090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227886 (Hartree/Particle)
Thermal correction to Energy= 0.243750
Thermal correction to Enthalpy= 0.244695
Thermal correction to Gibbs (Free) Energy= 0.184189
Sum of electronic and zero-point Energies= -826.099345
Sum of electronic and thermal Energies= -826.083481
Sum of electronic and thermal Enthalpies= -826.082536
Sum of electronic and thermal (Free) Energies= -826.143042

PC

C 1.2163320000 -0.8940860000 -0.6585430000
C 1.5127810000 -1.0240990000 0.7748480000
O 2.7317970000 -1.2715220000 1.1887410000
C 0.5111330000 -0.8355430000 1.8120300000
H 0.9143030000 -0.9722350000 2.8156910000
H 0.0639480000 0.1752300000 1.6772690000
H -0.3622960000 -1.4694640000 1.5963130000
C 0.9341120000 0.6560670000 -1.0542540000
C -0.4216380000 1.0831840000 -0.5515190000
C -0.3095000000 2.0914320000 0.3516430000
C 1.1181050000 2.5265370000 0.5506300000
O -1.4705590000 0.4239210000 -1.0021520000
H -1.1537760000 2.5375450000 0.8626860000
B -2.3815260000 -0.3678730000 -0.0880680000
F -1.7325160000 -1.6361350000 0.1036850000
F -3.5816540000 -0.5281840000 -0.7217950000
F -2.4787910000 0.2669550000 1.1488080000
H 1.2537040000 3.6072750000 0.4117070000
H 1.4785260000 2.3137470000 1.5698410000
H 0.9352510000 0.5917440000 -2.1482280000
C 1.9141970000 1.7239160000 -0.5227750000
H 2.8470350000 1.3062330000 -0.1235130000
H 2.2034210000 2.3854400000 -1.3449340000
C 2.2840580000 -1.5040850000 -1.5767400000
H 3.2248280000 -0.9337100000 -1.5732260000
H 2.4985860000 -2.5511600000 -1.3295640000
H 1.9216400000 -1.4872560000 -2.6078080000
H 0.2333050000 -1.3593980000 -0.8176130000
H 3.3384230000 -1.3874800000 0.4308010000

Zero-point correction= 0.230756 (Hartree/Particle)
Thermal correction to Energy= 0.245790
Thermal correction to Enthalpy= 0.246734
Thermal correction to Gibbs (Free) Energy= 0.188925
Sum of electronic and zero-point Energies= -826.112625
Sum of electronic and thermal Energies= -826.097592
Sum of electronic and thermal Enthalpies= -826.096648
Sum of electronic and thermal (Free) Energies= -826.154457

Entry 14

RC

C 1.4811120000 -1.5456860000 -0.3346090000
C 1.9184410000 -0.8888040000 0.7690180000
O 3.2162500000 -0.4472400000 0.8115810000
C 1.0680630000 -0.5889140000 1.9625060000
H 1.5035170000 -1.0375570000 2.8667360000
H 1.0008350000 0.4962980000 2.1351550000
H 0.0549620000 -0.9731980000 1.8289750000
C 0.7520210000 0.8986350000 -1.2255590000
C -0.5583130000 0.8985270000 -0.6736440000
C -0.6340350000 1.9992440000 0.1847780000
C 0.6158600000 2.8074240000 0.1933310000
O -1.4421020000 -0.0037310000 -0.9894030000
H -1.5252200000 2.2434410000 0.7484780000
B -2.4544960000 -0.5498070000 0.0304170000
F -1.7379310000 -1.4841250000 0.8056500000
F -3.4541380000 -1.1360500000 -0.6937350000
F -2.9006510000 0.5019380000 0.8330200000
H 0.4259300000 3.8233260000 -0.1856260000
H 1.0178390000 2.9472930000 1.2061890000
H 1.0333960000 0.2699910000 -2.0609960000
C 1.5722090000 2.0355800000 -0.7459250000
H 2.4786660000 1.6751910000 -0.2352350000
H 1.9306720000 2.6464030000 -1.5866160000
C 2.3544020000 -1.9982190000 -1.4679340000
H 3.3289290000 -1.5029960000 -1.4642760000
H 2.5275500000 -3.0810470000 -1.4000150000
H 1.8727730000 -1.8283510000 -2.4391020000
H 0.4421150000 -1.8620030000 -0.3182740000
H 3.4032510000 -0.1025830000 1.6989180000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227275 (Hartree/Particle)
Thermal correction to Energy= 0.244195
Thermal correction to Enthalpy= 0.245140
Thermal correction to Gibbs (Free) Energy= 0.181935
Sum of electronic and zero-point Energies= -826.100707

Sum of electronic and thermal Energies= -826.083787
Sum of electronic and thermal Enthalpies= -826.082843
Sum of electronic and thermal (Free) Energies= -826.146048

TS

C 1.4041790000 -1.4038500000 -0.4615290000
C 1.7598350000 -0.9642170000 0.7858390000
O 3.0634200000 -0.6520430000 1.0073670000
C 0.7938840000 -0.7327730000 1.8965220000
H 1.2077880000 -1.0756570000 2.8537420000
H 0.5677430000 0.3437100000 1.9884110000
H -0.1579200000 -1.2309770000 1.7030730000
C 0.8349400000 0.8016320000 -1.1829820000
C -0.4866080000 0.9337380000 -0.6420830000
C -0.4722260000 2.0030640000 0.2428950000
C 0.8505300000 2.6971430000 0.2842730000
O -1.4439800000 0.1237460000 -1.0051750000
H -1.3467960000 2.3269400000 0.7918230000
B -2.4624840000 -0.4548920000 -0.0169870000
F -1.8402510000 -1.5995850000 0.5322740000
F -3.5772530000 -0.7777520000 -0.7402150000
F -2.7076850000 0.4821050000 0.9873990000
H 0.7588790000 3.7398440000 -0.0543200000
H 1.2666480000 2.7570700000 1.2995180000
H 1.0122160000 0.2798030000 -2.1155620000
C 1.7393670000 1.8814210000 -0.6905090000
H 2.6418160000 1.4781530000 -0.2111010000
H 2.0951270000 2.4897210000 -1.5332520000
C 2.3984470000 -1.8220340000 -1.5107490000
H 3.3248300000 -1.2426520000 -1.4611680000
H 2.6635140000 -2.8792610000 -1.3764620000
H 1.9754890000 -1.7298220000 -2.5167910000
H 0.3681260000 -1.7130410000 -0.5697500000
H 3.1720550000 -0.3506520000 1.9240630000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227774 (Hartree/Particle)
Thermal correction to Energy= 0.243670
Thermal correction to Enthalpy= 0.244614
Thermal correction to Gibbs (Free) Energy= 0.183835
Sum of electronic and zero-point Energies= -826.099803
Sum of electronic and thermal Energies= -826.083907
Sum of electronic and thermal Enthalpies= -826.082963
Sum of electronic and thermal (Free) Energies= -826.143741

PC

C 1.2534740000 -0.8939010000 -0.6957420000
C 1.5126870000 -1.0454110000 0.7355460000
O 2.7596250000 -1.2729140000 1.0848600000
C 0.4746270000 -0.8832780000 1.7437850000
H 0.8219280000 -1.0467680000 2.7688810000
H 0.0472160000 0.1428250000 1.6246320000
H -0.4051230000 -1.4940240000 1.4883980000
C 0.9484410000 0.6665710000 -1.0601040000
C -0.4060480000 1.0692000000 -0.5390530000
C -0.2938880000 2.0504990000 0.3975000000
C 1.1327940000 2.4917700000 0.5911040000
O -1.4517900000 0.4122640000 -0.9955370000
H -1.1371090000 2.4773170000 0.9261840000
B -2.3996670000 -0.3528810000 -0.0946470000
F -1.7963300000 -1.6420360000 0.0912530000
F -3.6000560000 -0.4641960000 -0.7373470000
F -2.4844000000 0.2760940000 1.1476050000
H 1.2562140000 3.5778830000 0.4870330000
H 1.5074810000 2.2517640000 1.6001540000
H 0.9449240000 0.6155950000 -2.1541820000
C 1.9228040000 1.7307180000 -0.5158540000
H 2.8664020000 1.3099350000 -0.1498180000
H 2.1861650000 2.4198770000 -1.3240440000
C 2.3520850000 -1.4593090000 -1.6017830000
H 3.2863850000 -0.8965430000 -1.5103050000
H 2.5647980000 -2.5078370000 -1.3702240000
H 2.0202990000 -1.4038580000 -2.6423630000
H 0.2771850000 -1.3607860000 -0.8877440000
H 2.8441220000 -1.3256940000 2.0560630000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.230675 (Hartree/Particle)
Thermal correction to Energy= 0.245715
Thermal correction to Enthalpy= 0.246659
Thermal correction to Gibbs (Free) Energy= 0.188812
Sum of electronic and zero-point Energies= -826.111957
Sum of electronic and thermal Energies= -826.096917
Sum of electronic and thermal Enthalpies= -826.095973
Sum of electronic and thermal (Free) Energies= -826.153821

Entry 15

RC

C 1.7765690000 -0.5297510000 0.9411430000
C 1.9258620000 -1.4671130000 -0.0300900000
H 0.8321130000 -0.5498980000 1.4756390000
O 3.0991180000 -1.5033880000 -0.7324820000
C 2.8869150000 0.3407090000 1.4556100000
H 3.6750460000 0.4875700000 0.7110110000
H 2.5161170000 1.3206700000 1.7788310000
H 3.3556490000 -0.1152870000 2.3394140000
C 0.8962460000 -2.4911550000 -0.3965890000
H 0.5850640000 -2.3872160000 -1.4445090000
H 1.3154410000 -3.4995680000 -0.2670990000
H 0.0065600000 -2.3892140000 0.2245500000
C 0.7319860000 1.1313180000 -1.0220890000
C -0.6132000000 0.9257720000 -0.6181590000
C -1.0177740000 2.0870620000 0.0484240000
C 0.0516340000 3.1144230000 0.1124370000
O -1.2656640000 -0.1745430000 -0.8635160000
H -2.0089100000 2.2036730000 0.4684090000
B -2.2936190000 -0.7066180000 0.1534380000
F -1.5389950000 -1.1123810000 1.2706780000
F -2.9216310000 -1.7559210000 -0.4608910000
F -3.1617590000 0.3272170000 0.5008360000
H -0.2788770000 4.0703130000 -0.3198190000
H 0.3247220000 3.3443720000 1.1532710000
H 1.2675540000 0.4586600000 -1.6805660000
C 1.2192000000 2.4892680000 -0.6811400000
H 2.1633140000 2.4610280000 -0.1221800000
H 1.4406470000 3.0527690000 -1.6004690000
H 3.0628410000 -2.2347680000 -1.3685810000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227105 (Hartree/Particle)
Thermal correction to Energy= 0.244169
Thermal correction to Enthalpy= 0.245113
Thermal correction to Gibbs (Free) Energy= 0.180973
Sum of electronic and zero-point Energies= -826.099302
Sum of electronic and thermal Energies= -826.082238
Sum of electronic and thermal Enthalpies= -826.081294
Sum of electronic and thermal (Free) Energies= -826.145434

TS

C 1.6256670000 -0.4729740000 0.8109570000
C 1.6993750000 -1.5724760000 -0.0166960000
H 0.6979920000 -0.3910970000 1.3681290000
O 2.8695870000 -1.8005890000 -0.6524430000
C 2.8575440000 0.1988900000 1.3627400000
H 3.6438680000 0.3135680000 0.6107550000
H 2.6211810000 1.1803360000 1.7831230000
H 3.2764060000 -0.4034670000 2.1801860000
C 0.5798220000 -2.5215070000 -0.2940920000
H 0.2411090000 -2.4395730000 -1.3351720000
H 0.9292730000 -3.5506040000 -0.1268420000
H -0.2763400000 -2.3138500000 0.3469260000
C 0.9213130000 0.9304080000 -0.9056370000
C -0.4882860000 0.9423190000 -0.6111350000
C -0.7953840000 2.1566010000 -0.0291480000
C 0.3942330000 3.0480090000 0.0987010000
O -1.2416070000 -0.0996900000 -0.8657920000
H -1.7943410000 2.4177720000 0.2951350000
B -2.3215080000 -0.5090260000 0.1388060000
F -1.6208830000 -0.8984120000 1.3079180000
F -2.9830340000 -1.5691100000 -0.4282320000
F -3.1456240000 0.5765730000 0.4091860000
H 0.2182190000 4.0406400000 -0.3390190000
H 0.6506680000 3.2310530000 1.1532680000
H 1.3427230000 0.2765470000 -1.6603360000
C 1.5087460000 2.2846660000 -0.6541830000

H 2.4696800000 2.2636560000 -0.1317280000
H 1.7115120000 2.7523670000 -1.6291880000
H 2.7794420000 -2.5750650000 -1.2322780000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.228397 (Hartree/Particle)
Thermal correction to Energy= 0.244144
Thermal correction to Enthalpy= 0.245088
Thermal correction to Gibbs (Free) Energy= 0.184598
Sum of electronic and zero-point Energies= -826.097252
Sum of electronic and thermal Energies= -826.081505
Sum of electronic and thermal Enthalpies= -826.080561
Sum of electronic and thermal (Free) Energies= -826.141051

PC

C 1.3613380000 -1.2873150000 0.3455570000
C -0.1653320000 -1.3181880000 0.0765530000
H 1.4898950000 -1.1724090000 1.4303300000
O -0.3898800000 -1.7344170000 -1.2179200000
C 2.0907270000 -2.5437620000 -0.1289840000
H 1.9668350000 -2.6840180000 -1.2061260000
H 3.1605670000 -2.4583160000 0.0900620000
H 1.7193980000 -3.4424230000 0.3761590000
C -1.0195030000 -2.0278020000 1.1116780000
H -2.0764940000 -1.9873540000 0.8388860000
H -0.7107630000 -3.0772060000 1.1515600000
H -0.8967240000 -1.5781550000 2.0997080000
C 1.7788250000 0.0303310000 -0.3342990000
C 0.6231110000 0.9235740000 -0.0153880000
C 0.9206510000 2.2017400000 0.1928860000
C 2.4262000000 2.3588200000 0.0335330000
O -0.5341380000 0.1762910000 0.1545050000
H 0.2321780000 3.0017610000 0.4299830000
B -2.1477280000 0.7195410000 -0.0553410000
F -2.6775070000 0.6271120000 1.1861440000
F -2.6413330000 -0.2164450000 -0.9446220000
F -1.9840250000 1.9630410000 -0.5550040000
H 2.6881150000 2.8018020000 -0.9390100000
H 2.8574160000 3.0138350000 0.7998650000
H 1.8364170000 -0.1432240000 -1.4195080000
C 2.9615430000 0.8941910000 0.1494800000
H 3.1730020000 0.6713800000 1.2028700000
H 3.8814460000 0.7308380000 -0.4197570000
H -1.3300730000 -1.5621190000 -1.4157550000

