THE CHEMICAL IMPLICATION OF CHARGE DENSITY DISTRIBUTION FOR HETEROCYCLIC RINGS, AND THE CONFORMATIONAL CONSEQUENCES OF THE PACKING IN XPh_4 [X= C, Si, Ge, Sn, Pb] AND RELATED CRYSTALS. CRYSTALLOGRAPHY AND MOLECULAR MODELLING.

by

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Submitted in partial fulfilment of the requirements for the degree of Doctor of Philosophy

at

Dalhousie University

Halifax, Nova Scotia

August, 1992

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ISBN 0-315-80147-6

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To my late teachers and friends

Drs Barbara Wiktorowska and Boleslaw Wojciechowski

"The universe is full of magical things, patiently waiting for our wits to grow sharper."

Eden Phillpotts

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Abstract

The work reported here examines various aspects of a study of the fine details in X-ray structure determination. It is divided into three parts:

1) Charge density studies of the benzene clathrate of hexa(aziridinyl)cyclotriphosphazene. The object of this part was to investigate the bonding electron density in the phosphazene ring and to answer, from a charge density study, the long-debated question about the nature of the phosphazene -P=N- bonds. The charge densities on the benzene ring and aziridinyl groups were also examined and are exactly as predicted. These observations are used to validate the charge density observed for the phosphazene ring which confirms that Dewar's original island delocalization model for the -P=N-P- system is essentially correct.

2) Charge density studies of a supposed aromatic 10-electron $p\pi$-$p\pi$ system. The object of this part was to see if a proposed aromatic $3p\pi$-$3p\pi$ bonding in a hetero-bicyclic benzodithiaphospholium cation could be confirmed by an examination of the bonding electron density. The neutral non-aromatic analogue (benzodithiaphosphole) was also examined to provide the necessary comparison. While it was possible to confirm that the neutral analogue had all the expected bonding density features, disorder phenomena in the cation structure made the identification of the aromatic 10e $p\pi$-$p\pi$ system rather tentative.

3) Precise determination of the factors influencing the observed structures of the neutral series of compounds XPh_4 [X = C, Si, Ge, Sn, Pb]. The factors which control the fine details of the molecular structure were explored and the inter-relation between the molecular shape and the crystal packing is discussed.

Abbreviations and Symbols

MW	Formula weight
Z	Number of molecules in the unit cell
a,b,c	Unit cell dimensions
a*,b*,c*	Reciprocal unit cell dimensions
α,β,γ	Angles between crystal axes
V	Volume of unit cell
μ	Linear absorption coefficient
d_c	Calculated density
θ	Bragg angle
h,k,l	Miller indices of the reflecting plane
MoKα	Radiation used
λ	Wavelength of X-radiation
e.s.d., σ	Estimated standard deviation
I	Intensity of diffracted beam
x/a,y/b,z/c	Fractional coordinates
U_{iso}	Isotropic temperature factor
U_{eq}	Equivalent temperature factor; $U_{eq} = (U_{11}+U_{22}+ U_{33})/3$
U's	Anisotropic temperature factors
U_{ii}'s	U_{11}, U_{22} and U_{33}
U_{ij}	U_{23}, U_{13} and U_{12}
B	Temperature factors tensor related to **U** by $B_{ij} = 8\pi^2U_{ij}$

B_{eq}	Equivalent temperature factor;
	$B_{eq} = (B_{11}+B_{22}+ B_{33})/3$
TLS	Torsion/Libration/Screw
r.m.s.	Root mean square
F(000)	Number of electrons in the unit cell
F_o	Observed structure amplitude
F_c	Calculated structure factor
N_{me}	Total number of measured reflections
N_{un}	Number of unique reflections after merging
N_{ob}	Number of reflections considered observed
N_v	Number of parameters refined
R-value, R	Residual index, R-factor
R_w	Weighted R-value
R_m	Merging R-value for equivalent reflections
GOF	Goodness of fit parameter
w	Weight in minimised function
g,k	Factors in weighting scheme
$\rho(\mathbf{r})$	Electron density in molecule
$\Delta\rho(\mathbf{r})$	Difference electron density
$\mathbf{r}$	Vector determining the point in the unit cell
k	Scale factor
$\mathbf{H}(h_1,h_2,h_3)$	Scattering vector in the reciprocal space
$\lvert F_o(\mathbf{H})\rvert$	Amplitude of the diffracted beam in the direction of the scattering vector $\mathbf{H}(h_1,h_2,h_3)$
$\lvert F_c(\mathbf{H})\rvert$	Calculated structure factor in the reciprocal space

ρ_c	Core atomic density
ρ_ν	Valence density
$y_{lm}(\theta,\phi)$	Multipolar spherical harmonic angular functions in real form
κ' and κ''	Expansion-contraction parameters
P_c	Core population parameters
P_ν	Valence population parameters
P_{lm}	Multipole population parameters
R_l	$= N_l r^n \exp(-\kappa''\varsigma r)$; Slater-type radial functions
N_l	Normalization factor
$\delta\rho(\mathbf{r})$	Deformation electron density
$z^2_{A,B}$	Mean square displacement amplitude of atom A in the direction of atom B
t	Temperature (^{o}C) of measurement
LT	Low temperature
RT	Room temperature
conv. ref.	Conventional (spherical atom) refinement
mul.	Multipole
pdf	Probability density function
hex.	Hexagonal
rh.	Rhombohedral
d(C-H)	Carbon-Hydrogen distance
HO	High order
az	Aziridinyl= $-N(CH_2)_2$
Ph	Phenyl ring

X	Central atom in XPh_4 [X=C, Si, Ge, Sn, Pb]
TPMe	Tetraphenylmethane
TPSi	Tetraphenylsilane
TPGe	Tetraphenyl germanium
TPSn	Tetraphenyl tin
TPPb	Tetraphenyl lead
oTMe	Tetra(o-tolyl)methane
oTSi	Tetra(o-tolyl)silane
ϕ	Angle of rotation of the tetraphenyl molecule about crystallographic c axis
ψ	Angle of rotation of the phenyl ring relative to a D_{2d} position of the ring
α_1	Angle between the phenyl ring planes related by the 2-fold axis
α_2	Angle between the phenyl ring planes related by the S_4 axis
x,y,z	Fractional coordinates of atom
$x_{ref}, y_{ref}, z_{ref}$	Atomic coordinates from ref. 121
L_1, L_2, L_3	Principal axes of libration
l_1, l_2, l_3	Mean amplitudes about librational motions about L_1, L_2, L_3
E_s	Steric energy
E(l)	Stretching energy
K_l	Stretching constant
l_0	Standard values of bonds in MM3
$E(\Theta)$	Bending energy

K_θ	Bending constant
θ_0	Standard values of angles in MM3
$E(\varphi)$	Torsional energy
E_0	Torsional constant
$E(r)$	Energy of nonbonded (van der Waals) interactions
$E(q)$	Energy of electrostatic interactions
Ix,Iy,Iz	Principal axes of inertia
X',Y',Z'	Orthogonal axes in MM3
X_c, Y_c, Z_c	Orthogonal crystal axes (= a,b,c in tetragonal crystal system)
x_c, y_c, z_c	Cartesian coordinates of atom C1 in crystal system
X",Y",Z"	Common orthogonal axes for calculated and experimental molecules
x",y",z"	Cartesian coordinates of atoms in the X"Y"Z" system
α_m	Angle of rotation from the MM3 X'Y'Z' system to the X"Y"Z" system
α_c	Angle of rotation from the crystal system to the X"Y"Z" system

Acknowledgements

It gives me a great pleasure to express my gratitude to my supervisors Drs. T. S. Cameron and O. Knop for their guidance, support, encouragement, and assistance in any possible way. They have always been as helpful as any student could wish and I am very grateful.

I would also like acknowledge here the assistance of people who have contributed to the research reported in this thesis: Dr. P. R. Mallinson of the University of Glasgow, Scotland, for his hospitality, helpful discussions, and comments on the use of the multipole refinement program Molly; Dr. B. Vincent of the Molecular Structure Corporation, Texas, for collecting data for benzene clathrate of phosphazene on R-Axis II, automated X-ray Imaging System; Drs. N. Burford and B. Royan for preparing the compounds of benzodithiaphospholium tetrachloroaluminate and phenylbenzodithiaphosphole; Dr. T. B. Grindley for his assistance with the molecular mechanics calculations.

Many of my co-workers have provided support and inspiration along the way. Wanda Tacreiter and Dr. Antony Linden helped me immensely, especially during my first year at Dalhousie. I also appreciate the help of Ruth Cordes, Dr. Margaret James, and Pradip Bakshi, who were always ready to discuss problems and to give valuable suggestions.

I would like to acknowledge financial support by the Killam Foundation and Dalhousie University in the forms of Graduate Scholarship and Teaching Assistantship, respectively.

My thanks also go to all my friends, fellow graduate students, and my family, especially to my daughter Agnieszka and my friend Grzegorz Bednarz, for their continuous understanding, encouragement, and support.

1. General Introduction

While the general purpose of this project was to acquire a training in all aspects of research X-ray crystallography, the specific interest is an investigation of the finest details in the determination of a crystal structure by X-ray methods. This interest has three main strands.

1) The determination of the charge density in a phosphazene ring to locate the bonding (and non-bonding pair)

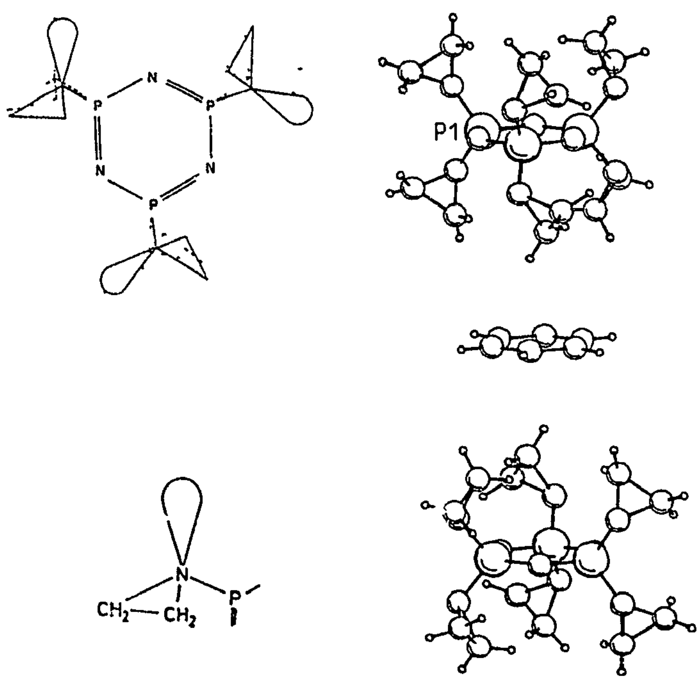

Figure 1. Structure of the benzene clathrate of hexa(aziridinyl)-cyclotriphosphazene (I).

electrons and to answer the long-debated questions about the bonding in that ring[1,2].

The benzene clathrate of hexa(1-aziridinyl)cyclotriphosphazene (I) (Figure 1) was chosen since the benzene molecule is tightly held in the lattice. The correct observations on the benzene ring and the expected observations on the three-membered aziridinyl groups all add credence to the observations on the phosphazene ring.

2) The determination of the charge density on two related molecules, a planar benzodithiaphospholium cation (II) (Figure 2) and the related benzodithiaphosphole (III)

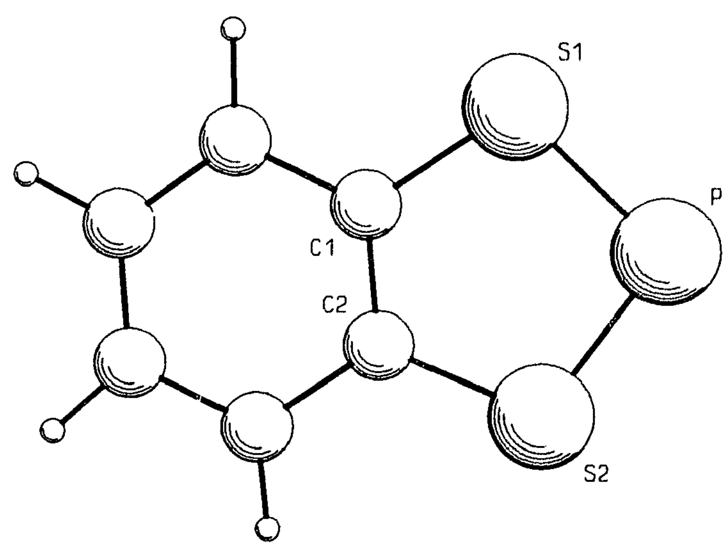

Figure 2. Benzodithiaphospholium cation (II).

(Figure 3), where the object of the investigation was to determine the nature of the bonding on the 10 electron π system of the cation.

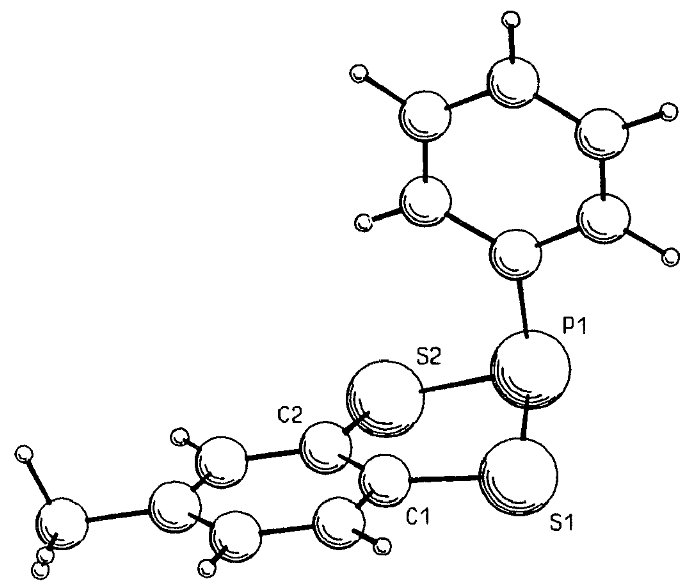

Figure 3. Benzodithiaphosphole molecule (III).

In this case the changes in the locations of the bonding and non-bonding pair electrons in the two similar molecules are highly significant and largely answer the questions about the bonding. However, it is possible to refine a parameter which measures the effect on the core electrons of an atom of the apparent charge on that atom. In this instance it should be possible to determine the extent of the spread of the charge on the cation which is nominally written all on the phosphorus atom.

3) The precise determination of the factors influencing the observed structures of the neutral series of compounds XPh_4 [X = C, Si, Ge, Sn, Pb] (IV) (Figure 4).

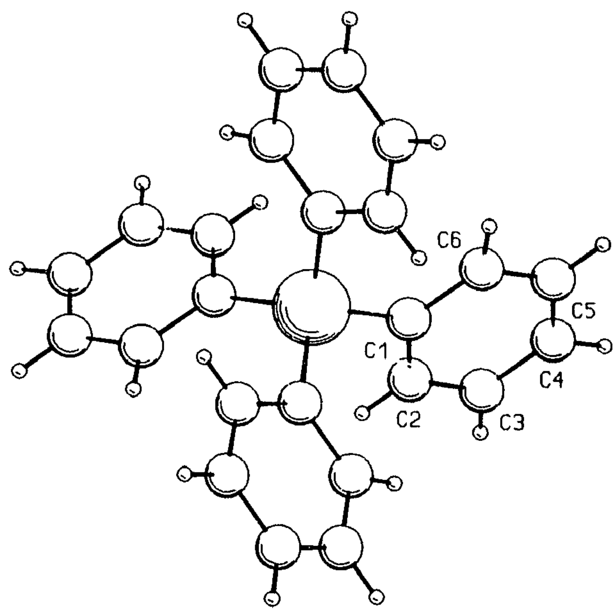

Figure 4. Molecule of XPh_4, [X= C, Si, Ge, Sn, Pb] (IV).

The compounds form an isomorphous series and are highly symmetric in the crystal with only one unique phenyl ring. The structural examination has two aspects. One is a thorough study of all the "vibrational" factors which might influence the observed dimensions and conformations of the system (and thus lead to spurious claims of structural differences or similarities between the various members of the series) and the other is the determination of the ideal conformations of an isolated molecule in this series, which leads then to a discussion on the reasons for the differences between the observed and predicted molecular arrangements.

2. Electron Density Studies

2.1. Introduction

Electron density maps have been used for years to illustrate an arrangement of the molecules in crystals. It has always been known that such maps can also give some information about the nature of the chemical bonds[3,4].

However, only with the recent development of automatic data collection and processing, that enabled a correct allowance for systematic errors and better experimental accuracy, and with the advancement of computing techniques. could the electron density distribution be interpreted with a real physical significance.

Electron or charge density determinations are based on the measurements of the intensity of X-ray photons elastically scattered by crystals[4,5]. The intensity of the diffracted radiation I(S) is proportional to the square of the scattering amplitude F(S)

$$I(\mathbf{S}) \propto |F(\mathbf{S})|^2$$

where **S** is the reciprocal lattice vector of magnitude $2\sin\theta/\lambda$, and θ is the angle of diffraction.

The scattering amplitude F(S) is given by

$$F(\mathbf{S}) = \int_V \langle\rho(\mathbf{r})\rangle \exp(2\pi i \mathbf{S}\cdot\mathbf{r})dv$$

where **r** is the vector determining the point in the unit cell.

Since the electron density in a crystal is the convolution of the density in the unit cell and a periodic lattice function, F(**S**) is observable only at the distinct points **H** in reciprocal space, representing the elastic Bragg reflections, and can be expressed by

$$F(\mathbf{H}) = \int_V \langle\rho(\mathbf{r})\rangle \exp(2\pi i \mathbf{H}\cdot\mathbf{r})d\mathbf{r}$$

The thermally averaged electron density is given by the inverse Fourier transform

$$\langle\rho(\mathbf{r})\rangle = 1/V \sum_{\mathbf{H}} F(\mathbf{H})\exp(-2\pi i \mathbf{H}\cdot\mathbf{r})$$

where the integral has been replaced by a sum over all reciprocal lattice points for which **S** = **H**, and V is the volume of the crystallographic unit cell.

The structure factor amplitude is generally a complex quantity and for the calculation of $\rho(\mathbf{r})$ both magnitude and phase are required. Only the former can be measured experimentally. For the centrosymmetric structures, the phase problem reduces to a question of the sign of the structure factor, but the difficulty in obtaining accurate structure factors increases when the phase is a continuous variable as in the non-centrosymmetric structures.

For a given model, structure factors (F_c) can be calculated and subtracted from the observed amplitudes (F_o) and the differences can be used as coefficients in the difference Fourier synthesis. Difference electron density, $\Delta\rho(\mathbf{r})$, is defined as the Fourier transform of the difference between the F_o and F_c:

$$\Delta\rho(\mathbf{r}) = 1/V \sum_{H} (|F_o(\mathbf{H})|/k - |F_c(\mathbf{H})|)\exp(-2\pi i\mathbf{H}\cdot\mathbf{r})$$

where, k is the scale factor, $|F_o(\mathbf{H})|$ is the amplitude of the diffracted beam in the direction of the scattering vector $\mathbf{H}(h_1,h_2,h_3)$.

This corresponds to a point-by-point subtraction of an F_c Fourier map from an F_o map calculated with the same phases. Thus the difference map shows peaks everywhere where the F_c model, based on the 'spherical' distribution of the electrons around the atomic centres, fails to provide the electron density implied by the F_o data and shows holes (negative difference density) where it provides too much. Hence, through the direct observation of the difference electron density maps, the bonds and their chemical significance in molecules can be studied.

Theoretical evaluations[6] of the differences in electron density distributions of atoms participating in chemical bonds and of the free atoms show that the calculated changes depend on the assumptions made for the wave functions of the molecules. Direct experimental information on these changes can be obtained by X-ray diffraction[7,5] and neutron diffraction or by joint X-ray and neutron diffraction experiment[8,5,9].

Two methods of the determination of the experimental deformation density, based on diffraction experiments, have been used in this study.

The $X-X_{HO}$ method[4,9,10,11] is an empirical method of separating the diffraction effects of the core and valence electrons. The highly resolved X-ray data set is separated into 'high-order' ($\sin\theta/\lambda > 0.7-0.8 Å^{-1}$) and 'low-order' sets (with the cut-off arbitrarily chosen at a $\sin\theta/\lambda$ value of 0.7-0.8$Å^{-1}$). At high angles the diffraction from the bonding and lone-pair electrons is negligible and the refinement is responding to the effect of the core electrons on each of the atoms. Thus the positional and thermal parameters obtained from the high order refinement give approximate positions of the nuclei. The electron density is determined by calculating a Fourier difference map (using only the 'low-order reflections), where the difference term represents the difference between the experimental, (F_o), and 'high-order' X-ray structure factors, (F_c), calculated from the parameters obtained by a least-squares refinement in which only high-angle data are used. This technique is useful in indicating whether the more time-consuming method, outlined below, is worth pursuing.

An alternative approach[12,13,14] is based on the concept of rigid pseudoatom[15,16] and has become the established tool in the analysis of charge density data.

The molecular charge density $\rho(\mathbf{r})$ in the crystal is described by a sum of rigid pseudoatom densities, where each pseudoatom is centred on an atomic nucleus. The pseudoatom is said to be rigid because its electron density is assumed to accompany the nucleus during thermal vibrations. Each pseudoatom has an invariant core, usually consisting of a neutral spherical Hartree-Fock atomic density, just as in conventional structure analysis. In addition, it has a series of nuclear-centred electron density terms, each with an adjustable weight (electron population parameters). These terms are intended to model the effects of the molecular and crystal environment, whereby the pseudoatom may become aspherical and carry a net charge.

The procedure, based on these ideas and modified by Hansen and Coppens[8] (program MOLLY[17]), uses the expansion of spherical harmonics to describe atomic deformations. It incorporates the expansion-contraction parameter kappa[18] which modifies the isolated-atom valence shell density and allows for the contraction of positively - and expansion of negatively - charged atoms, in agreement with theoretical concepts. This approach has the advantage of retaining the radial nodes of the atomic shells, allows for full treatment of extinction[19], and can be used for joint X-ray and neutron diffraction data[8], if necessary.

In a multipolar atomic density model used in MOLLY[17], electron densities at each atom are described by

$$\rho(\mathbf{r}) = P_c\rho_c(\mathbf{r}) + \kappa'^3 P_\nu\rho_\nu(\kappa'\mathbf{r}) + \sum_{l=0}^{3}\sum_{m=-l}^{+l}\{\kappa''^3 P_{lm}R_l(\kappa''\mathbf{r})y_{lm}(\theta,\phi)\}$$

where ρ_c and ρ_ν are spherically-averaged Hartree-Fock atomic core and valence densities, with the ρ_ν normalized to one electron; the $y_{lm}(\theta,\phi)$ are the multipolar spherical harmonic angular functions in real form; κ' and κ'' are expansion-contraction parameters, which can be refined together with the population parameters P_ν and P_{lm}. The core population P_c is fixed at 2 for first-row atoms. The valence-shell population parameters are constrained[8,17] to give an electrically neutral unit cell. Slater-type radial functions $R_l=N_l r^n \exp(-\kappa''\zeta r)$ are used, in which N_l is a normalization factor, $n=n(l)$ and ζ are parameters chosen according to Reference 8. The deformation functions with $l \geq 1$ are defined with respect to Cartesian axes local to each pseudoatom, which facilitates, if necessary, the use of any approximate chemical symmetry in the molecule.

From the multipole parameters obtained in the least-squares refinement, the molecular properties such as d-orbital populations[20], the electrostatic potential[21], atomic

Table 1. Electron density maps.

ELECTRON DENSITY MAPS:

DIRECT FOURIER MAPS:

$$\rho(\mathbf{r}) = 1/V \sum_H F(\mathbf{H}) \exp(-2\pi i\mathbf{H}\cdot\mathbf{r})$$

DIFFERENCE FOURIER MAPS:

general expression:

$$\Delta\rho(\mathbf{r}) = 1/V \sum_H [F_1(\mathbf{H})-F_2(\mathbf{H})] \exp(-2\pi i\mathbf{H}\cdot\mathbf{r})$$

(a) difference map (conventional refinement):

$F_1(H) = F_o(H)$
$F_2(H) = F_c(H)$ (conventional ref.)

(b) $X-X_{HO}$ deformation map

$F_1(H) = F_o(H)$
$F_2(H) = F_{c,sph}(H)$ (parameters from HO ref.)

(c) experimental deformation map

$F_1(H) = F_o(H)$
$F_2(H) = F_{c,sph}(H)$ (multipole ref.)

(d) dynamic deformation map

$F_1(H) = F_{c,mul}(H)$
$F_2(H) = F_{c,sph}(H)$ (multipole ref.)

(e) static deformation map

$\delta\rho(\mathbf{r}) = \rho_{mul}-\rho_{sph}$

(f) residual map

$F_1(H) = F_c(H)$
$F_2(H) = F_{c,mul}(H)$ (multipole ref.)

charges and dipole moments[22,23] can be obtained[24]. The use of the aspherical model gives structure factors closer to the true for non-centrosymmetric crystals. This permits mapping of the deformation densities in various ways[9] (Table 1).

The **experimental deformation map** is obtained using the calculated multipole phases with the observed structure amplitudes:

$$\delta\rho(\mathbf{r}) = 1/V \sum_{\mathbf{H}} [\,|F_o(\mathbf{H})|\exp(i\phi_{mul}) - |F_{sph}(\mathbf{H})|\exp(i\phi_{sph})\,]\exp(-2\pi i\mathbf{H}\cdot\mathbf{r})$$

$F_{sph}(\mathbf{H})$ is calculated with the atomic positions and thermal parameters obtained from the multipole refinement.

The **dynamic deformation map**, based more directly on the experimental data, is obtained from the calculated multipole factors, which include the effect of thermal motion. The density is smeared by the molecular vibrations and therefore referred to as 'dynamic'.

$$\delta\rho(\mathbf{r}) = 1/V \sum_{\mathbf{H}} [\,|F_{mul}(\mathbf{H})|\exp(i\phi_{mul}) - |F_{sph}(\mathbf{H})|\exp(i\phi_{sph})\,]\exp(-2\pi i\mathbf{H}\cdot\mathbf{r})$$

The **static deformation map** represents the difference between the total density, determined directly by the multipole parameters, and the total density of the same spherical-atom reference model. The multipole model allows for the deconvolution of the electron distribution from the thermal motion and hence the reference to the 'static' deformation density.

$$\delta\rho(\mathbf{r}) = \rho_{mul} - \rho_{sph}$$

Although the static density may be derived as described, and can be also calculated theoretically, it does not correspond to anything observable in nature.

The use of multipole phases makes the maps slightly model-dependent. The **residual map**, calculated with the least-squares parameters, allows us to test the success of the fitting procedure. It contains all features not accounted for in the model and for good data it should be a flat, featureless map.

$$\delta\rho(\mathbf{r}) = 1/V \sum_{H} [|F_o(\mathbf{H})|-|F_{mul}(\mathbf{H})|\exp(i\phi_{mul})]\exp(-2\pi i\mathbf{H}\cdot\mathbf{r})$$

Further, independent verification of the model and the anisotropic displacement parameters can be achieved by applying **Hirshfeld's rigid bond** test[13,25]. If the bond is to be considered as rigid, the component of the relative vibrational motion of a pair of bonded atoms vanishes in the direction of the bond (i.e. for the two atoms making the bond the components of the atomic vibration along the bond should be the same but of opposite sign).

$$\Delta_{A,B} = z^2_{A,B} - z^2_{B,A} = 0$$

where $z^2_{A,B}$ denotes the mean square displacement amplitude of atom A in the direction of atom B. If in parts of the molecule this is not fulfilled (to at least 0.001Å^2 for non-hydrogen atoms), the structural model used is insufficient.

The requirements of accuracy of the experimental observations in charge density studies are very severe. Symmetry equivalent reflections should be measured and should agree to better than 2% in the intensities. Systematic effects such as multiple reflections, absorption of X-rays in the crystals, extinction, and thermal diffuse scattering should be considered and eliminated experimentally or corrected for in data reduction or refinement. Furthermore, it is increasingly evident that, for the study of molecular crystals data should be collected at liquid nitrogen (77K) or liquid helium (4.2K) temperatures for a number of reasons:

- collection of high-order data will lead to an increase of resolution in the electron density maps and allow a more accurate determination of the positional and thermal parameters;

- reduction in temperature will reduce the anharmonicity of the external molecular vibrations so that introduction of a more complex model in the refinement can be avoided;

- effect of thermal diffuse scattering decreases relative to the intensity of the Bragg reflections when the temperature is lowered, thus one source of error in the temperature parameters is reduced.

This project involves two major studies of the deformation electron density in the benzene clathrate of hexa(1-aziridinyl)cyclotriphosphazene and comparative charge density studies of the phosphorus-sulphur bonding and of the extent of the aromatic system in a 1,3,2-benzodithiaphosphenium cation and the related 2-phenyl-1,3,2-benzodithiaphosphole.

2.2. Electron Density Distribution in the Benzene Clathrate of Hexa(1-aziridinyl)cyclotriphosphazene

2.2.1. Introduction

Cyclophosphazenes occupy a prominent place among inorganic heterocyclic compounds[1,2,26,27]. They contain an $[-N{=}PR_2-]$ repeating unit in a valence-unsaturated skeleton. The study on those compounds was initiated not only by their interesting chemical properties but also by their possible applications to serve as carriers for the medically active side groups.

Aziridinyl-substituted cyclophosphazenes have been recognized as cytostatic agents for more than 30 years[28]. They can be described as a combination of a biologically active group (1-aziridinyl) and an electron-directing (depending on other substituents) phosphazene ring as carrier material.

The hexa(1-aziridinyl)tricyclophosphazene $N_3P_3az_6$ (az = aziridinyl = $-N(CH_2)_2$) appears to be one of the most promising of these drugs. The structural study of this compound reveals that it can exist in several forms in crystals. When it is recrystallized from CCl_4, it forms an 'anticlathrate' complex[29] $N_3P_3az_6 \cdot 3CCl_4$. When recrystallized from m-xylene, it yields orthorhombic unsolvated crystals, whereas crystallization from CS_2 produces monoclinic unsolvated crystals[30]. The conformations of the aziridinyl groups in these compounds are similar (<u>trans</u>).

However, when $N_3P_3az_6$ is recrystallized from benzene it forms a very stable complex $2N_3P_3az_6 \cdot C_6H_6$ with a most unusual <u>cis</u> conformation at the geminal aziridinyl groups (Figure 5). The crystal structure of this complex was determined at room temperature (288K), refined to R=0.026 and has been published[31].

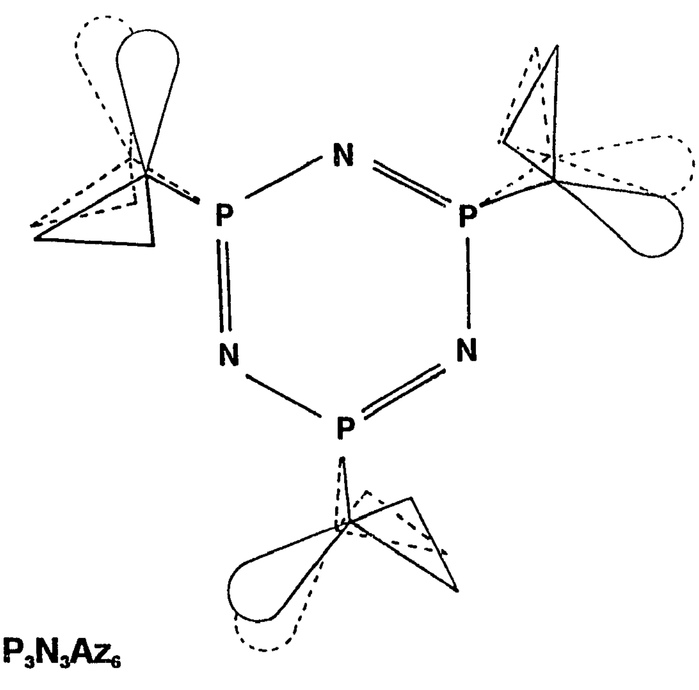

Figure 5. <u>Cis</u>-conformation of aziridinyl groups in cyclophosphazene.

The structure has been redetermined at 213 K to examine the deformation density of the phosphazene ring[32].

Detailed study of the electron distribution carried out at low temperature is reported here.

The molecule contains the well-known benzene ring and the three-member rings of the aziridinyl groups. The electron distribution features observed in those regions are used as an internal measure of the credibility of the electron density in the region of the P_3N_3 ring.

2.2.2. Experimental

Two independent sets of data have been used in the calculations. One set of data (set I) has been collected locally by a standard technique using the Enraf-Nonius CAD4 diffractometer. The second set (set II) has been collected for us by Bev Vincent at Molecular Structure Corporation[33], using R-Axis II, Rigaku automated X-ray Imaging System. The use of imaging plates allows accurate measurements of diffraction patterns with high dynamic range, high sensitivity, and low intrinsic background. This is the first example of using data from the X-ray Imaging System to calculate high accuracy deformation maps. The short time of data collection (6 hours as against about 3 months for the CAD-4) and the results, comparable with those obtained using the standard technique, allow us to predict that this technique can be widely used in the future.

2.2.3. Data Collection and Processing (Data Set I)

An Enraf-Nonius CAD4 diffractometer [$\lambda(MoK_{\alpha1})$=0.70926Å] was used to measure the unit cell dimensions and to collect the data. The crystal, which was mounted in a Mark-Röhrchen glass capillary, was a near perfect octahedron with edges in the range 0.10-0.12mm. The data were collected in the rhombohedral setting at 213K which is the lowest safe temperature the crystal will endure. At 150K[a] the crystal slowly (2 hours) crumbles, apparently transforming into a triclinic cell; the disintegration is slower at 170K but the crystal appears to be stable just above 200K. For reflections in the range $3^\circ<\theta<25^\circ$ the full ±h, ±k, ±l shell was collected but for $25^\circ<\theta<45^\circ$ only data in the range ±h, ±k, l ($h \geq k \geq l$) were collected. While the re-collection of certain portions of the data confuses the accounting of the total number of reflections measured, ultimately about 26000 were used to provide the unique data set. The crystal and data collection parameters are listed in Table 2. The unit cell constants were obtained by least-squares analysis of the diffractometer setting angles of 25 well-centred reflections in the range $2\theta=30^\circ-34^\circ$. The data were processed by routine procedures[34].

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[a] 150.2 K is the temperature at which the 2 0 0 reflection of KH_2PO_4 splits. It is thus a very precise probe for the actual crystal temperature. J.C. Slater, J. Chem. Phys. 9, 16, (1943); see also J. Phys C: Solid State Phys. 15, 37, (1982).

Lorentz and polarization corrections were applied and absorption corrections were performed[35]. Scattering factors for neutral atoms were taken from International Tables[36] and were corrected for the real part of anomalous dispersion.

2.2.4. Structure Solution (Data Set I)

The initial atomic parameters were taken from the original room temperature structure[31] and these were refined with full-matrix least-squares using SHELX-76[37] and CRYSTALS[38].

The space group was confirmed as $R\bar{3}$. Hydrogen atoms were placed in their geometrically calculated positions [d(C-H) = 1.08Å]. The final refinements were with anisotropic temperature factors on the non-hydrogen atoms and individual isotropic temperature factors on the hydrogen atoms. The function minimised was $\Sigma w(|F_o|-|F_c|)^2$ where w is the weight (Table 2). Final R-values[b] are R=0.0341 and R_w=0.0370. No correction for extinction was applied. The figures were produced with CHEMGRAF[39]. Slant Fourier F_o maps and difference F_o-F_c maps were calculated through the benzene, cyclotriphosphazene, and aziridinyl groups planes using CRYSTALS[38].

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[b] $R = \Sigma||F_o|-|F_c||/\Sigma|F_o|$;

$R_w = [(\Sigma w(|F_o|-|F_c|)^2/\Sigma wF_o^2)]^{½}$;

Table 2. Physical properties and parameters for data collection and refinement of $2P_3N_3(NC_2H_4)_6 \cdot C_6H_6$ (Data Set I).

Formula	$2P_3N_3(NC_2H_4)_6 \cdot C_6H_6$
Molecular weight	852.71
Crystal class	Trigonal
Space group	$R\bar{3}$ (rhombohedral) (No. 148)
Temperature (^oK)	213(1)
a (Å)	10.210(1)
α (^{o})	79.18(2)
V ($Å^3$)	1013.9
Z	1
d_c (g cm^{-3})	1.396
F(000)	450
μ (cm^{-1})	3.07
Crystal size (mm)	.12x .12x .12
Diffractometer	CAD-4
λ (Å) (MoKα)	0.70926
hkl range	h: -20 20
	k: -20 20
	l: 0 20
θ range (^{o})	0-45
$\sin\theta/\lambda$	1.00

Table 2. (cont.). Physical properties and parameters for data collection and refinement of $2P_3N_3(NC_2H_4)_6 \cdot C_6H_6$ (Data Set I).

Take off angle (°)	6.0
Detector width (mm):	
variable slit:	4(1.4 + tan Θ)
Scan speed (° min^{-1})	variable: 1.6-3.3
Scan type	$\omega/2\Theta$
Scan width (°)	1.0 + 0.35 tan Θ
Standards (period.)	5 5 5 / 6 1 2 / 3 6 1
orientation (200 refls.)	
intensity (2h)	no loss
No. of meas. refls.	≈26000
No. of unique refls.	5562
R_m	0.0371
No. of obs. refls., N_{ob}	2518
observed if $[I>3\sigma(I)]$	
No. of variables, N_v	118
Transmission coefficients	0.677-1.253
Weighting scheme	
$w=k/[\sigma^2(F)+gF^2]$ k,g	0.7940, 0.0092
Highest peak	
in final diff. Fourier (e $Å^{-3}$)	0.42
Agreement factors:	
$R=(\Sigma\|\|F_o\|-\|F_c\|\|)/(\Sigma\|F_o\|)$	0.0341
$R_w=[\Sigma w(\|F_o\|-\|F_c\|)^2/(\Sigma w\|F_o\|)^2]^{1/2}$	0.0370
$GOF=[\Sigma(\|F_o\|-\|F_c\|)^2/(N_{ob}-N_v)]^{1/2}$	1.0708

Table 3. Physical properties and parameters for data collection and refinement of $2P_3N_3(NC_2H_4)_6 \cdot C_6H_6$ (Data Set II).