Zero-point correction= 0.232834 (Hartree/Particle)
Thermal correction to Energy= 0.247637
Thermal correction to Enthalpy= 0.248581
Thermal correction to Gibbs (Free) Energy= 0.191708
Sum of electronic and zero-point Energies= -826.152440
Sum of electronic and thermal Energies= -826.137637
Sum of electronic and thermal Enthalpies= -826.136693
Sum of electronic and thermal (Free) Energies= -826.193566

Entry 16

RC

C 1.5742820000 -1.3605540000 0.4500440000
C 2.7597150000 -0.9174990000 -0.0194000000
H 1.0238850000 -2.0522900000 -0.1813310000
O 3.4855590000 -0.0166030000 0.7289350000
C 0.9907650000 -1.0526960000 1.7929410000
H 1.5105000000 -0.2290570000 2.2901370000
H -0.0797260000 -0.8301340000 1.7115040000
H 1.0678440000 -1.9353970000 2.4436170000
C 3.3784640000 -1.3305140000 -1.3235830000
H 3.5790060000 -0.4621050000 -1.9678440000
H 4.3387230000 -1.8389950000 -1.1566470000
H 2.7281500000 -2.0190670000 -1.8678630000
C 0.6450500000 0.9275470000 -1.0639010000
C -0.6437620000 0.6604290000 -0.5488370000
C -0.9216330000 1.6822900000 0.3749990000
C 0.1879570000 2.6559670000 0.5018040000
O -1.3570290000 -0.3674660000 -0.8945840000
H -1.8592220000 1.7533610000 0.9120350000
B -2.6750950000 -0.6243390000 -0.1222600000
F -2.3128930000 -0.7640680000 1.2267940000
F -3.2088490000 -1.7615340000 -0.6577220000
F -3.4738190000 0.5053730000 -0.2837720000
H -0.1411030000 3.6715070000 0.2341510000
H 0.5424840000 2.7282430000 1.5403730000
H 1.0641290000 0.3769940000 -1.8983260000
C 1.2670400000 2.1313490000 -0.4688060000
H 2.2042240000 1.8686100000 0.0474350000
H 1.5399020000 2.8669500000 -1.2393570000
H 4.3612290000 0.0997830000 0.3293420000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.226667 (Hartree/Particle)
Thermal correction to Energy= 0.243855
Thermal correction to Enthalpy= 0.244799
Thermal correction to Gibbs (Free) Energy= 0.180761
Sum of electronic and zero-point Energies= -826.099105
Sum of electronic and thermal Energies= -826.081917
Sum of electronic and thermal Enthalpies= -826.080972
Sum of electronic and thermal (Free) Energies= -826.145011

TS

C 1.3848000000 -0.9448580000 0.4359150000
C 2.6964170000 -0.9305260000 0.0241310000
H 0.7201750000 -1.6239030000 -0.0929880000
O 3.5928410000 -0.2547380000 0.7749180000
C 0.9500100000 -0.5251530000 1.8147130000
H 1.4114950000 0.4168040000 2.1269430000
H -0.1387950000 -0.4434940000 1.8528520000
H 1.2528130000 -1.2911880000 2.5405030000
C 3.2023780000 -1.5647840000 -1.2340130000
H 3.6618540000 -0.8186680000 -1.8985790000
H 3.9695490000 -2.3150730000 -1.0001280000
H 2.3978620000 -2.0641360000 -1.7772230000
C 0.7796130000 0.6504780000 -0.9236960000
C -0.6222670000 0.6214720000 -0.5689290000
C -0.9264750000 1.8088840000 0.0678030000
C 0.2517430000 2.7138250000 0.2054760000
O -1.3492250000 -0.4305080000 -0.8318250000
H -1.9306810000 2.0620550000 0.3834150000
B -2.6629530000 -0.6463350000 -0.0472170000
F -2.2983780000 -0.7528000000 1.3031900000
F -3.2002470000 -1.8052820000 -0.5432840000
F -3.4745730000 0.4680850000 -0.2455780000
H 0.0668020000 3.6972720000 -0.2502470000
H 0.4915540000 2.9164920000 1.2594320000
H 1.1128620000 0.1151930000 -1.8069920000
C 1.3915680000 1.9660310000 -0.5331600000
H 2.2911780000 1.8468860000 0.0835320000
H 1.7065370000 2.5098060000 -1.4337420000
H 4.4646880000 -0.2566380000 0.3461710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.228306 (Hartree/Particle)
Thermal correction to Energy= 0.244189
Thermal correction to Enthalpy= 0.245133
Thermal correction to Gibbs (Free) Energy= 0.184383
Sum of electronic and zero-point Energies= -826.095077
Sum of electronic and thermal Energies= -826.079194
Sum of electronic and thermal Enthalpies= -826.078250
Sum of electronic and thermal (Free) Energies= -826.139000

PC

C 1.2905250000 -0.6408110000 0.3051840000
C 2.6597990000 -0.9219620000 0.0008920000
H 0.6379680000 -1.4397740000 -0.0761410000
O 3.5819320000 -0.4671170000 0.8315380000
C 0.9571160000 -0.3039530000 1.7570190000
H 1.3794840000 0.6566250000 2.0659600000
H -0.1295290000 -0.2809320000 1.8652450000
H 1.3545680000 -1.0756850000 2.4249260000
C 3.1112370000 -1.6323050000 -1.2302900000
H 3.8525890000 -1.0398510000 -1.7848410000
H 3.5876160000 -2.5833870000 -0.9521420000
H 2.2712410000 -1.8562800000 -1.8892560000
C 0.8525030000 0.5646730000 -0.7640160000
C -0.6373580000 0.6671900000 -0.5752550000
C -0.9689110000 1.9045980000 -0.1139660000
C 0.2250500000 2.7862210000 0.0971320000
O -1.3355430000 -0.4125800000 -0.8149300000

H -1.9929930000 2.2152790000 0.0472340000
B -2.6221540000 -0.7014560000 -0.0054870000
F -2.2108160000 -0.8803080000 1.3235380000
F -3.1398150000 -1.8511110000 -0.5496920000
F -3.4722300000 0.3911320000 -0.1217800000
H 0.1300770000 3.7511090000 -0.4209150000
H 0.3667850000 3.0338030000 1.1603840000
H 1.1046540000 0.1785180000 -1.7559620000
C 1.4185040000 1.9637780000 -0.4713230000
H 2.2710380000 1.9422780000 0.2168620000
H 1.7791750000 2.4136320000 -1.4025580000
H 4.4819530000 -0.6324660000 0.4949190000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.230274 (Hartree/Particle)
Thermal correction to Energy= 0.246124
Thermal correction to Enthalpy= 0.247068
Thermal correction to Gibbs (Free) Energy= 0.186077
Sum of electronic and zero-point Energies= -826.098760
Sum of electronic and thermal Energies= -826.082910
Sum of electronic and thermal Enthalpies= -826.081966
Sum of electronic and thermal (Free) Energies= -826.142956

Entry 17

RC

C 1.7156780000 -0.5371030000 0.9205260000
C 2.0710180000 -1.3987320000 -0.0704920000
H 0.7152100000 -0.6632430000 1.3216080000
O 3.3049290000 -1.4216130000 -0.6477230000
C 2.6523340000 0.3990140000 1.6354550000
H 3.4767760000 0.7670270000 1.0067050000
H 2.1179860000 1.2813970000 2.0045500000
H 3.1074360000 -0.0771560000 2.5156490000
C 1.1588720000 -2.4250790000 -0.6620510000
H 1.0155430000 -2.2489100000 -1.7353750000
H 1.6129300000 -3.4180330000 -0.5577610000
H 0.1873500000 -2.4049140000 -0.1686420000
C 0.6534950000 1.1332540000 -1.0580980000
C -0.6817390000 0.9069310000 -0.6317880000
C -1.0946450000 2.0697040000 0.0311040000
C -0.0426870000 3.1156500000 0.0692730000
O -1.3220600000 -0.1995170000 -0.8681960000
H -2.0828960000 2.1775350000 0.4593390000
B -2.2962680000 -0.7944050000 0.1707160000
F -1.4758970000 -1.3556860000 1.1647860000
F -3.0345040000 -1.7334260000 -0.4937410000
F -3.0714760000 0.2371810000 0.7022730000
H -0.3944700000 4.0561550000 -0.3800120000
H 0.2335210000 3.3734250000 1.1025850000
H 1.1828590000 0.4629350000 -1.7242060000
C 1.1289240000 2.4979300000 -0.7246260000
H 2.0717760000 2.4819050000 -0.1619700000
H 1.3463590000 3.0614780000 -1.6446310000
H 3.8973980000 -0.8105660000 -0.1797480000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.226948 (Hartree/Particle)
Thermal correction to Energy= 0.244077
Thermal correction to Enthalpy= 0.245022
Thermal correction to Gibbs (Free) Energy= 0.180469
Sum of electronic and zero-point Energies= -826.098047
Sum of electronic and thermal Energies= -826.080917
Sum of electronic and thermal Enthalpies= -826.079973
Sum of electronic and thermal (Free) Energies= -826.144526

TS

C 1.5547920000 -0.4709480000 0.7950130000
C 1.8274510000 -1.5279680000 -0.0519470000
H 0.5661120000 -0.4980710000 1.2421640000
O 3.0499850000 -1.7490990000 -0.5697320000
C 2.6305870000 0.2918460000 1.5300100000
H 3.4938540000 0.5634910000 0.9054020000
H 2.2338880000 1.2238270000 1.9415130000
H 3.0112190000 -0.2922180000 2.3789240000
C 0.8108550000 -2.5009200000 -0.5433410000
H 0.5904920000 -2.3270340000 -1.6042820000
H 1.2155960000 -3.5157180000 -0.4560100000
H -0.1168220000 -2.4025050000 0.0193660000
C 0.8602240000 0.9268360000 -0.9330010000
C -0.5482670000 0.9259990000 -0.6268900000
C -0.8630850000 2.1460280000 -0.0597670000
C 0.3153420000 3.0556650000 0.0418490000
O -1.2916180000 -0.1230680000 -0.8712160000
H -1.8629660000 2.4036020000 0.2637320000
B -2.3251150000 -0.5877550000 0.1604870000
F -1.5658010000 -1.1046800000 1.2394260000
F -3.0666090000 -1.5639090000 -0.4508790000
F -3.0834720000 0.4992070000 0.5822630000
H 0.1248250000 4.0317750000 -0.4262270000
H 0.5712120000 3.2764100000 1.0890910000
H 1.2707180000 0.2720980000 -1.6931080000
C 1.4392530000 2.2879040000 -0.6944550000
H 2.3937130000 2.2801040000 -0.1581320000
H 1.6518590000 2.7467750000 -1.6712050000
H 3.6949620000 -1.1286310000 -0.1881940000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.228266 (Hartree/Particle)
Thermal correction to Energy= 0.244064
Thermal correction to Enthalpy= 0.245008
Thermal correction to Gibbs (Free) Energy= 0.184430
Sum of electronic and zero-point Energies= -826.095849
Sum of electronic and thermal Energies= -826.080051
Sum of electronic and thermal Enthalpies= -826.079107
Sum of electronic and thermal (Free) Energies= -826.139685

PC

C 1.5825650000 -1.0621550000 0.4034320000
C 0.1183440000 -1.3710840000 -0.0559440000
H 1.5363480000 -0.8706750000 1.4840960000
O 0.0372790000 -2.0345510000 -1.2784440000
C 2.5692470000 -2.1959180000 0.1325420000
H 2.6502170000 -2.4114580000 -0.9379880000
H 3.5654450000 -1.9259660000 0.4995820000
H 2.2672870000 -3.1218610000 0.6338470000
C -0.7159080000 -2.1557100000 0.9368910000
H -1.7080630000 -2.3390420000 0.5205960000
H -0.2350490000 -3.1190330000 1.1319660000
H -0.8145780000 -1.6037480000 1.8738050000
C 1.8649040000 0.2767440000 -0.2962550000
C 0.5166780000 0.9262300000 -0.2169700000
C 0.5390670000 2.2481650000 -0.0510000000
C 1.9911250000 2.6971740000 0.0103870000
O -0.4874260000 -0.0113860000 -0.2197940000
H -0.3148240000 2.9066530000 0.0354340000
B -2.5263030000 0.4900100000 0.0458290000
F -2.5320570000 0.4439970000 1.3776550000
F -3.0244310000 -0.5407440000 -0.6328400000
F -2.4371250000 1.6770710000 -0.5533650000
H 2.3208110000 3.1546260000 -0.9352660000
H 2.1623250000 3.4473040000 0.7919730000
H 2.1432290000 0.0849710000 -1.3488020000
C 2.7710520000 1.3739240000 0.2971210000
H 2.8514220000 1.2309180000 1.3818250000
H 3.7841370000 1.3753490000 -0.1167190000
H 0.5440560000 -1.5377180000 -1.9418730000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.231696 (Hartree/Particle)
Thermal correction to Energy= 0.247383
Thermal correction to Enthalpy= 0.248328
Thermal correction to Gibbs (Free) Energy= 0.187768
Sum of electronic and zero-point Energies= -826.145126
Sum of electronic and thermal Energies= -826.129438
Sum of electronic and thermal Enthalpies= -826.128494
Sum of electronic and thermal (Free) Energies= -826.189054

Entry 18

RC

C 2.4605180000 -1.5988220000 -0.1849990000
C 3.4005250000 -0.6614820000 0.0009600000
H 2.5517190000 -2.2049750000 -1.0836220000
O 3.3151920000 0.1928340000 1.0953190000
C 1.3242530000 -1.9112090000 0.7447790000

H 1.3654910000 -1.2954200000 1.6472770000
H 0.3415530000 -1.7724740000 0.2756160000
H 1.3667190000 -2.9643710000 1.0534630000
C 4.5706860000 -0.4117260000 -0.9079850000
H 4.5650180000 0.6152780000 -1.2984810000
H 5.5227360000 -0.5489630000 -0.3733090000
H 4.5672700000 -1.1021770000 -1.7548900000
C -0.7009960000 0.9091460000 -0.9597580000
C -1.2674270000 1.0443020000 0.3350360000
C -0.3889210000 1.8775970000 1.0480050000
C 0.8116610000 2.2613480000 0.2804390000
O -2.3558990000 0.5225080000 0.7980890000
H -0.5715870000 2.1785920000 2.0760220000
B -3.0106390000 -0.5886940000 -0.0686320000
F -3.4095900000 0.0114500000 -1.2623110000
F -4.0353710000 -1.0977540000 0.6685920000
F -1.9875860000 -1.5167980000 -0.3280440000
H 0.9132020000 3.3533690000 0.1911060000
H 1.7250160000 1.9069440000 0.7854450000
H -1.1885780000 0.3623900000 -1.7579110000
C 0.6048330000 1.5737710000 -1.0803770000
H 1.3845820000 0.8160370000 -1.2759030000
H 0.6386340000 2.2642160000 -1.9356840000
H 4.1992010000 0.5426490000 1.2860440000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.225756 (Hartree/Particle)
Thermal correction to Energy= 0.243371
Thermal correction to Enthalpy= 0.244315
Thermal correction to Gibbs (Free) Energy= 0.177777
Sum of electronic and zero-point Energies= -826.096453
Sum of electronic and thermal Energies= -826.078839
Sum of electronic and thermal Enthalpies= -826.077895
Sum of electronic and thermal (Free) Energies= -826.144433