Formula	$2P_3N_3(NC_2H_4)_6 \cdot C_6H_6$
Molecular weight	852.72
Crystal class	Trigonal
Space group	$R\bar{3}$ (hexagonal) (No. 148)
Temperature (^{o}K)	213(1)
a (Å)	13.026(1)
c (Å)	20.759(1)
$\alpha=\beta$ (^{o})	90.00
γ	120.00
V (Å^3)	3050.5(2)
Z	3
d_c (g cm^{-3})	1.393
F(000)	1350
μ (cm^{-1})	3.14
Crystal size (mm)	.02x .02x .02
Diffractometer	RAXIS II-c
λ (Å) (MoKα)	0.71069
θ range (^{o})	0-63
$\sin\theta/\lambda$	1.25

Table 3. (cont.). Physical properties and parameters for data collection and refinement of $2P_3N_3(NC_2H_4)_6 \cdot C_6H_6$ (Data Set II).

Take off angle (°)	2.8
Detector aperture (mm):	200x200
Crystal to detector dist.(mm)	59
Detector off-axis angle (°)	-28.5
Scan	6° oscillations
No. of meas. refls.	17639
No. of unique refls.	4596
R_m	0.0450
No. of obs. refls., N_{ob}	3215
observed if [$I>3\sigma(I)$]	
No. of variables, N_v	118
N_{ob}/N_v	27.25
Weighting scheme	$1/\sigma^2(F_o)$
Highest peak	
in final diff. Fourier (e $Å^{-3}$)	0.81
Agreement factors:	
$R=(\Sigma\|\|F_o\|-\|F_c\|\|)/(\Sigma\|F_o\|)$	0.0430
$R_w=[\Sigma w(\|F_o\|-\|F_c\|)^2/(\Sigma w\|F_o\|)^2]^{1/2}$	0.0490
$GOF=[\Sigma(\|F_o\|-\|F_c\|)^2/(N_{ob}-N_v)]^{1/2}$	1.910

2.2.5. HO Deformation Density Maps (Data Set I)

Once the refinement had converged, the structure was re-refined using those high-order (HO) reflections for which $25^\circ \leq \theta \leq 45^\circ$ ($\sin\theta/\lambda > 0.6\text{Å}^{-1}$). At these angles the diffraction from the bonding and lone-pair electrons is negligible[4] and the refinement is responding to the effect of just the core electrons on each of the atoms. The calculations were performed using CRYSTALS[38] and Dunitz-Seiler weights[40]. The parameters from the HO refinement were then used with the low-order data $3^\circ \leq \theta \leq 25^\circ$ ($\sin\theta/\lambda < 0.6\text{Å}^{-1}$) to calculate structure factors F_c for all the reflections in the low-angle data. The low-order data are more susceptible to bonding effects concentrated in the valence electrons. Thus when the structure factors (F_c), calculated with high-angle parameters, are subtracted from the low-angle F_o data, a significant portion of the difference should represent the valence electron density. Such difference maps, which are known as $X-X_{HO}$ maps, show areas of both positive and negative electron density.

The experimental deformation density maps were calculated by the Slant Fourier procedure in CRYSTALS[38] through the benzene, aziridinyl and phosphazene planes. As a compromise between reducing experimental noise in the deformation maps and getting the maximum of information in the lone-pair region, $\sin\theta/\lambda$ was limited to 0.6Å^{-1}. Only reflections with

$I>3\sigma(I)$ were used in calculations.

The deformation densities observed show most promising features. The expected features are seen on the benzene ring and aziridinyl group. The densities in the P_3N_3 ring have a very significant arrangement which should finally settle the arguments about the nature of the bonding in this ring[1,2].

2.2.6. Data Collection and Processing (Data Set II)

The data were collected on an R-Axis IIc imaging plate area detector[33] mounted on an RU200 rotating anode X-ray generator equipped with a Mo anode. The area detector was fitted on a 2θ stage which allows it to be moved around the ϕ axis to attain high 2θ reflections. A low temperature device was installed to lower the crystal temperature to 213K. The generator was set at 50kV and 180mA to give 9kW of power. The crystal to detector distance was set at 59mm and the detector was swung out to a 2θ value of -28.5°. This configuration allowed the direct beam image to be recorded on the plate while simultaneously giving full coverage out to 90° in a single positioning of the area detector.

The octahedral crystal having approximate dimensions of 0.02x0.02x0.02mm was mounted in a glass capillary and a standard xyz goniometer head was used to center the crystal in the beam. The X-ray filament was normal focus, but a 0.3mm collimator was used to reduce background on the imaging plate.

The position of the direct beam was recorded on one frame by removing the beam trap and opening the shutter for a fraction of a second.

Three 3° oscillation photographs were recorded at 0°, 45°, and 90° (in ϕ), respectively. These oscillation photographs were used by the indexing software to determine the unit cell and crystal orientation. Based on this information, it was determined that the data could be collected in frames of 6° of oscillation with a minimum of reflection overlap. (Overlapping reflections are totally rejected in the integration procedure.) A total of thirty 6° frames were collected to give a full 180° of data. Each frame was exposed for 10 minutes, so total data collection time was just over 5 hours. The crystal and data collection parameters are listed in Table 3.

Several different techniques[41,42] were used to integrate the data and compared. The one which gave the best results used an integration box of fixed size (roughly 4.5 mm square). After the integration box shape was optimized, the thirty frames were integrated to yield 17639 reflections. Data are divided into two categories: fulls and partials. Full reflections appear completely on one frame. Partials appear on more than one consecutive frame; partials which appear on more than 2 frames are rejected. The final refined mosaic spread of 0.344° (when compared to the total oscillation range per frame) was low enough to guarantee that the vast majority of the data (94%) were fully recorded on a single exposure.

The data were merged into one data file, brought to a common scale and averaged. Then a post-refinement procedure was undertaken which uses all data to refine the cell dimensions and camera constants (which include crystal to detector distance, 2θ offset, crystal orientation, mosaic spread and the plate deformation). Based on these new parameters, the frames were reintegrated, merged, scaled and averaged to produce the final data set. A total of 4596 unique reflections were produced, with a merging R-value of 4.5%. The data were corrected for Lorentz and polarization effects. No absorption correction was applied. The data are based on the hexagonal setting of the rhombohedral cell.

2.2.7. Structure Solution (Data Set II)

The structure was solved by direct methods[43] and expanded using Fourier techniques[44]. The non-hydrogen atoms were refined anisotropically. Hydrogen atoms were refined isotropically. The final cycle of full-matrix least-squares refinement[c] was based on 3215 observed reflections ($I>3.00\sigma(I)$ and $2\theta\leq180^{\circ}$) and 118 variable parameters, and converged with unweighted and weighted agreement factors of R=0.043 and

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[c] Least-Squares:
Function minimized: $\Sigma w(|F_o|-|F_c|)^2$
where: $w = 1/\sigma^2(F_o) = 4F_o^2/\sigma^2(F_o^2)$

R_w=0.049.

The standard deviation of an observation of unit weight[d] was 2.50. The weighting scheme was based on counting statistics and included a factor (p=0.02) to downweight the intense reflections. Plots of $\Sigma w(|F_o|-|F_c|)^2$ versus $|F_o|$, reflection order in data collection, sin θ/λ, and various classes of indices showed no unusual trends. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.81 and $-0.72e/Å^3$, respectively. No absorption nor extinction corrections were applied.

Neutral atom scattering factors were taken from Cromer and Waber[36]. Anomalous dispersion effects were included in F_c[45]; the values for $\Delta f'$ and $\Delta f''$ were those of Cromer[36].

All calculations were performed using the TEXSAN[46] crystallographic software package of Molecular Structure Corporation.

2.2.8. HO Deformation Density Maps (Data Set II)

Positional and thermal parameters of non-hydrogen atoms were re-refined based on high-order (HO) reflections with $\sin\theta/\lambda > 0.6Å^{-1}$ in order to avoid bias from the aspherical

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[d] Standard deviation of an observation of unit weight:

$\Sigma w(|F_o|-|F_c|)^2/(N_o-N_v)]^{1/2}$;

where: N_o = number of observations
N_v = number of variables

distribution of the valence electrons. The parameters from the HO refinement were then used with the low-order data ($\sin\theta/\lambda<0.6Å^{-1}$) to calculate structure factors F_c for all the reflections in the low angle data. The $X-X_{HO}$ deformation maps were calculated for the benzene, cyclotriphosphazene, and aziridinyl groups planes.

All calculations were performed using the TEXSAN[46] crystallographic software package of Molecular Structure Corporation.

2.2.9. Multipole Deformation Maps (Data Set II)

Multipole refinement was performed using program MOLLY[17]. Data Set II was converted to rhombohedral setting. The aspherical atomic density expansion of Hansen and Coppens[8] was used in calculations, as incorporated in the program MOLLY[17]. The valence-shell population parameters were constrained[8] to give an electrically neutral unit cell. For phosphorus, nitrogen, carbon, and hydrogen atoms, Slater-type functions were used for the multipole deformation functions. In the subsequent refinement, the overall scale factor, κ' , κ'', and multipole parameters, together with the positional and thermal parameters of non-hydrogen atoms were varied. Initially, hydrogen atoms were refined isotropically. Later, their coordinates were adjusted by extending along the C-H bond directions to bond length of 1.06Å for the $C_{tetrahedral}$-H bonds, and 1.08Å for the $C_{aromatic}$-H bonds[47]. Positional and thermal parameters of hydrogens were then fixed in the subsequent refinements. The multipole expansion was truncated at the octapole level for phosphorus, nitrogen, and carbon atoms and at the dipole level for hydrogen atoms. No site symmetry constraints were applied on the multipole functions since they were not required by the space group symmetry. The analysis of the agreement between model and experimental structure factors gave no indication that significant extinction was present therefore the extinction coefficient was not refined.

The multipole population parameters are listed in Appendix 1. The fractional coordinates and thermal parameters from this refinement are given on microfiches (Appendix 4).

The rigid-bond[13] test indicated that the multipole refinement produced a relatively effective deconvolution of the mean-square atomic displacements from the valence-electron density deformations. The differences between the mean-square displacements along interatomic directions were less than 0.001$Å^{-1}$ for nearly all the bonded pairs of non-hydrogen atoms (Appendix 4). The exceptions were bonds N3-C1, N3-C2, and C1-C2 of one of the aziridinyl group, where the $\Delta_{A,B}$ = 0.0013$Å^2$, 0.0014$Å^2$, and 0.0012$Å^2$, respectively. This fact and the shape of the thermal ellipsoid, as well as the observations of the electron density maps, suggest that the aziridinyl groups are not entirely rigid and that there is still some libration present.

The residual maps, experimental deformation maps, and dynamic deformation maps were calculated using program NF (local modification of NIELSAV[48]).

2.2.10. Molecule

The benzene clathrate of hexa(1-aziridinyl)cyclotriphosphazene crystallizes in space group $R\bar{3}$ with the three-fold axis passing through the centres of the planes of both

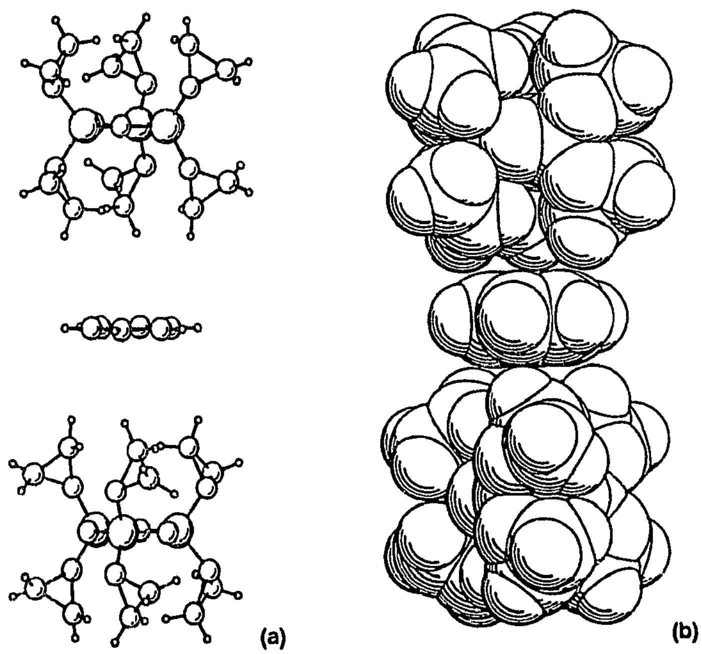


Figure 6. Crystal structure of $2N_3P_3az_6 \cdot C_6H_6$ shown with the C_3 axis vertical; (a) ball and stick model; (b) space filling model.

the benzene and the phosphazene rings (Figure 6). The single molecule of benzene is located at the centre of symmetry between two molecules of cyclophosphazene. The planes of three rings are parallel but their planarity is not required by symmetry and in fact the phosphazene ring is very slightly puckered with P and N atoms deviated by 0.016Å from the plane. The structure thus contains two unique aziridinyl groups, a phosphazene ring, and a benzene molecule which is very firmly held in the lattice (Figure 6).

The cyclotriphosphazene ring contains two unique exocyclic and two unique endocyclic P-N bonds: exocyclic (mean): 1.675(1)Å, endocyclic (mean): 1.593(1)Å.

The molecule has two aziridinyl groups bonded to each P atom. The aziridinyl groups are pyramidal and adopt an unusual <u>cis</u> conformation (Figure 5). Each group has a prominent electron lone-pair orbital which occupies space within the crystal lattice (Figure 7). The lone-pairs are arranged in such a way that their axes are almost parallel to the plane of P_3N_3 ring. Atomic positions, temperature factors, interatomic distances, interbond angles for both set of data are given in Appendix 1. The pertinent torsional angles are

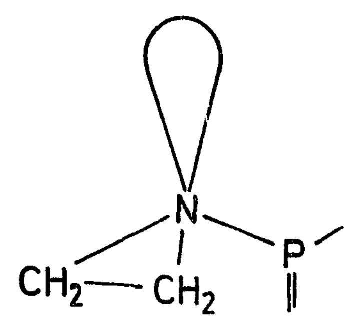


Figure 7. Aziridinyl group.

listed on microfiches (Appendix 4).

2.2.11. Bonding in the Phosphazene Ring

The problem of explaining the bonding arrangements in phosphazenes has occupied the attention of a number of investigators[1,2,49,50]. It seems generally agreed that two electrons of nitrogen occupy an sp^2 lone-pair orbital in the plane of the ring (or the local P-N-P plane), with the third electron occupying the p_z orbital. The situation with phosphorus is not so clear. The σ-bonds can be considered to result from the approximate sp^3 hybrids on the P atom, bonding to the p orbitals of the N from the aziridinyl groups, and sp^2 hybrid on the N in the ring. The disposition of the remaining electrons has been the subject of controversy. With the phosphorus 3s and 3p orbitals filled, there is a possibility of the involvement of 3d orbitals on P in π-bonding.

One type of out-of-plane p_π-d_π bonding (π) would involve a single occupied p_z orbital on N and d_{xz} (heteromorphic bonding) or d_{yz} (homomorphic bonding) orbitals on P. In addition, the nitrogen sp^2 lone-pair can be involved in the in-plane bonding (called π') to $d_{x^2-y^2}$ and d_{xy} orbitals on the P (Figure 8). The discussion centres on the questions whether delocalized π bonding occurs over the entire ring[51,52], or gives rise to a three-centre bond system[53] with the discontinuity of the electron cloud at each phosphorus atom.

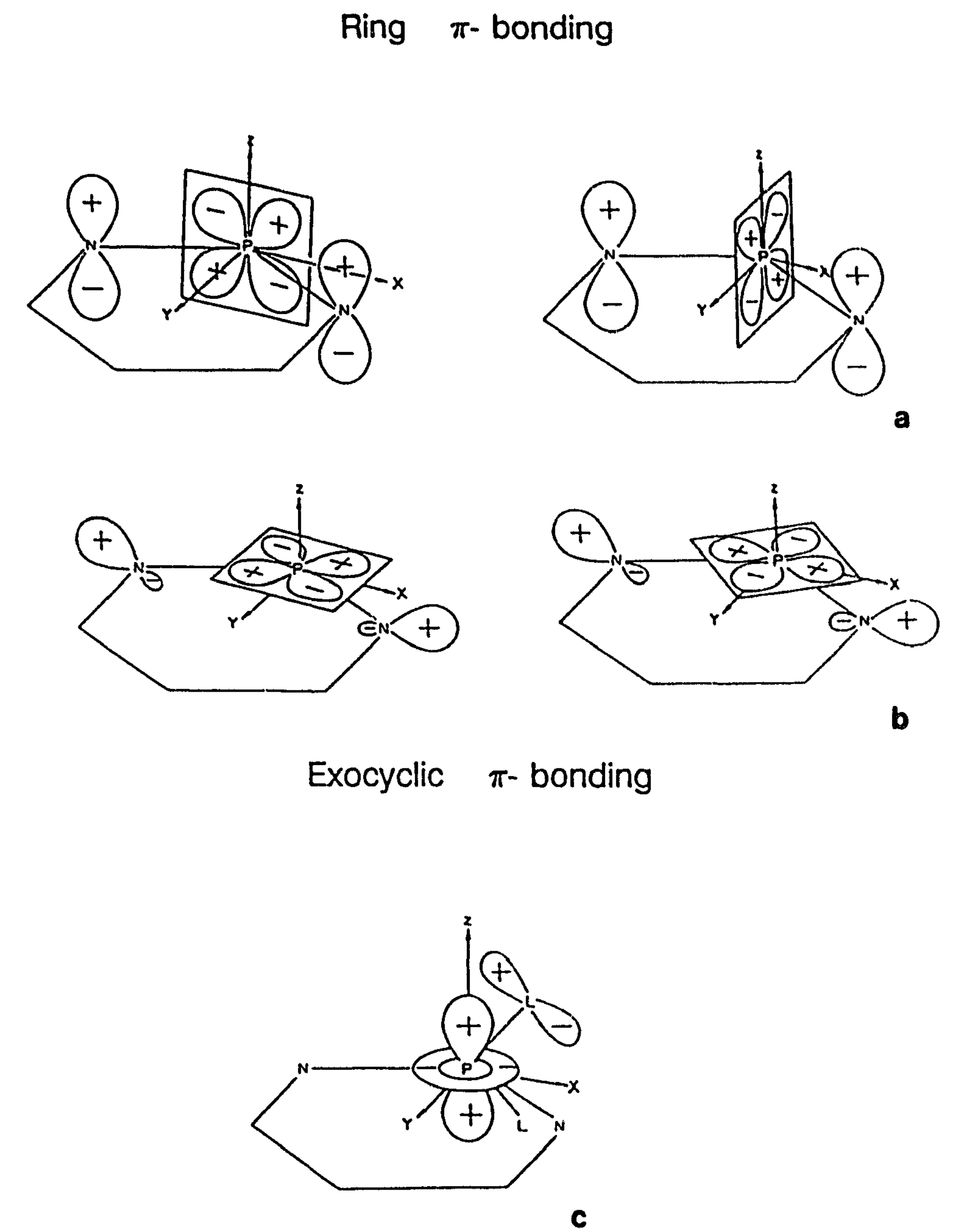


Figure 8. Bonding in the phosphazenes; (a) π-bonding; (b) π'-bonding; (c) exocyclic π-bonding.

Different effects are anticipated according to the relative participation of the d_{xz} and d_{yz} orbitals in the π bonding. If only the d_{xz} orbital gives rise to the bonding, a broadly delocalised, heteromorphic, 'pseudoaromatic' π orbital could be formed. Exclusive involvement by d_{yz} would generate a homomorphic π system. On the other hand, the approximately equal contributions from the two orbitals would tend to separate π orbitals into localized three-centre islands of π character interrupted at each P atom, and a broad delocalization would not be expected.

More detailed theoretical calculations[54,55] appear to support the delocalized model and indicate that conjugation beyond the three-center islands is of minor importance in the cyclotriphosphazene derivatives. The work of Doggett[56] suggests that the delocalized model of Craig and Paddock[52] and the three-center model of Dewar[53] et al. are fundamentally very similar and differ only in the choice of parameters.

The influence of the substituents on phosphorus in the phosphazenes has been also discussed[1,2,50,57,58]. The presence of a highly electronegative group will contract the phosphorus d orbitals and facilitate the donation of the nitrogen sp^2 lone-pair electron to the π'-system; whereas the electron-donating substituents can participate in the exocyclic π-bonding (Figure 8) by means of the d_{z^2} orbital on P. However, the aziridine derivatives of phosphazenes have pyramidal exocyclic nitrogen atom configurations and relatively long exocyclic P-N bond length and hence it is supposed that exocyclic lone-pair delocalization does not occur in these systems[55].

An additional complication to the electronic structure of cyclophosphazenes is the possibility of transannular phosphorus-phosphorus bonding[59].

Some experimental evidence[26,55] can be adducted to support all of the above theories. Thus, thermochemical measurements[60] have been cited in support the initial 'aromatic' theory; ultraviolet spectra[55,61] and some X-ray works[55,62] support the view about incomplete delocalization, at least in some structures; whilst the alternation of properties with the ring size appears to support the proposal on π'-bonding[63].

2.2.12. Electron Density Maps

Electron density calculations were performed to examine the deformation electron density of the phosphazene ring. However, the same structure should show the expected features for the deformation density of the benzene ring. It should also show the nitrogen lone-pair electrons for the two unique aziridinyl groups and the deformation density of the two three-membered rings. The presence of these expected features should give support to the observations on the phosphazene ring.

The $X-X_{HO}$ map through the plane of the benzene ring is

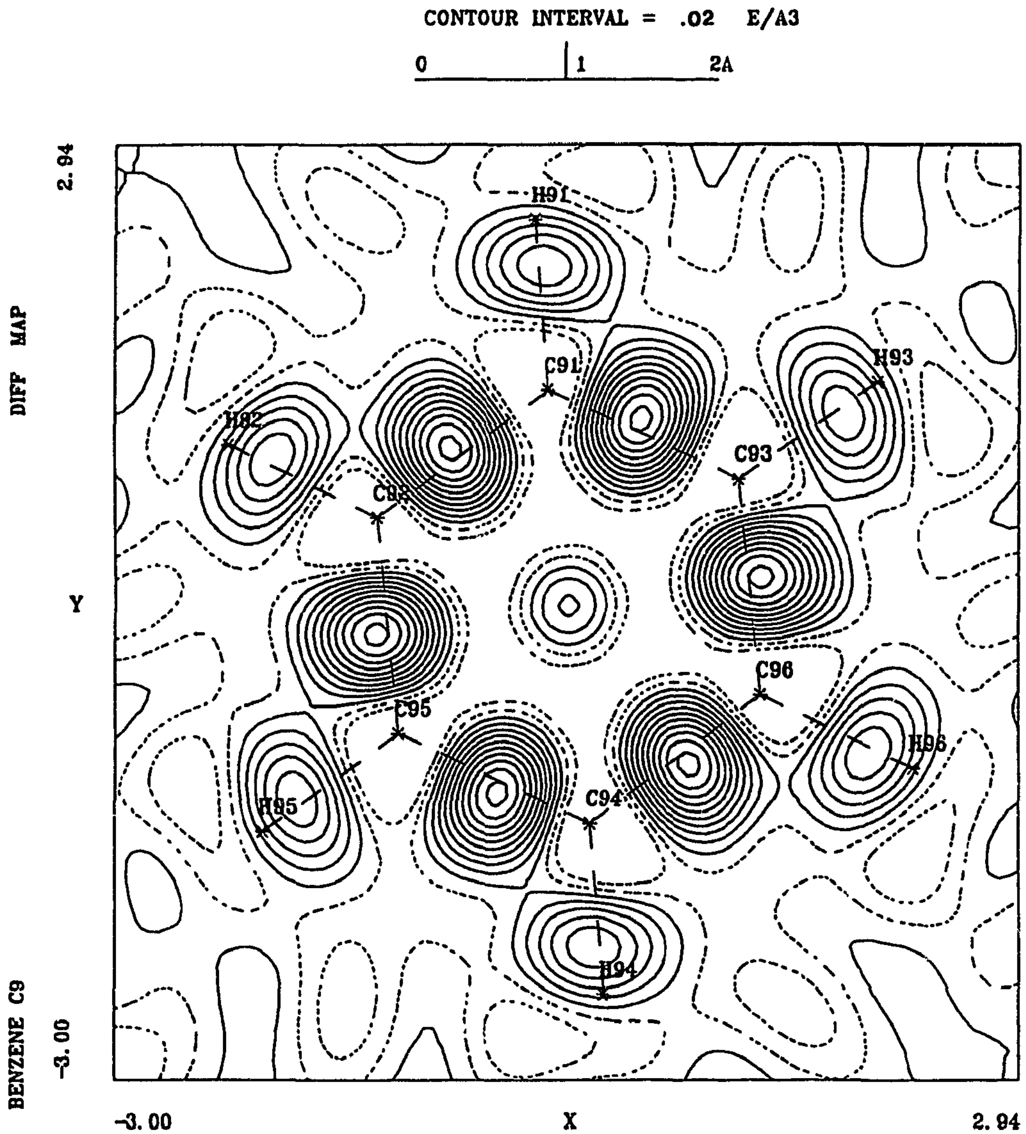
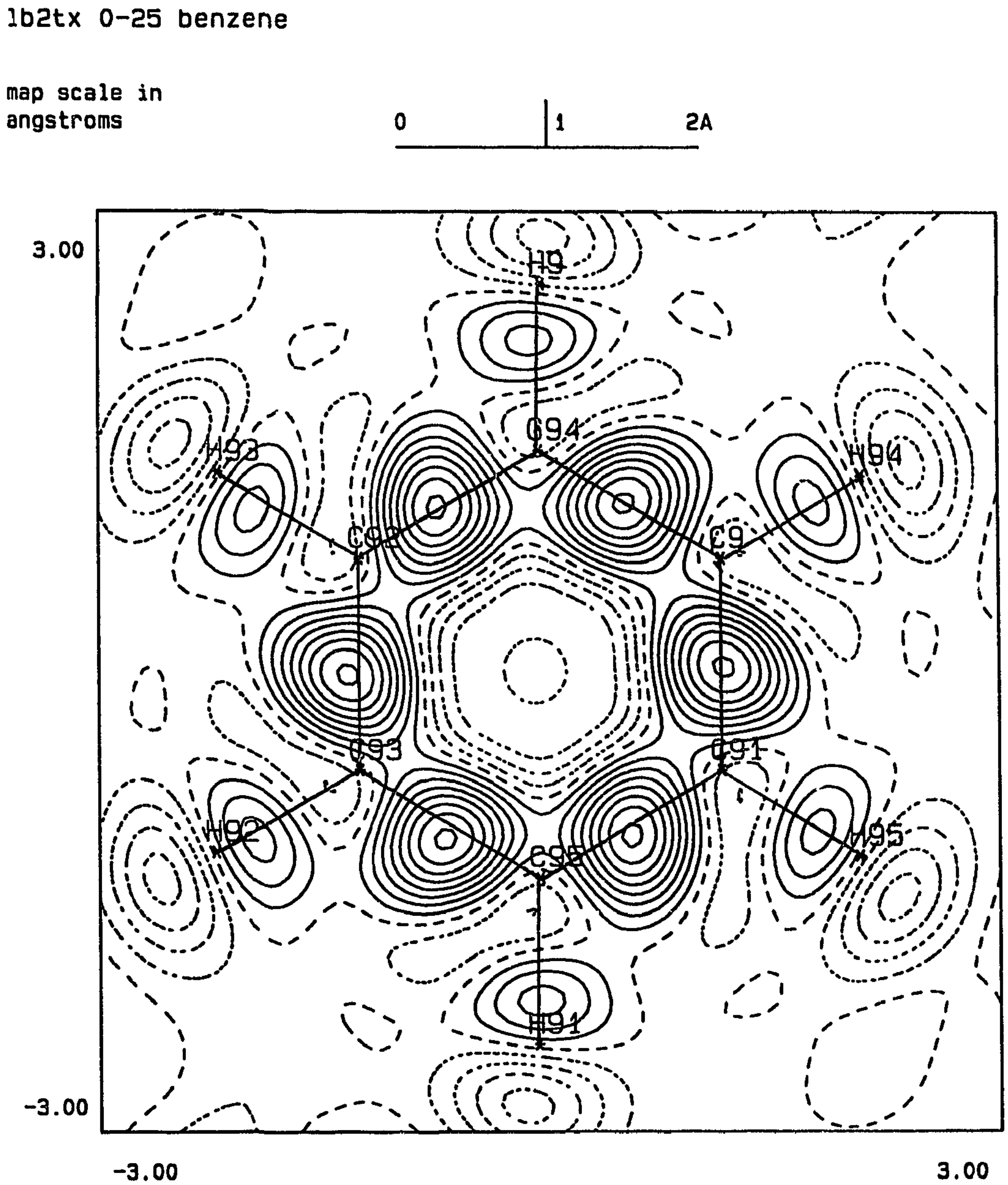


Figure 9. X-X_{HO} deformation density in the benzene ring (Data Set I).



plane defined by three atoms: C9 C92 C95
contour interval (e/A**3): 0.04
perpendicular offset: 0.00
origin translation along x (A): 1.30
origin translation along y (A): 0.70
map rotation (deg): 0.

Figure 10. $X-X_{HO}$ deformation density map in benzene (Data Set II).

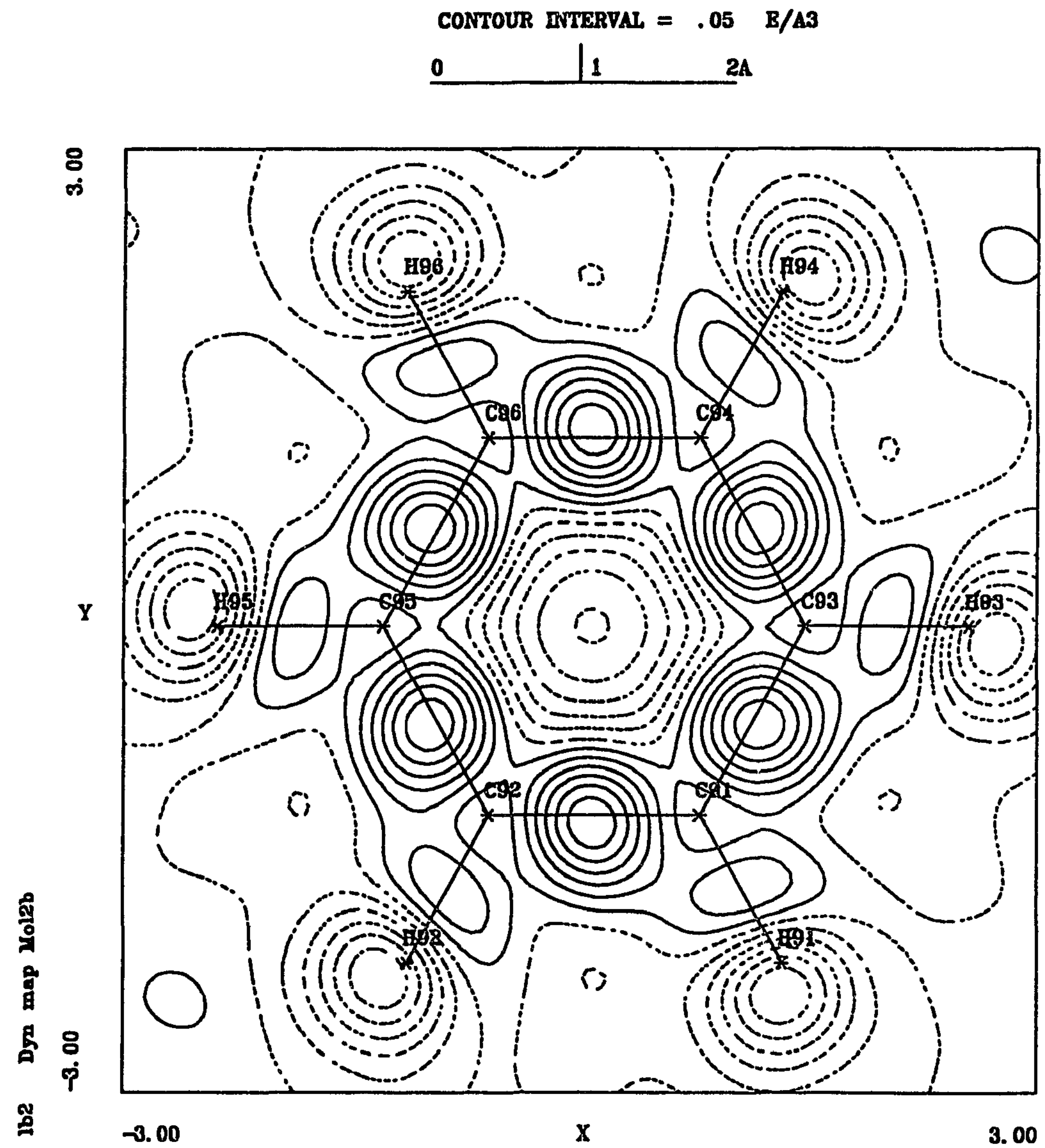


Figure 11. Dynamic deformation density map in the plane of the benzene ring.

shown in Figure 9 and Figure 10. The peaks of deformation density are clearly observed between the carbon atoms in the ring, and the level of density (see below) strongly indicates both σ and π bonding. This compares very favourably with the reported deformation density for naphthalene[64].

The dynamic multipole deformation density map for the benzene plane is shown in Figure 11. All maps presented for the benzene ring display similar features. The existence of the negative minima near the hydrogen atoms can be attributed to the experimental H-atom modelling. The hydrogens in the benzene ring were positioned to give 1.08Å C-H bond length and 120° C-C-H angles. Any error in the hydrogen position will produce strongly correlated errors in the hydrogen dipole population. The mean-square atomic displacement parameters are correlated with monopole populations and this can also bias the valence-shell population parameters.

Figure 12 and Figure 13 show the plane perpendicular to the benzene ring, exactly bisecting two opposite C-C bonds. Since the C-C bond in the benzene is formed with both σ and π bonds, the cross-section should be elliptical, with the long-axis perpendicular to the plane of the ring. The electron density in the bond should be squashed, by electron-electron repulsions, on the inside of the ring and somewhat elongated on the outside. All these features can be seen in Figure 12 and Figure 13.

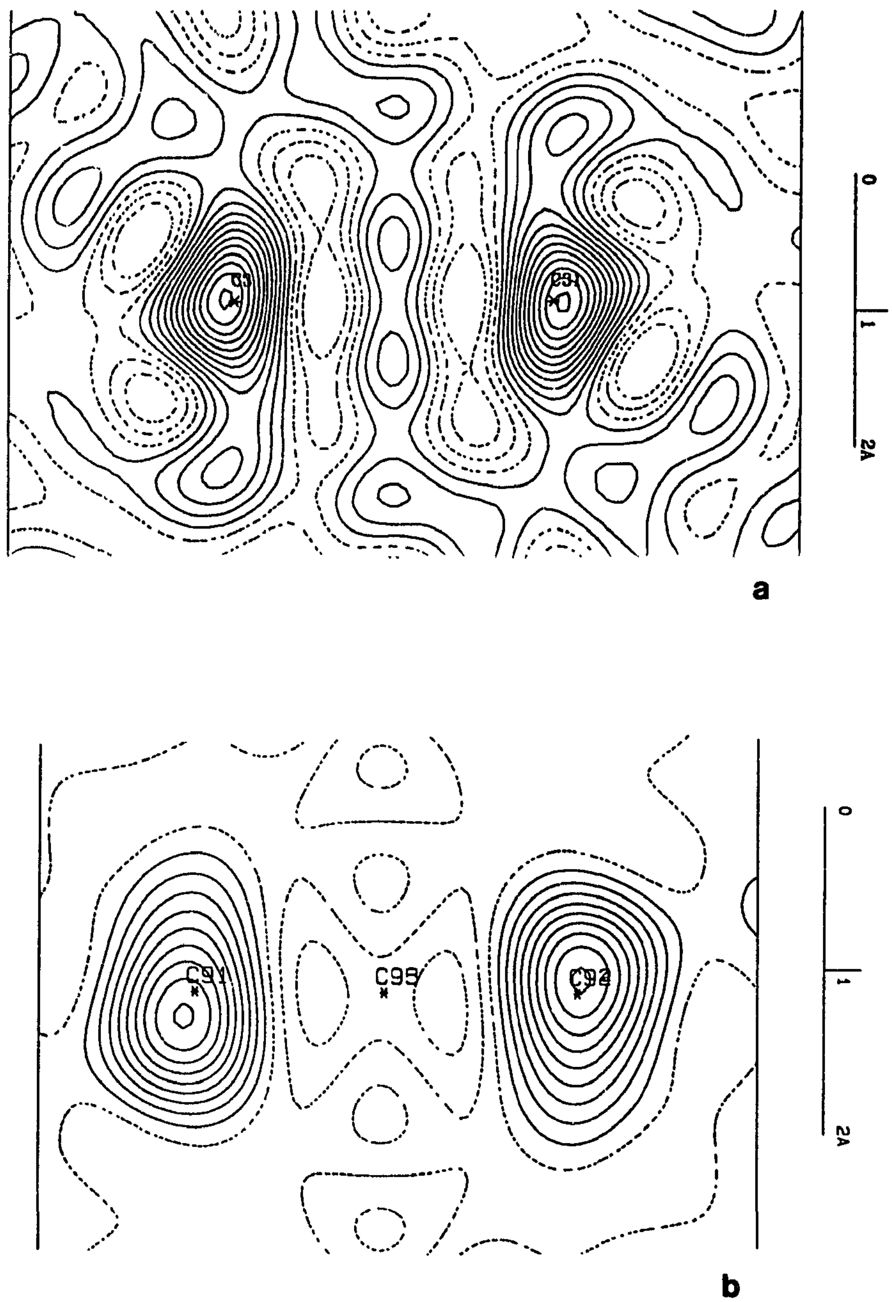


Figure 12. X-X_{HO} deformation density in the plane bisecting C-C bond in the benzene ring; (a) Data Set I; (b) Data Set II)

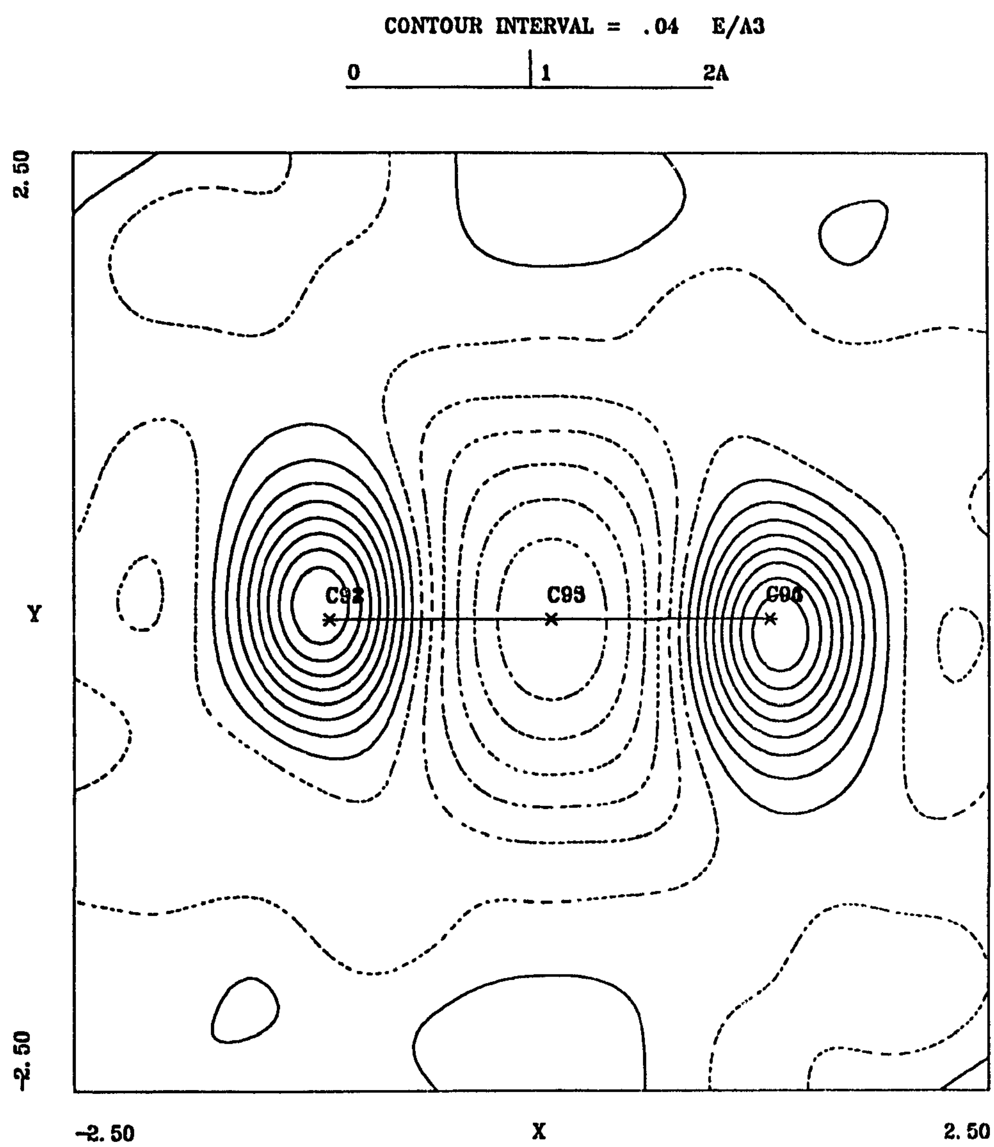


Figure 13. Dynamic deformation density in the plane bisecting two opposite C-C bonds in the benzene ring.

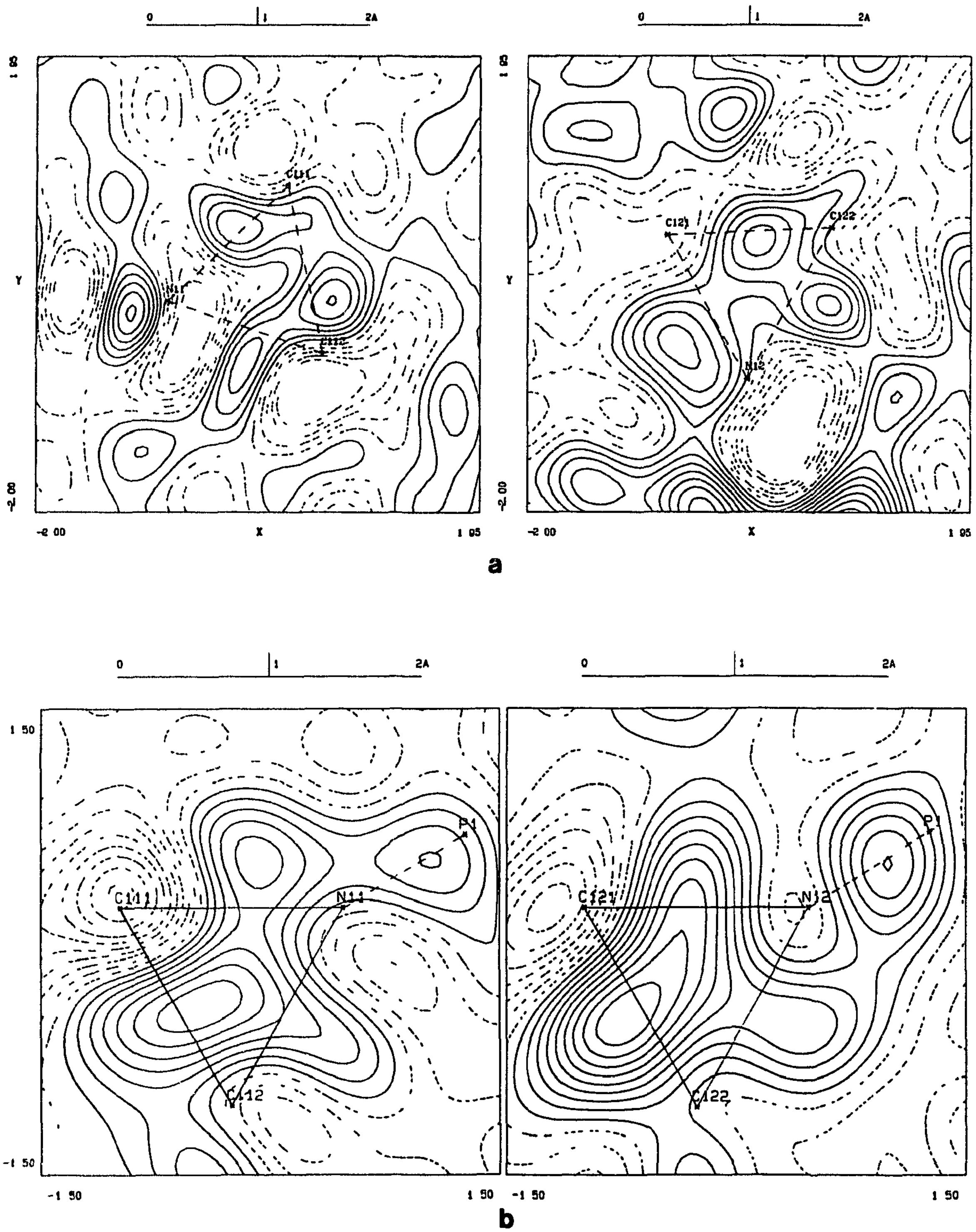


Figure 14. X-λ_{HO} deformation density in the three-member rings; (a) Data set I; (b) Data set II;

The $X-X_{HO}$ maps through the plane of each of the two aziridinyl rings are presented in Figure 14. Figure 15 shows the multipole dynamic deformation density map for aziridinyl groups.

In the three-membered ring the deformation density peaks appear outside the triangle sides and can be attributed to the

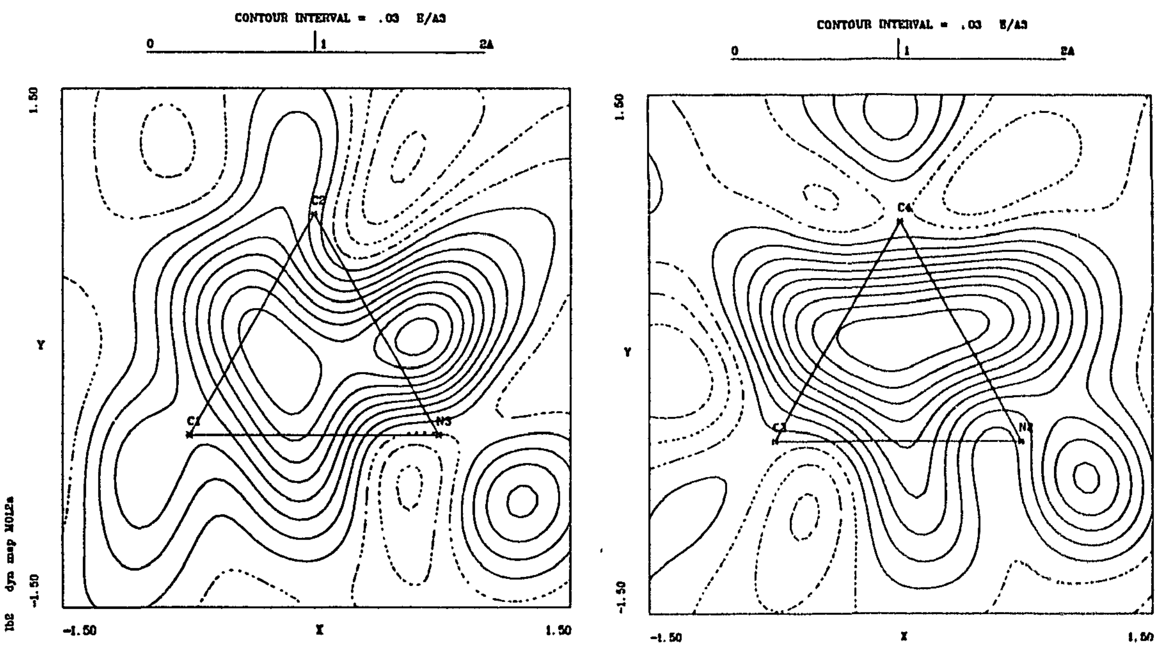
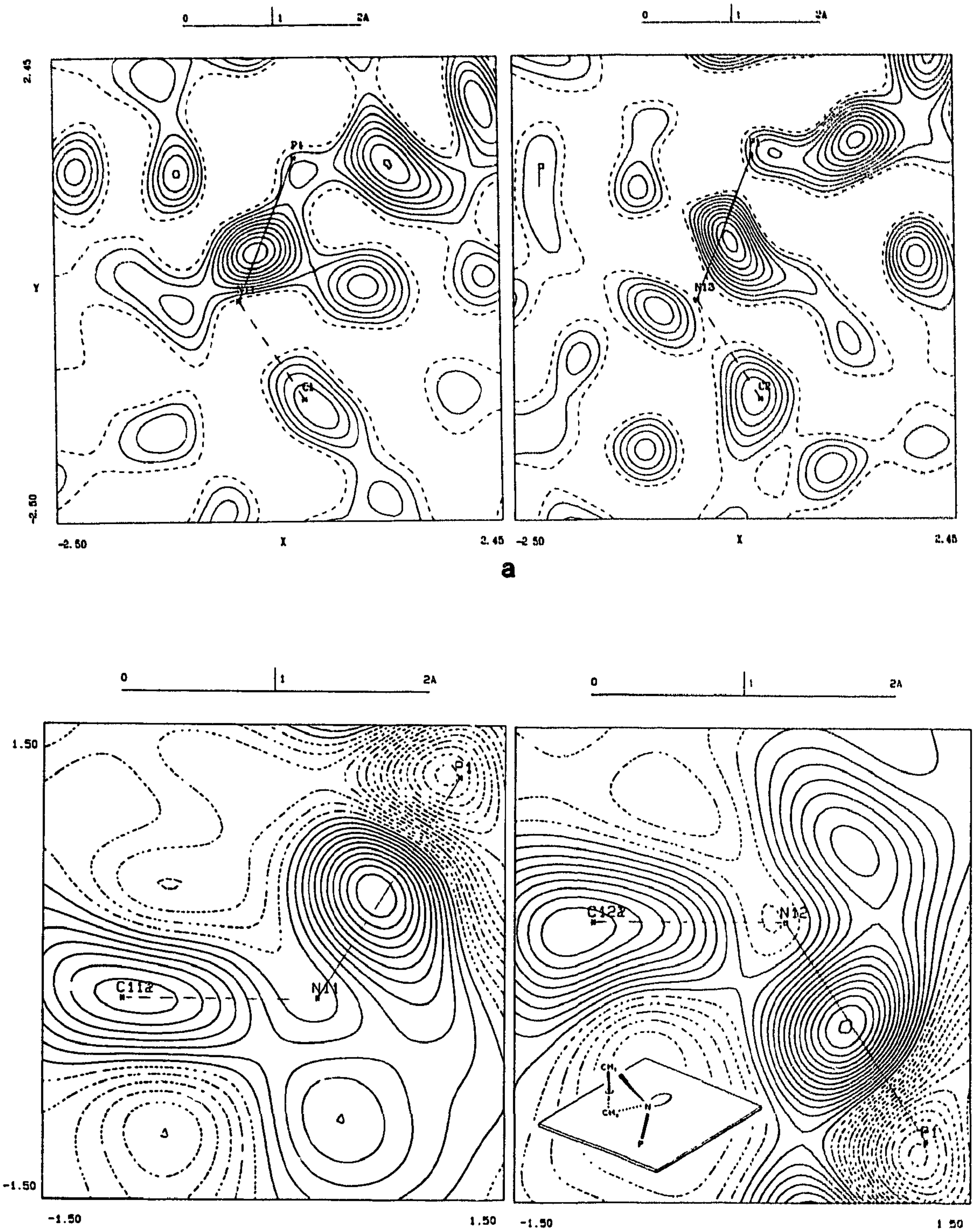


Figure 15. Dynamic deformation density in the aziridinyl rings.

'bent bond' concept, in accordance with the theoretical prediction for highly strained bonds[65,66,67]. Both rings show the expected 'bent' σ bonds with a much lower residual density (since they have no π bonding density) than that seen for the benzene. There is also an additional feature at the nitrogen atom in Figure 14a, which is probably the tail of the lone pair. However, there is still some libration present (suggested also by the rigid-bond test) in at least one of these aziridinyl groups (with N12) and the three-membered ring density while clear and confirming is not as good as the very best seen in these systems[67].

The lone-pair electrons are clearly visible on the aziridinyl nitrogen atoms. Peaks of the deformation density in the region of non-bonding orbitals represent the part of the lone-pair density which is in excess of the spherical atomic distribution rather than their total density. Figure 16 shows the $X-X_{HO}$ maps for the planes which pass through the phosphorus atom, the appropriate nitrogen atom, and then bisect the C-C bond of the aziridinyl group. The nitrogen lone-pair electrons should be found in this plane. The multipole dynamic deformation maps are presented in Figure 17. Both groups show the deformation density maxima in exactly the predicted positions.



b

Figure 16. X-X_{HO} deformation density in the region of the lone-pair at N11 and N12; (a) Data Set I; (b) Data Set II.

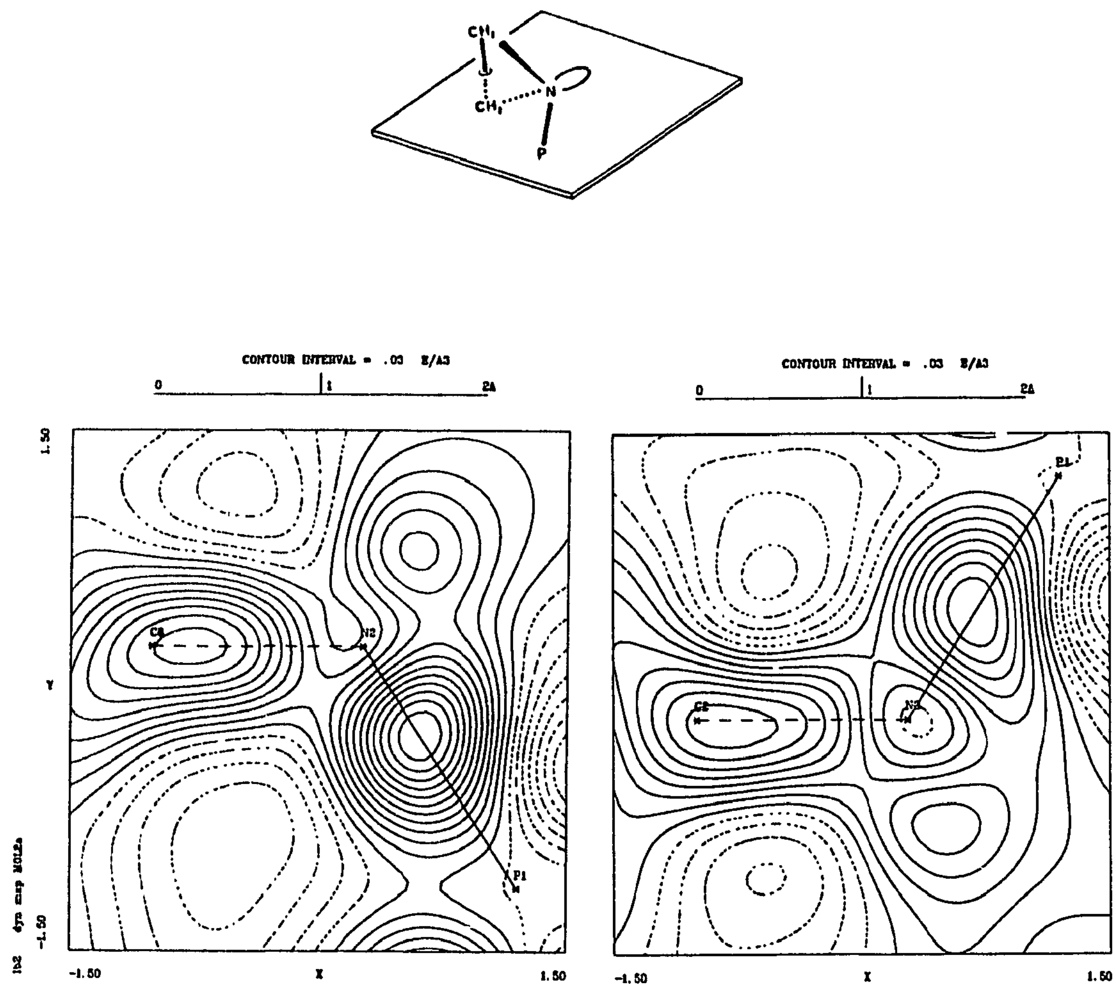


Figure 17. Dynamic multipole map in the regions of lone-pair electrons in the aziridinyl groups.

The X-X_{HO} calculations for the light-atom portions of the structure show the expected features very clearly. The multipole deformation maps for the benzene and aziridinyl groups are almost an exact copy of the X-X_{HO} calculations. Thus the expected deformation densities observed at those parts of the molecule support the chemical conclusions and credibility of data presented for the phosphazene ring.

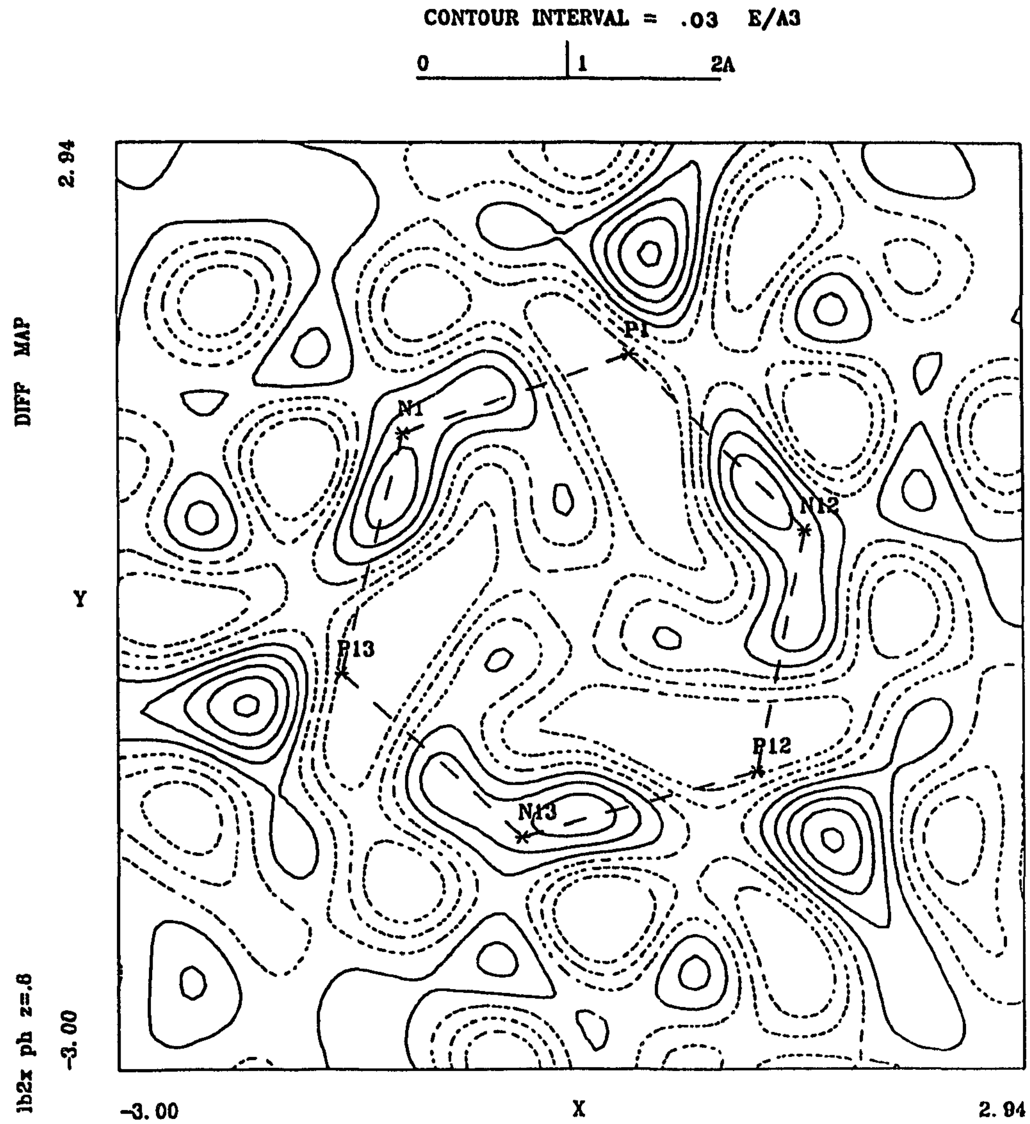
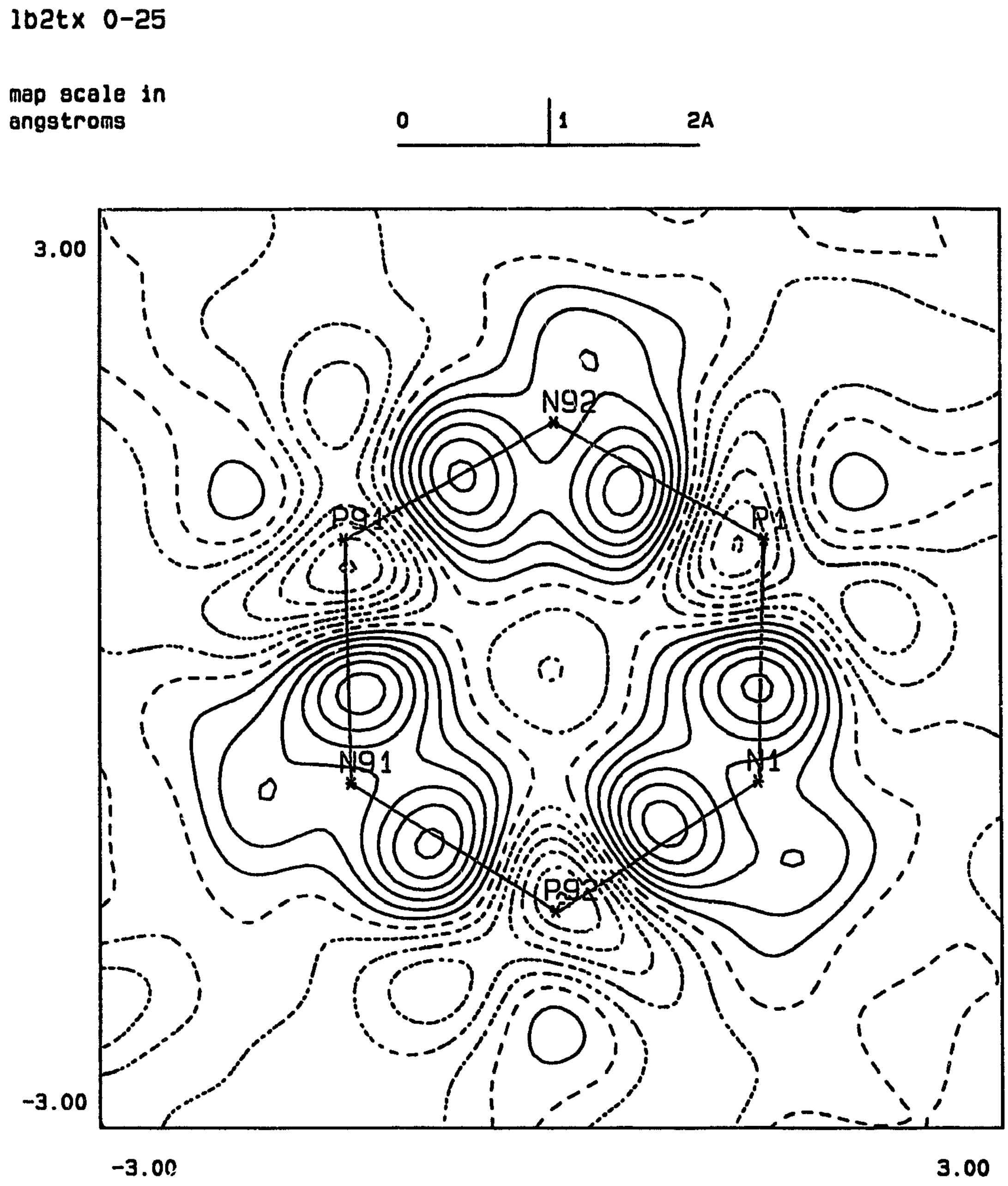


Figure 18. X-X_{HO} deformation density in the phosphazene ring (Data Set I).



plane defined by three atoms: P1 P91 P92
contour interval (e/A**3): 0.05
perpendicular offset: 0.30
origin translation along x (A): 1.40
origin translation along y (A): 0.80
map rotation (deg): 0.

Figure 19. X-X_{HO} deformation density in the phosphazene ring (Data Set II).

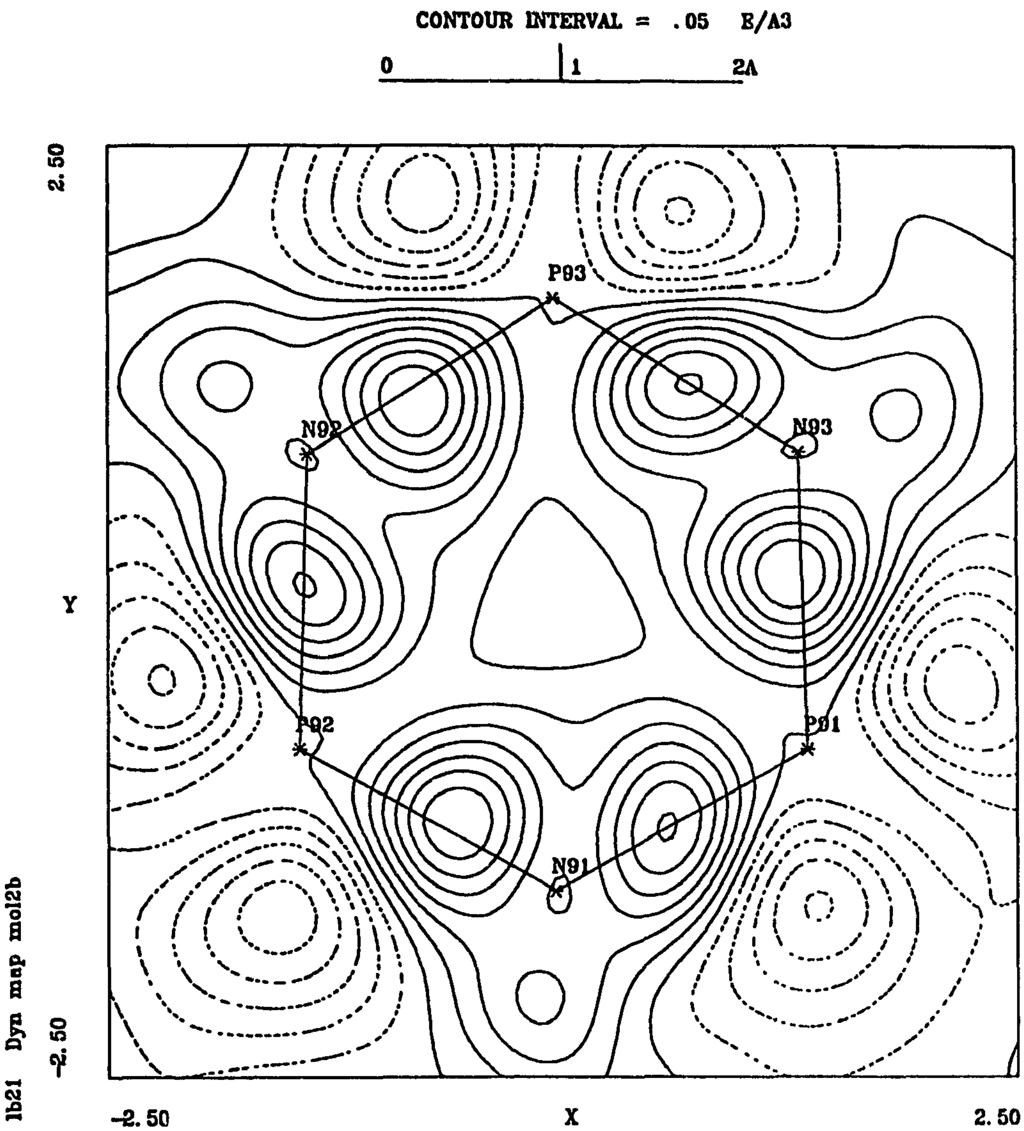


Figure 20. Dynamic deformation density in the phosphazene ring (Data Set II).

Figure 18 and Figure 19 show the $X-X_{HO}$ deformation density on the phosphazene ring. They clearly display the bonding through the nitrogen atoms with the in-plane lone pair and the node at phosphorus. Many minor changes in refinement parameters, data ranges, and distances from the plane have been performed for this ring, yet all the deformation maps show the same broad features. There is a clear reduction in the valence electron density at the phosphorus atom, and a clear increase in density at the nitrogen atom and this density appears to connect from one endocyclic P-N bond through the nitrogen atom to the second endocyclic P-N bond. This observation is also supported by the multipole dynamic deformation density of the phosphazene ring (Figure 20). The multipole parameters which are normalized in such a way that a value of unity corresponds to the transfer of one electron from the negative to positive regions of the corresponding charge deformation term also indicate this trend. The net valence charges (P_{ν}) obtained for P1 and N1 suggest that the N1 has an excess charge of 0.55(15) while the P1 has a deficiency of charges of 0.14(30) (Appendix 1). However, it should be noticed that the magnitudes of such charge shifts are model-dependent and no quantitative conclusions can be derived.

The cross-sections through the P-N and P-N' bonds are presented in Figure 21. The electron density is elongated in the direction normal to the plane of the ring, similarly to that in the benzene, which indicates the contribution of the π-bonding into the P-N bonding. This contribution seems to be slightly larger for one P-N bond than for another. Usually, the endocyclic P-N bonds in phosphazenes are considered as equivalent. The values of the P-N bond lengths in $2N_3P_3az_6 \cdot C_6H_6$ are significantly different (1.588(1)Å and 1.598(1)Å). Such a difference would be predicted from the cis geometry of the aziridinyl groups which requires the two cyclic P-N bonds to be non-equivalent because of their different local environments. (In the trans system these two bonds should be equal.)

Contrary to the case of benzene (Figure 13), in the phosphazene ring the deformation density is squashed from

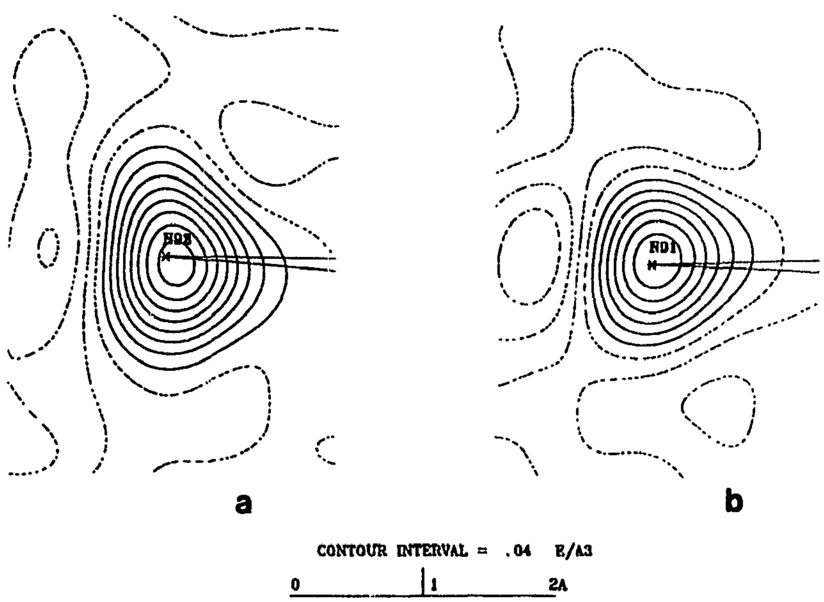


Figure 21. Dynamic deformation maps through the planes bisecting the P-N bonds; (a) P1-N1 bond; (b) P1-N1(1+z,x,y-1) bond.

outside the ring and elongated on the inside (Figure 21). This could indicate the contribution from the in-the-plane π'-bonding.

In the phosphazene system, the residual map through the phosphazene ring is essentially featureless (Figure 22). It shows a density range that seldom exceeds $\pm$ 0.1e/Å^3 and is never more than $\pm$ 0.15e/Å^3.

The observations of the deformation density of the phosphazene system, supported by the observation on the well-known molecular systems as benzene and three-member rings, are the first experimental observation on the bonding density for the system and are in agreement with the delocalization models[52,53,56] for bonding in the cyclotriphosphazene ring.

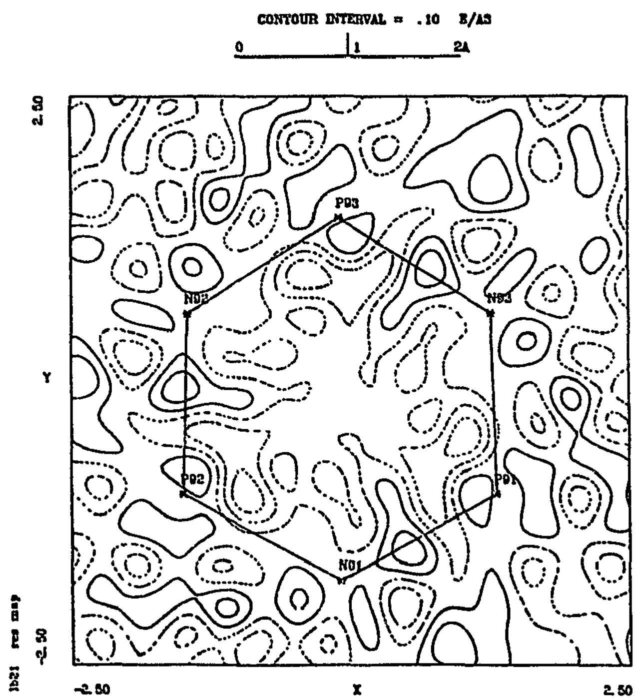


Figure 22. Residual multipole map in the region of the phosphazene ring.

2.2.13. Summary

The study of the deformation electron density in the benzene clathrate of hexa(1-aziridinyl)cyclotriphosphazene has been undertaken to locate the bonding and non-bonding lone-pair electrons in the phosphazene ring and to answer the long-debated questions about the bonding in this ring[1,2,26,55]. The compound contains well-known molecular fragments (like benzene and three-member rings of aziridinyl groups) for which the deformation density has already been examined. The expected observations on these fragments add credence to the observations on the phosphazene ring.

Two independent sets of data have been used in the calculations. One has been collected locally by a standard technique (CAD-4), while the second has been collected for us at MSC[33], using R-Axis II, Rigaku automated X-ray Imaging System. The use of imaging plates allows accurate measurements of diffraction patterns with high dynamic range, high sensitivity, and low intrinsic background. This is the first example of using data from the X-ray Imaging System to calculate high accuracy deformation maps. The low time of data collection (6 hours as against about 3 months for the CAD-4) and the results, comparable with those obtained using standard technique, allow us to predict that this technique can be widely used in the future.

The $X-X_{HO}$ calculations for the light-atom portions of the structure show the expected features very clearly. The multipole deformation maps for the benzene and aziridinyl groups are almost an exact copy of the $X-X_{HO}$ calculations. Thus the expected deformation densities observed at those parts of the molecule support the chemical conclusions and credibility of data presented for the phosphazene ring.

The observations of the deformation density of the phosphazene system are the first experimental observation on the bonding density for the system and are in agreement with the delocalization models[52,53,56] for bonding in the cyclotriphosphazene ring.

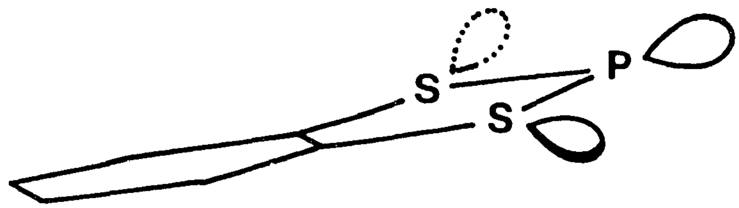
2.3. Comparative Charge Density Studies of the Phosphorus-Sulphur Bonding and of the Extent of the Aromatic System in a 1,3,2-Benzodithiaphosphenium Cation and the Related 5-Methyl-2-Phenyl-1,3,2-Benzodithiaphosphole.