TS

C -1.3307720000 -1.3758510000 0.6074800000
C -2.4036780000 -0.8899210000 -0.1166130000
H -1.5393520000 -1.5121210000 1.6669300000
O -2.2651510000 -0.8049470000 -1.4464750000
C -0.3052330000 -2.3097750000 0.0036340000
H -0.1033910000 -2.0707720000 -1.0409240000
H 0.6406400000 -2.2603180000 0.5424710000
H -0.6971100000 -3.3343030000 0.0609290000
C -3.7164390000 -0.4706120000 0.4770760000
H -4.0721410000 0.4876880000 0.0810630000
H -4.4767130000 -1.2285230000 0.2393110000
H -3.6555400000 -0.3982080000 1.5643170000
C -0.2478980000 0.4945650000 0.8482610000
C 0.3947260000 0.7518470000 -0.4361840000
C -0.2919800000 1.7734110000 -1.0549350000
C -1.3869420000 2.3352820000 -0.2051350000
O 1.4220630000 0.0995770000 -0.9130460000
H -0.0037340000 2.1820120000 -2.0175810000
B 2.6303480000 -0.1530690000 0.0087860000
F 3.0444330000 1.0799150000 0.4886410000
F 3.5620440000 -0.7987890000 -0.7579570000
F 2.1991650000 -0.9576430000 1.0963420000
H -1.3352050000 3.4297060000 -0.1345050000
H -2.3889580000 2.1141210000 -0.6041680000
H 0.3044940000 -0.0259740000 1.6218750000
C -1.1522090000 1.6524490000 1.1650600000
H -2.0648730000 1.3907340000 1.7082850000
H -0.5871570000 2.3295790000 1.8213540000
H -3.0362260000 -0.3750380000 -1.8522090000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.228495 (Hartree/Particle)
Thermal correction to Energy= 0.244145
Thermal correction to Enthalpy= 0.245089
Thermal correction to Gibbs (Free) Energy= 0.184976
Sum of electronic and zero-point Energies= -826.084944
Sum of electronic and thermal Energies= -826.069295
Sum of electronic and thermal Enthalpies= -826.068350
Sum of electronic and thermal (Free) Energies= -826.128463

PC

C 1.1422630000 -0.9255520000 -0.8045540000
C 2.1013530000 -0.9134700000 0.3031220000
H 1.7070010000 -1.0863640000 -1.7293060000
O 1.5585690000 -0.7589380000 1.4847430000
C 0.1080070000 -2.0714320000 -0.6380290000
H -0.4957820000 -1.9572270000 0.2619070000
H -0.5804190000 -2.0450200000 -1.4841820000
H 0.6211540000 -3.0397790000 -0.6209080000
C 3.5620400000 -1.1875850000 0.1732560000
H 4.1365670000 -0.8267770000 1.0338000000
H 3.7166930000 -2.2762840000 0.0986540000
H 3.9657370000 -0.7446500000 -0.7404880000
C 0.4046630000 0.5087620000 -0.9899840000
C -0.2688280000 1.0329400000 0.2728360000
C 0.5782390000 1.9347940000 0.8816670000
C 1.8281440000 2.1152210000 0.0928550000
O -1.4173670000 0.6693650000 0.7482540000
H 0.3480290000 2.4443550000 1.8101370000
B -2.5576590000 -0.1319330000 0.0946340000
F -3.7018350000 0.5945380000 0.3027840000
F -2.5793620000 -1.3650820000 0.7390840000
F -2.2849960000 -0.2923650000 -1.2757210000
H 2.2413190000 3.1304040000 0.1020490000
H 2.6520000000 1.4572380000 0.4717440000
H -0.3159520000 0.3161660000 -1.7830810000
C 1.4306570000 1.6081470000 -1.3052640000
H 2.2796790000 1.2558560000 -1.9053310000
H 0.9390370000 2.4118970000 -1.8631460000
H 2.2201360000 -0.7083290000 2.2002640000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.230374 (Hartree/Particle)
Thermal correction to Energy= 0.245699
Thermal correction to Enthalpy= 0.246643
Thermal correction to Gibbs (Free) Energy= 0.188190
Sum of electronic and zero-point Energies= -826.092473
Sum of electronic and thermal Energies= -826.077149
Sum of electronic and thermal Enthalpies= -826.076205
Sum of electronic and thermal (Free) Energies= -826.134657

Entry 19

RC

C -2.9029540000 -1.1614900000 1.0206750000
C -3.3252600000 -0.6677190000 -0.1483220000
H -3.6756020000 -1.4213350000 1.7411440000
O -2.3976950000 -0.2185600000 -1.0853710000
C -1.4759710000 -1.3891460000 1.4260380000
H -0.7863840000 -1.3750200000 0.5787380000
H -1.1356550000 -0.6339940000 2.1514370000
H -1.3705670000 -2.3597700000 1.9256540000
C -4.7606610000 -0.4889920000 -0.5520300000
H -4.9899990000 0.5660220000 -0.7546100000
H -4.9882560000 -1.0511620000 -1.4707630000
H -5.4377750000 -0.8471040000 0.2274400000
C 0.8553050000 1.9976260000 1.2724480000
C 1.4098490000 1.0089020000 0.4450400000
C 0.7661760000 1.1589500000 -0.8145950000
C -0.2779030000 2.1913610000 -0.8015990000
O 2.3155780000 0.1551210000 0.7914340000
H 1.0235240000 0.5586360000 -1.6785400000
B 2.6275260000 -0.9807730000 -0.2239290000
F 1.3934180000 -1.5847420000 -0.5068210000
F 3.5168890000 -1.8090850000 0.3894310000
F 3.1217830000 -0.3644000000 -1.3737440000
H -0.1547200000 2.9172700000 -1.6182590000
H -1.2511700000 1.6978880000 -0.9748990000
H 1.1579740000 2.1353420000 2.3068610000
C -0.1829410000 2.8108850000 0.6035830000
H -1.1340150000 2.7778920000 1.1557120000
H 0.0986650000 3.8744620000 0.5679010000
H -2.7593660000 -0.3659690000 -1.9738900000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.225495 (Hartree/Particle)
Thermal correction to Energy= 0.243271
Thermal correction to Enthalpy= 0.244215
Thermal correction to Gibbs (Free) Energy= 0.175815
Sum of electronic and zero-point Energies= -826.095042
Sum of electronic and thermal Energies= -826.077266

Sum of electronic and thermal Enthalpies= -826.076322
Sum of electronic and thermal (Free) Energies= -826.144722

TS

C 1.6251790000 -1.3671410000 -0.8113470000
C 1.9185840000 -1.1049930000 0.5117800000
H 2.4910810000 -1.3738890000 -1.4711250000
O 0.9175330000 -1.1666220000 1.3895350000
C 0.4352090000 -2.1962870000 -1.2358260000
H -0.4078200000 -2.0861700000 -0.5525280000
H 0.0951280000 -1.9240790000 -2.2392880000
H 0.7397540000 -3.2515130000 -1.2669330000
C 3.2806960000 -0.7407680000 1.0261880000
H 3.2492590000 0.1302600000 1.6913780000
H 3.6862030000 -1.5816690000 1.6059890000
H 3.9768800000 -0.5356160000 0.2108720000
C 0.9349190000 0.7023660000 -1.3045490000
C -0.2850230000 0.8896220000 -0.5471350000
C -0.0322330000 1.8418540000 0.4276710000
C 1.3523170000 2.3982110000 0.3463830000
O -1.3647160000 0.2268290000 -0.8468890000
H -0.7874800000 2.1841190000 1.1217320000
B -2.4723320000 -0.1104230000 0.1725130000
F -2.0515320000 -1.2708790000 0.8268350000
F -3.6109910000 -0.3063660000 -0.5684240000
F -2.5971880000 0.9491500000 1.0761090000
H 1.3477480000 3.4960590000 0.2944540000
H 1.9579390000 2.1552550000 1.2326470000
H 0.8969150000 0.2917920000 -2.3084290000
C 1.9283960000 1.7695420000 -0.9459770000
H 2.9587920000 1.4119280000 -0.8515370000
H 1.9405230000 2.5121430000 -1.7567720000
H 1.1833440000 -0.8597450000 2.2720060000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.228075 (Hartree/Particle)
Thermal correction to Energy= 0.243867
Thermal correction to Enthalpy= 0.244811
Thermal correction to Gibbs (Free) Energy= 0.184184
Sum of electronic and zero-point Energies= -826.086593
Sum of electronic and thermal Energies= -826.070801
Sum of electronic and thermal Enthalpies= -826.069857
Sum of electronic and thermal (Free) Energies= -826.130483

PC

C 1.5739620000 -0.8660740000 -0.9081480000
C 1.8730440000 -0.9392570000 0.5239860000
H 2.5169410000 -0.9519500000 -1.4592450000
O 0.8189040000 -0.9077700000 1.2837860000
C 0.5935730000 -1.9852980000 -1.3487630000
H -0.3265840000 -1.9611190000 -0.7630600000
H 0.3358150000 -1.8365390000 -2.4010610000
H 1.0740540000 -2.9647980000 -1.2467410000
C 3.2388100000 -1.0742140000 1.1067050000
H 3.2748880000 -0.7867420000 2.1629520000
H 3.5576790000 -2.1256490000 1.0308500000
H 3.9649110000 -0.4811400000 0.5440470000
C 0.9592440000 0.5956620000 -1.2884040000
C -0.3059390000 0.8973310000 -0.5177910000
C -0.0281280000 1.7855910000 0.4917760000
C 1.4150690000 2.1825470000 0.4777140000
O -1.4020720000 0.2782570000 -0.8549470000
H -0.7607360000 2.1324480000 1.2063300000
B -2.4719320000 -0.1557140000 0.1642070000
F -1.9701560000 -1.3314370000 0.7493750000
F -3.6134420000 -0.3849680000 -0.5626290000
F -2.6345980000 0.8388460000 1.1259770000
H 1.5924190000 3.2444330000 0.6879190000
H 2.0002930000 1.6329590000 1.2487680000
H 0.7758880000 0.4904890000 -2.3624180000
C 1.8942020000 1.7587670000 -0.9283170000
H 2.9602530000 1.5016960000 -0.9736020000
H 1.7274080000 2.5793640000 -1.6339840000
H 1.0125200000 -0.8910640000 2.2404470000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.333051 (Hartree/Particle)
Thermal correction to Energy= 0.356244
Thermal correction to Enthalpy= 0.357188
Thermal correction to Gibbs (Free) Energy= 0.281030
Sum of electronic and zero-point Energies= -1234.729962
Sum of electronic and thermal Energies= -1234.706770
Sum of electronic and thermal Enthalpies= -1234.705826
Sum of electronic and thermal (Free) Energies= -1234.781984

Entry 20

RC

C 2.0735130000 -1.1340740000 0.9815350000
C 2.9816760000 -0.7750080000 0.0572220000
H 2.1995980000 -0.6989870000 1.9711530000
O 2.8605500000 -1.2386430000 -1.2399310000
C 0.9672690000 -2.1321160000 0.8044520000
H 1.1570120000 -3.0136410000 1.4332220000
H -0.0039750000 -1.7281220000 1.1091640000
H 0.8838780000 -2.4649520000 -0.2322410000
C 4.1436040000 0.1455280000 0.3035900000
H 5.0979860000 -0.3613900000 0.0971090000
H 4.1052820000 1.0301360000 -0.3489860000
H 4.1703260000 0.4822170000 1.3430270000
C 0.5760850000 1.1130470000 -0.8362500000
C -0.7423710000 0.7710190000 -0.4702990000
C -1.1898020000 1.7995050000 0.3897510000
C -0.1752930000 2.8517410000 0.6014590000
O -1.3598500000 -0.2971800000 -0.8599110000
H -2.1801820000 1.8042150000 0.8291470000
B -2.6385250000 -0.7049220000 -0.0782050000
F -3.0776690000 -1.8656400000 -0.6417760000
F -3.5449260000 0.3517060000 -0.1921940000
F -2.2280180000 -0.8416360000 1.2540080000
H -0.5691700000 3.8492870000 0.3569770000
H 0.1154900000 2.9075110000 1.6622870000
H 1.1865740000 0.4917020000 -1.4848750000
C 1.0035080000 2.4217900000 -0.2937420000
H 1.9552080000 2.3449860000 0.2483740000
H 1.1840330000 3.1422040000 -1.1069150000
H 3.7113420000 -1.1424400000 -1.6943330000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.226049 (Hartree/Particle)
Thermal correction to Energy= 0.243605
Thermal correction to Enthalpy= 0.244549
Thermal correction to Gibbs (Free) Energy= 0.178348
Sum of electronic and zero-point Energies= -826.093758
Sum of electronic and thermal Energies= -826.076202
Sum of electronic and thermal Enthalpies= -826.075258
Sum of electronic and thermal (Free) Energies= -826.141459

TS

C 1.6619450000 -0.5659740000 0.7685190000
C 2.8343280000 -0.8157160000 0.0741130000
H 1.7488210000 0.2058860000 1.5301280000
O 2.8596720000 -1.8857130000 -0.7377810000
C 0.6572720000 -1.6655210000 1.0291570000
H 1.0636330000 -2.3353460000 1.7988940000
H -0.2955830000 -1.2704100000 1.3831770000
H 0.4572520000 -2.2565360000 0.1335290000
C 4.0621330000 0.0403370000 0.0941900000
H 4.9373290000 -0.5712300000 0.3532900000
H 4.2542660000 0.4870060000 -0.8922600000
H 3.9842950000 0.8420890000 0.8293760000
C 0.8180040000 0.7100700000 -0.7254670000
C -0.6013900000 0.6658100000 -0.4106640000
C -0.9200450000 1.8177770000 0.2861060000
C 0.2585460000 2.7094460000 0.4897550000
O -1.3418400000 -0.3400330000 -0.7812710000
H -1.9313820000 2.0590570000 0.5862390000
B -2.7117750000 -0.5492450000 -0.0995540000
F -3.2489160000 -1.6668750000 -0.6830020000
F -3.4756660000 0.5986330000 -0.3029490000
F -2.4468810000 -0.7212150000 1.2672610000
H 0.0410650000 3.7589410000 0.2520070000
H 0.6023570000 2.7055800000 1.5377130000
H 1.1738750000 0.1329300000 -1.5741640000
C 1.3234690000 2.1050180000 -0.4559970000
H 2.3446120000 2.1550650000 -0.0677930000