2.3.1. Introduction

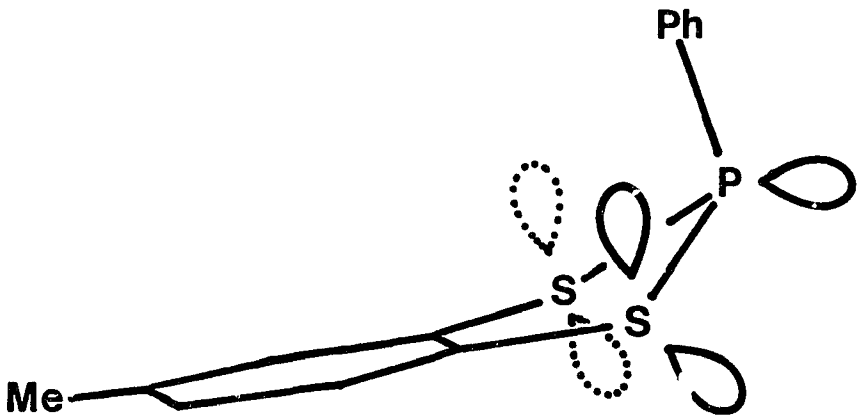
It has been suggested[68,69,70,71] that the 1,3,2-benzodithiaphosphenium cation (II) contains an extended ten electron pπ-pπ system analogous to naphthalene[64]. This suggestion was based initially on the spectroscopic evidence, structural observations on the bond lengths, and the planarity of the cation[70].

A preliminary examination of the charge density from data collected at room temperature indicated[72] that the situation might not be as simple as this since the electron density in the bonds was not distributed as evenly as might be expected.

The low-temperature deformation density studies of the cation (II) and the related neutral molecule of 5-methyl-2-phenyl-1,3,2-benzodithiaphosphole (III) are reported here. The electron distribution in these molecules should be predictably different (Figure 23) and the extent to which the deformation density studies show all the expected features in the two systems can be used as a measure of the validity of the conclusions derived for the cation (II).



II



III

Figure 23. Diagram of molecules (II) and (III).

If the cation (II) contains an extended 10 electron pπ-pπ system, a π-electron distribution like that of naphthalene[64] is expected to appear in the deformation density map for the cation, while the neutral molecule (III), which is not planar, will show an aromatic distribution for the phenyl ring only.

Similarly, the sulphur atoms of the cation will each have a single set of lone-pair electrons in the plane of the ring. The sulphur atoms in the neutral molecule, however, will each have two sets of lone-pair electrons which, together with the

S-C and S-P bonds, will make up an approximate tetrahedron (Figure 23).

The positive charge for the cation is formally written on the phosphorus atom. If the charge is predominantly on this atom[e], then the charge-density distribution will show little charge (or a charge hole) at the phosphorus atom and the single set of lone-pair electrons, which should be in the plane of the ring, may be lost in the hole.

2.3.2. Experimental and Refinement

The crystals of (II) and (III) were mounted in glass capillaries. An Enraf-Nonius CAD4 diffractometer was used to measure the unit cell dimensions and to collect the data at 213K. The crystal and data collection parameters for the phosphenium cation and the neutral molecule are listed in Table 4 and Table 5, respectively. The unit cell constants were obtained by the least-squares analysis of the diffractometer setting angles of 25 well-centred reflections in the range $2\theta = 20-30^{\circ}$. The intensities were reduced to a standard scale using routine procedures[34]. Lorentz and polarization corrections were applied. Absorption corrections were performed[35]. Scattering factors for neutral atoms were

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[e]Various theoretical calculations suggest that between 50-70% of the charge is on this phosphorus atom (see Reference 71 p. 39 and B.W. Royan, N. Burford, J. Waluk, & J. Michl, Organometallics, (1990), 9, 1085).

taken from International Tables[36] and were corrected for the real part of the anomalous dispersion. The calculations and refinements were performed by using SHELX-76[37].

The space group was confirmed as $P2_1/c$ for the cation and $P2_1/n$ for the neutral molecule. The initial positions of the non-hydrogen atoms were taken from the structure determination at room temperature[70]. The structure was refined by a full-matrix least-squares procedure initially with independent isotropic temperature factors on the atoms. Absorption corrections were then applied. Hydrogen atoms were placed in their geometrically calculated positions [d(C-H) = 1.08Å]. The final refinements were with anisotropic temperature factors on the non-hydrogen atoms and individual isotropic temperature factors on the hydrogen atoms. The function minimised was $\Sigma w(|F_o|-|F_c|)^2$ where w is the weight (Table 4 and Table 5). Final agreement factors for the cation and neutral molecule are given in Table 4 and Table 5, respectively. No correction for extinction was applied. The final difference map had no recognizable residual features. The figures were produced with CHEMGRAF[39]. Slant Fourier F_o maps and difference F_o-F_c maps were calculated through different molecular planes by using CRYSTALS[38]. Atomic positions, temperature factors, interatomic distances, and interbond angles for the benzodithiaphosphenium cation and benzodithiaphosphole molecule are given in Appendix 2. The pertinent torsional angles for both structures are listed on microfiches (Appendix 4).

The atomic positional and thermal parameters of the neutral molecule (III) were re-refined based on high-order (HO) reflections with $\sin\theta/\lambda > 0.6Å^{-1}$. The parameters from the HO refinement were then used with the low-order data ($\sin\theta/\lambda < 0.6Å^{-1}$) to calculate structure factors F_c for all the reflections in the low angle data. The $X-X_{HO}$ deformation maps were calculated using the TEXSAN[46] crystallographic software package of Molecular Structure Corporation.

Although the extended data set at 213K has also been collected for the cation (II), a careful examination of these data showed that a small number of reflections were present for the class h0l $l \neq 2n$. These reflections had $I > 6\sigma(I)$ and were present for all the symmetry equivalent reflections. Refinement of the structure produced an unsatisfactory result for the anion, $AlCl_4^-$, and it seems likely that at low temperatures the space group degrades from $P2_1/c$ to $P2_1$ with the four $AlCl_4^-$ anions splitting into two non-equivalent groups of two each. Despite many attempts, this space group anomaly was not satisfactory resolved, and so the study was suspended until another, a more temperature-stable, derivative could be prepared. At 230K the crystal appears to be well-behaved and the difference maps are shown for the data collected at this temperature. While these maps show many intriguing features, which will be discussed, the temperature is really too high for any definite conclusions to be drawn.

Table 4. Physical properties and parameters for data collection and refinement of $C_6H_4S_2P^+ \cdot AlCl_4^-$.

Formula	$C_6H_4AlCl_4PS_2$
Molecular weight	339.98
Crystal class	Monoclinic
Space group	$P2_1/c$ (No. 14)
a (Å)	6.589(3)
b (Å)	23.351(5)
c (Å)	8.657(3)
β (°)	100.25(3)
V (Å^3)	1310.7
Z	4
d_c (g cm^{-3})	1.723
F(000)	672
μ (cm^{-1})	13.62
Crystal size (mm)	.05 x .35 x .50
Temperature (°K)	230
Diffractometer	CAD-4
λ (Å) (MoKα)	0.70926
hkl range	h: -7 7,
	k: -1 25,
	l: -9 9
θ range (°)	2-23
$\sin\theta/\lambda$	0.55

Table 4. (cont.). Physical properties and parameters for data collection and refinement of $C_6H_4S_2P^+ \cdot AlCl_4^-$.

Take off angle (°)	6.0
Detector width (mm):	
variable slit:	4(1.4 + tanθ)
Scan speed (° min^{-1})	variable: 1.6-3.3
Scan type	ω/2θ
Scan width (°)	1.0 + 0.35tanθ
Standards (period.)	1 6 4 / -3 6 3 / -1 13 0
orientation (200 refls.)	
intensity (2h)	no loss
No. of meas. refls.	7578
No. of unique refls.	1816
R_m	0.0375
No. of obs. refls., N_{ob}	1265
observed if [$I>3\sigma(I)$]	
No. of variables, N_v	132
Transmission coefficients	0.777-1.143
Weighting scheme	
$w=k/[\sigma^2(F)+gF^2]$ k,g	1.0909, 0.0003
Highest peak	
in final diff. Fourier (e $Å^{-3}$)	-0.31
Agreement factors:	
$R=(\Sigma\|\|F_o\|-\|F_c\|\|)/(\Sigma\|F_o\|)$	0.0326
$R_w=[\Sigma w(\|F_o\|-\|F_c\|)^2/(\Sigma w\|F_o\|)^2]^{1/2}$	0.0328
$GOF=[\Sigma(\|F_o\|-\|F_c\|)^2/(N_{ob}-N_v)]^{1/2}$	1.4439

Table 5. Physical properties and parameters for data collection and refinement of $C_{13}H_{11}PS_2$.

Formula	$C_{13}H_{11}PS_2$
Molecular weight	262.32
Crystal class	Monoclinic
Space group	$P2_1/n$ (No. 14)
a (Å)	14.696(7)
b (Å)	6.244(7)
c (Å)	14.793(6)
β (°)	114.64(4)
V (Å^3)	1233.7
Z	4
d_c (g cm^{-3})	1.412
F(000)	544
μ (cm^{-1})	5.11
Crystal size (mm)	.15 x .25 x .25
Temperature (°K)	210
λ (Å) (MoKα)	0.70926
hkl range	h: -26 26,
	k: 0 11,
	l: -17 26
Θ range (°)	2-45
$\sin\Theta/\lambda$	1.0

Table 5 (cont). Physical properties and parameters for data collection and refinement of $C_{13}H_{11}PS_2$.

Take off angle (°)	6.0
Detector width (mm):	
variable slit:	$4(1.4 + \tan\theta)$
Scan speed (° min^{-1})	variable: 1.6-3.3
Scan type	$\omega/2\theta$
Scan width (°)	$1.0 + 0.35\tan\theta$
Standards (period.)	-2 0 8 / 2 3 -6 / -9 0 5
orientation (200 refls.)	
intensity (2h)	no loss
No. of meas. refls.	17035
No. of unique refls.	7081
R_m	0.0334
No. of obs. refls., N_{ob}	1915
observed if $[I>3\sigma(I)]$	
No. of variables, N_v	202
Transmission coefficients	0.650 - 1.233
Weighting scheme:	
$w=k/[\sigma^2(F)+gF^2]$ k,g	1.0503, 0.0013
Highest peak	
in final diff. Fourier (e $Å^{-3}$)	-0.44
Agreement factors:	
$R=(\Sigma\|\|F_o\|-\|F_c\|\|)/(\Sigma\|F_o\|)$	0.0466
$R_w=[\Sigma w(\|F_o\|-\|F_c\|)^2/(\Sigma w\|F_o\|)^2]^{1/2}$	0.0488
$GOF=[\Sigma(\|F_o\|-\|F_c\|)^2/(N_{ob}-N_v)]^{1/2}$	1.4743

2.3.3. Electron Density Maps

In the 10π-electron cation system, each sulphur atom should have one set of lone-pair electrons in the plane of the rings. The sulphur atoms in the neutral compound, on the other hand, should each have two sets of lone-pair electrons and these should be found in the plane bisecting the C-S-P angle and perpendicular to the C-S-S-C plane (Figure 23). However, a careful examination of the cation shows that, in fact, the ring is slightly saucer shaped, while the neutral molecule is distorted by a steric interaction which causes the whole ring to twist (Figure 24).

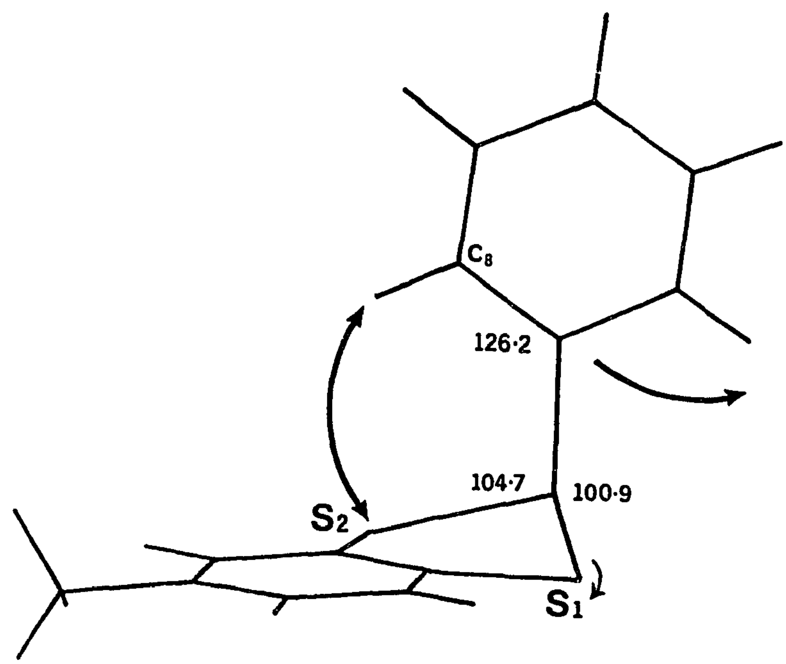


Figure 24. Diagram showing the twist of the phenyl ring in the neutral molecule (III).

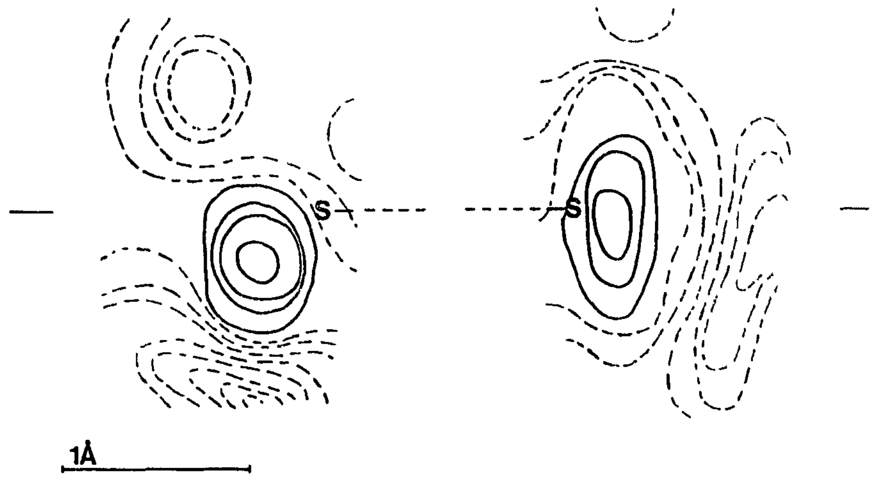


Figure 25. Sulphur lone-pairs in the cation (II).

The diagram (Figure 25) shows the electron distribution on the planes which bisect the two C-S-P angles in the phosphenium cation and are perpendicular to the ring. Interestingly, the lone-pairs follow the surface of the saucer.

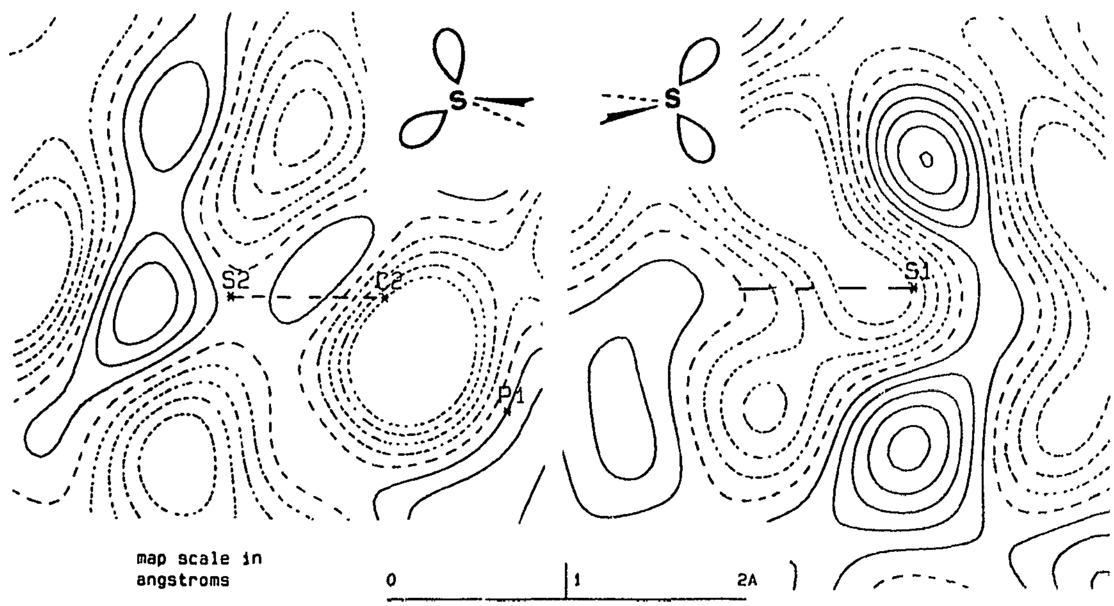


Figure 26. Sulphur lone-pairs in the neutral molecule (III).

Figure 26 shows the electron density on the planes perpendicular to the rings which bisect two C-S-P angles in the benzodithiophosphole molecule. In this case, two lone-pairs, clearly visible on each sulphur atom, are distorted in exactly the way that could be predicted from the twisting of the neutral molecule (Figure 24).

Thus the location of the sulphur lone-pairs supports the proposition that the cation is a 10π electron system.

While the observations of the deformation density in the cation in general terms support the proposed 10π-electron system, the fine details suggest that there is a large contribution from the "quinoid" structure (Figure 27).

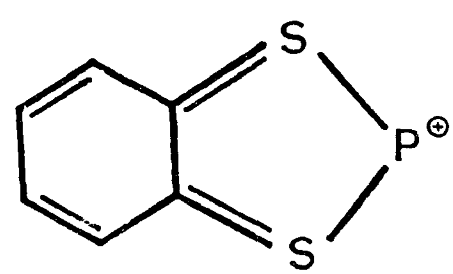
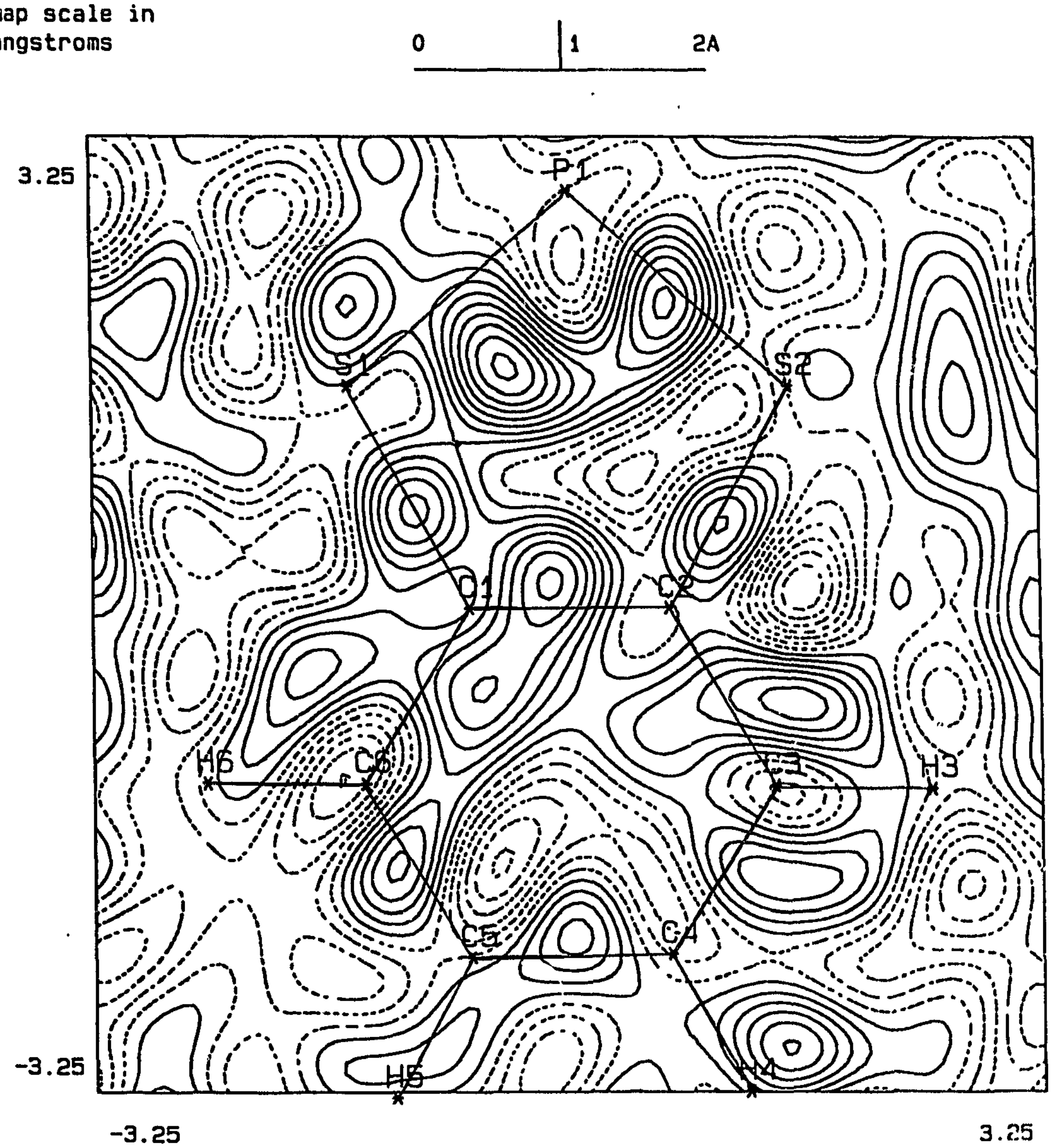


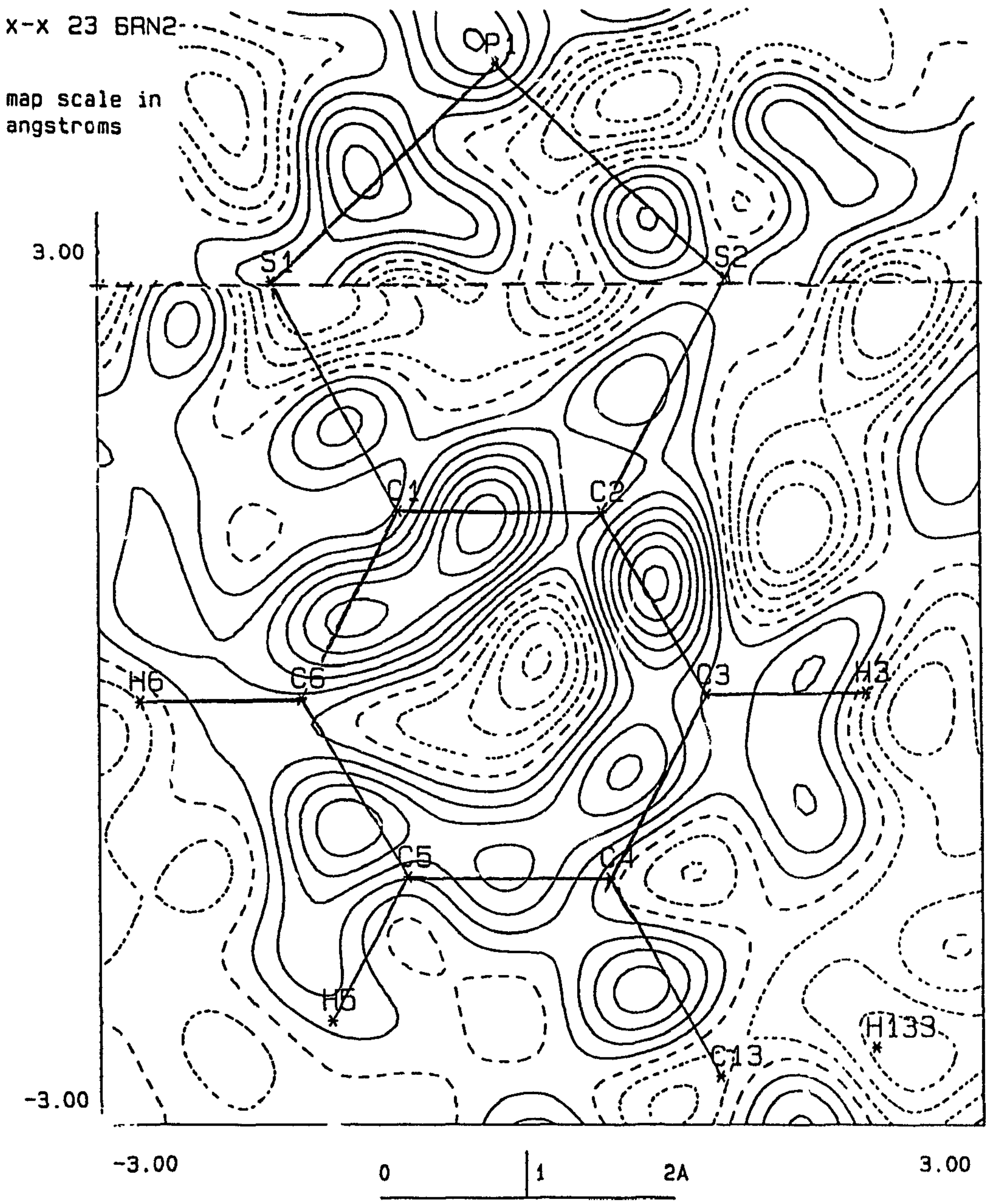
Figure 27. The "quinoid" structure proposed for the cation (II).

map scale in
angstroms



plane defined by three atoms: S1 S2 P1
contour interval (e/A**3): 0.03
perpendicular offset: 0.20
origin translation along x (A): 1.50
origin translation along y (A): -1.50
map rotation (deg): 180.

Figure 28. Difference electron density in the cation (II).



plane defined by three atoms: C2 C1 C5
contour interval (e/A**3): 0.05
perpendicular offset: -0.10
origin translation along x (A): 1.00
origin translation along y (A): 1.00
map rotation (deg): 0.

Figure 29. X-X_{HO} deformation density in the neutral molecule (III).

This is reflected perhaps most clearly in the interatomic distances (Appendix 2), though it can also be seen in the variation of the deformation density along the C-S, C3-C4 and C5-C6 bonds in the cation (Figure 28). Figure 29 shows the $X-X_{HO}$ deformation density map for the neutral phosphole molecule. There is a noticeable difference between the electron density distribution in both molecules. The deformation density map for the cation resembles that of naphthalene[64] with the 'aromatic' spread of the σ and π bonding density over the whole ring. However, the slight concentration of the deformation density along the C-S bonds, ascribed to the contribution from the "quinoid" structure, can be observed. Interestingly, there is considerably more bonding density along these bonds in the cation than in the neutral molecule. On the other hand, in the neutral molecule there is a greater concentration of the electron density in the C_6 ring.

If the "quinoid" type structure suggested by the ring density makes a major contribution to the bonding in the cation, then the phosphorus atom must receive a substantial portion of the positive charge. This is also supported by the deformation density observations. The phosphorus lone-pair for the cation is presented in Figure 30. The lone-pair electrons are also very clear for the neutral molecule (Figure 31).

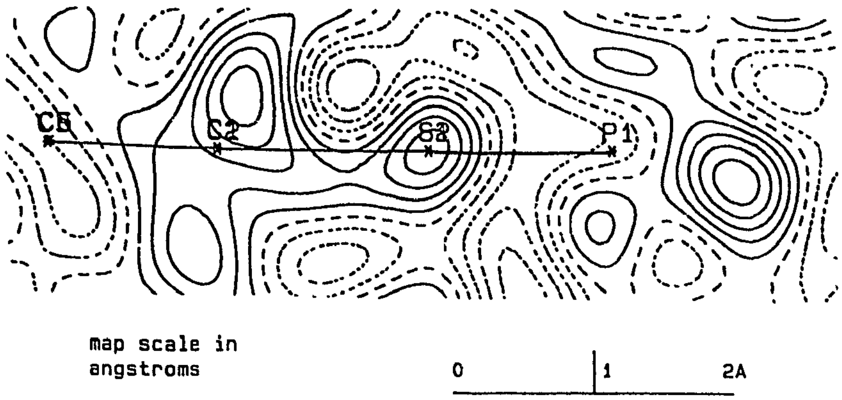


Figure 30. Phosphorus lone-pair in the cation (II).

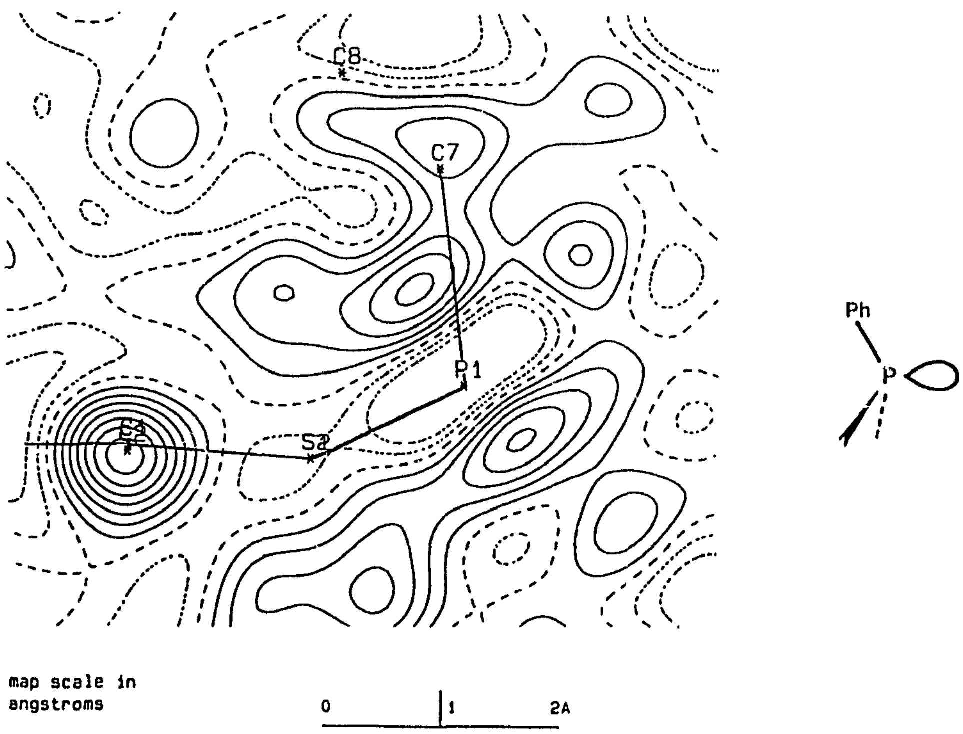


Figure 31. Phosphorus lone-pair in the neutral molecule (III).

2.3.4. Summary

The 1,3,2-benzodithiaphospholium cation (II) is one of the examples of a novel type of compounds containing the thermodynamically stable 3pπ-3pπ bonding between the phosphorus and sulphur[70]. The observed structural features, planarity, and a general aromatic behaviour indicate a bicyclic 10-π-electron system. The related molecule of 5-methyl-2-phenyl-1,3,2-benzodithiaphosphole represents the closest PS_2 σ-bonded analogue of (II) allowing direct structural comparison of both systems. The presence of the lone pairs on P and S atoms evident in the folded conformation of (III) and their absence in the planar cation of (II) support the delocalized pπ structure. However, there is a significant interaction between the sulphur centres and the benzo moiety in the cation, which suggest a contribution of the quinoid structure. The low-temperature deformation density studies of the cation (II) and the related neutral molecule of (III) reported here provide direct observable evidence supporting, in general, the existence of the delocalized 10-π-electron system in (II). However, the absence of really high-quality low-temperature data for (II) leaves some lingering doubt on the conclusions and this work cannot be completed until such data become available.

3. Conformational Consequences of the Packing in XPh_4 [X=C, Si, Ge, Sn, Pb] and Related Crystals. Crystallography and Molecular Modelling.

3.1. Introduction

The molecular symmetry, crystal packing and energetics of tetraaryl compounds of Group IV have been the subject of numerous investigations. The great increase of interest in these compounds has paralleled the overall growth of the whole field of organometallic chemistry[73]. The determination of molecular and lattice structures is a fundamental problem to chemists in general. Of the various methods which may be used, X-ray crystallography is now at this stage where, for most materials, the procurement of single crystals is virtually the only obstacle in completion of highly accurate structural identification.

All the elements of Group IV form a large number of organic derivatives. The relative simplicity and the isomorphism of tetraaryl compounds of the type XAr_4, where X is a Group IV element and Ar an organic aryl group, make them useful as model compounds for more complex derivatives.

Carbon, silicon, and germanium are the non-metallic elements of Group IV (the latter two are semiconductors) while the higher homologs, tin and lead, are metals. In the ground state, their atoms have the valence electron configuration s^2p^2, but the sp^3 excited state, arising from the promotion of one s-electron to a p orbital, accounts for the formation of most of the compounds. The sp^3 hybrid bonds with carbon give rise to the tetrahedral structures of the XAr_4 compounds. The elements heavier than carbon, especially silicon[74], have also empty d orbitals which can interact with filled lone pair orbitals, of π symmetry relative to the σ bonds, of the groups bound to them[75]. The difference in the size of the central atom can also influence the arrangement of aryl group in those compounds.

In the study of the stereochemistry of XPh_4 [X= C, Si, Ge, Sn, Pb] (Figure 4) and related systems the primary questions concern molecular symmetry.

Theoretical considerations[76] reveal that the superimposition of twofold rotors onto a skeleton of T_d symmetry removes all four three-fold symmetry axes. Such systems can therefore never adopt T_d symmetry but must belong to one of the seven subgroups of D_{2d}: D_{2d}, D_2, S_4, C_{2v}, C_2, C_s, and C_1. Thus the orientation of four equivalent aryl groups around central atom usually corresponds to S_4 symmetry if the Ar group of XAr_4 is a twofold rotor (e.g. phenyl ring). In the crystalline state, for symmetrical XAr_4 compounds this molecular symmetry is retained.

The existing crystallographic data on the tetraphenyl[77] and pentafluorotetraphenyl[78,79] derivatives of Group IV, as well as or salts of tetraphenylphosphonium[80,81] and -bismuthonium[82] ions (and in some cases of the tetraphenylarsonium[83,84] ion) all indicate that the molecular S_4 symmetry is adopted in the crystal. Infrared and Raman studies of XPh_4[85,86], and also an early gas-phase electron diffraction study of tetraphenylsilane[87] (TPSi) and tetraphenyl tin[88] (TPSn) indicate S_4 symmetry. However, a recent gas-phase electron diffraction study of molecular structures of tetraphenylsilane, tetraphenylgermane (TPGe), and tetraphenyl tin has shown that since several models (D_{2d}, S_4, D_2) fit the experimental data equally well, only a limited amount of reliable structural information could be derived from the results[89].

The tetraphenylborate anion, however, in the presence of unsymmetrical counterions[90,91], has S_4 symmetry in the crystal, but with potassium, tetramethylammonium[92] and ammonium[93] cations it has D_{2d} symmetry.

The packing of the XAr_4 molecules has been extensively studied on the basis of symmetry arguments[94]. It has been proposed that those molecules which retain S_4 symmetry in the solid state will crystallize in the space groups $I\bar{4}$, $P4_2/n$, or $P\bar{4}2_1c$. The other tetragonal space groups were considered[94] as unsuitable since they do not allow close packing of the XAr_4 molecules. In addition, it was predicted that as larger and more complex para substituents make the molecule less spherical, less symmetric space groups would be favoured, with an accompanying lowering of molecular symmetry.

These ideas are supported by observations on the phenyl and other derivatives of the Group IV elements. All the tetraphenyls of Group IV crystallize in the noncentrosymmetric space group $P\bar{4}2_1c$, with the central atoms in the special positions of $\bar{4}$ site symmetry. Tetra(o-tolyl)tin[95] also crystallizes in $P\bar{4}2_1c$. In tetra(p-tolyl)tin[96,97], tetra(p-methoxyphenyl)tin[98,99], and tetra(p-methylthiophenyl)tin[99] the space group is $I\bar{4}$ and in each case the symmetry of molecule is S_4. On the other hand, in the structures of the pentafluorophenyl derivatives of Si[79], Ge, and Sn[78], and also in tetra(m-tolyl)tin[100], the molecules retain S_4 symmetry, while the compounds crystallize in the centrosymmetric space group $I4_1/a$. In those compounds the close packing of molecules is not favoured because adjacent molecules are related by mirror planes[94]. In tetra(o-tolyl)germanium[101] the space group is $P\bar{1}$, however, while the molecule still retains pseudo S_4 symmetry. It is apparent that close packing is not a sufficient criterion for the retention of the highest molecular symmetry ($\bar{4}$) possible in the solid state. The tetra(p-methylsulphonylphenyl)tin[99] has been found to be the first fully characterized tetraaryl compound with a symmetry lower than fourfold. It crystallizes in the monoclinic space group $C2/c$, for which, however, $I4_1/a$ is a corresponding minimal non-isomorphic supergroup[79]. In contrast, tetra(p-methylsulphinylphenyl)tin monohydrate[102], with para groups of similar size and complexity, crystallizes in the previously not utilized close-packed tetragonal space group $P4_2/n$, and the molecule retains S_4 symmetry. The importance of bulky para substituents is shown also by the crystal data for $(p\text{-}EtOPh)_4Sn$[94]. However, in this case the space group ($P2_1/a$) is not related to any tetragonal space group and a more detailed analysis of this structure is clearly necessary.

The results of the first crude empirical force field calculations[103,104] and also of lattice dynamic calculations[105,106] for tetraphenylmethane (TPMe) were consistent with the crystallographic data and confirmed the molecular symmetry S_4. In contrast to these earlier results, the full relaxation empirical force field calculations[107,108] gave a ground state of D_{2d} symmetry for TPMe, but TPSi was found to have a ground state of S_4 symmetry, consistent with the symmetry found in the crystal. The energy of the calculated ground state of tetraphenylmethane was found to be approximately about 5 kcal/mol below that of a structure of S_4 symmetry with the same degree of twist of the phenyl ring as that reported for the molecule in the crystal. It has been suggested[107] that the influence of the central atom on the symmetry of the tetraphenyls is similar to that of the counterion in tetraphenylborates. However, a combined empirical force field

- extended Hückel molecular orbital calculations[145] have found two energy minima for tetraphenylmethane. One of these has D_{2d} symmetry and corresponds to the ground state, in agreement with the previous calculations. The other corresponds to the S_4 symmetry of the molecule and lies 0.4kcal/mol above the ground state.