H 1.3243190000 2.6557750000 -1.4070130000
H 3.6889630000 -1.9189890000 -1.2430040000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.228509 (Hartree/Particle)
Thermal correction to Energy= 0.244229
Thermal correction to Enthalpy= 0.245173
Thermal correction to Gibbs (Free) Energy= 0.184404
Sum of electronic and zero-point Energies= -826.086534
Sum of electronic and thermal Energies= -826.070814
Sum of electronic and thermal Enthalpies= -826.069870
Sum of electronic and thermal (Free) Energies= -826.130639

PC

C 1.3899030000 -0.6222690000 0.3912050000
C 2.8086510000 -0.7235970000 0.1372650000
H 1.2377630000 -0.1481940000 1.3638870000
O 3.1658630000 -1.4574290000 -0.8997290000
C 0.6296950000 -1.9648280000 0.3051890000
H 1.1359980000 -2.7163640000 0.9209640000
H -0.3876910000 -1.8285700000 0.6730960000
H 0.5800800000 -2.3308450000 -0.7230910000
C 3.8820170000 -0.0560160000 0.9271140000
H 4.4313490000 -0.8192750000 1.5007720000
H 4.6096860000 0.4546510000 0.2813900000
H 3.4677410000 0.6630370000 1.6341000000
C 0.8208730000 0.4520980000 -0.7444640000
C -0.6382100000 0.7073670000 -0.4483010000
C -0.7712030000 1.9231030000 0.1704990000
C 0.5438920000 2.6201770000 0.3376070000
O -1.5183370000 -0.1927630000 -0.7841300000
H -1.7297940000 2.3372890000 0.4509720000
B -2.7843410000 -0.4488770000 0.0574260000
F -3.5814090000 -1.2598450000 -0.7116500000
F -3.3856380000 0.7678920000 0.3635770000
F -2.3354660000 -1.0908920000 1.2230560000
H 0.4956680000 3.6931850000 0.1125700000
H 0.9332920000 2.5459150000 1.3687650000
H 0.9827100000 -0.0614810000 -1.6967240000
C 1.4510550000 1.8517550000 -0.6571460000
H 2.5122200000 1.8661450000 -0.3811970000
H 1.3698170000 2.3201690000 -1.6440990000
H 4.1252270000 -1.4108800000 -1.0663180000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.230364 (Hartree/Particle)
Thermal correction to Energy= 0.246062
Thermal correction to Enthalpy= 0.247006
Thermal correction to Gibbs (Free) Energy= 0.186391
Sum of electronic and zero-point Energies= -826.089848
Sum of electronic and thermal Energies= -826.074150
Sum of electronic and thermal Enthalpies= -826.073206
Sum of electronic and thermal (Free) Energies= -826.133821

9b

SEE RT (*gauche*)

C 2.6106990000 0.0047500000 0.0497640000
H 3.4531630000 -0.6313490000 0.3122890000
C 1.4361610000 -0.6042230000 -0.1633350000
C 2.8690380000 1.4786080000 -0.0580490000
H 3.2141380000 1.8966280000 0.8981460000
H 3.6558960000 1.6912140000 -0.7948660000
H 1.9675790000 2.0166700000 -0.3614800000
C 1.2374880000 -2.0931640000 -0.0686730000
H 0.5036130000 -2.3576000000 0.7048860000
H 0.8626200000 -2.4952160000 -1.0186320000
H 2.1763600000 -2.5982590000 0.1745490000
O 0.3362590000 0.1224900000 -0.5620610000
Si -1.2446430000 0.1751730000 0.0184070000
C -1.9338530000 1.7844760000 -0.6679960000
H -2.9864920000 1.9176790000 -0.3897220000
H -1.3748150000 2.6483370000 -0.2909460000
H -1.8731140000 1.8014180000 -1.7622460000
C -2.2545180000 -1.2807970000 -0.6345280000
H -1.9009550000 -2.2431990000 -0.2482360000
H -3.3084330000 -1.1768640000 -0.3462100000
H -2.2148420000 -1.3261380000 -1.7292710000
C -1.2462590000 0.1854980000 1.9057520000
H -0.6637600000 1.0279130000 2.2962430000
H -2.2688940000 0.2790850000 2.2922500000
H -0.8196660000 -0.7335510000 2.3244320000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.215435 (Hartree/Particle)
Thermal correction to Energy= 0.229586
Thermal correction to Enthalpy= 0.230530
Thermal correction to Gibbs (Free) Energy= 0.174371
Sum of electronic and zero-point Energies= -640.946086
Sum of electronic and thermal Energies= -640.931935
Sum of electronic and thermal Enthalpies= -640.930991
Sum of electronic and thermal (Free) Energies= -640.987150

SEE TS (*gauche* ↔ *anti* ↔ *gauche*)

C 2.7146360000 -0.0601310000 -0.0001190000
H 3.5295370000 -0.7801180000 -0.0001230000
C 1.4691100000 -0.5567710000 -0.0000480000
C 3.0781050000 1.3953560000 -0.0001920000
H 3.6809070000 1.6570020000 0.8807590000
H 3.6808370000 1.6569310000 -0.8812130000
H 2.1850310000 2.0248970000 -0.0001820000
C 1.1674730000 -2.0311100000 0.0000230000
H 0.5859370000 -2.3223710000 0.8843670000
H 0.5858660000 -2.3224410000 -0.8842510000
H 2.0931400000 -2.6128230000 0.0000090000
O 0.3973250000 0.3019420000 -0.0000410000
Si -1.2795650000 0.1799940000 0.0000510000
C -1.9079820000 -0.6967620000 -1.5501390000
H -3.0005840000 -0.6141010000 -1.6153940000
H -1.4881650000 -0.2443180000 -2.4561920000
H -1.6600480000 -1.7639720000 -1.5626630000
C -1.9078230000 -0.6966190000 1.5503860000
H -1.4879120000 -0.2440940000 2.4563540000
H -3.0004190000 -0.6139520000 1.6157470000
H -1.6598900000 -1.7638290000 1.5629820000
C -1.8482650000 1.9724690000 -0.0000020000
H -1.4787840000 2.5034680000 -0.8846280000
H -2.9429830000 2.0421320000 0.0000480000
H -1.4786970000 2.5035480000 0.8845400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.215448 (Hartree/Particle)
Thermal correction to Energy= 0.228694
Thermal correction to Enthalpy= 0.229638
Thermal correction to Gibbs (Free) Energy= 0.176770
Sum of electronic and zero-point Energies= -640.945540
Sum of electronic and thermal Energies= -640.932294
Sum of electronic and thermal Enthalpies= -640.931349
Sum of electronic and thermal (Free) Energies= -640.984218

SEE TS (*gauche* ↔ *syn* ↔ *gauche*)

C -2.3156900000 -0.5930950000 0.0000070000
H -3.3993660000 -0.4998950000 -0.0000040000
C -1.6475240000 0.5708800000 -0.0000410000
C -1.7960880000 -2.0004620000 0.0000720000
H -2.1528500000 -2.5529690000 0.8807370000
H -2.1528130000 -2.5530380000 -0.8805640000
H -0.7068220000 -2.0582370000 0.0000980000
C -2.3432270000 1.9069840000 -0.0001040000
H -2.0499240000 2.4911030000 0.8813010000
H -2.0499140000 2.4910250000 -0.8815560000
H -3.4304940000 1.7943420000 -0.0001050000
O -0.2925450000 0.7492340000 -0.0000410000
Si 1.2197980000 0.0288090000 0.0000090000
C 1.4988220000 -0.9947980000 -1.5618490000
H 2.5412800000 -1.3358510000 -1.6055800000
H 0.8585120000 -1.8806860000 -1.6227560000
H 1.3134540000 -0.3892380000 -2.4569410000
C 2.4067070000 1.4899400000 -0.0000540000
H 2.2587170000 2.1198170000 0.8845620000
H 3.4507920000 1.1530470000 -0.0000270000
H 2.2587340000 2.1197270000 -0.8847360000
C 1.4987910000 -0.9946400000 1.5619760000
H 0.8584750000 -1.8805190000 1.6229620000
H 2.5412470000 -1.3356950000 1.6057580000
H 1.3134120000 -0.3889890000 2.4570030000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.215376 (Hartree/Particle)
Thermal correction to Energy= 0.228769
Thermal correction to Enthalpy= 0.229714
Thermal correction to Gibbs (Free) Energy= 0.176107
Sum of electronic and zero-point Energies= -640.941422
Sum of electronic and thermal Energies= -640.928029
Sum of electronic and thermal Enthalpies= -640.927085
Sum of electronic and thermal (Free) Energies= -640.980691

Entry 30

RC

C -0.0924610000 -1.3531340000 0.9884810000
C -0.8204410000 -0.6867150000 0.0557620000
O -2.0117670000 -0.1159470000 0.4019700000
Si -3.5358230000 -0.1204890000 -0.3619780000
C -0.3482250000 -0.4972680000 -1.3555480000
H -1.0244780000 -0.9944000000 -2.0639450000
H -0.3354710000 0.5680210000 -1.6237260000
H 0.6551040000 -0.9072260000 -1.4881240000
C -3.9457910000 -1.8719150000 -0.9171300000
H -4.9520740000 -1.9100910000 -1.3524780000
H -3.2468750000 -2.2431980000 -1.6751700000
H -3.9226510000 -2.5702460000 -0.0727900000
C -3.5567230000 1.0799490000 -1.8154470000
H -3.2595930000 2.0888110000 -1.5051270000
H -2.8908900000 0.7681360000 -2.6271720000
H -4.5702470000 1.1512750000 -2.2301710000
C -4.7008520000 0.4682180000 0.9884760000
H -5.7314560000 0.5293170000 0.6184000000
H -4.6930610000 -0.2148230000 1.8451990000
H -4.4201970000 1.4634400000 1.3521150000
C 1.0526470000 1.0974540000 1.4694340000
C 2.1557220000 0.9090390000 0.5950060000
C 2.0976090000 1.9386760000 -0.3505850000
C 0.9743270000 2.8816450000 -0.1042990000
O 3.0020080000 -0.0689530000 0.7423660000
H 2.8178710000 2.0381540000 -1.1526250000
B 3.6653150000 -0.7543980000 -0.4641630000
F 2.6706470000 -1.5810790000 -1.0210840000
F 4.7184130000 -1.4702080000 0.0333280000
F 4.0527970000 0.2238590000 -1.3825470000
H 1.3534530000 3.8925840000 0.1108120000
H 0.3260710000 2.9954360000 -0.9837300000
H 0.9363810000 0.5445170000 2.3932010000
C 0.2437260000 2.2872300000 1.1213400000
H -0.7956670000 1.9975350000 0.9020890000
H 0.1846920000 2.9876300000 1.9668120000
C -0.5588830000 -1.6939310000 2.3721420000
H -1.4387540000 -1.1140850000 2.6634420000
H -0.8194740000 -2.7598660000 2.4339040000
H 0.2351190000 -1.5348540000 3.1128650000
H 0.8645750000 -1.7466600000 0.6569770000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.329281 (Hartree/Particle)
Thermal correction to Energy= 0.354037
Thermal correction to Enthalpy= 0.354981
Thermal correction to Gibbs (Free) Energy= 0.272900
Sum of electronic and zero-point Energies= -1234.716636
Sum of electronic and thermal Energies= -1234.691880
Sum of electronic and thermal Enthalpies= -1234.690935
Sum of electronic and thermal (Free) Energies= -1234.773016

TS

C -0.0252870000 -1.0269690000 -1.3761800000
C 0.7617610000 -0.7340130000 -0.2909350000
O 2.0103870000 -0.2734080000 -0.5040940000
Si 3.4433000000 -0.2069310000 0.4360080000
C 0.2535080000 -0.8327850000 1.1121050000
H 0.9517190000 -1.3950770000 1.7433040000
H 0.1464750000 0.1691820000 1.5545550000
H -0.7260050000 -1.3136350000 1.1417100000
C 3.8988170000 -1.9483690000 0.9827030000
H 4.8728910000 -1.9415910000 1.4877480000
H 3.1724270000 -2.3787360000 1.6806660000
H 3.9771700000 -2.6230760000 0.1226390000
C 3.2265000000 0.9541340000 1.9026860000
H 2.8845970000 1.9455590000 1.5824350000
H 2.5148080000 0.5734030000 2.6424000000
H 4.1887860000 1.0910820000 2.4121960000
C 4.6974630000 0.4790800000 -0.7792880000
H 5.6850800000 0.5707440000 -0.3113910000
H 4.8009050000 -0.1742040000 -1.6527480000
H 4.4066600000 1.4731430000 -1.1375500000
C -1.0110650000 1.1728590000 -1.3878090000
C -2.0736860000 0.9875500000 -0.4441210000
C -1.8662650000 1.8795690000 0.5992010000
C -0.6829360000 2.7628470000 0.3740610000
O -3.0109010000 0.1032390000 -0.6560180000
H -2.5283620000 1.9533530000 1.4518900000
B -3.6231220000 -0.7393010000 0.4675410000
F -2.7115040000 -1.7959910000 0.6834790000
F -4.8287470000 -1.1915050000 0.0034510000
F -3.7365910000 0.0415110000 1.6183870000
H -0.9840940000 3.8198660000 0.3223420000
H 0.0477290000 2.7073880000 1.1927290000
H -1.1049830000 0.8473570000 -2.4165090000
C -0.1081420000 2.2890290000 -0.9854890000
H 0.9400700000 1.9674730000 -0.9205080000
H -0.1312050000 3.0840610000 -1.7437210000
C 0.4961620000 -1.1350300000 -2.7822600000
H 1.3309190000 -0.4529280000 -2.9663550000
H 0.8542970000 -2.1557900000 -2.9742960000
H -0.2934540000 -0.9392840000 -3.5160110000
H -1.0023070000 -1.4469440000 -1.1523650000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.329630 (Hartree/Particle)
Thermal correction to Energy= 0.353504
Thermal correction to Enthalpy= 0.354448
Thermal correction to Gibbs (Free) Energy= 0.274842
Sum of electronic and zero-point Energies= -1234.715844
Sum of electronic and thermal Energies= -1234.691971
Sum of electronic and thermal Enthalpies= -1234.691026
Sum of electronic and thermal (Free) Energies= -1234.770632