The aim of this project is to identify factors influencing the observed structures of compounds XPh_4 [X= C, Si, Ge, Sn, Pb] and to explore the inter-relation between the molecular shape and crystal packing. As part of a general study of the geometric deformation in tetraphenyl complexes, careful redeterminations of the crystal structures of tetraphenyls by modern methods of X-ray crystallography and accurate structure calculation by molecular mechanics[109,110] are required. Such crystal-structure redeterminations of the tetraphenyls and the results of MM3 calculations for tetraphenylmethane, silane and their o-tolyl derivatives are reported in the following.

3.2. Previous Crystallographic Reports

The first study was done in 1927 by George[111] who, from single-crystal rotation X-ray photographs, determined the cell dimensions and predicted $P\bar{4}2_1c$ as the space group for TPMe, TPSi, TPGe, TPSn, and tetraphenyl lead (TPPb).

As part of an investigation of the nature of the organometallic bonds TPSi, TPSn, and TPPb were studied by Giacomello[112] (1938). He noticed that the configuration of the phenyl rings retained the S_4 symmetry in all three compounds. However, the angle of rotation of the phenyl group remained undetermined.

Sumsion and McLachlan[113] (1949) determined the crystal structure of TPMe from powder, rotation, and Weissenberg X-ray data. Assuming, in the trial structure, that the distances between the central carbon and its nearest atoms were 1.49Å, while the C-C distances in the phenyl ring were 1.39Å, they estimated the angle of rotation of the phenyl ring about the tetragonal bonds of the central atoms (φ), and the angle of rotation of the entire molecule about the c axis (ϕ) as 55° and 7.5°, respectively. They also determined positions of carbon atoms in final structure and carbon-carbon distances as 1.47Å (C-C0) and 1.39Å for bonds in the ring.

The results obtained by Ismailzade and Zhdanov[114,115,116] for the TPSi, TPSn, and TPPb, on the basis of Laue and Weissenberg photographs and geometrical analysis of the intermolecular distances between the hydrogen atoms, were in disagreement with previous findings[112]. The reported φ and ϕ angles were: TPSi, 37° and 8°; TPSn, 42° and 7°; TPPb, 50° and 5.5°, respectively. The suggestion was made that the valence angles might be deformed by 4-5°. Ismailzade[117] calculated also the crystal structure of TPGe by considering the closest approach of the phenyl hydrogens. He obtained the values of 52.5° and 6.5° for φ and ϕ angles, respectively. However, subsequent crystal structure determinations of TPGe[118,119] and TPPb[120] have shown the geometrical analysis of those compounds to be in error.

The apparent deficiencies of the early two-dimensional and geometrical analyses led to reexamination of the structures and geometrical considerations for the tetraphenyls by modern crystallographic methods. The development of single-crystal diffractometry and crystallographic computational methods made possible a better refinement of the structures and a higher accuracy. In particular, there exists a reliable set of three independent structure determinations of TPMe[121] with a discussion of the accuracy of the results. There are no systematic differences in the atomic positions or thermal parameters between those three groups of data. Results from this study are used here for comparison with the other structures of the tetraphenyls.

The TPSi structure has been investigated by several authors[77,122,123] but their studies yielded only moderate R value of about 7%. A significant deviation from a local hexagonal symmetry of phenyl rings, involving a small displacement of the carbon attached to silicon has been noted. More accurate analysis[124], focused on the determination of electron density, was undertaken in connection with the investigation of the physical properties of TPSi[125].

There have been two almost simultaneous recent structure determinations of TPGe by Chieh[118], and by Karipides and Haller[119]. Both studies have given similar results. The former analysis concentrated on the comparison of the different techniques of data collection. Karipides and Haller[119] reexamined the geometrical considerations of Ismailzade[117] and found that their results from the X-ray analysis were in agreement with calculations.

The structure of TPSn has been reported several times[103,126,77,127,95]. Earlier determinations derived from film[103] or limited diffractometer data[126] were of unsatisfactory accuracy and inappropriate for comparative purposes. The redetermination done by Engelhardt et al.[127] offered a significant improvement in precision but no discussion of conformation of the molecule. Belsky et al.[95] reported and compared the structure of TPSn with that of tetra(o-tolyl)tin.

The structure of TPPb has been determined by Busetti et al.[120] The results, obtained from the precession and Weissenberg photographs, are in disagreement with previous geometrical analysis[117] of this compound. However, the precise values of bond lengths as well as atomic coordinates were not reported.

As part of the general study of the geometric deformations in tetraphenyl complexes precise values of bond and angles are required. The existence of discrepancies in the results of earlier determinations of tetraphenyl derivatives of Group IV, obtained by different authors, justifies the need for a structure redetermination of tetraphenyl compounds for comparative and confirmative reasons.

The introduction of substituents into <u>ortho</u> or <u>meta</u> positions of the phenyl groups of tetraaryls can lead to a significant lowering of the symmetry of the molecule. Although the results of the conformational analysis of the substituted tetraphenyls have been extensively discussed[107], crystal structure data are scarce. There have been no crystallographic reports on tetra(o-tolyl)methane and silane. The structures of tetra(o-tolyl)germanium[101] and tetra(o-tolyl)tin[95] have been studied by Belsky et al. The tetra(o-tolyl)germane[101] crystallizes in the space group $P\bar{1}$, while the tetra(o-tolyl)tin[95] retains the molecular conformation and the packing mode of TPSn and crystallizes in the same space group, $P\bar{4}2_1c$. The tetra(o-tolyl)germanium molecule has almost a C_2 symmetry but would closely approximate the S_4 symmetry in the absence of the substituents. The introduction of the methyl group in the ortho position causes a lengthening of the central C-Ge and C-Sn bonds. The steric factor also influences the geometry of the o-tolyl groups.

Among para-methyl substituted derivatives only tetra(p-tolyl)tin[96,97] has been studied by X-ray analysis. The first study was done by Ismailzade and Zhdanov[96]. The structure was determined from a two-dimensional electron density projection. The compound was found to crystallize in the space group $I\bar{4}$. The determined values of φ and ϕ angles were 44° and 14°, respectively. Free rotation of the methyl group was absent in crystal. A later study of this compound by Karipides et al.[97] (1975) confirmed the space group and gave an accurate description of the function of the methyl group in the molecular packing and the conformation of the aryl rings. The rotation of the phenyl ring about the C-Sn bond measured from the vertical plane through the c axis (φ) was 49.3° and the rotation of the molecule about the c axis (ϕ) measured from the a axis was -14.5°. The crystal packing was found to be different from that of the TPSn owing to the extensive involvement of the methyl group in intermolecular interactions in the crystal. All three methyl hydrogens were found to take part in the close H...H interactions which require the methyl group to be rigidly oriented in the crystal lattice.

Recently, tetra(p-methoxyphenyl)tin and tetra(p-methylthiophenyl)tin have been prepared and characterized by X-ray analysis[99]. Both complexes crystallize in the tetragonal space group $I\bar{4}$ and the molecules have $\bar{4}$ molecular symmetry. It was concluded from steric considerations in an early study of the tetrakis(p-methoxyphenyl)tin[98] that the p-methoxy group must lie in a plane perpendicular to the phenyl ring. This is in variance with more recent results[99] where the CH_3O and CH_3S groups are found to have the <u>exo</u>[107] conformation almost coplanar with the phenyl ring. Increasing the size of the <u>para</u> substituent from CH_3 to CH_3O causes a decrease of the Sn-C distance with respect to tetra(p-tolyl)tin. The φ and ϕ angles are 48.4° and 14.5° for tetra(p-methylthiophenyl)tin, and 52.1° and 15.5° for tetra(p-methoxyphenyl)tin, respectively.

Recent studies in aryltin chemistry[102] have yielded the determination of crystal and molecular structures of tetra(p-methylsulphonylphenyl)tin, $[p\text{-}CH_3S(O)_2C_6H_4]_4Sn$, and tetra(p-methylsulphinylphenyl)tin monohydrate, $[p\text{-}CH_3S(O)C_6H_4]_4Sn\cdot n\text{-}H_2O$. Tetra(p-methylsulphonylphenyl)tin crystallizes in the monoclinic space group C2/c and is the first example of a tetraaryl compound with a lower than fourfold symmetry. Nevertheless, the space group C2/c is related to the tetragonal space group $I4_1/a$[79] and the deviation from the S_4 symmetry is small. Tetra(p-methylsulphinylphenyl)tin monohydrate, however, crystallizes in the close-packed tetragonal space group $P4_2/n$, and the molecule retains S_4 symmetry. Both structures are found to be disordered.

The crystal structure of tetra(m-tolyl)tin has been determined by Karipides and Oertel[100] (1977). The compound crystallizes in the tetragonal space group $I4_1/a$. The crystal structure consists of the discrete molecules with crystallographically imposed S_4 symmetry. Unlike in tetra(p-tolyl)tin, the methyl group in the tetra(m-tolyl)tin was found to be twofold-disordered due to more flexible intermolecular environment created by the long-range, weak methyl H interactions. The angle of rotation of the phenyl ring from the C-Sn-C plane is 41°, which differs considerably from the value of 140.3° predicted by a geometrical analysis[128]. The observed conformation of the molecule is <u>exo</u>[107], where the methyl groups are relatively remote from the plane through the centre of the molecule and normal to the $\bar{4}$ axis.

The crystal structure investigation of the several tetrakis(pentafluorophenyl) derivatives of Group IV have been undertaken by Karipides et al.[78,79] in order to compare the structure and packing with those of the corresponding tetraphenyl derivatives. The crystal structures of tetrakis(pentafluorophenyl)silane[79], germanium[78], and tin[78] have been determined. The compounds crystallize in the tetragonal space group $I4_1/a$. The molecules have the crystallographically imposed molecular symmetry S_4. The conformation of the pentafluorophenyl ring in the molecule is specified by the rotation angle (φ) measured from the vertical plane through the c axis and unlike in the tetraphenyls seems to be independent of the central-atom size. The pentafluorophenyl rings in all the compounds are planar but deviate substantially from the ideal D_{6h} symmetry in a way consistent with the deformations of substituted benzene[129,130].

3.3. X-ray Structure Determination

The crystal structures of TPSi, TPGe, TPSn, and TPPb have been redetermined by single crystal X-ray crystallography. Crystals of suitable size were mounted on glass fibres. An Enraf-Nonius CAD4 diffractometer (MoK_α graphite-monochromated) was used to measure the unit cell dimensions and to collect the data at room temperature. For TPGe data were also collected at 213K. The crystal and data collection parameters are listed in Table 6. The unit cell constants were obtained by least-squares analysis of the diffractometer setting angles of 25 well-centred reflections in the range $2\theta=28-32^\circ$ and $2\theta=20-30^\circ$ for TPSi, TPSn, TPPb and for TPGe, respectively. The intensities were reduced to a standard scale using routine procedures[34]. Lorentz and polarization corrections were applied. Absorption corrections (DIFABS)[35] were performed except in the case of TPSi for which the linear absorption coefficient was small (1.32 cm^{-1}). Scattering factors for neutral atoms were taken from the International Tables[36] and were corrected for the real and imaginary parts of anomalous dispersion. The refinements were performed by using SHELX-76[37].

All the tetraphenyls studied crystallize in the acentric space group $P\bar{4}2_1c$. The initial isotropic positions of most of the atoms were taken from the previous reports. The structures were refined by a full-matrix least-squares procedure, initially with independent isotropic temperature factors on the non-hydrogen atoms. Absorption corrections were then applied. Hydrogen atoms were placed in their geometrically calculated positions [d(C-H)=1.08Å] and then refined free. Some of the C-C and C-H distances had to be constrained during refinement. The final refinements were with anisotropic temperature factors on the non-hydrogen atoms and individual isotropic temperature factors on the hydrogen atoms. The function minimised was $\Sigma w(|F_o|-|F_c|)^2$ where w is the weight. Final agreement factors are given in Table 6. No correction for extinction was applied. The final difference maps had no recognizable residual features. The figures were produced with CHEMGRAF[39]. The best planes through phenyl rings were calculated using CRYSTALS[38]. Thermal motion analyses were performed by using CRYSTALS[38] TLS routine. The TLS calculations[131,132] were done for the whole molecule and also for two other models. In the first model the movement of the central atom and the phenyl ring was considered as rigid-body. In the second model only the phenyl ring was treated as a rigid body.

Multipole refinement was performed for TPSi and TPGe by using the program MOLLY[17]. For silicon, germanium, carbon and hydrogen atoms, Slater-type functions were used for the multipole deformation functions. Positional and thermal parameters of hydrogens were fixed during refinement. The multipole expansion was truncated at the octapolar level for carbon atoms and monopolar level for silicon and germanium atoms. The final agreement factor for TPSi was better than from the conventional refinement (R=0.0260) but for TPGe the results obtained by performing the multipole refinement (R=0.0413) did not improve with respect to conventional refinement (R=0.0326). Since the collected data did not include the high order reflections (only the low order data have been collected $\theta<30^{\circ}-40^{\circ}$) that are responsible for the core position of atoms, the multipole refinement served as a test rather than as a source of structural data. These results are not conclusive and are not presented here.

The crystal data for TPMe[113,77], given in this report for comparison, are taken from ref. 121.

The fractional coordinates of atoms, bonds and angles determined by conventional refinement for TPSi, TPGe, TPSn, and TPPb are listed in Table 7, Table 9, Table 10, Table 13, and Table 14, respectively. The atomic and thermal parameters for hydrogen atoms as well as the pertinent torsional angles are given in tables on microfiches (Appendix 4).

Table 6. Physical properties and parameters for data collection and refinement of tetraphenyls.

1) tetraphenylsilane

$C_{24}H_{20}Si$	MW = 336.5	t = 18 °C
tetragonal	$P\bar{4}2_1c$ (No. 114)	noncentrosymmetric
a = 11.461(2) Å	b = 11.461(2) Å	c = 7.054(1) Å
$\alpha = 90°$	$\beta = 90°$	$\gamma = 90°$
F(000) = 356 e	$\mu = 1.32\ cm^{-1}$	$V = 926.7\ Å^3$
Z = 2	$d_c = 1.206\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 1242$	N_{un} = 11[illegible]2	$N_{ob} = 540$
obs. if $I > 3\sigma(I)$	$N_v = 77$	$N_{ob}/N_v = 7.0$
$2° < \theta < 35°$	R = 0.0461	$R_w = 0.0483$

2) Tetraphenyl germanium

$C_{24}H_{20}Ge$	MW = 380.9	t = 18 °C
tetragonal	$P\bar{4}2_1c$ (No. 114)	noncentrosymmetric
a = 11.619(1) Å	b = 11.619(2) Å	c = 6.900(2) Å
$\alpha = 90°$	$\beta = 90°$	$\gamma = 90°$
F(000) = 392 e	$\mu = 16.21\ cm^{-1}$	$V = 931.4\ Å^3$
Z = 2	$d_c = 1.358\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 3264$	$N_{un} = 1627$	$N_{ob} = 522$
obs. if $I > 3\sigma(I)$	$N_v = 77$	$N_{ob}/N_v = 6.8$
$2° < \theta < 40°$	R = 0.0326	$R_w = 0.0310$

3) Tetraphenyl germanium

$C_{24}H_{20}Ge$	MW = 380.9	t = -60 °C
tetragonal	$P\bar{4}2_1c$ (No. 114)	noncentrosymmetric
a = 11.649(3) Å	b = 11.649(3) Å	c = 6.794(2) Å
$\alpha = 90°$	$\beta = 90°$	$\gamma = 90°$
F(000) = 392 e	$\mu = 16.37\ cm^{-1}$	$V = 922.0\ Å^3$
Z = 2	$d_c = 1.372\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 4041$	$N_{un} = 1614$	$N_{ob} = 639$
obs. if $I > 3\sigma(I)$	$N_v = 77$	$N_{ob}/N_v = 8.3$
$2° < \theta < 40°$	R = 0.0350	$R_w = 0.0350$

Table 6 (cont.). Physical properties and parameters for data collection and refinement of tetraphenyls.

4) Tetraphenyl tin		
$C_{24}H_{20}Sn$	MW = 427.0	t = 18 °C
tetragonal	$P\bar{4}2_1c$ (No. 114)	noncentrosymmetric
a = 12.063(2) Å	b = 12.063(2) Å	c = 6.543(2) Å
α = 90°	β = 90°	γ = 90°
F(000) = 428 e	μ = 13.52 cm^{-1}	V = 952.0 $Å^3$
Z = 2	d_c = 1.490 g/cm^3	λ = 0.70926 Å
N_{me} = 2142	N_{un} = 965	N_{ob} = 696
obs. if I> 3σ(I)	N_v = 77	N_{ob}/N_v = 9.0
$2° < \theta < 30°$	R = 0.0257	R_w = 0.0266
5) Tetraphenyl lead		
$C_{24}H_{20}Pb$	MW = 515.6	t = 18 °C
tetragonal	$P\bar{4}2_1c$ (No. 114)	noncentrosymmetric
a = 12.140(2) Å	b = 12.140(2) Å	c = 6.530(2) Å
α = 90°	β = 90°	γ = 90°
F(000) = 492 e	μ = 86.41 cm^{-1}	V = 962.8 $Å^3$
Z = 2	d_c = 1.778 g/cm^3	λ = 0.70926 Å
N_{me} = 1296	N_{un} = 1216	N_{ob} = 581
obs. if I> 3σ(I)	N_v = 77	N_{ob}/N_v = 7.5
$2° < \theta < 35°$	R = 0.0270	R_w = 0.0302

Table 7. Fractional atomic positional parameters and equivalent isotropic temperature factors ($Å^2$) for $SiPh_4$ with e.s.d.s in parentheses.

Atom	x/a	y/b	z/c	U_{eq}
Si1	0.0000(0)	0.0000(0)	0.0000(0)	0.0424
C1	0.1318(2)	-0.0162(2)	-0.1563(4)	0.0435
C2	0.1331(3)	-0.0998(2)	-0.2991(4)	0.0560
C3	0.2303(3)	-0.1148(3)	-0.4144(5)	0.0644
C4	0.3265(3)	-0.0457(3)	-0.3910(5)	0.0641
C5	0.3270(2)	0.0388(3)	-0.2534(5)	0.0632
C6	0.2309(2)	0.0531(2)	-0.1373(4)	0.0540

Table 8. Interatomic distances (Å) and interbond angles (degrees) for $SiPh_4$.

Si1 -C1	1.879(3)	C1 -Si1 -C1'	108.2(1)
Si1 -C1'	1.879(3)	C1 -Si1 -C1''	110.1(1)
Si1 -C1''	1.879(3)	Si1 -C1 -C2	120.1(2)
Si1 -C1'''	1.879(3)	Si1 -C1 -C6	122.9(2)
C1 -C2	1.391(4)	C2 -C1 -C6	117.0(3)
C1 -C6	1.393(4)	C1 -C2 -C3	121.2(3)
C2 -C3	1.389(5)	C2 -C3 -C4	120.3(4)
C3 -C4	1.368(6)	C3 -C4 -C5	119.8(4)
C4 -C5	1.371(5)	C4 -C5 -C6	120.0(3)
C5 -C6	1.382(5)	C1 -C6 -C5	121.7(3)

Primed atoms have symmetry operations:

' - -x, -y, z,

'' - y, -x, -z,

''' - -y, x, -z,

Table 9. Fractional atomic positional parameters and equivalent isotropic temperature factors (Å^2) for $GePh_4$ with e.s.d.'s in parentheses.

Atom	x/a	y/b	z/c	U_{eq}
Ge1	0.0000 (0)	0.0000 (0)	0.0000 (0)	0.0429
C1	0.1353 (2)	-0.0174 (2)	-0.1641 (5)	0.0408
C2	0.1394 (3)	-0.1018 (3)	-0.3065 (6)	0.0551
C3	0.2347 (4)	-0.1156 (3)	-0.4218 (5)	0.0620
C4	0.3288 (3)	-0.0445 (4)	-0.3993 (6)	0.0617
C5	0.3262 (3)	0.0399 (3)	-0.2631 (6)	0.0605
C6	0.2314 (3)	0.0539 (3)	-0.1458 (5)	0.0532

Table 10. Fractional atomic positional parameters and equivalent isotropic temperature factors (Å^2) for $GePh_4$ (LT) with e.s.d.'s in parentheses.

Atom	x/a	y/b	z/c	U_{eq}
Ge1	0.0000 (0)	0.0000 (0)	0.0000 (0)	0.0325
C1	0.1355 (2)	-0.0170 (2)	-0.1666 (5)	0.0324
C2	0.1400 (3)	-0.1030 (3)	-0.3090 (5)	0.0413
C3	0.2368 (3)	-0.1167 (3)	-0.4261 (5)	0.0462
C4	0.3301 (3)	-0.0441 (3)	-0.4027 (5)	0.0490
C5	0.3262 (2)	0.0410 (3)	-0.2660 (6)	0.0465
C6	0.2303 (3)	0.0551 (2)	-0.1479 (5)	0.0393

Table 11. Interatomic distances (Å) for $GePh_4$.

	288 K	213 K
Ge1 -C1	1.948(3)	1.952(3)
Ge1 -C1'	1.948(3)	1.952(3)
Ge1 -C1''	1.948(3)	1.952(3)
Ge1 -C1'''	1.948(3)	1.952(3)
C1 -C2	1.388(6)	1.393(5)
C1 -C6	1.397(5)	1.394(5)
C2 -C3	1.373(6)	1.389(6)
C3 -C4	1.379(7)	1.387(6)
C4 -C5	1.359(6)	1.359(5)
C5 -C6	1.377(6)	1.385(5)

Table 12. Interbond angles (degrees) for $GePh_4$.

	288 K	213 K
C1 -Ge1 -C1'	108.90(14)	109.10(13)
C1 -Ge1 -C1''	109.76(14)	109.65(13)
Ge1 -C1 -C2	120.8 (3)	120.4 (2)
Ge1 -C1 -C6	122.1 (3)	121.8 (2)
C2 -C1 -C6	117.1 (3)	117.8 (3)
C1 -C2 -C3	121.4 (4)	120.7 (3)
C2 -C3 -C4	120.3 (4)	120.1 (4)
C3 -C4 -C5	119.5 (4)	119.8 (4)
C4 -C5 -C6	120.7 (4)	120.6 (4)
C1 -C6 -C5	121.1 (4)	121.0 (3)

Primed atoms have symmetry operations:

' - -x, -y, z,

'' - y, -x, -z,

''' - -y, x, -z,

Table 13. Fractional atomic positional parameters and equivalent isotropic temperature factors ($Å^2$) for $SnPh_4$ with e.s.d.'s in parentheses.

Atom	x/a	y/b	z/c	U_{eq}
Sn1	0.0000(0)	0.0000(0)	0.0000(0)	0.0375
C1	0.1445(3)	-0.0194(2)	-0.1857(5)	0.0376
C2	0.1531(4)	-0.1047(4)	-0.3284(8)	0.0480
C3	0.2483(4)	-0.1168(4)	-0.4462(8)	0.0560
C4	0.3346(4)	-0.0409(5)	-0.4260(8)	0.0586
C5	0.3267(3)	0.0424(4)	-0.2888(7)	0.0574
C6	0.2337(3)	0.0538(3)	-0.1666(7)	0.0480

Table 14. Fractional atomic positional parameters and equivalent isotropic temperature factors ($Å^2$) for $PbPh_4$ with e.s.d.'s in parentheses.

Atom	x/a	y/b	z/c	U_{eq}
Pb1	0.0000(0)	0.0000(0)	0.0000(0)	0.0382
C1	0.1480(7)	-0.0201(5)	-0.1917(12)	0.0357
C2	0.1567(9)	-0.1051(8)	-0.3352(18)	0.0502
C3	0.2514(10)	-0.1160(9)	-0.4538(14)	0.0567
C4	0.3360(9)	-0.0415(10)	-0.4336(18)	0.0611
C5	0.3294(8)	0.0432(8)	-0.2958(16)	0.0578
C6	0.2368(8)	0.0533(7)	-0.1770(18)	0.0489

Table 15. Interatomic distances (Å) and interbond angles (degrees) for $SnPh_4$.

Sn1	-C1	2.137(4)	C1	-Sn1	-C1'		110.70(13)
C1	-C2	1.393(6)	C1	-Sn1	-C1''		108.86(13)
C1	-C6	1.398(6)	Sn1	-C1	-C2		121.5 (3)
C2	-C3	1.390(8)	Sn1	-C1	-C6		120.5 (3)
C3	-C4	1.393(8)	C2	-C1	-C6		118.0 (4)
C4	-C5	1.351(7)	C1	-C2	-C3		120.7 (5)
C5	-C6	1.385(7)	C2	-C3	-C4		119.7 (5)
			C3	-C4	-C5		119.9 (5)
			C4	-C5	-C6		121.0 (5)
			C1	-C6	-C5		120.6 ([illegible])

Primed atoms have symmetry operations:

'	-	-x,	-y,	z,
''	-	y,	-x,	-z,
'''	-	-y,	x,	-z,

Table 16. Interatomic distances (Å) and interbond angles (degrees) for $PbPh_4$.

Pb1	-C1	2.203(8)	C1	-Pb1	-C1'	110.8 (3)
C1	-C2	1.398(14)	C1	-Pb1	-C1''	108.8 (3)
C1	-C6	1.402(13)	Pb1	-C1	-C2	121.6 (7)
C2	-C3	1.39 (2)	Pb1	-C1	-C6	121.2 (6)
C3	-C4	1.38 (2)	C2	-C1	-C6	117.2 (8)
C4	-C5	1.37 (2)	C1	-C2	-C3	120.3 (10)
C5	-C6	1.371(15)	C2	-C3	-C4	120.0 (10)
			C3	-C4	-C5	120.9 (11)
			C4	-C5	-C6	119.2 (10)
			C1	-C6	-C5	122.3 (9)

Primed atoms have symmetry operations:

'	-	-x,	-y,	z,
''	-	y,	-x,	-z,
'''	-	-y,	x,	-z,

3.4. Molecule

All the Group IV tetraphenyls studied crystallize in the noncentrosymmetric space group $P\bar{4}2_1c$. The molecules have S_4 symmetry with the two central atoms per unit cell in the special positions (0,0,0) and (0.5,0.5,0.5), related by a twofold screw axis, and one unique phenyl ring in the asymmetric unit. The projection of the crystal packing of molecules along the c axis is shown in Figure 32.

The distance between the central atom and C1 increases from C to Pb. For TPMe this distance (corrected for thermal motion)[121] is 1.553(3)Å, for TPSi - 1.879(3)Å, for TPGe - 1.950(3)Å (mean), for TPSn - 2.137(4)Å, and for TPPb - 2.203(8)Å (Table 8, Table 11, Table 15, Table 16). The determined values are in good agreement with the bond lengths at the central atoms previously reported (Table 17). They also compare well with the recent electron diffraction study[89] of the gas phase of TPSi, TPGe and TPSn. A comparison of all the data is presented in Table 17.

The effect of substitution at the phenyl ring for various tetraaryls is summarised in Table 18. In the case of para substituents a shortening of the central bond lengths can be observed as para hydrogen is replaced by CH_3O and by CH_3S. This has been ascribed to an increase in intermolecular repulsions in these close-packed structures with the size of

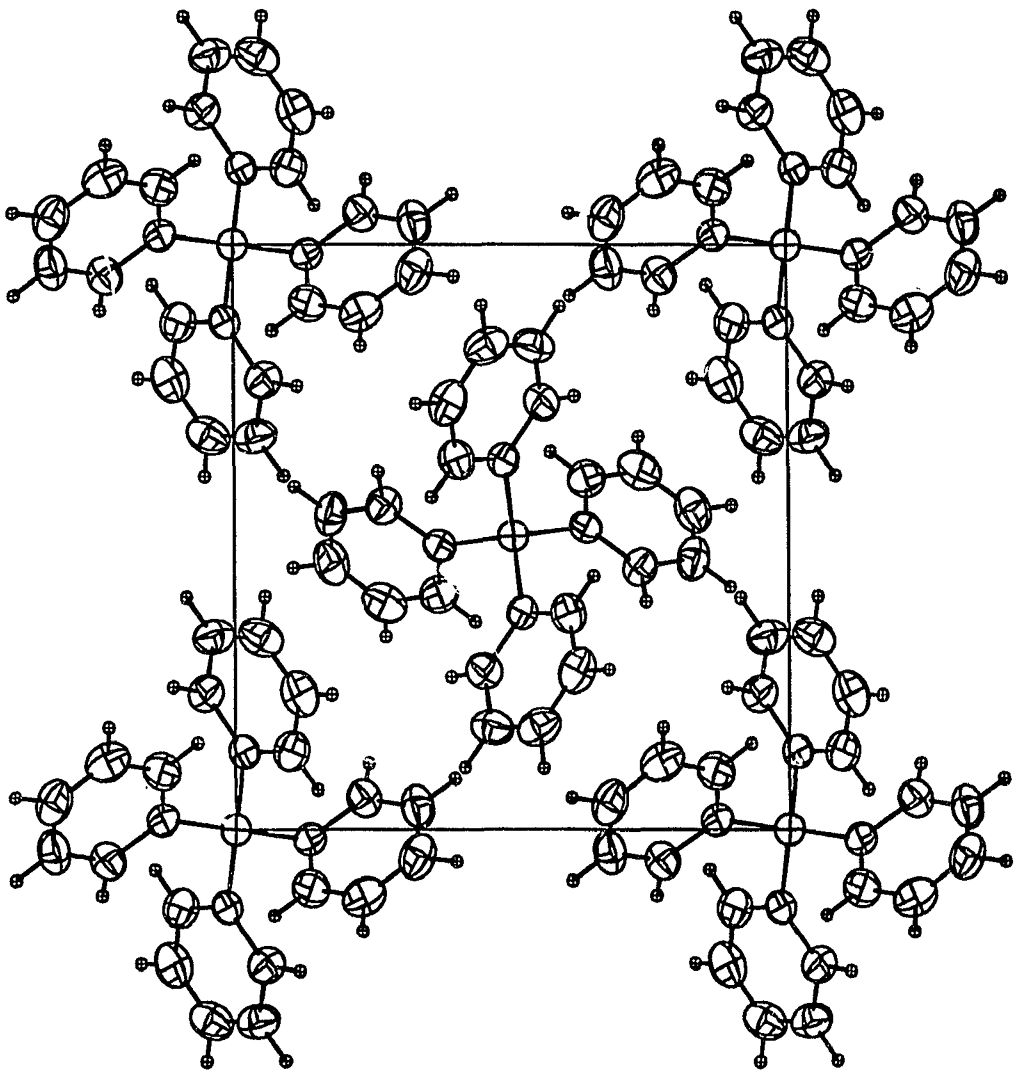


Figure 32. Packing diagram of tetraphenylsilane - projection along c-axis.

Table 17. Structural parameters for the tetraphenyls.

param.	TPMe	TPSi	TPGe (RT)	TPGe (LT)	TPSn	TPPb
X-C (Å)	1.553(3)[121]	1.878(2)[124]	1.957(4)[119]	-	2.139(4)[95]	2.19(3)[120]
	-	1.871(4)[89]	1.960(4)[89]	-	2.137(5)[89]	-
	-	1.879(3)	1.948(3)	1.952(3)	2.137(4)	2.203(8)
θ_1 (°)	106.7(2)[121]	108.1(1)[124]	109.0(2)[119]	-	111.2(2)[95]	111.5[120]
	-	-	-	-	-	-
	-	108.2(1)	108.9(1)	109.1(1)	110.7(1)	110.8(3)
θ_2 (°)	110.9(2)[121]	110.1(1)[124]	-	-	108.6(1)[95]	108.4[120]
	-	-	-	-	-	-
	-	110.1(1)	109.8(1)	109.7(1)	108.7(1)	108.8(3)
α (°)	117.5(3)[121]	117.2(2)[124]	118.4(4)[119]	-	117.6(4)[95]	120.0[120]
	-	118.2(4)[89]	119.5(3)[89]	-	119.5(3)[89]	-
	-	117.3(3)	117.1(3)	117.8(3)	118.0(3)	117.2(8)
ψ (°)	40.8[121]	37.67[124]	35.5[119]	-	31.9[95]	31.1[120]
	-	-	-	-	-	-
	-	37.7	35.5	34.8	31.8	31.3
φ (°)	49.2(2)[121]	52.33[124]	54.1[119]	-	58.1[95]	58.9[120]
	-	-	-	-	-	-
	-	52.3	54.5	54.2	58.2	58.7
ϕ (°)	7.5[121]	6.97[124]	7.2[119]	-	7.5[95]	7.5[120]
	-	-	-	-	-	-
	-	7.6(1)	7.6(1)	7.5(1)	7.3(1)	7.3(1)

Table 18. Structural parameters for the various substituted tetraphenyls.

Compound	X-C (Å)	θ_1 (°)	θ_2 (°)	α (°)	φ (°)	ϕ (°)
$GePh_4$[a] ($P\bar{4}2_1c$)	1.948(3)	108.9(1)	109.8(1)	117.1(3)	54.5	7.6
$Ge(o\text{-}CH_3Ph)_4$[101] ($P\bar{1}$)	1.966(3)	–	–	118.8	–	–
$SnPh_4$[a] ($P\bar{4}2_1c$)	2.137(4)	110.7(1)	108.9(1)	117.2(8)	58.1	7.3
$Sn(o\text{-}CH_3Ph)_4$[95] ($P\bar{4}2_1c$)	2.152(5)	107.9(1)	112.6(3)	118.1(5)	53.1	11.2
$Sn(m\text{-}CH_3Ph)_4$[100] ($I4_1/a$)	2.150(3)	109.3	109.5	118.4(3)	40.7	37.5
$Sn(p\text{-}CH_3Ph)_4$[97] ($I\bar{4}$)	2.147(7)	114.4(3)	107.0(2)	116.4(6)	48.4	14.5
$Sn(p\text{-}CH_3OPh)_4$[99] ($I\bar{4}$)	2.136(4)	106.2(3)	111.1(3)	116.1(6)	52.1	15.5
$Sn(p\text{-}CH_3SPh)_4$[99] ($I\bar{4}$)	2.123(7)	112.5(1)	108.0(1)	116.8(3)	49.2	13.8
$Sn(p\text{-}CH_3S(O)Ph)_4$[102] ($P4_2/n$)	2.136(8)	113.3(3)	107.6(3)	–	–	–
$Sn(p\text{-}CH_3S(O_2)Ph)_4$[102] ($C2/c$)	2.150(3) 2.134(3)	110.8(1) 106.2(3)	114.7(1) 108.9(1)	–	–	–

a - present work.

para substituent[99]. However, in the case of *ortho* and *meta* substituents an *increase* in the distance at the central atom is observed instead. This has usually been explained by the steric effects caused by the presence of substituent[95,101].

The distortion of the tetrahedral bond configuration at the central atom can be described by the valence angles θ_1=C1-X-C1' (bisected by the S_4 axis) and θ_2=C1-X-C1" (Figure 33). The central atom valence angles are listed in Table 17 and Table 19. The angle θ_1 increases while the angle θ_2 decreases as the central atom gets larger. The molecule becomes flatter, and it appears that the distortion from the ideal tetrahedron becomes smaller as the central atom changes from C to Ge then increases again. The valence angles observed for TPGe are practically tetrahedral (Table 17 and Table 19).

The experimental values of the valence angles θ_1 and θ_2 are plotted against the carbon- central atom distances in the tetraphenyls in Figure 34, together with the fitted curve obtained from the least-squares fitting procedure[133]. The two fits, linear and parabolic, were used in analysis. The standard deviations of the linear fits are 0.37° and 0.15° for θ_1 and θ_2, respectively. The coefficients of determination for the linear fit are 0.97 and 0.98 for θ_1 and θ_2, respectively. A slightly better fit has been obtained using parabolic regression analysis. In this case, the coefficients of determination are 0.99, while the standard deviations of the fits are 0.29° and 0.12°, for θ_1 and θ_2, respectively.

VALENCE ANGLES:

Θ_1 = C1-X-C1'; Θ_2 = C1-X-C1''

Primed atoms have symmetry operations:
'   -   -x, -y, z;
'' -   y, -x, -z;

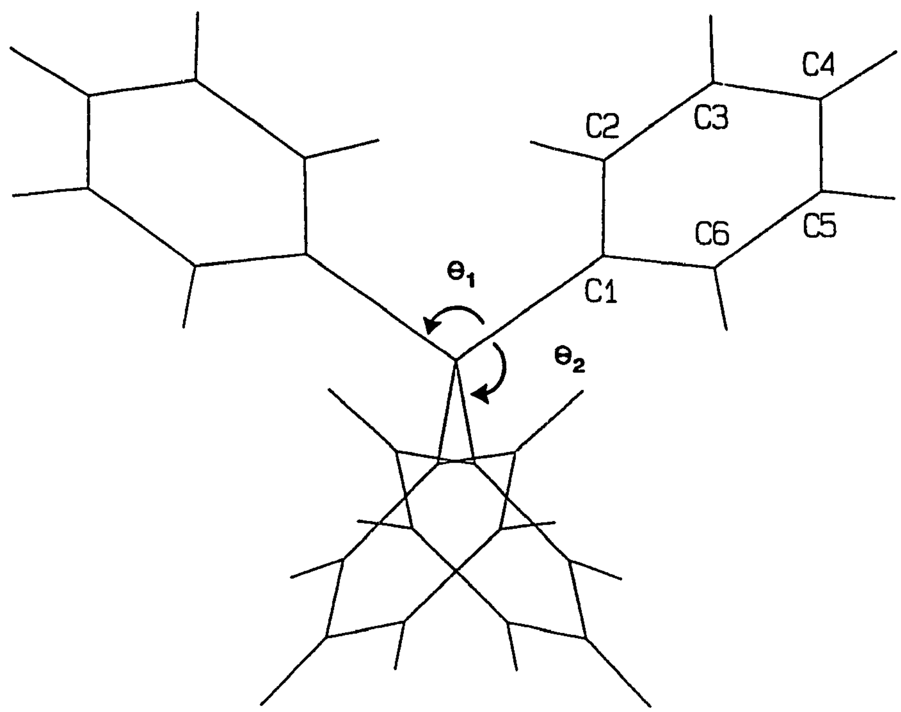


Figure 33. Valence angles.