PC

C 0.2440300000 0.3998560000 1.4557900000
C -0.6479090000 -0.2510420000 0.4757900000
O -1.9168160000 -0.0183280000 0.5879270000
Si -3.3738490000 -0.5162640000 -0.2756560000
C -0.0917460000 -1.0807080000 -0.5947540000
H -0.8386870000 -1.5482450000 -1.2355360000
H 0.5980170000 -0.4424470000 -1.1922340000
H 0.6217080000 -1.8057190000 -0.1758890000
C -3.5297120000 -2.3754460000 -0.0884260000
H -4.4943540000 -2.7051980000 -0.4942300000
H -2.7452770000 -2.9277200000 -0.6155540000
H -3.5003210000 -2.6699110000 0.9666900000
C -3.2331020000 0.0717380000 -2.0509240000
H -2.9678500000 1.1341740000 -2.0972000000
H -2.4929270000 -0.4867580000 -2.6323680000
H -4.2025130000 -0.0454360000 -2.5515120000
C -4.6892030000 0.4110830000 0.6769550000
H -5.6846900000 0.1955680000 0.2705220000
H -4.6911670000 0.1249880000 1.7343720000
H -4.5337560000 1.4940780000 0.6210040000
C 1.0685630000 1.6192320000 0.7828010000
C 2.1408690000 1.0961750000 -0.1423770000
C 1.9127790000 1.4855660000 -1.4231620000
C 0.6910270000 2.3583460000 -1.5432790000
O 3.0806890000 0.3357150000 0.3853970000
H 2.5384120000 1.2016300000 -2.2604040000
B 3.3254930000 -1.0902840000 -0.0479110000
F 2.4084390000 -1.8957310000 0.7074980000
F 4.6194380000 -1.4131800000 0.2602380000
F 3.0245500000 -1.2358120000 -1.4037830000
H 0.8880120000 3.2957930000 -2.0805530000
H -0.1179790000 1.8628120000 -2.1073160000
H 1.5212110000 2.0798720000 1.6679750000
C 0.2765840000 2.6352870000 -0.0670200000
H -0.8074090000 2.5806010000 0.0881920000
H 0.5777260000 3.6487730000 0.2161860000
C -0.4693130000 0.8665120000 2.7285850000

H -1.1695380000 1.6834320000 2.5273380000
H -1.0284050000 0.0512190000 3.1996770000
H 0.2748180000 1.2233180000 3.4466620000
H 1.0413640000 -0.3218930000 1.6808710000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.332495 (Hartree/Particle)
Thermal correction to Energy= 0.355638
Thermal correction to Enthalpy= 0.356582
Thermal correction to Gibbs (Free) Energy= 0.279754
Sum of electronic and zero-point Energies= -1234.731883
Sum of electronic and thermal Energies= -1234.708740
Sum of electronic and thermal Enthalpies= -1234.707796
Sum of electronic and thermal (Free) Energies= -1234.784625

Entry 31

RC

C 0.2359390000 -1.3502120000 -0.1053440000
C 1.2965400000 -0.8149670000 -0.7490510000
H -0.3988170000 -2.0222020000 -0.6775580000
O 2.1114650000 0.0930350000 -0.1196460000
Si 3.7417340000 -0.0470380000 0.3512900000
C -0.1168900000 -1.1551630000 1.3351420000
H 0.4466170000 -0.3329370000 1.7854800000
H -1.1926460000 -0.9800030000 1.4543240000
H 0.1060720000 -2.0683390000 1.9057810000
C 1.6437700000 -1.1087480000 -2.1833200000
H 1.7363600000 -0.1808260000 -2.7626370000
H 2.6099320000 -1.6249300000 -2.2592690000
H 0.8874310000 -1.7447230000 -2.6512260000
C 4.8746120000 0.3483030000 -1.1033400000
H 5.9218780000 0.3680170000 -0.7760830000
H 4.7974480000 -0.3915970000 -1.9078760000
H 4.6453780000 1.3316630000 -1.5304680000
C 4.0494670000 -1.7888550000 0.9949150000
H 3.4034190000 -2.0168540000 1.8501240000
H 3.8637680000 -2.5491450000 0.2273200000
H 5.0901730000 -1.9007060000 1.3230810000
C 3.9381820000 1.2465200000 1.6993800000
H 4.9698460000 1.2731460000 2.0705410000
H 3.6954910000 2.2491130000 1.3282500000
H 3.2821040000 1.0362200000 2.5514540000
C -1.0189470000 1.0165680000 -1.2966220000
C -2.1766660000 0.6890990000 -0.5551690000
C -2.2884070000 1.6612710000 0.4537230000
C -1.1944700000 2.6593000000 0.4092950000
O -2.9249190000 -0.3415520000 -0.8064690000
H -3.1028180000 1.6808950000 1.1671300000
B -4.0699430000 -0.6619360000 0.1847070000
F -3.4594530000 -0.8553440000 1.4345740000
F -4.6812610000 -1.7847270000 -0.2954160000
F -4.8992740000 0.4565120000 0.2320460000
H -1.5893610000 3.6760490000 0.2622140000
H -0.6451490000 2.6949580000 1.3615360000
H -0.7512670000 0.5086160000 -2.2160070000
C -0.3164040000 2.2087760000 -0.7763350000
H 0.7089660000 1.9467070000 -0.4698080000
H -0.2122260000 2.9839190000 -1.5494360000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.328630 (Hartree/Particle)
Thermal correction to Energy= 0.353664
Thermal correction to Enthalpy= 0.354608
Thermal correction to Gibbs (Free) Energy= 0.270736
Sum of electronic and zero-point Energies= -1234.716069
Sum of electronic and thermal Energies= -1234.691035
Sum of electronic and thermal Enthalpies= -1234.690091
Sum of electronic and thermal (Free) Energies= -1234.773963

TS

C -0.0123370000 -0.9648520000 0.1785960000
C 1.2393030000 -0.8655420000 -0.3814720000
H -0.7158860000 -1.6323840000 -0.3120870000
O 2.1778550000 -0.1541420000 0.2584180000
Si 3.8928290000 -0.0609220000 0.2302650000
C -0.3261270000 -0.5867760000 1.5984470000
H 0.1521720000 0.3529810000 1.8913520000
H -1.4075510000 -0.5215310000 1.7420770000
H 0.0485440000 -1.3663240000 2.2760280000
C 1.5804960000 -1.4513350000 -1.7214570000
H 1.8889020000 -0.6698140000 -2.4278350000
H 2.4150820000 -2.1581600000 -1.6350940000
H 0.7275440000 -1.9886250000 -2.1418500000
C 4.4971800000 0.5703460000 -1.4376820000
H 5.5722950000 0.7832370000 -1.3810050000
H 4.3511380000 -0.1528570000 -2.2469440000
H 3.9956570000 1.5031340000 -1.7206200000
C 4.5895710000 -1.7623210000 0.6276860000
H 4.1857650000 -2.1424790000 1.5728040000
H 4.3749250000 -2.5026440000 -0.1512020000
H 5.6804020000 -1.7074430000 0.7321970000
C 4.2575430000 1.1747180000 1.5911320000
H 5.3381320000 1.3218320000 1.7064090000
H 3.8106210000 2.1516200000 1.3747810000
H 3.8616980000 0.8314510000 2.5532010000
C -0.8474940000 0.7147250000 -1.1027950000
C -2.1823700000 0.6233550000 -0.5708570000
C -2.4306010000 1.7782910000 0.1508310000
C -1.2711080000 2.7154400000 0.1625530000
O -2.9158300000 -0.4368310000 -0.7755860000
H -3.3877930000 1.9860030000 0.6120780000
B -4.1327170000 -0.6888250000 0.1400000000
F -3.6272980000 -0.8052380000 1.4436310000
F -4.7012440000 -1.8505200000 -0.3133080000
F -4.9805380000 0.4134580000 0.0466950000
H -1.5427400000 3.7045980000 -0.2341060000
H -0.9025650000 2.8971550000 1.1826820000
H -0.5857730000 0.1853540000 -2.0121600000
C -0.2177940000 2.0246040000 -0.7399230000
H 0.7519010000 1.8969960000 -0.2419600000
H -0.0205310000 2.6095000000 -1.6486310000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.330020 (Hartree/Particle)
Thermal correction to Energy= 0.353857
Thermal correction to Enthalpy= 0.354801
Thermal correction to Gibbs (Free) Energy= 0.274573
Sum of electronic and zero-point Energies= -1234.712830
Sum of electronic and thermal Energies= -1234.688993
Sum of electronic and thermal Enthalpies= -1234.688049
Sum of electronic and thermal (Free) Energies= -1234.768277

PC

C -0.1360580000 -0.5293060000 0.0504380000
C 1.2217610000 -0.7225130000 -0.4034290000
H -0.7663410000 -1.3665610000 -0.2842160000
O 2.1933850000 -0.2610100000 0.3230830000
Si 3.9414720000 -0.1229350000 0.2244150000
C -0.3274370000 -0.2764040000 1.5442740000
H 0.0639060000 0.6978690000 1.8518580000
H -1.3946870000 -0.3313040000 1.7710230000
H 0.1898780000 -1.0453690000 2.1287850000
C 1.5206170000 -1.3946440000 -1.7064890000
H 2.2117660000 -0.8034710000 -2.3181670000
H 2.0009300000 -2.3624220000 -1.5084940000
H 0.6062900000 -1.5825580000 -2.2713310000
C 4.3337350000 1.0827820000 -1.1593750000
H 5.4038520000 1.3248330000 -1.1408180000
H 4.1089480000 0.6847490000 -2.1547180000
H 3.7829560000 2.0218590000 -1.0358190000
C 4.6574960000 -1.8356460000 -0.0547920000
H 4.2682190000 -2.5574920000 0.6722040000
H 4.4674500000 -2.2237490000 -1.0607720000
H 5.7460980000 -1.7968950000 0.0779910000
C 4.3585760000 0.5584710000 1.9131650000
H 5.4397690000 0.7111150000 2.0142760000
H 3.8667560000 1.5219410000 2.0854780000
H 4.0415060000 -0.1264060000 2.7071570000
C -0.7585610000 0.6659610000 -0.8939610000
C -2.2294300000 0.6788360000 -0.5533160000
C -2.5874760000 1.8801290000 -0.0310210000
C -1.4338220000 2.8328630000 0.0818020000
O -2.8828440000 -0.4398720000 -0.7554550000
H -3.6044440000 2.1200150000 0.2505540000
B -4.0503320000 -0.8348140000 0.1676080000
F -3.4973790000 -1.0258750000 1.4442910000

F -4.5507820000 -2.0036220000 -0.3578750000
F -4.9823550000 0.1972020000 0.1808510000
H -1.6345380000 3.7972050000 -0.4071210000
H -1.2028780000 3.0753500000 1.1308180000
H -0.6001770000 0.3441250000 -1.9284510000
C -0.2516190000 2.0927870000 -0.6125440000
H 0.6560660000 2.1047670000 0.0020870000
H 0.0033560000 2.5853600000 -1.5571140000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.332281 (Hartree/Particle)
Thermal correction to Energy= 0.356057
Thermal correction to Enthalpy= 0.357002
Thermal correction to Gibbs (Free) Energy= 0.277119
Sum of electronic and zero-point Energies= -1234.720107
Sum of electronic and thermal Energies= -1234.696330
Sum of electronic and thermal Enthalpies= -1234.695386
Sum of electronic and thermal (Free) Energies= -1234.775268

Entry 32

RC

C 0.1225660000 0.5493990000 1.4159510000
C 0.9795910000 -0.1989020000 0.6658580000
H -0.7996900000 0.0591990000 1.7124060000
O 2.1531760000 0.3531490000 0.2669600000
Si 3.6506580000 -0.2647800000 -0.2643330000
C 0.4690910000 1.8700040000 2.0382380000
H 1.2601300000 2.3880420000 1.4881240000
H -0.4070430000 2.5253610000 2.1089870000
H 0.8269840000 1.7275700000 3.0683250000
C 0.6685730000 -1.6021390000 0.2340980000
H 0.6265770000 -1.6828890000 -0.8589430000
H 1.4477550000 -2.2905890000 0.5868060000
H -0.2954750000 -1.9190770000 0.6325090000
C 3.4734320000 -1.1738390000 -1.9047210000
H 4.4667630000 -1.4245760000 -2.2985690000
H 2.9107680000 -2.1084000000 -1.8124380000
H 2.9722570000 -0.5518780000 -2.6557760000
C 4.3836750000 -1.3791890000 1.0650000000
H 4.4441840000 -0.8582040000 2.0274100000
H 3.8014090000 -2.2948070000 1.2160420000
H 5.4014730000 -1.6807110000 0.7868850000
C 4.6837430000 1.2886870000 -0.4844630000
H 5.6972580000 1.0410460000 -0.8226000000
H 4.2403440000 1.9598640000 -1.2289020000
H 4.7717390000 1.8438430000 0.4561520000
C -1.0250600000 1.3476970000 -0.9299740000
C -2.2087130000 0.5867300000 -0.7283710000
C -3.2114630000 1.4861120000 -0.3567600000
C -2.7311890000 2.8906700000 -0.2985710000
O -2.2504940000 -0.7057500000 -0.8883630000
H -4.2250790000 1.1742020000 -0.1398540000
B -3.1205360000 -1.5813000000 0.0309610000
F -2.4719630000 -1.5715930000 1.2806840000
F -3.1389800000 -2.8264730000 -0.5371860000
F -4.3882180000 -1.0089300000 0.1360230000
H -3.3285870000 3.5494120000 -0.9459280000
H -2.8305370000 3.3089270000 0.7141310000
H -0.1280070000 0.9417680000 -1.3801410000
C -1.2603430000 2.8027490000 -0.7620620000
H -0.5518680000 3.2590930000 -0.0593150000
H -1.1003060000 3.3221220000 -1.7192530000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.329266 (Hartree/Particle)
Thermal correction to Energy= 0.354112
Thermal correction to Enthalpy= 0.355056
Thermal correction to Gibbs (Free) Energy= 0.272129
Sum of electronic and zero-point Energies= -1234.714731
Sum of electronic and thermal Energies= -1234.689885
Sum of electronic and thermal Enthalpies= -1234.688941
Sum of electronic and thermal (Free) Energies= -1234.771868