Table 19. Valence angles C1-X-C1' and C1-X-C1'' for tetraphenyls [X= C, Si, Ge, Sn, Pb].

C	106.7(2)	110.9(2)
Si	108.2(1)	110.1(1)
Ge (RT)	108.9(1)	109.8(1)
Sn	110.7(1)	108.9(1)
Pb	110.8(3)	108.8(3)

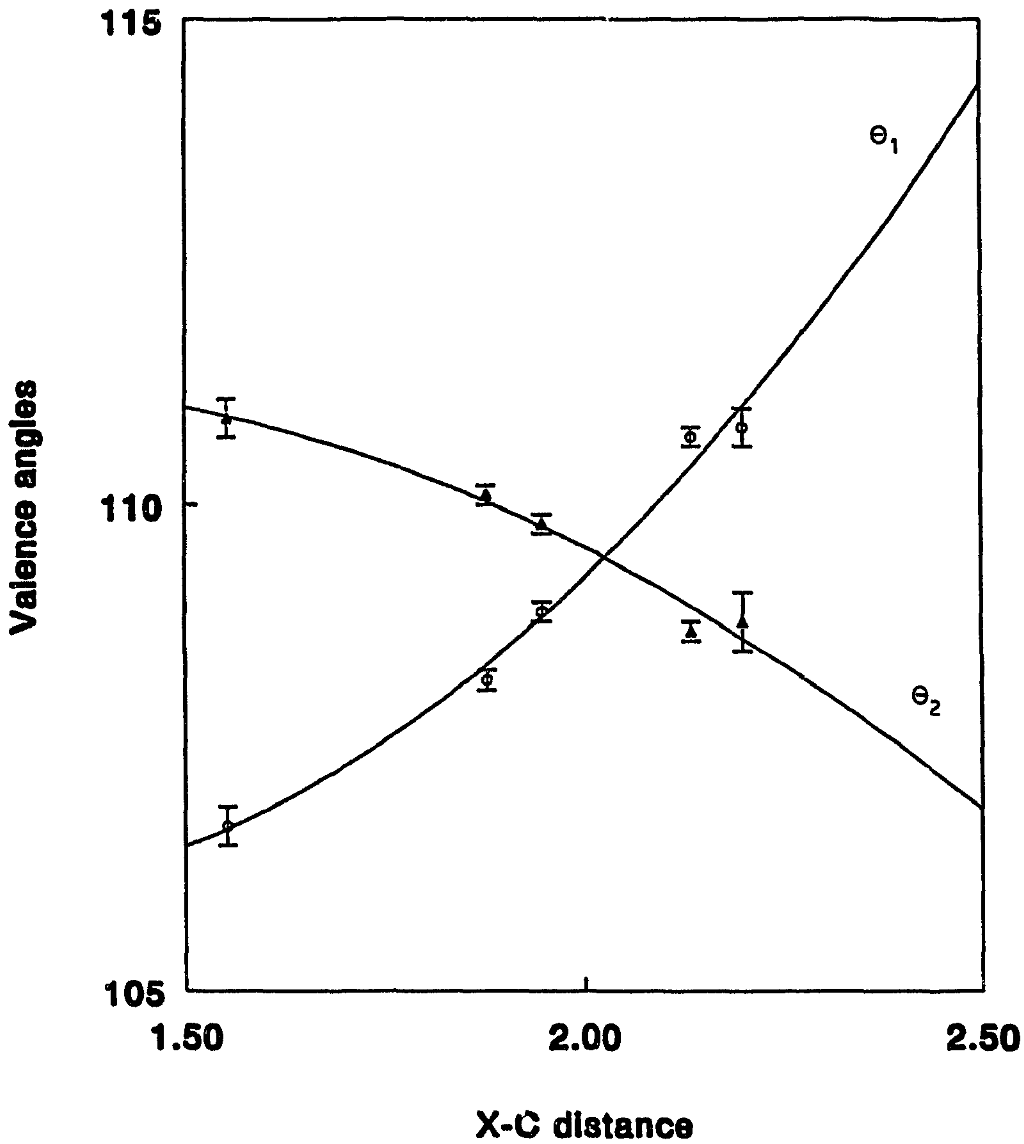


Figure 34. Relationship between the valence angles and X-C distances for tetraphenyls.

The phenyl rings are planar, with the mean deviations of the central atom from the least-squares planes through the six carbon atoms of 0.011Å for TPMe[121], 0.025Å for TPSi, 0.022Å for TPGe, 0.008Å for TPSn, and 0.010Å for TPPb.

For all the tetraphenyls studied the average C-C-C angle in the phenyl ring is 120°, but the ring is slightly distorted from hexagonal symmetry; the decrease of the α angle at C1, α = C2-C1-C6, from 120° is compensated for by an increase of the _endo_ angles at C2 and C6.

The effect on the internal geometry of a phenyl ring caused by introduction of a substituent has been comprehensively studied[129,130,143,134]. Any primary distortion is such as to lower the symmetry of the phenyl ring from D_{6h} to approximately C_{2v}. Further lowering to C_s geometry may occur with substituents that depart strongly from axial symmetry, like the methoxy group. Deviations from the ideal D_{6h} symmetry depend on the electronic properties of the substituent[129,130,143,134].

The angular distortion of monosubstituted phenyl rings is primarily characterized by the _ipso_ bond angle α=C2-C1-C6[129,130,143,134]. This angle is consistently, although only slightly, smaller than 120° in all the derivatives studied. The internal angles at C1 are equal to 117.6° for TPMe[121], 117.3(3)° for TPSi, 117.1(3)° for TPGe (RT), 117.8(3)° for TPGe (LT), 118.0(4)° for TPSn, and 117.2(8)° for TPPb (Table 12, Table 15, Table 16). This direction of angular deformation generally occurs with electron-releasing substituents. A similar effect has also been observed in the substituted tetraphenyls (Table 18) with the largest deviation in α angle for <u>para</u>-substituted derivatives[143].

The mean carbon-carbon distances in the ring are: 1.393Å (corrected for riding-motion) for TPMe[121], 1.385Å for TPSi, TPSn and TPPb, and 1.382Å for TPGe. All those distances are shorter than the reported[135] value of 1.395(3)Å in the aromatic ring. Usually the C4-C5 distances are shorter than the other C-C distances in the phenyl ring (Table 8, Table 11, Table 15, Table 16).

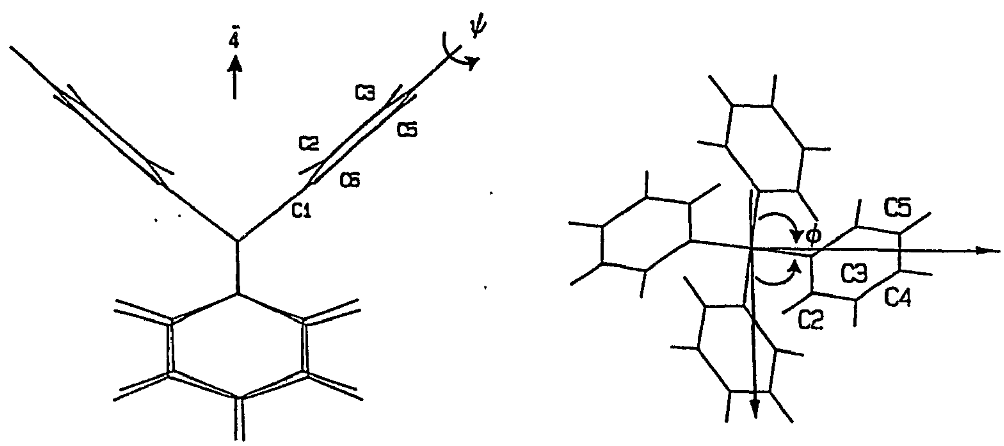


Figure 35. Molecular angles, ψ and ϕ, determining the orientation of the phenyl ring.

Table 20. The rotational displacement angles, ϕ, and the twist angles, ψ, for tetraphenyls.

XPh_4	ϕ	ψ
C	7.5(2)°	40.8°
Si	7.6(1)°	37.7°
Ge (RT)	7.6(1)°	35.5°
Ge (LT)	7.5(1)°	34.8°
Sn	7.3(1)°	31.8°
Pb	7.3(1)°	31.3°

The molecular orientation of the phenyl ring can be conveniently described by the two angles ϕ and ψ (Figure 35), where ϕ is the angle between the vector joining the central atom and the projection of the centroid of the phenyl ring on (001) plane, and the nearest tetragonal a axis; ψ is defined as the angle of rotation (twist) of the phenyl ring plane relative to D_{2d} position of the ring; for the D_{2d} conformation, the $\psi=0$. (The angles given in references 77, 103, 107, and 121 are the complements of ψ, $\psi=90^{\circ}-\varphi$).

Table 21. The angles (deg.) between the planes of phenyl rings related by S_4.

XPh_4	α_1	α_2
C	111.6	74.7
Si	114.8	80.7
Ge (RT)	116.3	83.4
Ge (LT)	117.2	85.1
Sn	119.2	88.5
Pb	119.3	91.3

The angle ϕ measures the rotational displacement of the molecule about its S_4 axis. All the tetraphenyl molecules studied are rotated about the S_4 axis by an angle of about 7-8°. The values obtained for these angles (Table 20) are in accordance with the typical values observed previously (Table 17).

The values of ψ vary from 40.8° for TPMe to 31.3° for TPPb (Table 20).

The angles between the least-squares best planes of the phenyl rings connected by the S_4 axis are listed in Table 21. The angles α_1 and α_2 are the angles between the normal of the planes of the phenyl rings related by symmetry operations:

α_1 - (x,y,z,) and (-x, -y, z); and

α_2 - (x,y,z) and (y,-x,-z), respectively.

3.5. Analysis of Thermal Motion - TLS Calculations.

3.5.1. Thermal Motion of Atoms

A full description of the motion of atoms in the free molecule or in the crystal is not a simple matter and requires knowledge of the dynamics of the systems[136] studied. From X-ray diffraction studies[137,138,132] it is possible to obtain information about the mean atomic positions and also about the probability density function (pdf), averaged over time and over all unit cells in the crystal. The pdf describes the relative probability of finding an atom displaced by the vector **u** from its equilibrium position. The time-averaged motion of a combination of simple harmonic oscillators (in thermal equilibrium at temperature T) that corresponds to the motion of an atom in the harmonic potential in crystal, is represented by the Gaussian probability function[139] centred at the atomic position **r**

$$D(\mathbf{u}) = [(\det \mathbf{U}^{-1})/(2\pi)^3]^{1/2} \exp[(-1/2)\mathbf{u}^T\mathbf{P}\mathbf{u}]$$

where $\mathbf{P}=\mathbf{U}^{-1}$ is the inverse of the symmetric second-moment matrix $\mathbf{U}=\langle\mathbf{u}\mathbf{u}^T\rangle$ of the pdf; the atomic position is defined as the mean value of this distribution. If $\mathbf{U}$ is positive definite, the surfaces of the set of equations

$$\mathbf{u}^T\mathbf{U}^{-1}\mathbf{u} = \text{const.}$$

are ellipsoids. Thermal ellipsoids, which are often used in graphical presentations of crystal structures, are surfaces of constant probability density, centred on the mean position of atom and usually drawn at the 50% probability level.

The Fourier transform of the corresponding pdf, often referred to as atomic 'anisotropic temperature factors', takes the form

$$T_H = \exp\left(-2\pi^2\, \mathbf{H}^T\mathbf{U}\mathbf{H}\right)$$

where $\mathbf{H}$ is a reciprocal-lattice vector. The mean square displacement amplitude of an atom along the direction defined by the unit vector $\mathbf{n}$ (referred to the unit vectors of the reciprocal-lattice axis) is then given by

$$\langle u^2 \rangle_n = \mathbf{n}^T\mathbf{U}\mathbf{n}$$

and has the dimension (length)^2. The surface the radius of which along $\mathbf{n}$ is proportional to $\mathbf{n}^T\mathbf{U}\mathbf{n}$ has a peanut shape rather than ellipsoidal[132,136].

The six components of $\mathbf{U}$ for each atom are measures of the mean-square displacement (of the second moments of the pdf's) and are included, together with positional parameters, in the least-squares analysis. Examination of $\mathbf{U}$ can provide information about pdf in crystals and create a basis for a partial analysis of the overall thermal motion in terms of contributions from different sources.

3.5.2. Analysis of Thermal Motion

Generally, anisotropic thermal parameters (components of U) are treated as independent variables. The movement of the atoms is considered as independent and the actual correlations in the motion of different atoms are ignored. However, if the crystal contains rigid groups of atoms with fixed interatomic separations, the translational and librational oscillations of those groups introduce strong correlations among the U_{ij} parameters of different atoms. The full analysis of the thermal motion of the atoms in crystal requires consideration of the correlations among the motions of a large number of atoms or groups and, in general, involves dynamics of the entire crystal. In the solid state, however, where the contributions from internal vibrations are smaller than those from the translational and librational motions, the motion of rigid groups can often be approximated by simplified models of the vibrating systems.

The rigid-body model[140,131,132] most commonly used assumes that the interatomic distances within the rigid-body group remain constant during the movement and describes the simplest correlation among the motions of all different atoms within a molecule. Analysis of such motion is based on calculation of overall rigid body motion tensors **T**, **L**, and **S**[140,131,132,38], by a least-squares fit to the individual anisotropic temperature factor components, given atomic positions and the atomic **U**'s. The translation vector **T** describes the translational motion of the molecule. The libration tensor **L** depicts the librational motion of the molecule, and the screw correlation tensor **S** represents the correlation between the translational and librational motions of the molecule. Once the **T** and **L** tensors have been determined, they may be diagonalized to yield magnitudes and directions of their principal axes. The eigenvectors of the **L** tensor represent the three principal libration axes, and their eigenvalues represent the mean-squares librational amplitudes about these axes. The librational axes are perpendicular to each other but do not necessarily intersect[131]. Pertinent transformations help to relate those axes to the internal geometry of the molecule or to the crystal coordinate system and to the intermolecular packing.

The R-values[f] and the r.m.s. discrepancy serve to evaluate the fit of the chosen model to observed **U**'s. However, a good least-squares fit of the parameters of the model to observed atomic displacement parameters does not necessarily mean that the molecule or its parts are rigid,

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[f] $R(U_{ij}) = \Sigma\Sigma U_{ijobs} - U_{ijcalc} / \Sigma\Sigma U_{ijobs}$;

$R_w(U_{ij}) = [\Sigma\Sigma w(U_{ijobs} - U_{ijcalc})^2 / \Sigma\Sigma w U_{ijobs}^2]^{1/2}$;

since these parameters can absorb some of the effect of internal motion[141].

3.5.3. Effect of Thermal Vibrations on Bonds

The general effect of thermal motion on bond lengths estimated from diffraction measurement has been thoroughly discussed[131,132,136,138,140,142]. The atomic coordinates obtained by X-ray analysis refer to the centroid of an electron density distribution arising from the combined effect of external and internal atomic vibrations. The separation between atomic centroids cannot be interpreted directly as interatomic distances[142]. Correlations between the motions of pairs of atoms, which are usually unknown, can lead to an apparent shortening in the distances determined by a crystal-structure analysis. If proper corrections are to be made the joint distribution of motions of the atoms should be known or assumed. The rigid-body motion is one of the cases where the correlations are well defined. The TLS procedure[38] produces also the corrected values of bond lengths for a molecular fragment in libration model. Appropriate corrections are made to every coordinate of every atom and corrected interatomic distances are calculated.

3.5.4. TLS Calculations

In an attempt to explain the thermal motion of the molecules studied the rigid-body motion was analyzed by routine TLS[38] calculations. TLS calculations for TPMe are based on crystal coordinates and temperature factors from ref. 121. The fractional coordinates of atoms given in this reference are related to our set of coordinates by symmetry: $x_{ref}=-y$, $y_{ref}=x$, $z_{ref}=-z$. This corresponds to a different choice of an unique phenyl ring in the molecule.

First the rigid-body model was calculated to fit the whole molecule. For TPMe, the vibrational tensors **TLS**, calculated from the lattice-dynamics, have been reported[106]

Table 22. TLS details for XPh_4 - whole molecule; centroid of libration at (000); l_1, l_2, l_3 - mean amplitudes of libration about the principal libration axes L_1, L_2, L_3.

X	l_1	l_2 (°)	l_3	$R(U_{ij})$ %	$R_w(U_{ij})$ %	r.m.s. ($Å^2$)
C	2.3	2.3	2.9	9.61	9.10	0.0032
Si	1.8	1.8	2.9	15.64	14.26	0.0059
Ge(RT)	1.4	1.4	3.0	16.66	15.29	0.0061
Ge(LT)	1.3	1.3	2.6	16.09	14.35	0.0044
Sn	1.4	1.4	2.8	13.03	12.64	0.0047
Pb	1.4	1.4	2.9	19.89	18.88	0.0071

together with the corresponding values derived from the X-ray analysis[121]. The evaluated rigid-body model values of TLS tensors were higher than the values derived from the lattice-dynamic calculations since in the TLS model the contributions from internal vibrations are interpreted also in terms of rigid-body translation and rotation. This should also be true for the other tetraphenyl molecules.

Two other models were used in calculations. In the first

Table 23. TLS details for XPh_4 - model 1; l_1, l_2, l_3 - mean amplitudes of librational motions about L_1, L_2, L_3.

X	l_1	l_2 (°)	l_3	$R(U_{ij})$ %	$R_w(U_{ij})$ %	r.m.s. (Å)	centroid (cryst. fractions)
C	2.1	3.6	5.1	4.00	3.85	0.0013	0.0106 0.0803 0.0470
Si	1.5	3.8	6.1	8.01	6.83	0.0028	0.0959 -0.0090 -0.0348
Ge(RT)	1.7	3.6	6.3	8.58	7.71	0.0030	0.1054 -0.0191 -0.0454
Ge(LT)	1.7	3.3	5.4	7.58	6.74	0.0020	0.1043 -0.0034 -0.0819
Sn	1.9	2.9	5.8	7.06	6.44	0.0023	0.0860 -0.0294 -0.0481
Pb	1.0	3.8	5.6	13.45	12.43	0.0046	0.0577 -0.0541 -0.1546

model the central atom and the phenyl ring were assumed to move as a rigid body. In the second model only the phenyl ring was considered as a rigid body.

The results of the TLS calculations for all three models are given in Table 22, Table 23 and Table 24.

When the whole molecule is considered as a rigid body the centre of libration is placed in the central atom at the

Table 24. TLS details for XPh_4 - model 2; l_1, l_2, l_3 - mean amplitudes of librational motions about L_1, L_2, L_3.

X	l_1	l_2 (°)	l_3	$R(U_{ij})$ %	$R_w(U_{ij})$ %	r.m.s. Å^2	centroid (cryst. fractions)
C	4.4	6.3	7.9	3.10	3.00	0.0011	0.0237 0.1675 0.1935
Si	5.5	6.7	9.0	4.29	3.97	0.0017	0.1979 -0.0235 -0.2302
Ge(RT)	5.4	6.6	9.0	6.19	5.48	0.0022	0.2016 -0.0254 -0.2375
Ge(LT)	4.5	5.6	7.6	5.01	4.75	0.0015	0.1960 -0.0203 -0.2449
Sn	4.7	6.5	8.5	4.98	4.54	0.0017	0.2019 -0.0246 -0.2679
Pb	4.1	6.6	9.0	10.08	9.20	0.0035	0.2018 -0.0217 -0.2620

origin (000). The axis corresponding to the largest mean librational amplitude, L_3, coincides with the crystallographic axis c. The librational axes L_1 and L_2 are perpendicular to L_3 and to each other, and are rotated with respect to the crystallographic axes a and b. Since in tetragonal crystal system axis a is equivalent by symmetry to b and the molecules are at sites of symmetry $\bar{4}$ (S_4), the libration axes L_1 and L_2 are equivalent and the librational amplitudes about those axes are equal. The $R(U_{ij})$ values change from 9% for TPMe to almost 20% for TPPb, with r.m.s. discrepancies of 0.0032Å^2 to 0.0071Å^2 for TPMe and TPPb, respectively.

The average librational corrections based on this model are relatively small (max 0.003Å) compared to the calculated e.s.d's for the pertinent bonds. The differences in corrected and uncorrected bond lengths cannot therefore be considered as significant.

The presumption that the tetraphenyl molecules behave as rigid bodies seems to be unjustified, and in modelling of thermal motion of such molecules more flexibility should be allowed for. Not only can the molecule librate as a whole but also the phenyl groups can experience librations which can be visualized as yawing, pitching and rolling[143]. Because of this motion atoms outside the ring (opposite C1) will have the highest thermal motion and the distances C3-C4, C4-C5, and C1-C2, C1-C6 will be shortened.

An assumption that the central atom and the phenyl ring perform as a rigid body entails restricting the motion of the ring in the direction of the bond. The $R(U_{ij})$ ranges from about 7% for TPSn to 13% for TPPb and 4% for TPMe. An r.m.s. discrepancy between observed and calculated anisotropic temperature factors changes from $0.0020Å^2$ for TPGe (LT) to $0.0046Å^2$ for TPPb and is equal $0.0013Å^2$ for TPMe. As would be expected, from the two determined structures of TPGe the one collected at low temperature gives better fit with the model.

The librational movement about one of the axes is larger

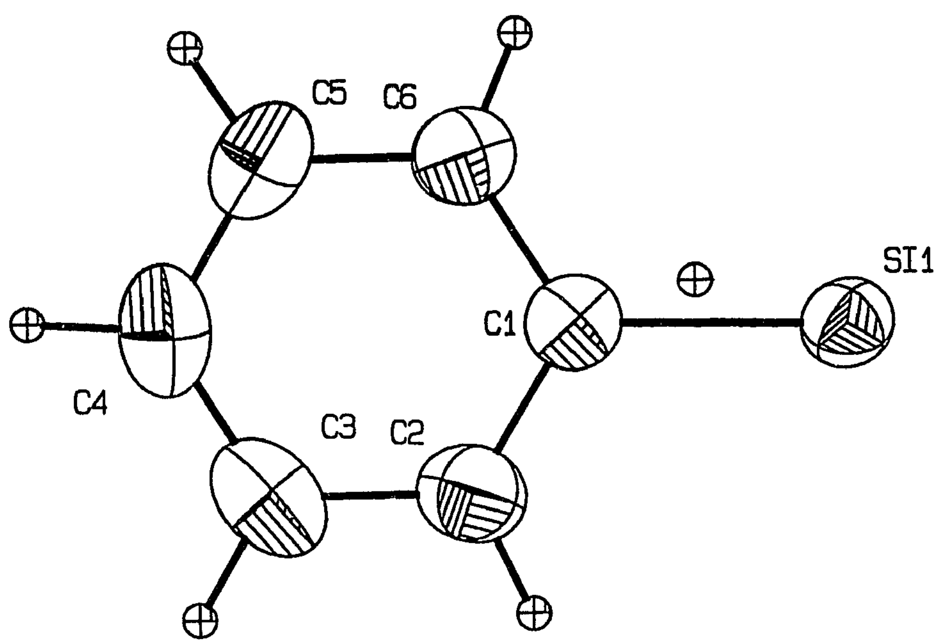

Figure 36. The typical location of the centre of libration in model 1 (TPSi).

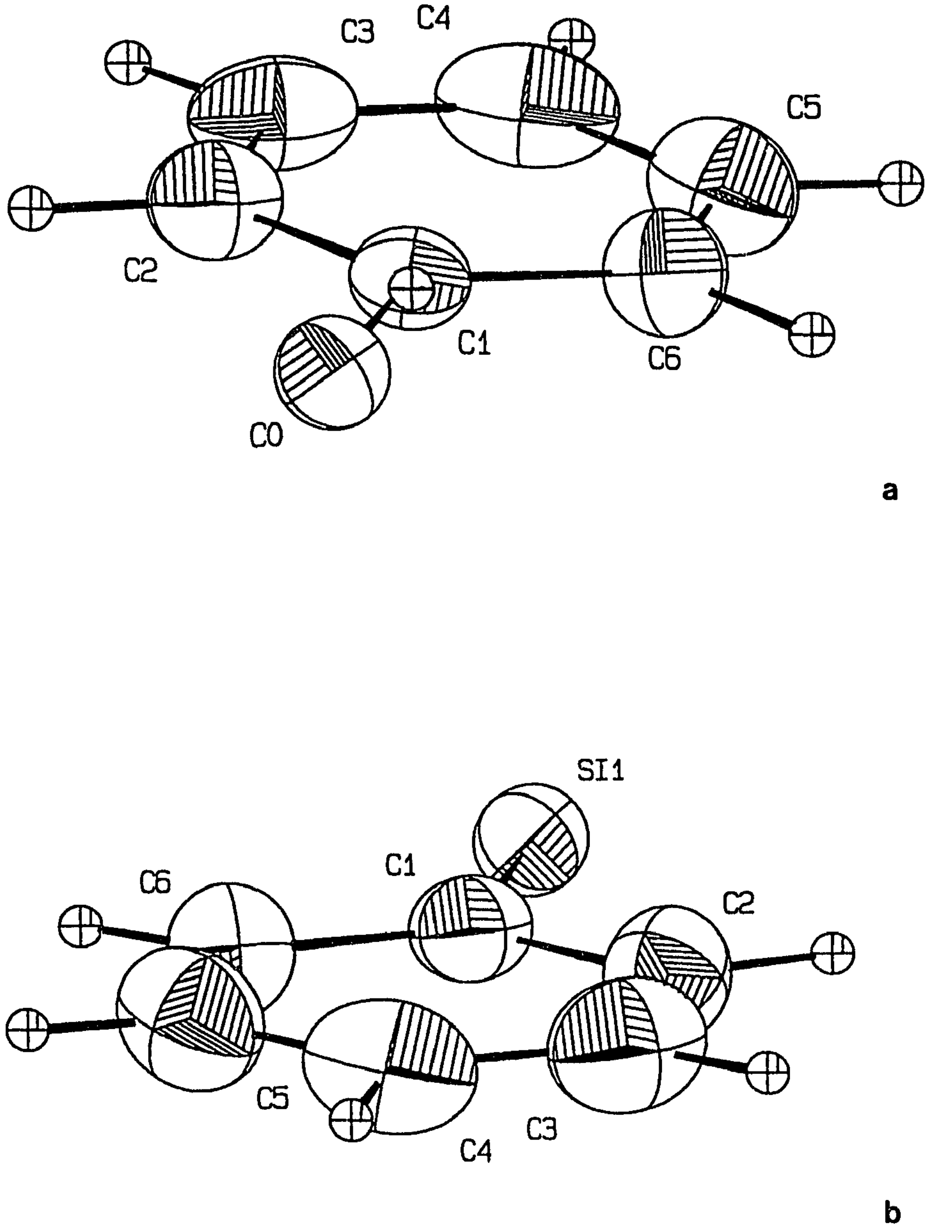

Figure 37. View of the phenyl ring (model 1) along the largest libration axis (L_3); (a) - TPMe; (b) - TPSi.

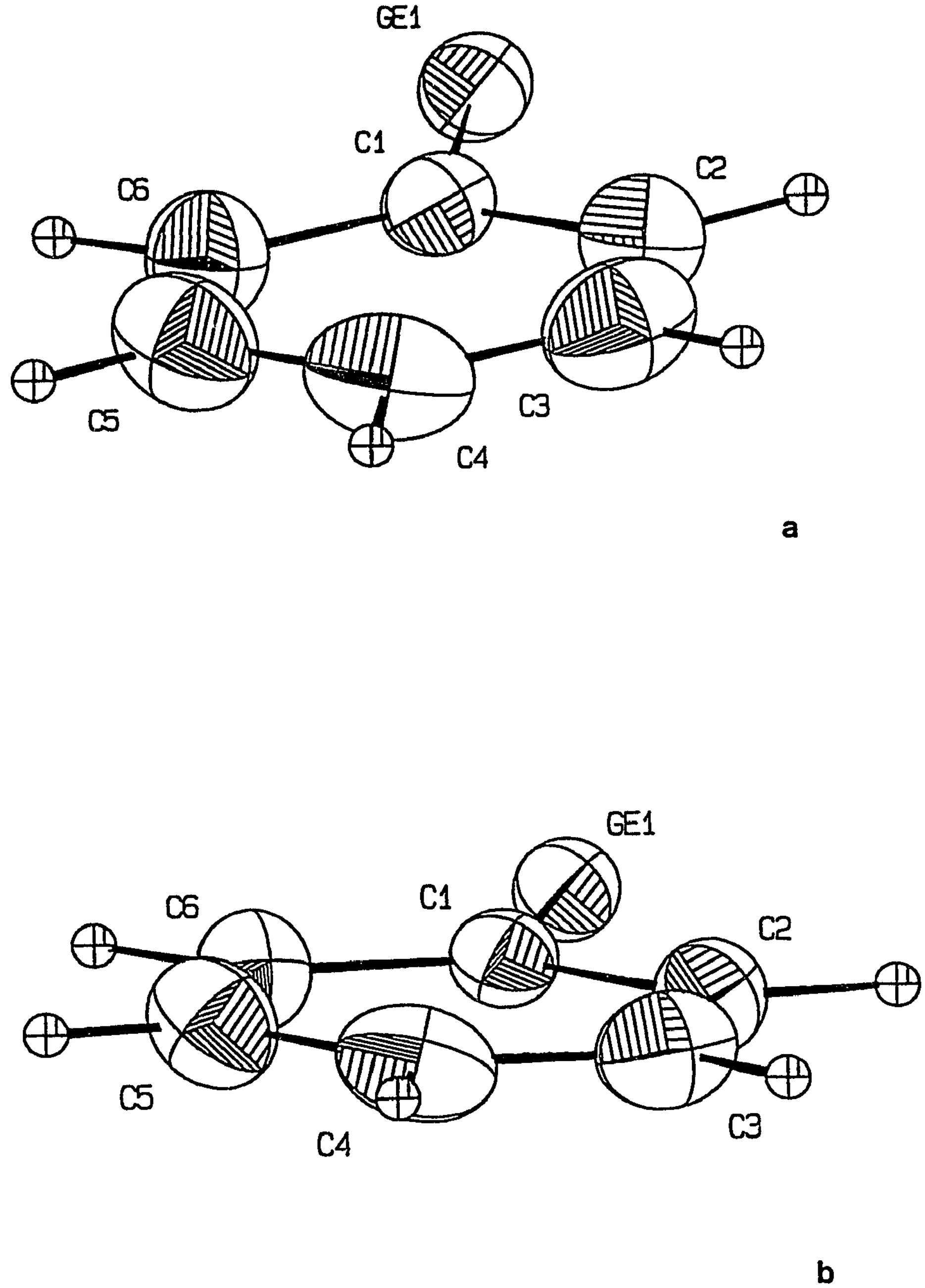

Figure 38. Libration axes for TPGe (model 1); (a) - room temperature structure; (b) - low temperature structure.

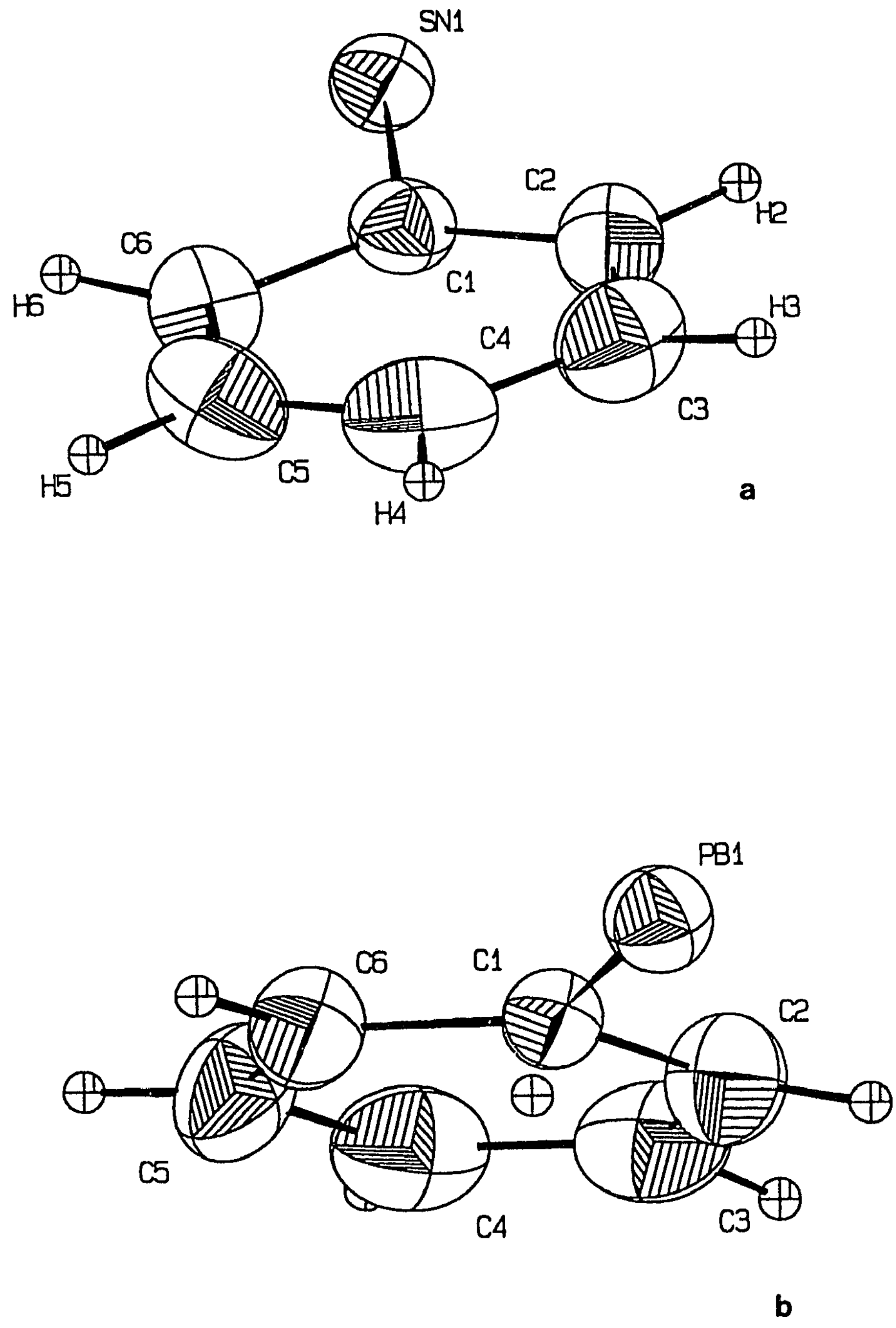

Figure 39. Libration axes (model 1) for TPSn - (a) and TPPb - (b).

than along the other two orthogonal axes. The rigid part of the molecule has the major libration about the axis inclined to the plane of the ring which runs through the libration centre below the ring plane between the C1 and the central atom (Figure 36). The coordinates of the libration centre are given in crystal fraction units with respect to the real crystal axes in Table 23. Figure 37, Figure 38, and Figure 39 show the view of the phenyl ring along the axis around which the largest libration occurs (L_3). This axis is perpendicular to the page and passes through the centroid. The L_1 and L_2 axes are perpendicular to L_3 and run down and across the page respectively, but do not necessarily intersect either with L_3 or with each other.

The average librational corrections based on this model increase the C-C distance in TPMe by 0.006Å, in TPSi by 0.007Å, in TPGe(RT) by 0.008Å, in TPGe(LT) by 0.006Å, in TPSn by 0.006Å, and in TPPb by 0.007Å. Similarly, the corrected X-C distances increase by 0.006Å in TPMe, by 0.006Å in TPSi, by 0.005Å in TPGe(RT), by 0.003Å in TPGe(LT), by 0.006Å in TPSn, and by 0.004Å in TPPb.

The assumption that only the phenyl ring behaves as a rigid body gives more freedom in movement of the ring. Although this model gives larger amplitudes of libration, it gives better agreement between the observed and calculated anisotropic temperature factors. The $R(U_{ij})$ values range from about 3% for TPMe to 10% for TPPb and the r.m.s. discrepancy varies from 0.0011Å^2 for TPMe to 0.0035Å^2 for TPPb. Here again better results were obtained for TPGe(LT) than for TPGe(RT).

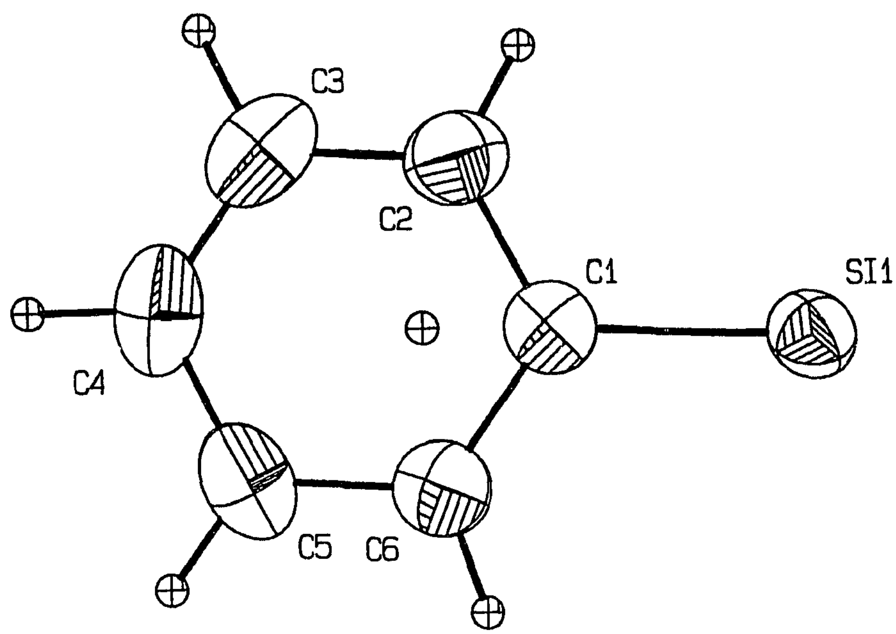

Figure 40. Location of the centre of libration for model 2 (TPSi).

Now the centre of libration is located in the plane of the ring along the line connecting central atom, C1, and C4, closer to C1 (Figure 40). The rigid phenyl ring librates about an axis running approximately along the plane of the ring (Figure 41, Figure 42). The librational movement is larger about L_3 than along the other orthogonal axes.