TS

C 0.0290230000 0.6649050000 1.3086610000
C 0.9343860000 -0.1608620000 0.6820170000
H -0.8929770000 0.1860640000 1.6224830000
O 2.1325860000 0.3468990000 0.3481290000
Si 3.6056570000 -0.2870040000 -0.2614600000
C 0.4143900000 1.9693270000 1.9497440000
H 1.1794540000 2.5025990000 1.3778790000
H -0.4535400000 2.6223550000 2.0840680000
H 0.8274680000 1.7880030000 2.9521750000
C 0.6242630000 -1.5829220000 0.3259600000
H 0.5804670000 -1.7193650000 -0.7614620000
H 1.4083380000 -2.2448620000 0.7148450000
H -0.3405490000 -1.8790780000 0.7373580000
C 3.3408350000 -1.1178530000 -1.9290350000
H 4.3130480000 -1.3642780000 -2.3748410000
H 2.7685990000 -2.0480510000 -1.8547820000
H 2.8197140000 -0.4556380000 -2.6302970000
C 4.3456530000 -1.4676740000 1.0029570000
H 4.4251590000 -0.9931810000 1.9876920000
H 3.7619960000 -2.3872230000 1.1185860000
H 5.3574920000 -1.7594090000 0.6942570000
C 4.6595410000 1.2553500000 -0.4428320000
H 5.6598400000 1.0036810000 -0.8154390000
H 4.2111740000 1.9645240000 -1.1478300000
H 4.7804740000 1.7688940000 0.5174970000
C -0.9371190000 1.3227600000 -0.8317870000
C -2.1558640000 0.5751000000 -0.7174990000
C -3.1718350000 1.4677130000 -0.4157580000
C -2.6894600000 2.8747280000 -0.3162490000
O -2.1799280000 -0.7236200000 -0.8763310000
H -4.1999220000 1.1612740000 -0.2737110000
B -3.0606250000 -1.5906740000 0.0288500000
F -2.4712390000 -1.5149130000 1.3122920000
F -3.0024680000 -2.8606100000 -0.4849610000
F -4.3514110000 -1.0697800000 0.0585820000
H -3.2594960000 3.5523850000 -0.9677090000
H -2.8110440000 3.2734270000 0.7021160000
H -0.0672350000 0.9340630000 -1.3464190000
C -1.2051310000 2.7884930000 -0.7423670000
H -0.5186490000 3.3181700000 -0.0737350000
H -1.0531860000 3.2341840000 -1.7370260000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.329938 (Hartree/Particle)
Thermal correction to Energy= 0.353711
Thermal correction to Enthalpy= 0.354656
Thermal correction to Gibbs (Free) Energy= 0.274904
Sum of electronic and zero-point Energies= -1234.713858
Sum of electronic and thermal Energies= -1234.690085
Sum of electronic and thermal Enthalpies= -1234.689140
Sum of electronic and thermal (Free) Energies= -1234.768892

PC

C -1.0467920000 1.5528430000 1.0932740000
C 0.0936290000 0.4987730000 0.9692870000
H -1.7308800000 1.1839040000 1.8695550000
O 1.1249390000 1.0186530000 0.2395500000
Si 2.4792640000 0.4403870000 -0.6255400000
C -0.5536530000 2.9490370000 1.4675120000
H 0.1294240000 3.3386230000 0.7078520000
H -1.4041920000 3.6342520000 1.5536740000
H -0.0290680000 2.9503940000 2.4296820000
C 0.5146490000 -0.1249790000 2.2884800000
H 1.3071860000 -0.8583150000 2.1480860000
H 0.8851100000 0.6772060000 2.9348040000
H -0.3329790000 -0.6140940000 2.7721150000
C 3.6112010000 -0.6192110000 0.4421880000
H 4.5417300000 -0.8226660000 -0.1035890000
H 3.8829750000 -0.1132160000 1.3759110000
H 3.1515480000 -1.5808090000 0.6860050000
C 3.3444060000 2.0450920000 -1.0930570000
H 2.6910650000 2.6912640000 -1.6903450000
H 3.6500020000 2.6082450000 -0.2037500000
H 4.2453790000 1.8437140000 -1.6855130000
C 1.9130650000 -0.4798380000 -2.1640830000
H 2.7808740000 -0.7518940000 -2.7785770000
H 1.3748480000 -1.3991960000 -1.9171690000
H 1.2547790000 0.1445380000 -2.7793670000
C -1.7582980000 1.4326750000 -0.2621300000
C -1.7179950000 -0.0443010000 -0.4896070000
C -2.7885010000 -0.5604120000 -1.0878090000
C -3.7623370000 0.5735160000 -1.3696730000

O -0.5920650000 -0.6018730000 0.1034480000
H -2.9597890000 -1.5985250000 -1.3346360000
B -0.4386020000 -2.3215950000 0.3154390000
F -1.1929610000 -2.5792290000 1.4105870000
F 0.9088670000 -2.4599490000 0.4836290000
F -0.9171970000 -2.7859000000 -0.8647610000
H -3.7403040000 0.8745420000 -2.4280930000
H -4.7990630000 0.2923450000 -1.1492470000
H -1.1603400000 1.9589240000 -1.0220500000
C -3.2617550000 1.7267670000 -0.4427280000
H -3.7683840000 1.6535840000 0.5276600000
H -3.4636920000 2.7214130000 -0.8516420000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.334779 (Hartree/Particle)
Thermal correction to Energy= 0.357505
Thermal correction to Enthalpy= 0.358449
Thermal correction to Gibbs (Free) Energy= 0.283615
Sum of electronic and zero-point Energies= -1234.764788
Sum of electronic and thermal Energies= -1234.742062
Sum of electronic and thermal Enthalpies= -1234.741118
Sum of electronic and thermal (Free) Energies= -1234.815952

10a

ENL RT (*anti*)

C -0.7638060000 -0.6493060000 0.0000000000
C 0.4613270000 -0.1093200000 0.0000000000
O 1.5462980000 -0.9690780000 0.0000000000
H 2.3608890000 -0.4461850000 0.0000020000
C -2.0809830000 0.0711530000 0.0000000000
H -2.6815930000 -0.1976770000 -0.8802720000
H -2.6815930000 -0.1976780000 0.8802710000
H -1.9732710000 1.1601350000 0.0000000000
C 0.8210230000 1.3495530000 0.0000000000
H 1.4217270000 1.6017230000 -0.8857100000
H -0.0582180000 1.9955410000 0.0000000000
H 1.4217270000 1.6017230000 0.8857100000
H -0.8054150000 -1.7374330000 0.0000000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.112636 (Hartree/Particle)
Thermal correction to Energy= 0.119523
Thermal correction to Enthalpy= 0.120468
Thermal correction to Gibbs (Free) Energy= 0.082079
Sum of electronic and zero-point Energies= -232.327591
Sum of electronic and thermal Energies= -232.320703
Sum of electronic and thermal Enthalpies= -232.319759
Sum of electronic and thermal (Free) Energies= -232.358148

ENL TS (*anti* ↔ *syn*)

C -0.7458290000 -0.6466750000 -0.0180050000
C 0.4662170000 -0.0812000000 -0.0125710000
O 1.6029790000 -0.8956920000 -0.0964110000
H 1.8384490000 -1.1921140000 0.7960280000
C -2.0801550000 0.0419600000 0.0163850000
H -2.6751260000 -0.2118190000 -0.8715140000
H -2.6671740000 -0.2793500000 0.8877000000
H -1.9956610000 1.1314060000 0.0582650000
C 0.8077620000 1.3813330000 0.0043530000
H 1.4241710000 1.6272010000 -0.8691100000
H -0.0754200000 2.0244770000 -0.0020710000
H 1.4063290000 1.6283830000 0.8918620000
H -0.7673690000 -1.7351660000 -0.0608420000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.112132 (Hartree/Particle)
Thermal correction to Energy= 0.118211
Thermal correction to Enthalpy= 0.119155
Thermal correction to Gibbs (Free) Energy= 0.083099
Sum of electronic and zero-point Energies= -232.323635
Sum of electronic and thermal Energies= -232.317556
Sum of electronic and thermal Enthalpies= -232.316612
Sum of electronic and thermal (Free) Energies= -232.352669

ENL RT (*syn*)

C 0.7460160000 -0.6420030000 0.0000000000
C -0.4750700000 -0.0863010000 0.0000000000
O -1.6314530000 -0.8358940000 0.0000000000
H -1.3886570000 -1.7759730000 0.0000000000
C 2.0737680000 0.0615790000 0.0000000000
H 2.6710150000 -0.2118200000 0.8810380000
H 2.6710150000 -0.2118200000 -0.8810380000
H 1.9727800000 1.1506300000 0.0000000000
C -0.8237180000 1.3722240000 0.0000000000
H -1.4295410000 1.6138940000 0.8817150000
H 0.0619470000 2.0091240000 0.0000000000
H -1.4295410000 1.6138940000 -0.8817150000
H 0.7966310000 -1.7337650000 0.0000000000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.113314 (Hartree/Particle)
Thermal correction to Energy= 0.119740
Thermal correction to Enthalpy= 0.120685
Thermal correction to Gibbs (Free) Energy= 0.083960
Sum of electronic and zero-point Energies= -232.330270
Sum of electronic and thermal Energies= -232.323843
Sum of electronic and thermal Enthalpies= -232.322899
Sum of electronic and thermal (Free) Energies= -232.359623

Entry 21

RC

C 1.7988610000 -1.7452390000 -0.6715110000
C 2.1645340000 -1.0818630000 0.4503470000
H 2.5330990000 -1.7787630000 -1.4822040000
O 3.3864010000 -0.4522620000 0.5467370000
C 0.5579140000 -2.5653350000 -0.8770790000
H 0.8032710000 -3.6367900000 -0.8497200000
H -0.2138540000 -2.3640470000 -0.1330500000
H 0.1171110000 -2.3648930000 -1.8601620000
C 1.3793000000 -0.9215400000 1.7126060000
H 1.7824720000 -1.5808860000 2.4918810000
H 1.4848190000 0.1050060000 2.0843930000
H 0.3186250000 -1.1358830000 1.5760930000
C 0.8283220000 1.0011190000 -1.2972160000
C -0.4086170000 0.9591060000 -0.6072330000
C -0.3515750000 1.9717560000 0.3657680000
C 0.9201700000 2.7327620000 0.3265700000
O -1.3519520000 0.1164750000 -0.9010190000
H -1.1700670000 2.1744500000 1.0451580000
B -2.4492270000 -0.2709550000 0.1129080000
F -1.8317050000 -1.1375960000 1.0312600000
F -3.4304410000 -0.8856430000 -0.6120090000
F -2.8875280000 0.8881790000 0.7560500000
H 0.7336840000 3.7890050000 0.0773540000
H 1.4230030000 2.7492310000 1.3035050000
H 1.0223220000 0.4072380000 -2.1830160000
C 1.7461980000 2.0345410000 -0.7743100000
H 2.6551690000 1.5661080000 -0.3611630000
H 2.0872250000 2.7175650000 -1.5651850000
H 3.9300910000 -0.7025760000 -0.2195270000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227121 (Hartree/Particle)
Thermal correction to Energy= 0.243943
Thermal correction to Enthalpy= 0.244887
Thermal correction to Gibbs (Free) Energy= 0.182262
Sum of electronic and zero-point Energies= -826.100595
Sum of electronic and thermal Energies= -826.083773
Sum of electronic and thermal Enthalpies= -826.082829
Sum of electronic and thermal (Free) Energies= -826.145454

TS

C 1.5922560000 -1.4837290000 -0.7319800000
C 1.7481100000 -1.2307430000 0.6156060000
H 2.5165960000 -1.4687970000 -1.3171520000
O 2.9435890000 -0.8333420000 1.1100430000
C 0.4545650000 -2.2594570000 -1.3485420000
H 0.7052320000 -3.3290130000 -1.3577690000
H -0.4919210000 -2.1165740000 -0.8259850000
H 0.3027110000 -1.9574470000 -2.3902400000
C 0.6782910000 -1.2023880000 1.6404860000
H 1.0596610000 -1.5733870000 2.5961460000
H 0.3606030000 -0.1548120000 1.7920970000

H -0.2182530000 -1.7408620000 1.3363590000
C 1.0578050000 0.7046570000 -1.2497640000
C -0.1871870000 0.9785620000 -0.5768240000
C 0.0427380000 1.9898970000 0.3430760000
C 1.4547850000 2.4758220000 0.3291600000
O -1.2689980000 0.3174170000 -0.8829370000
H -0.7356140000 2.4109760000 0.9650760000
B -2.3946890000 -0.0342970000 0.1032280000
F -2.2215560000 -1.4031470000 0.3840880000
F -3.5830630000 0.2130830000 -0.5306560000
F -2.2295120000 0.7179220000 1.2684740000
H 1.5062350000 3.5546880000 0.1234190000
H 1.9539680000 2.3333930000 1.2974260000
H 1.0616340000 0.2611700000 -2.2394790000
C 2.1215450000 1.6610170000 -0.8069620000
H 3.0408000000 1.1621180000 -0.4775330000
H 2.4124900000 2.3037620000 -1.6491630000
H 3.6323020000 -0.9388750000 0.4311220000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.228184 (Hartree/Particle)
Thermal correction to Energy= 0.243704
Thermal correction to Enthalpy= 0.244649
Thermal correction to Gibbs (Free) Energy= 0.185469
Sum of electronic and zero-point Energies= -826.096739
Sum of electronic and thermal Energies= -826.081219
Sum of electronic and thermal Enthalpies= -826.080275
Sum of electronic and thermal (Free) Energies= -826.139454

PC

C 1.5446760000 -0.9125050000 -0.8415950000
C 1.7417870000 -1.1274980000 0.6068640000
H 2.5251340000 -1.0236140000 -1.3325460000
O 2.9494640000 -1.3459470000 1.0767830000
C 0.5750480000 -1.9581370000 -1.4506810000
H 0.9916110000 -2.9663510000 -1.3506100000
H -0.4110450000 -1.9171550000 -0.9877910000
H 0.4590430000 -1.7388130000 -2.5163710000
C 0.6900730000 -1.0128280000 1.5960350000
H 1.0248570000 -1.2775090000 2.5993020000
H 0.3535040000 0.0595280000 1.5544190000
H -0.2401640000 -1.5183070000 1.2986700000
C 1.0806070000 0.5943720000 -1.1769570000
C -0.2194390000 0.9992050000 -0.5146940000
C -0.0035250000 1.9756780000 0.4146930000
C 1.4397880000 2.3965420000 0.4734290000
O -1.3066260000 0.3567500000 -0.8709630000
H -0.7871940000 2.4086190000 1.0214880000
B -2.3950070000 -0.1134230000 0.0873070000
F -2.0488310000 -1.4644250000 0.3973560000
F -3.5890410000 -0.0516480000 -0.5770140000
F -2.3653120000 0.6430130000 1.2539530000
H 1.5667120000 3.4853370000 0.4141880000
H 1.9234340000 2.0962390000 1.4183390000
H 0.9581470000 0.5436650000 -2.2651270000
C 2.0845230000 1.6871560000 -0.7495460000
H 3.0869140000 1.2951360000 -0.5334860000
H 2.2027800000 2.4006120000 -1.5710320000
H 3.6060350000 -1.3610630000 0.3535210000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.230878 (Hartree/Particle)
Thermal correction to Energy= 0.245793
Thermal correction to Enthalpy= 0.246737
Thermal correction to Gibbs (Free) Energy= 0.188888
Sum of electronic and zero-point Energies= -826.108361
Sum of electronic and thermal Energies= -826.093447
Sum of electronic and thermal Enthalpies= -826.092502
Sum of electronic and thermal (Free) Energies= -826.150352