The average librational bond corrections based on this model increase the C-C distance by 0.013Å for TPMe, by

0.020Å for TPSi, by 0.019Å for TPGe (RT), by 0.014Å for TPGe (LT), by 0.017Å for TPSn, and by 0.017Å for TPPb.

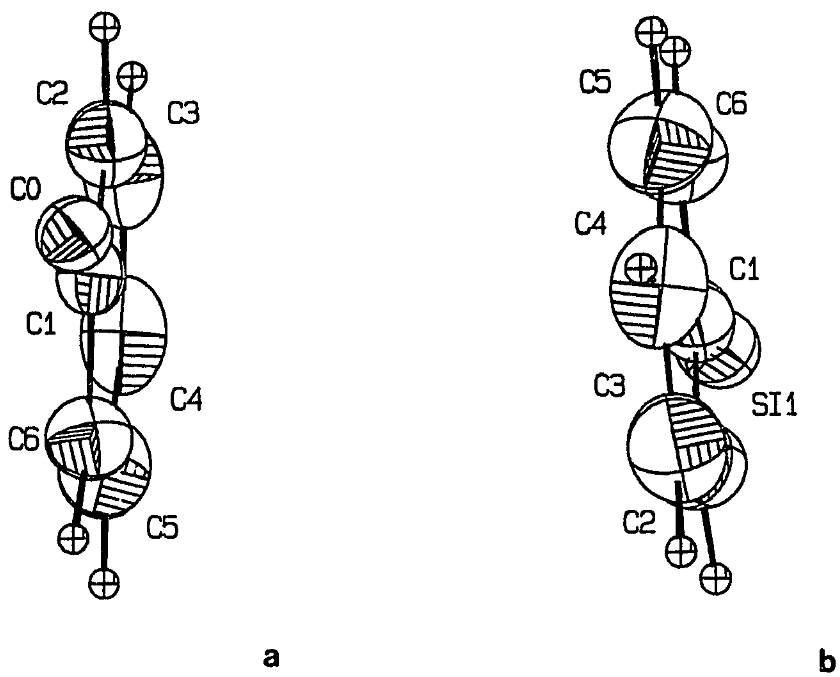

Figure 41. Libration axes (model 2) for (a) - TPMe; (b) - TPSi.

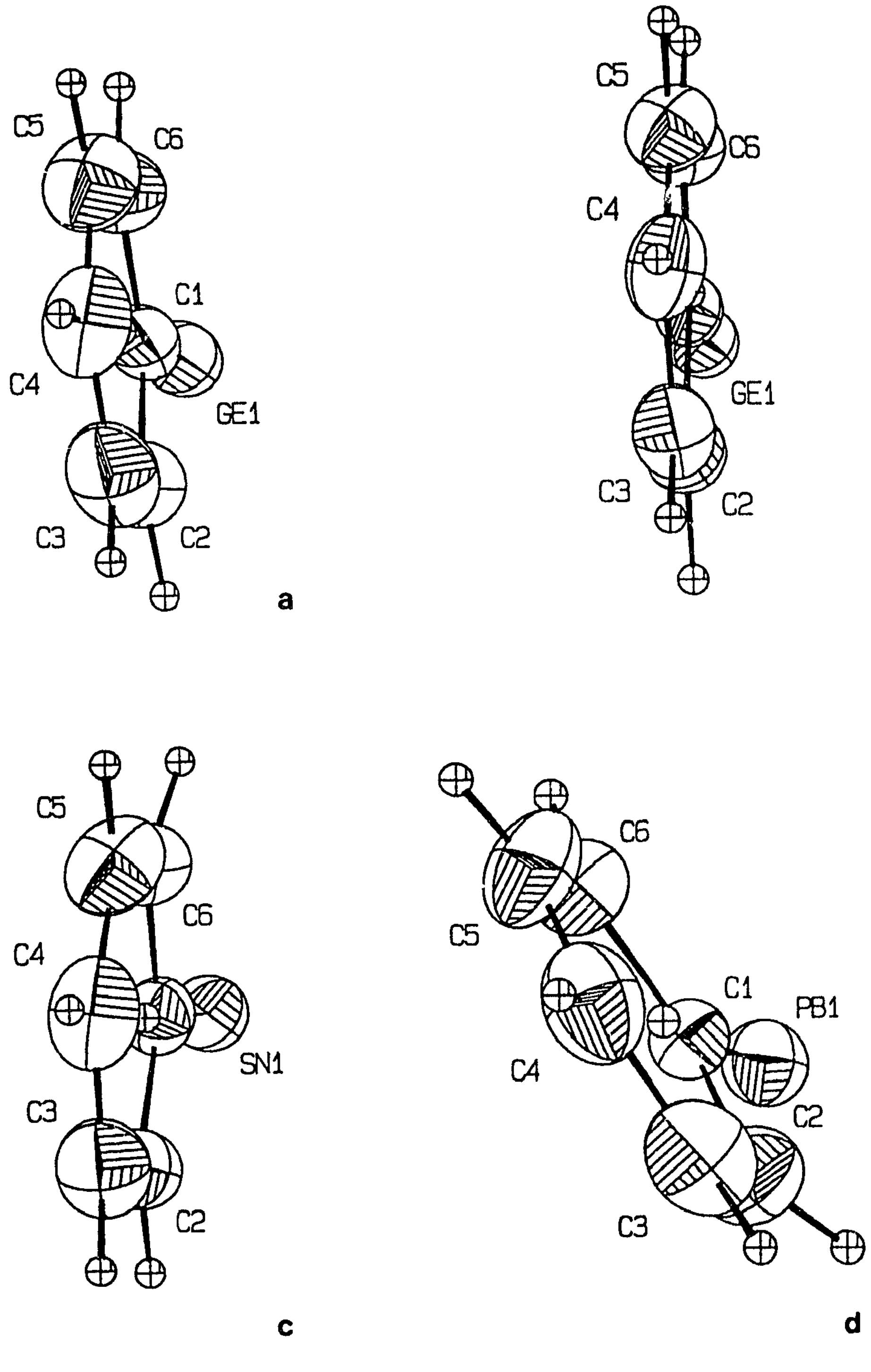

Figure 42. Libration axes (model 2) for TPGe (RT) - (a); TPGe (LT) -(b); TPSn - (c); and TPPb - (d).

3.6. Molecular Mechanics Calculations

3.6.1. Introduction

Conformational analysis involves examination of the geometric (bond lengths, valence and torsional angles, non-bonded contacts) and energetic (the relative energies of the conformers and isomers, rotational barriers etc.) characteristics of molecules. The conformers can be studied by experimental methods and by calculation.

The calculation methods for studying the conformation of molecules include semi-empirical and non-empirical quantum-chemical methods, and empirical methods, which use a mechanical model of the molecule, based on atom-atom approximation (molecular mechanics, force field methods). Recently, the accessibility of all these methods has increased considerably with the significant development of computer technology.

The possibility of examining a wide range of materials and the considerable saving of computing time (compared with quantum-chemical methods) has enabled the molecular mechanics method to occupy an important position among methods used to study molecular conformations.

The molecular mechanics method uses an empirical approximation based on the Born-Oppenheimer principle, which makes possible separation and independent study of the motions of the electrons and the nuclei in atoms. In this model, the molecule is regarded as a system of interacting atoms. The intramolecular and non-bonded interactions are central in character. For each type of atom there are 'ideal' values of the valence angles and bond lengths, deviation from which leads to an increase in the energy of molecules. To reproduce the experimental values of the dihedral angles and the barriers of rotation about the bonds in the molecules, the model is usually supplemented by a so-called torsional component characterising the expenditure of energy due to the relative rotation about chemical bonds. Where necessary, the model also takes into account the energy of electrostatic interaction, hydrogen bonds, etc.

Thus the steric energy of a molecule can be written as

$$E_s = \Sigma E(l) + \Sigma E(\theta) + \Sigma E(\varphi) + \Sigma E(r) + \Sigma E(q) \ldots$$

where the sums extend over all bonds, bond angles, torsion angles,and nonbonded interactions between all atoms not bound to each other or to a common atom.

The terms $E(l)$ (stretching energy) and $E(\theta)$ (bending energy) are the energies required to deform all bonds and valence angles in the molecule from the ideal values (l_0 and θ_0) to the actual values (l and θ). For the small deformations usually observed with change in the conformation, Hooke's law (the harmonic approximation) is applicable:

$$E(l) = 0.5K_l(l-l_0)^2,$$

$$E(\theta) = 0.5K_\theta(\theta-\theta_0)^2,$$

where K_l and K_θ are the force constants of the bond and angles. For larger deformations, additional terms (cubic, quadratic) are added or a Morse potential is substituted.

The torsional energy $E(\varphi)$ is written as

$$E(\varphi) = 0.5E_0(1+\cos n\varphi)$$

where E_0 is the torsional constant, φ the dihedral (torsional) angle for the k-th bond, and n the multiplicity of the barrier of rotation.

The energy E(r) of the nonbonded (van der Waals) interactions, is the sum of the paired interactions of all the atoms (atom-atom approximation), and is most frequently described by the Lennard-Jones or Buckingham potentials:

$$E(r) = -Cr^{-6} + Ar^{-12},$$

$$E(r) = -Cr^{-6} + A\exp(-Br),$$

where r represents the interatomic distances, and A, B, and C are empirical constants, obtained from an experiment.

The energy E(q) of the electrostatic interactions is taken into account fairly infrequently, sometimes in the dipole-dipole or, more often, in the monopole approximation:

$$E(q) = q_i q_j / \varepsilon r_{ij},$$

where q_i and q_j are the charges on the ith and jth atoms (obtained from the quantum mechanics calculations) situated at a distance r_{ij} from one another, and ε the dielectric constant.

The geometry of an isolated (free) molecule corresponds to a conformational energy minimum. Thus the determination of the optimal molecular conformation involves the search for a minimum value of E_s. A variety of mathematical techniques of minimising of E_s, of which the steepest-descent and the Newton-Raphson methods are the most common, can be used. In the general case, the problem of determining the optimal geometry of a molecule reduces to the search for a minimum of a function of (3N-6) variables, where N is the number of atoms in the molecule. However, it is often possible to fix most of the geometric parameters of the molecule and to simplify the problem by scanning the values of E_s over several variables.

The choice of the parameters for conformational calculations (the constants in the expressions for components of E_s) is based on their variation, for a series of simple compounds of the same type, to achieve the best agreement between the calculated and experimental data or corresponding data obtained in a non-empirical quantum-mechanics calculation.

The success of the calculations depends on the ability of the model to approximate the systems under consideration. Most molecular geometries are calculated now with an accuracy comparable to the precision of the experimental methods (0.005Å in bond lengths and 1° in angles). Thus in most cases the molecular mechanics represents the best approach to the calculation of molecular energies, even when the molecules of interest have not yet been prepared.

3.6.2. Molecular Conformations of the Tetraphenyls

The first theoretical calculations[117,116] on tetraphenyl compounds were based on geometrical considerations of crystal packing and the closest approach of phenyl hydrogens. Although the results so obtained were not very accurate (see ref 119, 120), they all confirmed the existence of fourfold symmetry in the molecules and were in agreement with the results from X-ray determinations. The conformational analysis of molecules based only on a simple consideration of van der Waals contacts is very limited[119]. The crystal lattice (packing) energy is a more sensitive probe in predicting a probable structure.

Because of the rigid nature of the phenyl ring the structures of tetraaryl compounds of Group IV can be described in terms of two angular parameters, ϕ and φ, where ϕ is the angle of rotation of the entire molecule about the S_4 axis, and φ is defined as the angle of rotation of the phenyl ring about the central bond. The total potential energy of the all pairs of the nonbonded and bonded atoms becomes then a function of these parameters.

In the first crude calculations[103] of nonbonded potential energy of TPSn the atom-atom potential approximation[94] was used, with all conformational changes of the molecule reduced to one rotation of the phenyl ring about the tetrahedral Sn-C bonds and the packing restricted only to the experimentally established symmetry of the space group.

Similar calculations based on the same model were also performed for all the tetraphenyls[104]. For all the compounds studied, the energy minima corresponded to S_4 symmetry and the values of the ϕ and φ angles were in fair agreement with the experimental data.

With the progress in modern computational techniques, the empirical force field method (molecular mechanics) has developed into a valuable source of data on structures and energies for the compounds containing aromatic rings[109, 110]. The study of the static[107] and dynamic[108] stereochemistry of tetraaryl derivatives of Group IV was undertaken utilizing the approach of full relaxation empirical force field calculations. A mathematical model has also been proposed[76] to represent the behaviour of the tetraaryls. The molecular mechanics force fields used included bond stretching, angle bending, torsion, and van der Waals energy interactions summarized over all bonds, bond angles, torsion angles, and nonbonded interactions between all atoms not bound to each other or to a common atom[144]. The steric energies and geometries of structures corresponding to minima on the potential hypersurfaces for the series of tetraarylmethanes and tetraarylsilanes were calculated[107].

Tetraphenylmethane was found to have a ground state of D_{2d} symmetry, unlike TPSi, which appeared to have two stable conformers, one of S_4 symmetry consistent with the symmetry found in the crystal and another of D_{2d} symmetry and of roughly equal energy.

More refined calculations[145] using a combined empirical force field and extended Hückel molecular orbital method have shown the existence of two energy minima for TPMe: one of D_{2d} symmetry corresponding to the ground state found previously and the other (0.4kcal/mol above the ground state) corresponding to the S_4 symmetry of the molecule. The D_{2d} conformation of TPSi was found to correspond to an energy maximum.

A search for the most favourable conformation has also been carried out for ortho-substituted tetraaryl derivatives[107,108]. The results of calculations on tetra(o-tolyl) derivatives of carbon and silicon as well as on tetra(2,6-xylyl)methane indicated a ground state of S_4 symmetry, with all the substituents oriented exo, for all the molecules studied.

The results of conformational analysis confirm the preference for the S_4 symmetry for the tetraaryl compounds.

3.6.3. MM3 Calculations

Molecular Mechanics calculations were performed for TPMe and TPSi using the MM3 Allinger Force Field program[109, 110]. Input structures for these calculations were taken from X-ray determinations reported in ref. 121 and from our redeterminations, for TPMe and TPSi respectively.

Initially the block-diagonal minimisation method was employed; later the full-matrix Newton-Raphson method was used. Minimisation was continued until atomic movements (all shifts in positional coordinates) converged with the following values: average movement at 0.00113Å and maximum movement at 0.01132Å. During minimisation of TPMe and TPSi structures S_4 symmetry restraints were employed for all symmetry-equivalent carbon and hydrogen atoms in the different phenyl rings. The motion of the central atom was restricted in all directions.

Only the parameters included in the MM3 program package were used in calculations.

The MM3 driver routine was used to drive a selected angle of TPMe and TPSi through a range of values and minimise all other degrees of freedom at each point. The scanning of the torsional angle chosen (C7-X-C1-C2 or =C1-X-C7-C8 [C7=C1', C8=C2'...]) corresponded to the rotation of the phenyl ring about the central bond by this angle. The ring was rotated about the C-X bond by increments of 15°, 5° and 1° through the range of -100° to 100°. At each stage, the structure was subjected to the full MM3 calculations, with the exception that the dihedral angle was held constant during energy minimisation. The steric energies of TPMe and TPSi (as a function of the angle through which a phenyl ring was driven) are depicted in Figure 45 and Figure 46, respectively.

Unfortunately, the MM3 force field at present does not contain the parameters that would enable us to calculate the structures of the other tetraphenyls.

MM3 calculations were also performed to determine the structures of the o-tolyl derivatives of tetraphenylmethane and silane. The structures of tetra(o-tolyl)methane (oTMe) and tetra(o-tolyl)silane (oTSi) were calculated using MM3. The procedure employed was the same as in the case of TPMe and TPSi.

3.6.4. MM3 Calculations of TPMe and TPSi

The minimised structure of TPMe has the symmetry D_{2d} (molecular shape - prolate symmetric rotor). The final steric energy is 28.100 kcal/mol. The phenyl rings are planar, with a mean deviation of the central carbon atom from the plane through the carbon atoms of 0.093Å. The mean C-C-C angle in the phenyl ring is 120°. The angle at C1 is equal to 117.6°.

The mean carbon-carbon bond length in the ring is 1.340Å, and the distances between the central carbon and the carbons C1 are 1.530Å. The bond lengths and angles of the calculated structure are listed in Table 25.

The valence angles are 102.3° and 113.2°.

The angles between the planes of the phenyl rings related by the S_4 axis are 93.2° and 121.9°.

For TPSi the final structure obtained from MM3 calculations has the symmetry S_4 (molecular shape - prolate symmetric rotor). The final steric energy was found to be 18.975 kcal/mol.

The deviation of the silicon atom from the best phenyl-ring plane through the carbon atoms is 0.034Å. The average C-C-C angle in the phenyl ring is 120.0°. The angle at C1 is equal to 119.2°. The average carbon-carbon bond length in the phenyl ring is 1.398Å. The Si-C1 distances are 1.865Å.

The valence angles are 108.5° and 110.0°.

The bond lengths and angles of the calculated structure

Table 25. Interatomic distances (Å) and interbond angles (degrees) for TPMe (MM3).

C0	-C1	1.530	C1	-C0	-C1'	102.3
C1	-C2	1.407	C1	-C0	-C1''	113.2
C1	-C6	1.406	C0	-C1	-C2	120.8
C2	-C3	1.396	C0	-C1	-C6	120.8
C3	-C4	1.395	C2	-C1	-C6	117.6
C4	-C5	1.394	C1	-C2	-C3	121.1
C5	-C6	1.397	C2	-C3	-C4	120.1
			C3	-C4	-C5	119.6
			C4	-C5	-C6	120.2
			C1	-C6	-C5	121.7

Primed atoms have symmetry operations:
' - -x, -y, z,
'' - y, -x, -z,
''' - -y, x, -z,

Table 26. Interatomic distances (Å) and interbond angles (degrees) for TPSi (MM3).

Si1	-C1	1.865	C1	-Si1	-C1'	108.5
C1	-C2	1.402	C1	-Si1	-C1''	110.0
C1	-C6	1.400	Si1	-C1	-C2	119.7
C2	-C3	1.396	Si1	-C1	-C6	121.1
C3	-C4	1.396	C2	-C1	-C6	119.2
C4	-C5	1.396	C1	-C2	-C3	120.4
C5	-C6	1.397	C2	-C3	-C4	120.1
			C3	-C4	-C5	119.8
			C4	-C5	-C6	120.1
			C1	-C6	-C5	120.4

Primed atoms have symmetry operations:
' - -x, -y, z,
'' - y, -x, -z,
''' - -y, x, -z,

are listed in Table 26.

The angles between the phenyl rings related by S_4 are 106.2° and 73.8°. The twist angle of the phenyl ring, ψ, is 50.4°.

After completion of the energy minimisation the program reorients the molecule so that the centre of mass is at the origin and the principal axes of inertia correspond to the Cartesian axes ($Ix < Iy < Iz$). Because of this transformation the crystallographic axis Z_c was interchanged with the MM3 axis X'.

In order to be able to compare the calculated structures with the structures obtained from the X-ray determinations it was necessary to bring both molecules to a common orthogonal system of coordinates.

The new orthogonal system (X",Y",Z") is related to the tetraphenyl molecule in such a way that the origin is placed at the central atom; the X" axis passes through the origin and the atom C1; the Z" axis coincides with the crystallographic axis, Z_c, and with the MM3 X' axis; and Y" is orthogonal to X" and Z". The transformation from the MM3 system, after interchanging the X' and Z" axes, is a simple rotation about Z" by an angle α_m= 72.96° for TPMe and 37.88° for TPSi. This angle is defined by $\tan \alpha_m = y_1/x_1$, where x_1, y_1, z_1 are the coordinates of C1 in the MM3 system (after interchanging X' and Z").

Table 27. Cartesian coordinates (Å) of TPMe in the X"Y"Z" system.

	X-ray (S_4)			MM3 (D_{2d})		
Atom	x"	y"	z"	x"	y"	z"
C0	0.000	0.000	0.000	0.000	0.000	0.000
C1	1.244	0.000	0.925	1.191	0.000	0.959
C2	1.298	-0.917	1.982	1.687	-1.204	1.492
C3	2.384	-0.967	2.834	2.711	-1.205	2.441
C4	3.442	-0.101	2.665	3.234	0.000	2.909
C5	3.397	0.830	1.649	2.711	1.204	2.442
C6	2.309	0.880	0.784	1.687	1.204	1.492
H2	0.529	-1.536	2.118	1.264	-2.171	1.176
H3	2.366	-1.627	3.567	3.095	-2.161	2.835
H4	4.228	-0.142	3.247	4.037	0.000	3.665
H5	4.131	1.449	1.529	3.095	2.160	2.835
H6	2.300	1.585	0.066	1.263	2.171	1.176

Table 28. Cartesian coordinates (Å) of TPSi in the X"Y"Z" system.

	X-ray (S_4)			MM3 (S_4)		
Atom	x"	y"	z"	x"	y"	z"
Si1	0.000	0.000	0.000	0.000	0.000	0.000
C1	1.522	0.000	1.103	1.513	0.000	1.090
C2	1.654	-0.949	2.110	1.535	-0.789	2.248
C3	2.780	-0.983	2.923	2.670	-0.820	3.060
C4	3.778	-0.062	2.758	3.794	-0.067	2.720
C5	3.665	0.900	1.789	3.781	0.717	1.566
C6	2.552	0.927	0.969	2.636	0.748	0.752
H2	0.983	-1.563	2.230	0.656	-1.394	2.529
H3	2.840	-1.642	3.626	2.679	-1.443	3.971
H4	4.580	-0.061	3.252	4.692	-0.090	3.362
H5	4.362	1.542	1.714	4.670	1.314	1.295
H6	2.587	1.614	-0.325	2.656	1.375	-0.155

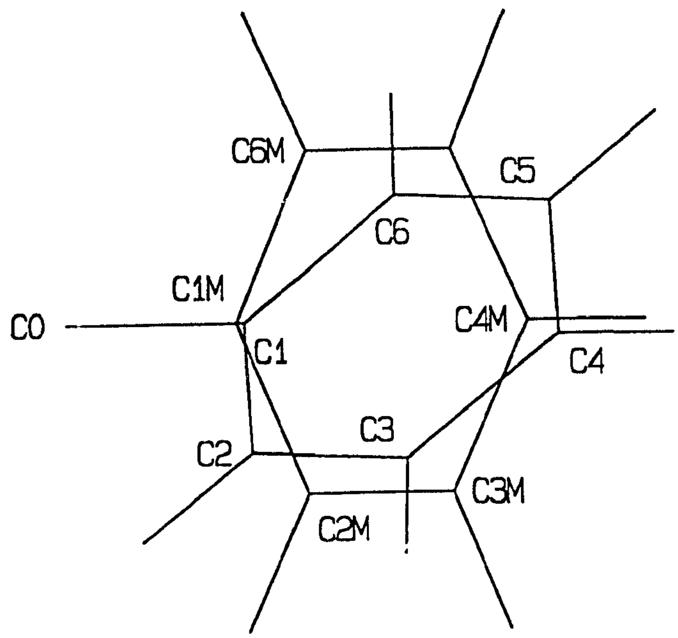

Figure 43. Projection of the phenyl ring of TPMe on the X"Y" plane.

Similarly, the transformation from the crystal coordinates system is a rotation about $Z"=Z_c$ by an angle α_c= 82.60° for TPMe and 82.99° for TPSi ($\tan \alpha_c = y_c/x_c$, where x_c, y_c, z_c, are the Cartesian coordinates of C1 in the crystal system). The transformed coordinates of both structures are given in Table 27 and Table 28. The projection of both phenyl rings on the X"Y" plane is shown in Figure 43 for TPMe and in Figure 44 for TPSi.

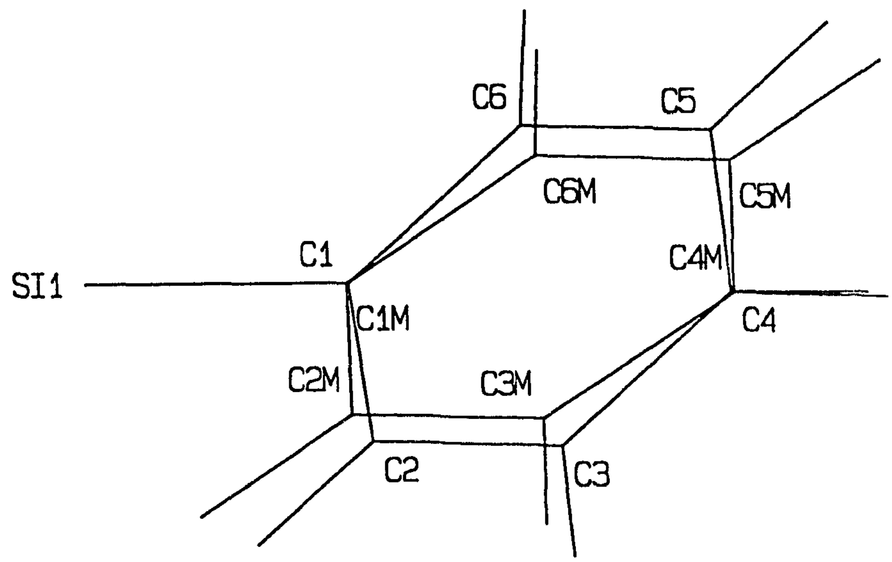

Figure 44. Projection of the phenyl ring of TPSi on the X"Y" plane.

Of particular interest is a comparison between the calculated molecular structures of TPMe and TPSi and the molecular structures found in the crystals.

The calculated structure of TPMe has the symmetry D_{2d} while the symmetry in the crystal is S_4. The difference between the calculated and the experimental structures is clearly shown in Figure 43. Table 29 lists the results of the calculation and of the X-ray experiment for TPMe. The distances calculated by MM3 are shorter than those obtained from crystallography. The valence angles, the angles between

Table 29. TPMe: comparison of results from MM3 and X-ray.

	MM3		X-ray	
C-C	1.340 Å		1.393 Å	
C0-C1	1.530 Å		1.553(3)Å	
C2-C1-C6	117.6°		117.6°	
C1-C0-C1'	102.3°		106.7(2)°	
C1-C0-C1"	113.2°		110.9(2)°	
ψ	0.0°	(D_{2d})	40.8°	(S_4)
α_1	93.2°		111.6°	
α_2	121.9°		74.7°	

the phenyl rings, and the twist angle of the phenyl ring are dissimilar because of the different molecular conformations. The angle C2-C1-C6 is the same in both cases. This might suggest that the distortion inside the phenyl ring has the same character for both conformations.

A possible explanation for the difference between the calculated molecular symmetry and that observed in the crystal might be provided by the analogy with tetraphenylborates, where the symmetry assumed by the anion is a function of the associated cation[107]. The intermolecular forces dictated by crystal packing play the dominant role in determining the anion stereochemistry in potassium and tetramethylammonium[92] tetraphenylborates. This statement is reinforced by the existing similarity of the distortions which the two systems suffer at the central atom. In the case of TPMe the intramolecular forces are apparently strong enough to overcome the energy which is needed to effect the conformational change from the symmetry in the free state to the symmetry in the crystal.

Table 30. TPSi: comparison of results from MM3 and X-ray.

	MM3		X-ray	
C-C	1.398 Å		1.385 Å	
Si-C1	1.865 Å		1.879(3)Å	
C2-C1-C6	119.2°		117.3°	
C1-Si-C1'	108.5°		108.2(1)°	
C1-Si-C1"	110.0°		110.1(1)°	
ψ	50.4°	(S_4)	37.7°	(S_4)
α_1	106.2°		114.8°	
α_2	73.8°		80.7°	

In the case of TPSi, the symmetry of the calculated and experimental structures is the same. The difference between these two structures is shown in Figure 44. Table 30 compares results obtained from calculation and experiment for TPSi. The principal difference is in the twist angle, ψ. This angle is larger in the calculated structure. The angles between the phenyl ring planes also differ. The average C-C distance in the ring is greater in the calculated structure but the Si-C1 distance is less than in the crystal. The valence angles have the same values in both structures but the α angle (at C1) in the phenyl ring is greater in the case of the calculated structure.

The MM3 driver routine has been used to determine that the conformations obtained for the tetraphenyls studied are located in the global minimum of the energy surface. The steric energies of TPMe and TPSi (as a function of the angle through which a phenyl ring was driven) are shown in Figure 45 and Figure 46, respectively. Because of the high symmetry of the phenyl ring only a limited range of angles needs to be considered.

Two energy minima for TPMe in the range of angles studied (-100° to 100°) have been found: one at about -85° and another at 85°. Both correspond to structures with D_{2d} symmetry, with the phenyl ring rotated by 180° about the C-X bond. Thus in one case, C7-X-C1-C2=85° and C7-X-C1-C6=-85°, while in another these values are inverted. There are also two 'discontinuity' (sudden energy change) regions, at 0° and at about 55°-60°. All attempts to minimise structures with these values of torsional angles led to the conformations with D_{2d} symmetry or to the transition structures with a higher energy. An explanation of the behaviour of TPMe in these angle regions would require a detailed dynamic analysis of all the transition conformations and is out of scope of this work.

In case of TPSi, the energy surface shows four minima located at -98°, -41°, 20°, and 80° in the range of angles studied. All the conformations corresponding to these minima posses S_4 symmetry and are in fact equivalent since the values of the torsional angles C7-Si-C1-C2, C13-Si-C1-C2, C19-Si-C1-C2, C7-Si-C1-C6, C13-Si-C1-C6, and C19-Si-C1-C6 (related to C1-C6 and C1-C2) permute.

The MM3 force field does not contain the parameters which would enable us to calculate the structures of TPGe, TPSn, and TPPb. However, attempts have been made to model these structures by adjusting the existing l_0 and K_l parameters to values observed in these compounds or given in MM3 for the $X(sp^3)$-$C(sp^3)$ bonds. The results of the MM3 calculations with new parameters are given in Table 31. Of course, such a treatment is unsatisfactory, because of the lack of other parameters involved in the calculations. Nonetheless, despite the deficiency of such an approach the symmetry of all the structures minimised (although C_1) turns out to be very close to S_4 observed in the crystals.

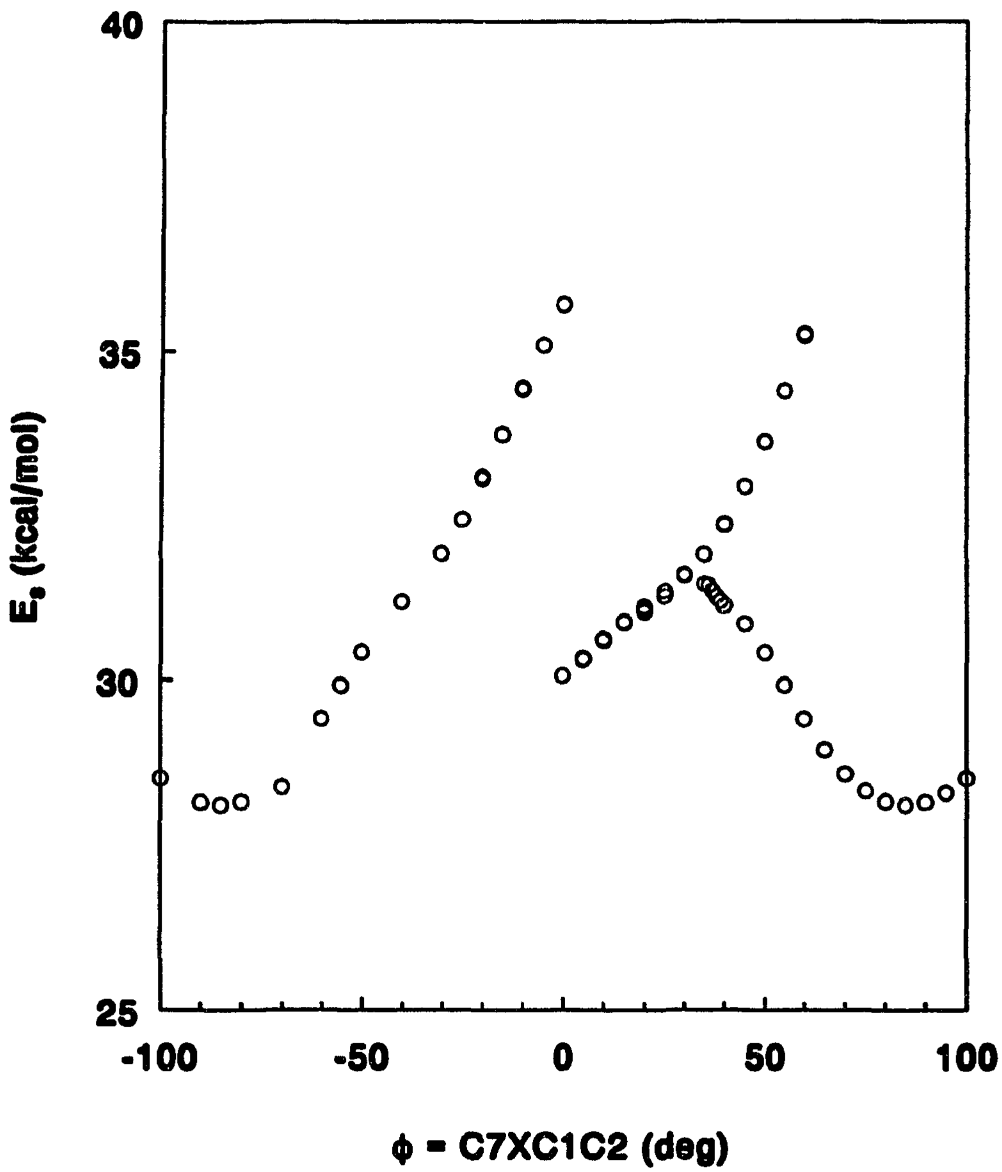

Figure 45. Steric energy E_s as a function of the angle of driven ring (C7-X-C1-C2) for TPMe.

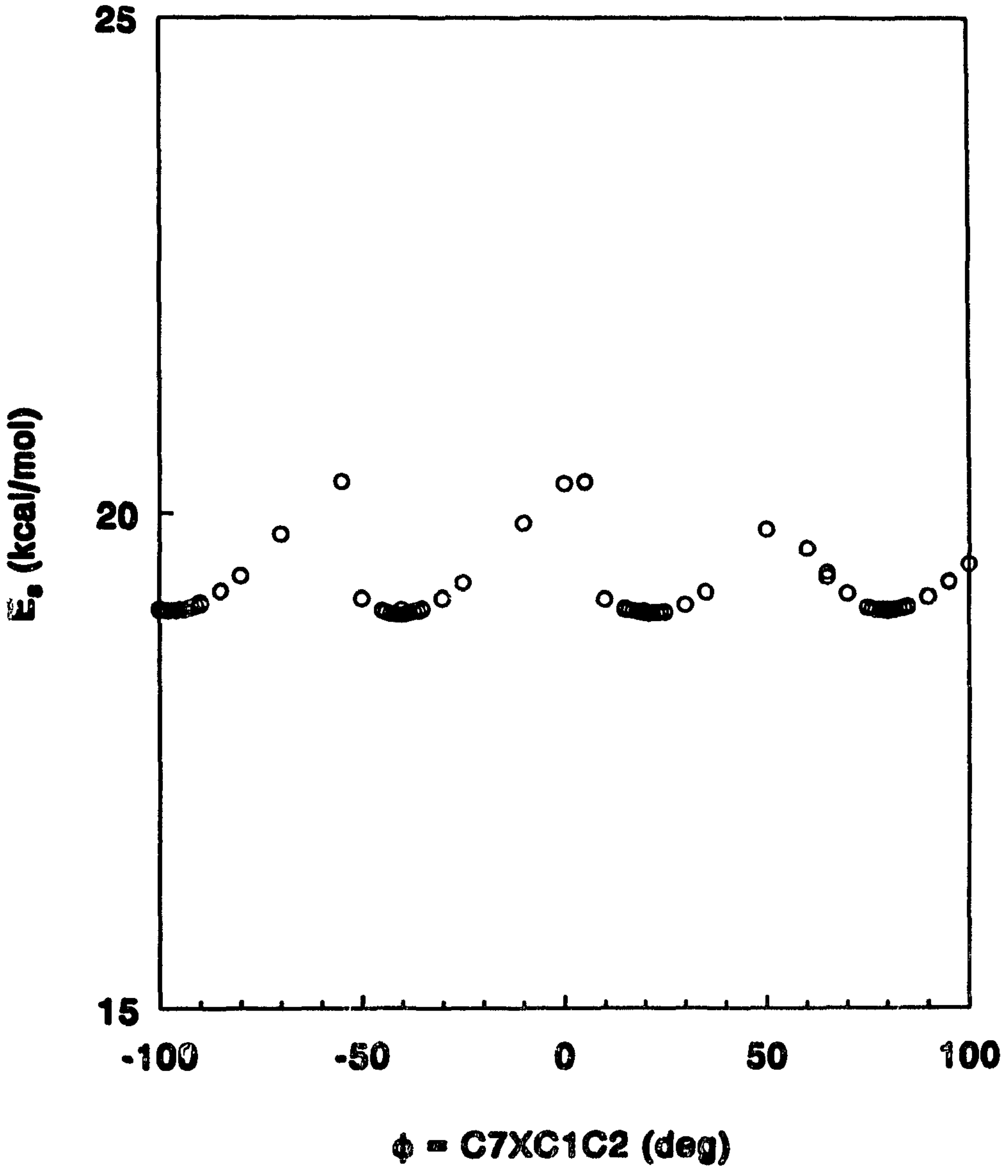

Figure 46. Steric energy E_s as a function of the angle of driven ring (C7-X-C1-C2) for TPSi.

Table 31. Results of MM3 calculations with changed l_0 and K_l.