Entry 22

RC

C 1.9017090000 -0.8780630000 0.9571760000
C 2.9362750000 -0.7015750000 0.1134140000
H 1.7857030000 -0.1149120000 1.7262770000
O 3.6971040000 0.4462030000 0.2689170000
C 0.9600470000 -2.0441190000 1.0298690000
H 1.1782610000 -2.6521950000 1.9194930000
H -0.0787430000 -1.7099270000 1.1211850000
H 1.0225390000 -2.7000270000 0.1570590000
C 3.3769450000 -1.6097520000 -0.9968790000
H 3.3979180000 -1.0772900000 -1.9587120000
H 4.3929670000 -1.9851000000 -0.8095670000
H 2.7180690000 -2.4721620000 -1.1038590000
C 0.5655840000 1.0835140000 -0.9631770000
C -0.7316200000 0.7583420000 -0.5115910000
C -1.0760250000 1.7492200000 0.4295890000
C 0.0030620000 2.7410050000 0.6341280000
O -1.4045350000 -0.2720960000 -0.9199340000
H -2.0339080000 1.7712220000 0.9349440000
B -2.6705560000 -0.6684160000 -0.1196150000
F -3.1817850000 -1.7717760000 -0.7392500000
F -3.5305180000 0.4303190000 -0.1317660000
F -2.2270040000 -0.9148440000 1.1875500000
H -0.3548180000 3.7689270000 0.4761830000
H 0.3646330000 2.7171080000 1.6744670000
H 1.0727140000 0.5160340000 -1.7360350000
C 1.0983430000 2.3247120000 -0.3673100000
H 2.0847450000 2.1488350000 0.0860430000
H 1.2597080000 3.0914430000 -1.1412820000
H 4.4502900000 0.4142790000 -0.3401060000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.226046 (Hartree/Particle)
Thermal correction to Energy= 0.243555
Thermal correction to Enthalpy= 0.244499
Thermal correction to Gibbs (Free) Energy= 0.178708
Sum of electronic and zero-point Energies= -826.096049
Sum of electronic and thermal Energies= -826.078539
Sum of electronic and thermal Enthalpies= -826.077595
Sum of electronic and thermal (Free) Energies= -826.143387

TS

C 1.6565680000 -0.4873950000 0.7989440000
C 2.8254770000 -0.7589890000 0.1063890000
H 1.7465760000 0.3321300000 1.5103290000
O 3.8230230000 0.1424190000 0.1997210000
C 0.6602460000 -1.5629060000 1.1694900000
H 1.0581030000 -2.1443480000 2.0116440000
H -0.2960690000 -1.1341120000 1.4736650000
H 0.4439160000 -2.2483060000 0.3465210000
C 3.0545770000 -1.9221620000 -0.8045700000
H 3.3950300000 -1.5805800000 -1.7928290000
H 3.8364700000 -2.5754350000 -0.3940370000
H 2.1510150000 -2.5167160000 -0.9385440000
C 0.8293950000 0.7110390000 -0.7397900000
C -0.5900500000 0.6658230000 -0.4249130000
C -0.9097700000 1.8228010000 0.2580970000
C 0.2689100000 2.7219180000 0.4447160000
O -1.3165840000 -0.3588760000 -0.7796700000
H -1.9185620000 2.0629670000 0.5677600000
B -2.6901990000 -0.5684510000 -0.1101110000
F -3.2075190000 -1.7045530000 -0.6786250000
F -3.4639480000 0.5657850000 -0.3422910000
F -2.4420220000 -0.7155030000 1.2637720000
H 0.0528120000 3.7616120000 0.1650740000
H 0.5935350000 2.7599540000 1.4979170000
H 1.1784750000 0.1432240000 -1.5973080000
C 1.3521830000 2.0955870000 -0.4657740000
H 2.3638230000 2.1119020000 -0.0483850000
H 1.3991090000 2.6398750000 -1.4193870000
H 4.5314290000 -0.0641280000 -0.4335170000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.228417 (Hartree/Particle)
Thermal correction to Energy= 0.244179
Thermal correction to Enthalpy= 0.245123
Thermal correction to Gibbs (Free) Energy= 0.184375
Sum of electronic and zero-point Energies= -826.088825
Sum of electronic and thermal Energies= -826.073063
Sum of electronic and thermal Enthalpies= -826.072119
Sum of electronic and thermal (Free) Energies= -826.132867

PC

C 1.4636380000 -0.4661310000 0.5352380000

C 2.8360670000 -0.6940080000 0.1517330000
H 1.4399440000 0.1388880000 1.4459290000
O 3.7570140000 0.0631250000 0.7165110000
C 0.6410420000 -1.7591580000 0.6977930000
H 1.1478770000 -2.4371860000 1.3941160000
H -0.3492080000 -1.5231920000 1.0911260000
H 0.4886720000 -2.2744390000 -0.2550610000
C 3.2540350000 -1.6871470000 -0.8749540000
H 4.1789540000 -1.3931240000 -1.3856230000
H 3.4258540000 -2.6593100000 -0.3895810000
H 2.4644940000 -1.8399180000 -1.6152160000
C 0.8628470000 0.5270330000 -0.6640280000
C -0.6210530000 0.7009030000 -0.4193820000
C -0.8465320000 1.9173100000 0.1601410000
C 0.4167970000 2.7034860000 0.3417650000
O -1.4259440000 -0.2651760000 -0.7709000000
H -1.8382590000 2.2805600000 0.3933030000
B -2.7452340000 -0.5190880000 -0.0181930000
F -3.3951190000 -1.4925170000 -0.7378620000
F -3.4618970000 0.6701730000 0.0568500000
F -2.3800000000 -0.9616030000 1.2649000000
H 0.3115820000 3.7552220000 0.0453420000
H 0.7551450000 2.7217930000 1.3921500000
H 1.0531230000 0.0169630000 -1.6134190000
C 1.4290640000 1.9509060000 -0.5615590000
H 2.4581120000 2.0013730000 -0.1903070000
H 1.4222110000 2.3997490000 -1.5611840000
H 4.6368170000 -0.0791680000 0.3190180000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.230295 (Hartree/Particle)
Thermal correction to Energy= 0.245997
Thermal correction to Enthalpy= 0.246941
Thermal correction to Gibbs (Free) Energy= 0.186257
Sum of electronic and zero-point Energies= -826.091492
Sum of electronic and thermal Energies= -826.075791
Sum of electronic and thermal Enthalpies= -826.074846
Sum of electronic and thermal (Free) Energies= -826.135530

Entry 23

RC

C 1.5855680000 -1.3339900000 0.1768820000
C 2.8086090000 -0.8875330000 -0.1824030000
H 0.9542430000 -1.7184060000 -0.6213120000
O 3.1092800000 -0.8679950000 -1.5280420000
C 1.0373520000 -1.4638180000 1.5669600000
H 1.5895450000 -0.8776720000 2.3089230000
H -0.0170970000 -1.1670050000 1.5913910000
H 1.0633280000 -2.5141540000 1.8899780000
C 3.8955900000 -0.3835740000 0.7208440000
H 4.7987710000 -1.0020400000 0.6197610000
H 4.1784100000 0.6472280000 0.4607430000
H 3.5993640000 -0.4029090000 1.7703960000
C 0.6164120000 1.0860660000 -0.9142180000
C -0.6835260000 0.7415330000 -0.4763170000
C -1.0595240000 1.7116260000 0.4690310000
C -0.0081050000 2.7292740000 0.6974300000
O -1.3324760000 -0.3042250000 -0.8888120000
H -2.0275970000 1.7155660000 0.9543810000
B -2.6276980000 -0.6894010000 -0.1295190000
F -3.0767500000 -1.8411460000 -0.7072300000
F -3.5098650000 0.3827250000 -0.2453200000
F -2.2492640000 -0.8512460000 1.2136630000
H -0.3847960000 3.7478230000 0.5227870000
H 0.3317220000 2.7203210000 1.7443960000
H 1.1335850000 0.5783610000 -1.7205000000
C 1.1116740000 2.3368560000 -0.2884890000
H 2.0872160000 2.1984680000 0.1967090000
H 1.2718670000 3.1103220000 -1.0550590000
H 4.0441170000 -0.6427670000 -1.6485100000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.226462 (Hartree/Particle)
Thermal correction to Energy= 0.243844
Thermal correction to Enthalpy= 0.244789
Thermal correction to Gibbs (Free) Energy= 0.179844
Sum of electronic and zero-point Energies= -826.095213
Sum of electronic and thermal Energies= -826.077831
Sum of electronic and thermal Enthalpies= -826.076887
Sum of electronic and thermal (Free) Energies= -826.141832

TS

C 1.4161140000 -0.9867330000 0.3208590000
C 2.7245710000 -0.9464250000 -0.0964990000
H 0.7409480000 -1.5878670000 -0.2862720000
O 2.9886330000 -1.4057410000 -1.3421770000
C 0.9673730000 -0.7377190000 1.7388250000
H 1.4183070000 0.1578990000 2.1809490000
H -0.1210750000 -0.6392020000 1.7674710000
H 1.2311080000 -1.5921530000 2.3758010000
C 3.8859860000 -0.3966070000 0.6709500000
H 4.6287650000 -1.1859930000 0.8507610000
H 4.3869180000 0.4024660000 0.1053380000
H 3.5812580000 0.0031180000 1.6384020000
C 0.7481920000 0.7268360000 -0.9115660000
C -0.6422230000 0.6463130000 -0.5397230000
C -0.9611200000 1.7881930000 0.1772420000
C 0.1995360000 2.7052470000 0.3551280000
O -1.3614420000 -0.3988600000 -0.8412270000
H -1.9643770000 1.9974300000 0.5264540000
B -2.6675190000 -0.6505580000 -0.0531400000
F -3.1892810000 -1.8096420000 -0.5606860000
F -3.4966180000 0.4549850000 -0.2284650000
F -2.2921800000 -0.7669160000 1.2951410000
H -0.0248500000 3.7269220000 0.0174280000
H 0.4824070000 2.7997430000 1.4144770000
H 1.1223100000 0.2035500000 -1.7858240000
C 1.3166840000 2.0553430000 -0.4970700000
H 2.2732950000 1.9786070000 0.0316590000
H 1.5154550000 2.6526240000 -1.3979310000
H 3.9216220000 -1.2600750000 -1.5685680000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.227996 (Hartree/Particle)
Thermal correction to Energy= 0.243985
Thermal correction to Enthalpy= 0.244930
Thermal correction to Gibbs (Free) Energy= 0.183927
Sum of electronic and zero-point Energies= -826.092014
Sum of electronic and thermal Energies= -826.076025
Sum of electronic and thermal Enthalpies= -826.075081
Sum of electronic and thermal (Free) Energies= -826.136084

PC

C 1.3015890000 -0.6598540000 0.2041760000
C 2.6731140000 -0.9393610000 -0.1173260000
H 0.6478510000 -1.4432430000 -0.2070310000
O 2.8874920000 -1.5160320000 -1.2878330000
C 0.9815250000 -0.4166030000 1.6802690000
H 1.3772630000 0.5382450000 2.0439100000
H -0.1052960000 -0.4158130000 1.7992170000
H 1.3875910000 -1.2185670000 2.3070310000
C 3.8529150000 -0.5901830000 0.7226980000
H 4.1593030000 -1.4696900000 1.3092740000
H 4.7109610000 -0.2829440000 0.1110960000
H 3.6127050000 0.2028450000 1.4323590000
C 0.8286910000 0.5921240000 -0.7780950000
C -0.6547560000 0.6780080000 -0.5577690000
C -0.9896110000 1.8943130000 -0.0377820000
C 0.2000360000 2.7737460000 0.1937440000
O -1.3595210000 -0.3910160000 -0.8209340000
H -2.0134800000 2.1887710000 0.1524130000
B -2.6331070000 -0.6994480000 0.0015810000
F -3.1565060000 -1.8401230000 -0.5529400000
F -3.4883570000 0.3927360000 -0.0801430000
F -2.2006000000 -0.8990560000 1.3224880000
H 0.0841010000 3.7678740000 -0.2606820000
H 0.3673260000 2.9572980000 1.2667740000
H 1.0814870000 0.2386400000 -1.7821320000
C 1.3809890000 1.9922360000 -0.4509750000
H 2.2632600000 1.9711560000 0.1989870000
H 1.6924150000 2.4814570000 -1.3800140000
H 3.8385000000 -1.5909600000 -1.4872520000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.230116 (Hartree/Particle)
Thermal correction to Energy= 0.245987

Thermal correction to Enthalpy= 0.246932
Thermal correction to Gibbs (Free) Energy= 0.185623
Sum of electronic and zero-point Energies= -826.096671
Sum of electronic and thermal Energies= -826.080799
Sum of electronic and thermal Enthalpies= -826.079855
Sum of electronic and thermal (Free) Energies= -826.141163

10b

SEE RT (*gauche*)

C 2.0150690000 0.7214780000 -0.2780960000
C 1.3199130000 -0.4237440000 -0.3360320000
O 0.0115340000 -0.4383250000 -0.7872530000
Si -1.3614460000 0.1013210000 0.0294360000
C -2.7933200000 -0.5072330000 -1.0262540000
H -3.7579150000 -0.2046040000 -0.6006560000
H -2.7336550000 -0.0998480000 -2.0420080000
H -2.7891830000 -1.6002110000 -1.1058300000
C -1.4147830000 -0.6533650000 1.7590890000
H -0.5246510000 -0.3841680000 2.3401560000
H -2.2902960000 -0.2963020000 2.3156780000
H -1.4706560000 -1.7474630000 1.7183580000
C -1.3913290000 1.9839990000 0.1566740000
H -1.3249910000 2.4511880000 -0.8329360000
H -2.3249450000 2.3240320000 0.6229720000
H -0.5617100000 2.3642760000 0.7632580000
C 3.4456250000 0.9021970000 0.1454230000
H 3.9220410000 -0.0333620000 0.4511800000
H 4.0475670000 1.3290800000 -0.6688000000
H 3.5228560000 1.6014630000 0.9894780000
H 1.4946840000 1.6256600000 -0.5891470000
C 1.8153620000 -1.8082610000 -0.0245560000
H 1.2304610000 -2.2530990000 0.7906350000
H 1.6792220000 -2.4522120000 -0.9021300000
H 2.8699190000 -1.8267520000 0.2582270000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.215451 (Hartree/Particle)
Thermal correction to Energy= 0.229574
Thermal correction to Enthalpy= 0.230518
Thermal correction to Gibbs (Free) Energy= 0.174444
Sum of electronic and zero-point Energies= -640.944915
Sum of electronic and thermal Energies= -640.930792
Sum of electronic and thermal Enthalpies= -640.929848
Sum of electronic and thermal (Free) Energies= -640.985921

SEE TS (*gauche* ↔ *anti* ↔ *gauche*)

C -2.4814980000 0.7892380000 -0.0000010000
C -1.4104880000 -0.0178400000 -0.0000010000
O -0.1697980000 0.5787280000 -0.0000040000
Si 1.4383810000 0.0956640000 0.0000000000
C 2.3841570000 1.7210230000 -0.0000050000
H 3.4678550000 1.5510600000 -0.0000030000
H 2.1382680000 2.3196070000 -0.8844250000
H 2.1382660000 2.3196130000 0.8844100000
C 1.8653400000 -0.8978610000 1.5491160000
H 1.3934910000 -1.8867780000 1.5618120000
H 2.9501790000 -1.0528890000 1.6125170000
H 1.5545890000 -0.3665360000 2.4563380000
C 1.8653440000 -0.8978720000 -1.5491080000
H 1.5545950000 -0.3665550000 -2.4563340000
H 2.9501830000 -1.0529010000 -1.6125040000
H 1.3934950000 -1.8867900000 -1.5617970000
C -3.9310220000 0.3977300000 0.0000010000
H -4.0855930000 -0.6851760000 0.0000020000
H -4.4503920000 0.8023760000 0.8800850000
H -4.4503930000 0.8023730000 -0.8800840000
H -2.2719570000 1.8575730000 -0.0000020000
C -1.4247740000 -1.5219660000 0.0000000000
H -0.9111150000 -1.9201750000 -0.8842040000
H -0.9111130000 -1.9201740000 0.8842020000
H -2.4416720000 -1.9184530000 0.0000010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.215412 (Hartree/Particle)
Thermal correction to Energy= 0.228660
Thermal correction to Enthalpy= 0.229605
Thermal correction to Gibbs (Free) Energy= 0.176698
Sum of electronic and zero-point Energies= -640.942687
Sum of electronic and thermal Energies= -640.929439
Sum of electronic and thermal Enthalpies= -640.928494
Sum of electronic and thermal (Free) Energies= -640.981401

SEE RT (*syn*)

C 1.8500420000 -0.6964210000 -0.0000040000
C 1.3696010000 0.5572390000 -0.0000050000
O 0.0277500000 0.8574460000 -0.0000100000
Si -1.3746360000 -0.0814990000 0.0000010000
C -2.7562660000 1.1942940000 -0.0000040000
H -3.7415290000 0.7120490000 0.0000020000
H -2.6988100000 1.8384160000 0.8847640000
H -2.6988150000 1.8384040000 -0.8847810000
C -1.4710800000 -1.1456790000 -1.5560160000
H -0.6649090000 -1.8848350000 -1.6118420000
H -2.4237280000 -1.6893200000 -1.5906450000
H -1.4121300000 -0.5235390000 -2.4568300000
C -1.4710690000 -1.1456580000 1.5560320000
H -1.4121190000 -0.5235050000 2.4568370000
H -2.4237130000 -1.6893040000 1.5906730000
H -0.6648930000 -1.8848080000 1.6118650000
C 3.2926940000 -1.1199750000 0.0000020000
H 3.9860960000 -0.2747570000 0.0000060000
H 3.5258460000 -1.7349620000 0.8805940000
H 3.5258540000 -1.7349600000 -0.8805900000
H 1.1327040000 -1.5148760000 -0.0000080000
C 2.1712220000 1.8288540000 -0.0000010000
H 1.9173050000 2.4308630000 -0.8811530000
H 1.9173000000 2.4308610000 0.8811510000
H 3.2475850000 1.6497490000 0.0000010000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.215367 (Hartree/Particle)
Thermal correction to Energy= 0.229664
Thermal correction to Enthalpy= 0.230608
Thermal correction to Gibbs (Free) Energy= 0.173457
Sum of electronic and zero-point Energies= -640.945182
Sum of electronic and thermal Energies= -640.930885
Sum of electronic and thermal Enthalpies= -640.929941
Sum of electronic and thermal (Free) Energies= -640.987092

SEE TS (*syn* ↔ *gauche* ↔ *gauche*)

C 1.9466820000 0.7182510000 -0.2448440000
C 1.3339090000 -0.4741170000 -0.2928460000
O 0.0099270000 -0.5974390000 -0.6666390000
Si -1.3637320000 0.0912940000 0.0297550000
C -2.7866920000 -0.9142830000 -0.6781770000
H -3.7532750000 -0.5508080000 -0.3082600000
H -2.8043180000 -0.8542370000 -1.7724920000
H -2.6981550000 -1.9718450000 -0.4050140000
C -1.2678950000 -0.0705170000 1.9067860000
H -0.3611210000 0.4035920000 2.2996030000
H -2.1288800000 0.4102160000 2.3874630000
H -1.2571150000 -1.1219000000 2.2171630000
C -1.5596340000 1.9054850000 -0.4560860000
H -1.4981770000 2.0330830000 -1.5432640000
H -2.5376450000 2.2847960000 -0.1327000000
H -0.7937280000 2.5428580000 0.0000550000
C 3.3787870000 0.9948470000 0.1183490000
H 3.9345350000 0.0909900000 0.3824780000
H 3.9110930000 1.4790900000 -0.7121730000
H 3.4447370000 1.6818540000 0.9734540000
H 1.3533080000 1.5900680000 -0.5144380000
C 1.9454510000 -1.8214630000 -0.0290100000
H 1.4455670000 -2.3105050000 0.8169470000
H 1.7977580000 -2.4679820000 -0.9026580000
H 3.0145890000 -1.7670870000 0.1853400000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.215376 (Hartree/Particle)
Thermal correction to Energy= 0.228644
Thermal correction to Enthalpy= 0.229588
Thermal correction to Gibbs (Free) Energy= 0.176537
Sum of electronic and zero-point Energies= -640.944935
Sum of electronic and thermal Energies= -640.931667
Sum of electronic and thermal Enthalpies= -640.930723
Sum of electronic and thermal (Free) Energies= -640.983774

Entry 33

RC

C -0.4443210000 1.1782020000 1.6832700000
C -1.3211440000 1.2355540000 0.6486990000
O -1.3019610000 0.2704320000 -0.3135180000
Si -2.0485330000 -1.2767680000 -0.3125200000
C -2.3350180000 2.3173730000 0.3921940000
H -2.2411150000 2.6894800000 -0.6357120000
H -3.3516820000 1.9136730000 0.4823140000
H -2.2425130000 3.1595100000 1.0810270000
C -3.8381300000 -1.0221880000 -0.8684320000
H -3.8904060000 -0.5134410000 -1.8382860000
H -4.3467940000 -1.9888500000 -0.9749910000
H -4.4152920000 -0.4306420000 -0.1472130000
C -2.0041180000 -2.0386190000 1.4019730000
H -0.9703870000 -2.2161320000 1.7098460000
H -2.4899330000 -1.4028570000 2.1513990000
H -2.5329100000 -3.0003100000 1.3930090000
C -1.0968600000 -2.2681830000 -1.5853870000
H -1.5068880000 -3.2830360000 -1.6618560000
H -1.1647120000 -1.8129530000 -2.5812050000
H -0.0408610000 -2.3492530000 -1.3084490000
C 1.4357340000 2.2018180000 -0.1701610000
C 1.8352580000 0.8760980000 -0.4498350000
C 1.4263140000 0.6060750000 -1.7646560000
C 0.8169610000 1.7830500000 -2.4302780000
O 2.4491800000 0.1276360000 0.4209900000
H 1.5772510000 -0.3541920000 -2.2397500000
B 2.3478280000 -1.3982700000 0.4573900000
F 1.1601880000 -1.6916560000 1.1513560000
F 3.4590960000 -1.8492280000 1.1122060000
F 2.2576860000 -1.8887650000 -0.8560430000
H 1.3663250000 2.0523070000 -3.3447020000
H -0.2108680000 1.5670150000 -2.7486690000
H 1.6674450000 2.7013580000 0.7639000000
C 0.8757850000 2.8915790000 -1.3577840000
H -0.1021390000 3.3453620000 -1.1542060000
H 1.5301260000 3.7247000000 -1.6578160000
H 0.1946020000 0.2992580000 1.7269040000
C -0.3519610000 2.1298110000 2.8411690000
H 0.6940440000 2.3853870000 3.0533400000
H -0.9063920000 3.0610510000 2.6922080000
H -0.7380720000 1.6575470000 3.7551670000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.329579 (Hartree/Particle)
Thermal correction to Energy= 0.354129
Thermal correction to Enthalpy= 0.355073
Thermal correction to Gibbs (Free) Energy= 0.275506
Sum of electronic and zero-point Energies= -1234.718981
Sum of electronic and thermal Energies= -1234.694432
Sum of electronic and thermal Enthalpies= -1234.693488
Sum of electronic and thermal (Free) Energies= -1234.773055

TS

C -0.2271360000 1.3406740000 1.4618120000
C -1.2659420000 1.2838900000 0.5539830000
O -1.3480770000 0.2659310000 -0.3001700000
Si -2.0598140000 -1.3128030000 -0.2279680000
C -2.3083350000 2.3494090000 0.3600450000
H -2.4288280000 2.5670380000 -0.7067310000
H -3.2794670000 1.9804580000 0.7171250000
H -2.0817190000 3.2726640000 0.8963330000
C -3.8553420000 -1.0731610000 -0.7634260000
H -3.9212520000 -0.6119390000 -1.7557260000
H -4.3679890000 -2.0421420000 -0.8158070000
H -4.4188820000 -0.4462830000 -0.0615990000
C -1.9833720000 -1.9582510000 1.5307540000
H -0.9446780000 -2.1178090000 1.8299250000
H -2.4598680000 -1.2749840000 2.2442940000
H -2.5137620000 -2.9170280000 1.5929450000
C -1.1167820000 -2.3313480000 -1.4770610000
H -1.4909260000 -3.3630110000 -1.4791520000
H -1.2447630000 -1.9335090000 -2.4909370000
H -0.0482680000 -2.3556720000 -1.2418940000
C 1.2972350000 2.0932540000 -0.0541970000
C 1.8213180000 0.8235730000 -0.4754440000
C 1.4721190000 0.6349630000 -1.7999860000
C 0.7599650000 1.8125260000 -2.3809440000
O 2.4869770000 0.0642550000 0.3612360000
H 1.7324580000 -0.2543740000 -2.3584270000
B 2.3105440000 -1.4401800000 0.4140700000
F 1.0945770000 -1.6639170000 1.1079100000
F 3.3829350000 -1.9519980000 1.0917540000
F 2.1955320000 -1.9534530000 -0.8870890000
H 1.2612890000 2.1851760000 -3.2854240000
H -0.2634120000 1.5584030000 -2.6847370000
H 1.6951980000 2.6026760000 0.8166200000
C 0.7894280000 2.8594540000 -1.2399380000
H -0.1690590000 3.3605760000 -1.0730400000
H 1.5108400000 3.6589480000 -1.4637600000
H 0.3487350000 0.4240220000 1.5749880000
C -0.1323530000 2.3346870000 2.5922430000
H 0.9024430000 2.4183660000 2.9406750000
H -0.4817460000 3.3371190000 2.3244030000
H -0.7250990000 1.9962540000 3.4523750000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.330365 (Hartree/Particle)
Thermal correction to Energy= 0.353900
Thermal correction to Enthalpy= 0.354844
Thermal correction to Gibbs (Free) Energy= 0.277726
Sum of electronic and zero-point Energies= -1234.716848
Sum of electronic and thermal Energies= -1234.693313
Sum of electronic and thermal Enthalpies= -1234.692369
Sum of electronic and thermal (Free) Energies= -1234.769487

PC

C -0.3740300000 1.7962010000 -1.1604600000
C 0.9475280000 1.4102320000 -0.6246060000
O 1.0661780000 0.2124240000 -0.2267110000
Si 2.1677790000 -1.1357860000 0.1630830000
C 2.0928810000 2.3708860000 -0.5284270000
H 2.8600910000 2.0209230000 0.1615540000
H 2.5439720000 2.4882090000 -1.5245280000
H 1.7422880000 3.3626330000 -0.2297980000
C 3.8280710000 -0.4149240000 0.6939590000
H 3.7453350000 0.2370030000 1.5713350000
H 4.4806640000 -1.2502440000 0.9807880000
H 4.3422960000 0.1320280000 -0.1039880000
C 2.2814830000 -2.0498550000 -1.4612560000
H 1.2731880000 -2.3440510000 -1.7653470000
H 2.7343000000 -1.4403510000 -2.2518710000
H 2.8952460000 -2.9513490000 -1.3416110000
C 1.3338060000 -2.0467090000 1.5514280000
H 1.8764750000 -2.9818290000 1.7431200000
H 1.3377450000 -1.4628620000 2.4784530000
H 0.2976010000 -2.2883590000 1.2924710000
C -1.4717210000 1.8999540000 0.0193090000
C -1.7981050000 0.5211840000 0.5345450000
C -1.3967510000 0.3781510000 1.8230770000
C -0.7563540000 1.6334620000 2.3529120000
O -2.3627680000 -0.3026900000 -0.3278630000
H -1.5108900000 -0.5324140000 2.3950340000
B -2.0084160000 -1.7601050000 -0.4457840000
F -0.7885480000 -1.8217420000 -1.1743510000
F -3.0239100000 -2.3790850000 -1.1297930000
F -1.8026250000 -2.3242110000 0.8257960000
H -1.1295390000 1.9277350000 3.3430440000
H 0.3367860000 1.5235250000 2.4736280000
H -2.3262270000 2.3305230000 -0.5153500000
C -1.1002890000 2.7032810000 1.2809560000
H -0.2987640000 3.4362630000 1.1267200000
H -1.9797850000 3.2703840000 1.6027070000
H -0.7412820000 0.9285210000 -1.7266030000
C -0.3715270000 3.0622960000 -2.0250630000
H -1.3585640000 3.1811720000 -2.4814400000
H -0.1706190000 3.9675430000 -1.4409290000
H 0.3613750000 3.0090430000 -2.8381370000

Temperature 298.150 Kelvin. Pressure 1.00000 Atm.
Zero-point correction= 0.333051 (Hartree/Particle)
Thermal correction to Energy= 0.356244
Thermal correction to Enthalpy= 0.357188
Thermal correction to Gibbs (Free) Energy= 0.281030

Sum of electronic and zero-point Energies= -1234.729962
Sum of electronic and thermal Energies= -1234.706770
Sum of electronic and thermal Enthalpies= -1234.705826
Sum of electronic and thermal (Free) Energies= -1234.781984