	TPMe	TPMe	TPSi	TPSi	TPGe	TPSn	TPPb
K_l	6.300	6.300	3.000	3.000	2.700	2.124	1.900
l_0	1.530	1.553	1.856	1.865	1.948	2.137	2.203
X-C (Å)	1.557	1.578	1.878	1.886	1.966	2.152	2.219
θ_1 (°)	102.5	102.7	109.0	109.0	109.2	109.4	109.5
θ_2 (°)	113.0	112.9	109.7	109.7	109.6	109.5	109.5
α (°)	117.8	118.0	119.3	119.3	119.5	119.7	119.7
ψ (°)	0.0	0.0	36.6	36.6	36.1	35.3	35.0
φ (°)	90.0	90.0	53.4	53.4	53.9	54.7	55.0
E_s (kcal/mol)	25.8	24.2	13.3	13.2	12.3	12.1	12.3
Symm.	D_{2d}	D_{2d}	C_1	C_1	C_1	C_1	C_1

3.6.5. MM3 Calculations of oTMe and oTSi

Introduction of substituents into *ortho* or *para* positions of the phenyl group of TPMe and TPSi can lead to further lowering of the symmetry of the molecule[107,100,101]. The conformations of the oTMe and oTSi molecules were calculated, using MM3, to observe the effect of the substituent on the preferred geometry.

For these molecules, only six diastereomeric conformers with S_4 or pseudo-S_4 symmetry are possible (Figure 47). To distinguish the different edges of the phenyl rings in the molecule the *endo*-*exo* nomenclature introduced by Mislow et al. is adopted. If a molecule in an S_4 conformation is represented by a Fischer projection where the central atom lies in the reference plane (the plane perpendicular to the S_4 axis), then the edges of the aryl groups inclined toward this plane are labelled *endo* (n), while those inclined away from the plane *exo* (x). According to this description, of the six diastereomers the (xxxx) and (nnnn) forms have S_4 symmetry, the (xxnn) form has C_2 symmetry, and the other four forms are asymmetric though of pseudo-S_4 symmetry.

The results of the MM3 calculations for oTMe and oTSi are presented in Table 32 and Table 33, respectively. Only six diastereomeric structures corresponding to energy minima were found for both oTMe and oTSi. In each case, the ground-state structure has S_4 symmetry ((xxxx) isomer) and relatively lower energy than the other conformers. The *endo* (nnnn) isomer has the highest conformational energy.

The phenyl rings are planar, with a maximum deviation from the plane through the carbon atoms of 0.044Å (for carbons) for oTMe and of 0.029Å for oTSi. The deviation of the central atom from this plane varies from 0.007Å for the (nnnn) form of oTMe to 0.038Å for the (xxxx) isomer, and from

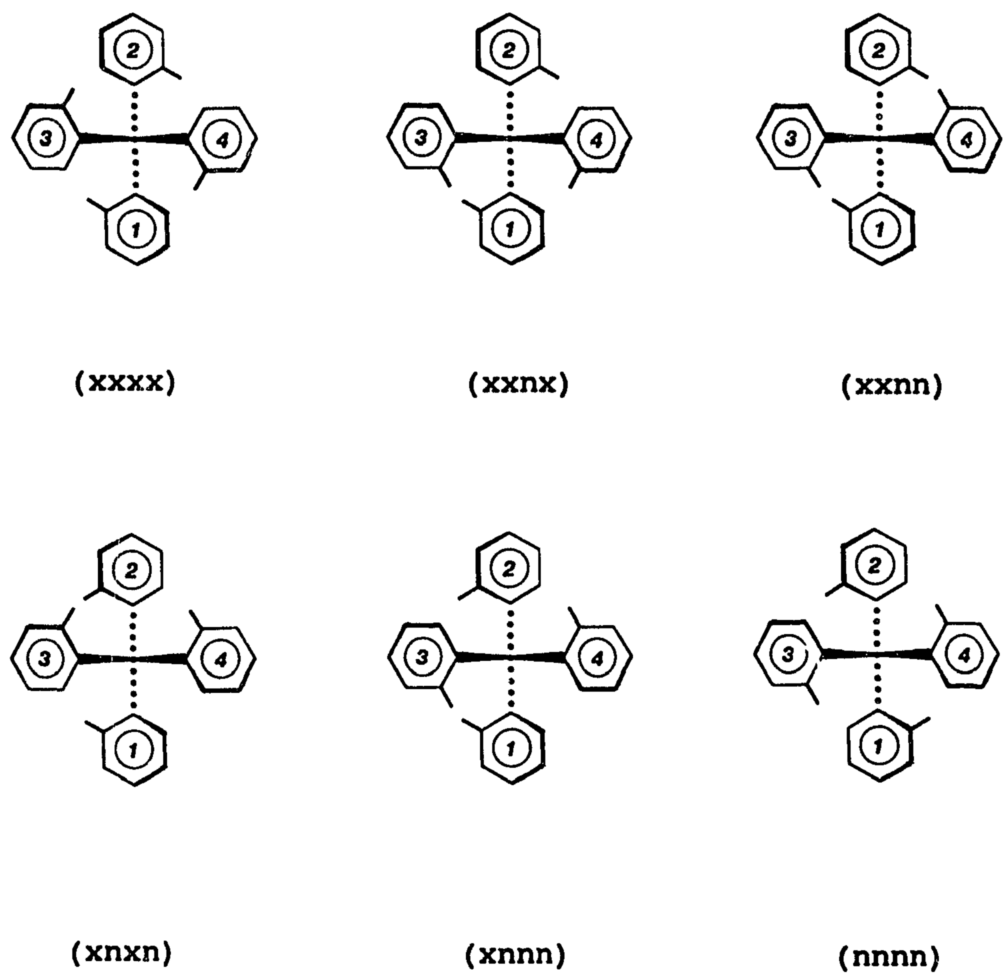

Figure 47. The six diastereomeric conformations of oTMe.

0.007Å for the (xxxx) conformer of oTSi to 0.020Å for the (xxnn) form. The methyl carbons in both cases are also deviated from the phenyl ring plane. The maximum deviation of the methyl carbons from the ring plane is observed in the (nnnn) form (0.162Å) for oTMe, while for oTSi in the (nnxn) isomer (0.139Å). The deviation is minimal in the (xxxx) isomer of oTMe (0.048Å) and the (nnnn) form of oTSi (0.009Å).

The ipso α angle at C1 is smaller than 120° for all the conformers studied. However, the deformation of the phenyl ring is greater in the case of oTMe, where the values of α range from 117.1°, for the (xxxx) isomer, to 116.9° for the (nnnn) form. In oTSi the deviation of α from 120° is less and varies from 119.2°, for the (xxxx) form, to 118.2° for the (nnnn) isomer.

The mean carbon-carbon distance in the ring is 1.403Å and 1.401Å in all the conformers of oTMe and of oTSi, respectively. These distances do not differ substantially and are longer than observed in the calculated structure of TPMe and TPSi and the related structures determined by X-ray.

The mean distance between the central carbon and the carbon C1 in oTMe conformers is 1.545Å. In this case, the shortest X-C distance of 1.543Å is observed in the (nnnn) conformer. However, for oTSi this conformer has the longest Si-C distance (1.896Å) of all forms, while for the (xxxx) isomer this bond lengths is 1.877Å and is the shortest of all. The calculated distance for oTMe is longer than for TPMe, but

Table 32. MM3 data for oTMe.

param.	(xxxx)	(xxnx)	(xxnn)	(xnxn)	(xnnn)	(nnnn)
X-C (Å)	1.546	1.546	1.545	1.547	1.545	1.543
Me-C (Å)	1.513	1.513	1.513	1.512	1.513	1.514
θ_1 (°)	104.3	103.5	100.6	102.0	100.7	99.7
θ_2 (°)	112.1	111.7	113.6	111.7	111.6	114.6
α (°)	117.1	117.0	116.9	116.9	116.8	116.9
ψ (°)	37.8	37.2	23.4	32.1	21.8	17.9
φ (°)	52.2	52.8	66.6	57.9	68.2	72.1
E_s (kcal/mol)	47.1	51.3	52.5	55.3	56.2	56.1
Symm.	S_4	C_1	C_2	C_1	C_1	S_4

Table 33. MM3 data for oTSi.

param.	(xxxx)	(xxnx)	(xxnn)	(xnxn)	(xnnn)	(nnnn)
X-C (Å)	1.877	1.880	1.880	1.882	1.881	1.896
Me-C (Å)	1.512	1.511	1.511	1.511	1.510	1.508
θ_1 (°)	106.3	105.7	102.7	104.3	102.2	104.8
θ_2 (°)	111.1	110.8	113.2	109.4	110.4	111.9
α (°)	119.2	118.8	118.8	118.8	118.7	118.2
ψ (°)	39.8	41.2	21.1	41.4	29.0	35.5
φ (°)	50.2	48.8	68.1	48.6	61.0	54.5
E_s (kcal/mol)	29.0	31.4	32.9	33.8	35.9	38.9
Symm.	S_4	C_1	C_2	C_1	C_1	S_4

for oTSi the reverse relationship exists.

In all conformers of oTMe and oTSi, the methyl groups are bent away from the central atom by at least 4-5° from the ideal value of 120°. In the system X-C-C-Me, the exocyclic angles are more, and the endocyclic angles less, than 120°.

Deformation of the central bond valence angles follows a characteristic pattern for most conformers and seems larger for oTMe than for oTSi. The θ_1 angles are smaller than the θ_2 angles in all cases. The valence angles θ_1 for the (nnnn) isomers of oTMe and oTSi are slightly smaller than the corresponding angles for the (xxxx) conformers. This is in disagreement with the observations of Mislow et al. that isomers of the highest energy (nnnn), adopt the exact reverse central angles with respect to (xxxx) isomers.

The tendency of the aryl rings to avoid positions corresponding to the most severe interactions between the adjacent methyl groups influences also the rotation angles of the aryl rings. These angles are generally smaller in the case of the (nnnn) conformers.

There exist only two X-ray structure determinations of the <u>ortho</u>-substituted derivatives of the tetraphenyls. Both compounds, tetra(o-tolyl)germanium and tetra(o-tolyl)tin, as well as tetra(m-tolyl)tin, have the more stable (xxxx) conformation of S_4 symmetry (or pseudo-S_4 in the case of tetra(o-tolyl)germanium) in crystals.

3.7. Summary

The previous crystallographic data on the tetraaryl derivatives of Group IV have shown that the molecular S_4 symmetry is preferred in crystals. However, earlier structure determinations of the tetraphenyl derivatives, obtained by different authors, contain discrepancies and require more accurate structural analysis. Therefore the structures of the complete series of the tetraphenyl derivatives (with the exception of TPMe, where a structure of very high standard was already available) were carefully redetermined under standardized conditions to produce a consistent set of structural parameters. The structures of TPMe, TPSi, and their o-tolyl derivatives were then further examined with molecular mechanics calculations.

The present crystallographic results provide more precise structural parameters (eg. bond lengths, angles) and allow for detailed analyses of these structures. The structures now display rational and understandable trends in their fine details. First, the well-known tendency of tetraphenyl molecules to retain S_4 symmetry has been confirmed. Second, the general trend in the distortion of the tetrahedral bond configuration at the central atom has also been confirmed; it can be described by a parabolic relationship between the valence angles and central atom-carbon distances. In addition, the thermal motion of the molecules in the crystals has been analyzed and described.

As part of a continued interest in tetraaryl compounds, the structures of some Group I tetraphenylborates have been determined by X-ray crystallography (Appendix 3). Attempts are continuing to obtain crystals of the corresponding tetraphenylaluminates.

The results of molecular mechanics calculations are, in general, consistent with the crystallographic data and confirm the molecular symmetry S_4 for all the tetraphenyls calculated, except for the tetraphenylmethane molecule, which has D_{2d} symmetry in the ground state. These results are in agreement with the previous empirical force field calculations but they indicate that in the present application this technique has been pushed to its limit.

MM3 calculations are restricted to an examination of a single molecule, uninfluenced by any neighbours. Any realistic extension of the molecular mechanics technique to crystals must simulate the crystal field by taking account of additional molecules placed according to the characteristics of the unit cell[146]. This kind of calculation, when performed for TPMe and TPSi, could provide additional evidence of the influence of the crystal packing on the symmetry of the molecule.

APPENDICES

Appendix 1

Fractional Atomic Positional Parameters and Equivalent Isotropic Temperature Factors ($Å^2$) for $2N_3P_3Az_6 \cdot C_6H_6$; Data Set I; (e.s.d.s in parentheses).

Atom	x/a	y/b	z/c	U_{eq}
P	0.28421(3)	0.24869(3)	0.05368(3)	0.0181
N1	0.1432 (0)	0.3312 (1)	0.1076 (1)	0.0219
N11	0.2815 (1)	0.2312 (1)	-0.1046 (1)	0.0268
C111	0.3720 (1)	0.1185 (1)	-0.1620 (1)	0.0378
C112	0.2259 (1)	0.1167 (1)	-0.1271 (1)	0.0407
N12	0.4017 (1)	0.3494 (1)	0.0247 (1)	0.0315
C121	0.4857 (1)	0.3401 (2)	0.1290 (2)	0.0510
C122	0.5448 (1)	0.2878 (1)	0.0036 (2)	0.0492
C9	0.5716 (1)	0.5502 (1)	0.3778 (1)	0.0434

Hydrogen Atom Positional Parameters for $2N_3P_3Az_6 \cdot C_6H_6$; Data Set I.

Atom	x/a	y/b	z/c	U_{iso}
H1	0.415 (1)	0.146 (1)	-0.261 (1)	0.067 (1)
H2	0.433 (1)	0.052 (1)	-0.100 (1)	0.056 (1)
H3	0.190 (1)	0.052 (1)	-0.045 (1)	0.057 (1)
H4	0.176 (1)	0.143 (1)	-0.197 (1)	0.065 (1)
H5	0.502 (1)	0.430 (1)	0.142 (1)	0.060 (1)
H6	0.468 (1)	0.279 (1)	0.208 (1)	0.055 (1)
H7	0.608 (1)	0.338 (1)	-0.062 (1)	0.063 (1)
H8	0.569 (1)	0.185 (1)	0.008 (1)	0.051 (1)
H9	0.617 (1)	0.587 (1)	0.295 (1)	0.058 (1)

Anisotropic Temperature Factors (Å^2) for $2N_3P_3Az_6 \cdot C_6H_6$; Data Set I; (e.s.d.s in parentheses).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P	0.0169 (1)	0.0189 (1)	0.0184 (1)	-0.0016 (1)	-0.0023 (1)	-0.0042(1)
N1	0.0209 (4)	0.0206 (4)	0.0215 (4)	-0.0008 (3)	-0.0015 (3)	-0.0012(3)
N11	0.0297 (5)	0.0293 (5)	0.0197 (4)	-0.0038 (3)	-0.0032 (3)	-0.0012(4)
C111	0.0399 (7)	0.0433 (7)	0.0288 (6)	-0.0155 (5)	0.0001 (5)	0.0010(6)
C112	0.0425 (7)	0.0516 (8)	0.0354 (6)	-0.0201 (6)	-0.0069 (6)	-0.0123(6)
N12	0.0229 (4)	0.0285 (5)	0.0429 (6)	0.0002 (4)	-0.0046 (4)	-0.0102(4)
C121	0.0407 (7)	0.0525 (8)	0.0708 (9)	-0.0053 (7)	-0.0253 (7)	-0.0232(6)
C122	0.0204 (5)	0.0448 (8)	0.0781(10)	0.0009 (7)	-0.0035 (6)	-0.0091(5)
C9	0.0431 (7)	0.0430 (7)	0.0351 (6)	0.0027 (6)	0.0039 (6)	-0.0032(6)

Fractional Atomic Positional Parameters and Equivalent Isotropic Temperature Factors (Å^2) for $2N_3P_3Az_6 \cdot C_6H_6$; Data Set II (hex.); (e.s.d.s in parentheses).

Atom	x/a	y/b	z/c	B_{eq}
P	0.7553(1)	0.2780(1)	0.0289(1)	1.22(1)
N1	0.6155(1)	0.1959(1)	0.0274(1)	1.51(2)
N11	0.8124(1)	0.2380(1)	-0.3070(5)	1.86(2)
C111	0.9293(1)	0.3239(1)	-0.0572(1)	2.60(4)
C112	0.8207(1)	0.2881(1)	-0.0949(1)	2.87(4)
N12	0.8[illegible]98(1)	0.2423(1)	0.0921(1)	2.16(3)
C121	0.8339(2)	0.3113(2)	0.1519(1)	3.54(5)
C122	0.9329(1)	0.3241(1)	0.1123(1)	3.47(5)
C9	0.9281(1)	0.0503(1)	0.0001(1)	3.00(4)

Hydrogen Atom Positional Parameters for $2N_3P_3Az_6 \cdot C_6H_6$; Data Set II (hex.).

Atom	x/a	y/b	z/c	B_{iso}
H1	0.969(2)	0.403(2)	-0.038(1)	3.5(4)
H2	0.980(2)	0.291(2)	-0.068(1)	4.0(5)
H3	0.795(2)	0.342(2)	-0.101(1)	4.1(5)
H4	0.802(2)	0.231(2)	-0.127(1)	3.4(4)
H5	0.823(2)	0.376(2)	0.151(1)	3.4(4)
H6	0.817(2)	0.268(2)	0.190(1)	4.4(5)
H7	0.980(2)	0.401(2)	0.089(1)	4.5(5)
H8	0.979(2)	0.294(2)	0.126(1)	5.1(6)
H9	0.884(2)	0.090(2)	0.002(1)	3.9(4)

Anisotropic Temperature Factors (Å^2) for $2N_3P_3Az_6 \cdot C_6H_6$; Data Set II; (hex.) (e.s.d.s in parentheses).

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
P	0.0134(1)	0.0137(1)	0.0201(1)	0.0076(1)	-0.0016(1)	-0.0004(1)
N1	0.0145(3)	0.0137(3)	0.0291(4)	0.0070(2)	-0.0003(3)	0.0005(3)
N11	0.0201(3)	0.0217(3)	0.0309(4)	0.0119(3)	0.0032(3)	-0.0034(3)
C111	0.0218(4)	0.0348(5)	0.0406(6)	0.0130(4)	0.0089(4)	-0.0024(5)
C112	0.0353(6)	0.0501(7)	0.0266(5)	0.0236(6)	0.0047(4)	-0.0014(5)
N12	0.0254(4)	0.0246(4)	0.0321(5)	0.0125(3)	-0.0106(3)	0.0021(3)
C121	0.0573(9)	0.0466(8)	0.0289(6)	0.0246(7	-0.0182(6)	0.0032(5)
C122	0.0307(5)	0.0368(6)	0.057(1)	0.114(5)	-0.0245(6)	0.0027(6)
C9	0.0293(5)	0.0309(5)	0.059(1)	0.0191(4)	0.0002(5)	0.0003(5)

Interatomic Distances (Å) for $2N_3P_3Az_6 \cdot C_6H_6$

Data Set	I	II
P -N1	1.583(1)	1.588(1)
P -N1'	1.597(1)	1.598(1)
P -N11	1.665(1)	1.671(1)
P -N12	1.673(1)	1.678(1)
N11 -C111	1.474(2)	1.472(2)
N11 -C112	1.462(2)	1.464(2)
C111-C112	1.470(3)	1.473(2)
N12 -C121	1.467(3)	1.470(2)
N12 -C122	1.471(2)	1.474(2)
C121-C122	1.461(3)	1.466(3)
C9 -C9''	1.382(3)	1.386(1)
C9 -C9'''	1.382(3)	1.386(1)

Primed atoms have symmetry operations:

' - y, z, x

'' - -y+1, -z+1, -x+1

''' - -z+1, -x+1, -y+1

'''' - z, x, y

Interbond Angles (degrees) for $2N_3P_3Az_6 \cdot C_6H_6$

Data Set	I	II
N1 - P - N1'	116.7 (1)	116.8 (1)
N1 - P - N11	107.6 (1)	107.7 (1)
N1 - P - N12	108.7 (1)	108.7 (1)
N1' - P - N11	111.8 (1)	111.6 (1)
N1' - P - N12	111.3 (1)	111.3 (1)
N11 - P - N12	99.3 (1)	99.2 (1)
P - N1 - P''''	123.2 (1)	123.1 (1)
P - N11 - C111	119.1 (1)	119.2 (1)
P - N11 - C112	118.3 (1)	118.3 (1)
C111- N11 - C112	60.1 (1)	60.2 (1)
N11 - C111 - C112	59.6 (1)	59.6 (1)
N11 - C112 - C111	60.3 (1)	60.2 (1)
P - N12 - C121	118.3 (1)	118.2 (1)
P - N12 - C122	118.5 (1)	118.5 (1)
C121- N12 - C122	59.6 (1)	59.7 (1)
N12 - C121 - C122	60.3 (1)	60.3 (1)
N12 - C122 - C121	60.0 (1)	60.0 (1)
C9''- C9 - C9'''	120.0 (2)	120.0 (0)

Primed atoms have symmetry operations:

' - y, z, x

'' - -y+1, -z+1, -x+1

''' - -z+1, -x+1, -y+1

'''' - z, x, y

Multipole Population Coefficients for $2N_3P_3Az_6 \cdot C_6H_6$; Data Set II; (rh.)

atom	P_v	P_{00}	P_{11}	P_{1-1}	P_{10}	P_{20}	P_{21}	P_{2-1}	P_{22}	P_{2-2}
P1	4.86(30)	0.00(0)	0.21(9)	- 0.20(9)	0.16(10)	0.11(8)	0.11(7)	0.02(6)	0.09(7)	0.18(8)
N1	5.55(15)	0.00(0)	0.01(5)	0.02(5)	- 0.07(5)	- 0.01(4)	0.03(4)	0.06(4)	- 0.06(3)	0.02(4)
N2	5.46(14)	0.00(0)	- 0.09(5)	- 0.06(6)	- 0.13(6)	- 0.01(5)	0.03(4)	0.06(5)	0.07(5)	0.01(4)
N3	5.31(13)	0.00(0)	- 0.01(5)	0.09(7)	- 0.09(6)	- 0.11(5)	0.01(4)	0.12(5)	- 0.01(5)	- 0.03(4)
C1	4.80(17)	0.00(0)	0.03(9)	0.06(9)	0.09(9)	0.12(8)	- 0.06(7)	0.11(8)	- 0.15(9)	0.04(8)
C2	4.61(16)	0.00(0)	- 0.26(10)	0.15(10)	0.20(9)	0.26(10)	0.15(8)	- 0.07(8)	- 0.18(8)	0.02(9)
C3	4.52(15)	0.00(0)	0.04(8)	0.10(8)	0.04(8)	0.14(7)	- 0.01(6)	- 0.05(6)	- 0.19(6)	- 0.11(7)
C4	4.41(15)	0.00(0)	- 0.01(8)	0.01(9)	0.03(9)	0.02(8)	0.00(7)	0.13(8)	- 0.16(6)	0.08(7)
C9	4.41(10)	0.00(0)	0.00(14)	- 0.18(16)	0.07(6)	0.13(5)	- 0.13(9)	0.07(11)	0.00(4)	0.28(5)
H1	0.65(7)	0.00(0)	0.05(4)	- 0.02(4)	0.07(4)					
H2	0.52(8)	0.00(0)	- 0.13(4)	- 0.06(5)	0.06(5)					
H3	0.43(6)	0.00(0)	- 0.02(3)	- 0.02(4)	0.04(4)					
H4	0.52(7)	0.00(0)	0.13(4)	- 0.03(4)	0.06(4)					
H5	0.62(6)	0.00(0)	- 0.03(3)	0.03(4)	0.07(4)					
H6	0.57(6)	0.00(0)	0.06(4)	0.00(4)	0.08(4)					
H7	0.59(7)	0.00(0)	0.01(4)	- 0.11(4)	0.09(4)					
H8	0.60(6)	0.00(0)	- 0.04(3)	- 0.02(4)	0.13(4)					
H9	0.58(6)	0.00(0)	0.02(4)	0.01(4)	0.09(4)					

Multipole Population Coefficients for $2N_3P_3Az_6 \cdot C_6H_6$ (cont.); Data Set II; (rh.) (e.s.d.s in parentheses).

atom	P_{30}	P_{31}	P_{3-1}	P_{32}	P_{3-2}	P_{33}	P_{3-3}
P1	0.62(11)	0.09(6)	-0.11(6)	-0.05(6)	-0.04(6)	-0.11(6)	0.35(7)
N1	0.09(4)	0.07(4)	0.00(4)	-0.04(4)	-0.11(4)	0.10(4)	0.02(3)
N2	0.12(5)	0.00(4)	-0.10(5)	-0.16(5)	-0.16(5)	-0.03(4)	0.12(5)
N3	0.03(5)	0.02(4)	-0.16(5)	-0.07(5)	0.06(4)	-0.05(4)	0.12(5)
C1	0.50(9)	-0.04(8)	-0.21(9)	0.13(8)	0.07(8)	-0.03(8)	0.11(8)
C2	0.50(9)	-0.04(8)	-0.17(10)	0.23(8)	0.09(8)	0.25(8)	0.30(8)
C3	0.44(7)	0.09(7)	0.00(7)	0.08(6)	-0.01(7)	-0.11(7)	0.12(6)
C4	0.41(8)	-0.03(7)	-0.12(9)	0.05(7)	-0.12(7)	-0.15(7)	0.23(7)
C9	0.41(6)	-0.01(10)	-0.12(12)	0.05(5)	-0.22(5)	0.13(10)	0.01(10)

Appendix 2

Fractional Atomic Positional Parameters and Equivalent Isotropic Temperature Factors (Å^2) for $C_6H_4S_2P^+$ $AlCl_4^-$ (e.s.d.'s in parentheses).

Atom	x/a	y/b	z/c	U_{eq}
Al1	0.0326 (2)	0.1512 (1)	0.2461 (2)	0.0417
Cl1	-0.0682 (2)	0.2223 (1)	0.3679 (1)	0.0584
Cl2	0.0669 (2)	0.0783 (1)	0.3957 (1)	0.0576
Cl3	-0.1813 (2)	0.1336 (1)	0.0384 (1)	0.0573
Cl4	0.3274 (2)	0.1701 (1)	0.1893 (1)	0.0629
S1	0.3381 (2)	0.3155 (1)	0.2365 (2)	0.0542
S2	0.6778 (2)	0.3694 (1)	0.0898 (2)	0.0658
P1	0.5535 (2)	0.2917 (1)	0.1103 (2)	0.0619
C1	0.3764 (6)	0.3886 (1)	0.2552 (4)	0.0443
C2	0.5326 (6)	0.4128 (1)	0.1882 (4)	0.0482
C3	0.5668 (7)	0.4724 (2)	0.1989 (5)	0.0689
C4	0.4413 (9)	0.5041 (2)	0.2754 (6)	0.0777
C5	0.2869 (8)	0.4794 (2)	0.3406 (6)	0.0747
C6	0.2518 (7)	0.4218 (2)	0.3334 (5)	0.0577

Hydrogen Atom Positional Parameters for $C_6H_4S_2P^+$ $AlCl_4^-$

Atom	x/a	y/b	z/c	U_{iso}
H3	0.679 (1)	0.489 (0)	0.151 (1)	0.074 (3)
H4	0.483 (1)	0.545 (0)	0.277 (1)	0.087 (3)
H5	0.193 (1)	0.502 (0)	0.398 (1)	0.083 (3)
H6	0.138 (1)	0.400 (0)	0.386 (1)	0.083 (3)

Anisotropic Temperature Factors ($Å^2$) for $C_6H_4S_2P^+$ $AlCl_4^-$ (e.s.d.'s in parentheses).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Al1	0.0400(6)	0.0433(7)	0.0412(7)	-0.0057(6)	0.0055(5)	0.0023(5)
Cl1	0.0645(7)	0.0489(7)	0.0643(7)	-0.0108(6)	0.0183(6)	0.0081(5)
Cl2	0.0668(7)	0.0526(7)	0.0523(6)	0.0036(5)	0.0076(5)	0.0126(6)
Cl3	0.0533(6)	0.0681(8)	0.0461(6)	-0.0018(6)	-0.0028(5)	-0.0056(6)
Cl4	0.0452(6)	0.0636(8)	0.0823(8)	-0.0111(6)	0.0183(6)	-0.0054(5)
S1	0.0545(7)	0.0507(7)	0.0579(7)	0.0050(6)	0.0115(5)	-0.0100(6)
S2	0.0619(8)	0.0818(10)	0.0576(7)	0.0059(7)	0.0214(6)	-0.0125(7)
P1	0.0662(8)	0.0631(9)	0.0569(8)	-0.0044(7)	0.0123(6)	-0.0022(7)
C1	0.048 (2)	0.045 (2)	0.039 (2)	0.007 (2)	0.002 (2)	0.000 (2)
C2	0.054 (2)	0.052 (2)	0.034 (2)	0.008 (2)	-0.003 (2)	-0.012 (2)
C3	0.077 (3)	0.063 (3)	0.060 (3)	0.019 (2)	-0.008 (2)	-0.025 (2)
C4	0.115 (3)	0.040 (2)	0.067 (3)	0.004 (2)	-0.010 (3)	-0.001 (3)
C5	0.093 (3)	0.068 (3)	0.060 (3)	0.003 (2)	0.007 (2)	0.018 (3)
C6	0.066 (2)	0.058 (3)	0.048 (2)	0.006 (2)	0.007 (2)	0.004 (2)

Interatomic Distances (Å) for $C_6H_4S_2P^+\ AlCl_4^-$

S1	-P1	2.017 (2)	Al1	-Cl1	2.134 (2)
S1	-C1	1.728 (4)	Al1	-Cl2	2.127 (2)
S2	-P1	2.010 (2)	Al1	-Cl3	2.118 (2)
S2	-C2	1.720 (5)	Al1	-Cl4	2.133 (2)
C1	-C2	1.389 (6)			
C1	-C6	1.391 (6)			
C2	-C3	1.409 (7)			
C3	-C4	1.366 (8)			
C4	-C5	1.375 (8)			
C5	-C6	1.364 (7)			

Interbond Angles (degrees) for $C_6H_4S_2P^+\ AlCl_4^-$

P1	-S1	-C1	102.6 (2)	Cl1	-Al1	-Cl2	109.3 (1)
P1	-S2	-C2	102.5 (2)	Cl1	-Al1	-Cl3	110.6 (1)
S1	-P1	-S2	97.9 (1)	Cl1	-Al1	-Cl4	109.2 (1)
S1	-C1	-C2	118.0 (3)	Cl2	-Al1	-Cl3	110.1 (1)
S1	-C1	-C6	120.5 (3)	Cl2	-Al1	-Cl4	107.7 (1)
C2	-C1	-C6	121.4 (4)	Cl3	-Al1	-Cl4	109.9 (1)
S2	-C2	-C1	119.0 (3)				
S2	-C2	-C3	121.2 (4)				
C1	-C2	-C3	119.8 (4)				
C2	-C3	-C4	117.6 (5)				
C3	-C4	-C5	121.9 (5)				
C4	-C5	-C6	121.7 (5)				
C1	-C6	-C5	117.6 (5)				

Fractional Atomic Positional Parameters and Equivalent Isotropic Temperature Factors ($Å^2$) for $C_{13}H_{11}PS_2$ (e.s.d.s in parentheses).

Atom	x/a	y/b	z/c	U_{eq}
P1	0.8654 (1)	0.2956 (1)	0.4908 (1)	0.0410
S1	0.7938 (1)	0.1001 (1)	0.5579 (1)	0.0465
S2	0.7567 (1)	0.5391 (1)	0.4501 (1)	0.0409
C1	0.7267 (2)	0.2988 (4)	0.5898 (2)	0.0361
C2	0.7081 (2)	0.4938 (4)	0.5394 (2)	0.0337
C3	0.6445 (2)	0.6421 (5)	0.5533 (2)	0.0387
C4	0.6009 (2)	0.6010 (5)	0.6184 (2)	0.0429
C13	0.5316 (3)	0.7599 (6)	0.6332 (3)	0.0618
C5	0.6230 (2)	0.4079 (6)	0.6699 (2)	0.0485
C6	0.6855 (2)	0.2596 (5)	0.6564 (2)	0.0444
C7	0.9696 (2)	0.3999 (4)	0.6000 (2)	0.0339
C8	0.9732 (2)	0.5984 (4)	0.6451 (2)	0.0418
C9	1.0569 (2)	0.6561 (5)	0.7282 (2)	0.0471
C10	1.1384 (2)	0.5196 (6)	0.7680 (2)	0.0481
C11	1.1362 (2)	0.3265 (6)	0.7232 (2)	0.0503
C12	1.0535 (2)	0.2674 (5)	0.6397 (2)	0.0454

Hydrogen Atom Positional Parameters for $C_{13}H_{11}PS_2$

Atom	x/a	y/b	z/c	U_{iso}
H3	0.632 (2)	0.785 (2)	0.514 (2)	0.044 (2)
H131	0.511 (2)	0.698 (2)	0.685 (2)	0.058 (2)
H132	0.470 (2)	0.786 (2)	0.568 (2)	0.059 (2)
H133	0.569 (2)	0.906 (2)	0.660 (2)	0.054 (2)
H134	0.464 (2)	0.711 (2)	0.616 (2)	0.045 (2)
H135	0.564 (2)	0.810 (2)	0.710 (2)	0.049 (2)
H136	0.527 (2)	0.907 (2)	0.590 (2)	0.046 (2)
H5	0.595 (2)	0.371 (2)	0.716 (2)	0.065 (2)
H6	0.700 (2)	0.115 (2)	0.696 (2)	0.053 (2)
H8	0.916 (2)	0.701 (2)	0.613 (2)	0.060 (2)
H9	1.062 (2)	0.807 (2)	0.762 (2)	0.061 (2)
H10	1.199 (2)	0.563 (2)	0.832 (2)	0.057 (2)
H11	1.195 (2)	0.222 (2)	0.749 (2)	0.078 (2)
H12	1.053 (2)	0.118 (2)	0.610 (2)	0.060 (2)

Anisotropic Temperature Factors (Å^2) for $C_{13}H_{11}PS_2$ (e.s.d.s in parentheses).

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
P1	0.0445(4)	0.0413(4)	0.0390(4)	-0.0068(3)	0.0192(4)	0.0007(3)
S1	0.0487(5)	0.0296(4)	0.0599(5)	-0.0010(3)	0.0213(4)	-0.0021(3)
S2	0.0424(4)	0.0450(4)	0.0351(4)	0.0063(3)	0.0159(3)	0.0031(3)
C1	0.0298(12)	0.0338(12)	0.0412(13)	-0.0013(11)	0.0112(11)	-0.0041(10)
C2	0.0285(12)	0.0368(12)	0.0321(12)	-0.0011(10)	0.0090(10)	-0.0043(10)
C3	0.0301(12)	0.0374(12)	0.0430(13)	-0.0039(11)	0.0097(11)	-0.0049(11)
C4	0.0313(13)	0.0488(14)	0.0486(14)	-0.0139(12)	0.0167(11)	-0.0085(11)
C13	0.0459(14)	0.0672(16)	0.0831(16)	-0.0196(14)	0.0377(13)	-0.0074(13)
C5	0.0388(13)	0.0669(16)	0.0439(13)	-0.0033(13)	0.0213(11)	-0.0139(13)
C6	0.0377(13)	0.0486(14)	0.0443(13)	0.0058(12)	0.0145(12)	-0.0094(12)
C7	0.0355(12)	0.0359(12)	0.0353(12)	0.0025(10)	0.0198(10)	0.0022(10)
C8	0.0419(13)	0.0373(13)	0.0483(13)	-0.0013(11)	0.0210(11)	0.0028(11)
C9	0.0419(13)	0.0492(13)	0.0508(14)	-0.0073(12)	0.0198(12)	-0.0075(12)
C10	0.0369(13)	0.0695(15)	0.0367(13)	0.0016(12)	0.0141(11)	-0.0069(13)
C11	0.0382(13)	0.0685(15)	0.0444(13)	0.0128(13)	0.0175(11)	0.0123(13)
C12	0.0470(13)	0.0450(13)	0.0467(13)	0.0027(12)	0.0219(12)	0.0091(12)

Interatomic Distances (Å) for $C_{13}H_{11}PS_2$

P1	-S1	2.112 (1)
P1	-S2	2.104 (1)
P1	-C7	1.821 (3)
S1	-C1	1.767 (3)
S2	-C2	1.767 (3)
C1	-C2	1.394 (5)
C1	-C6	1.376 (5)
C2	-C3	1.391 (5)
C3	-C4	1.385 (5)
C4	-C13	1.503 (6)
C4	-C5	1.391 (5)
C5	-C6	1.376 (5)
C7	-C8	1.398 (5)
C7	-C12	1.395 (5)
C8	-C9	1.375 (5)
C9	-C10	1.385 (5)
C10	-C11	1.371 (5)
C11	-C12	1.374 (5)

Interbond Angles (degrees) for $C_{13}H_{11}PS_2$

S1	-P1	-S2	94.8 (1)
S1	-P1	-C7	100.9 (1)
S2	-P1	-C7	104.7 (1)
P1	-S1	-C1	99.4 (1)
P1	-S2	-C2	99.5 (1)
S1	-C1	-C2	118.5 (3)
S1	-C1	-C6	121.8 (3)
C2	-C1	-C6	119.5 (3)
S2	-C2	-C1	119.3 (2)
S2	-C2	-C3	120.6 (2)
C1	-C2	-C3	119.8 (3)
C2	-C3	-C4	120.9 (3)
C3	-C4	-C13	121.2 (3)
C3	-C4	-C5	118.2 (3)
C13	-C4	-C5	120.7 (3)
C4	-C5	-C6	121.4 (4)
C1	-C6	-C5	120.2 (3)
P1	-C7	-C8	126.2 (3)
P1	-C7	-C12	115.5 (2)
C8	-C7	-C12	118.3 (3)
C7	-C8	-C9	120.0 (3)
C8	-C9	-C10	120.7 (3)
C9	-C10	-C11	119.6 (4)
C10	-C11	-C12	120.3 (4)
C7	-C12	-C11	121.0 (3)

Appendix 3

Other Structures Solved

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1)

1,2,3,4-dibenzo-trans-6,7-dibromo-1,3-cyclooctadiene

$C_{16}H_{14}Br_2$	MW = 366.1	t = 18 °C
orthorhombic	$C222_1$ (No. 20)	noncentrosymmetric
a = 10.913(3) Å	b = 9.179(3) Å	c = 27.906(3) Å
$\alpha = 90°$	$\beta = 90°$	$\gamma = 90°$
F(000) = 1440 e	$\mu = 61.20\ cm^{-1}$	$V = 2795.2\ Å^3$
Z = 8	$d_c = 1.740\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 4396$	$N_{un} = 1985$	$N_{ob} = 828$
obs. if $I > 2\sigma(I)$	$N_v = 178$	$N_{ob}/N_v = 5.6$
$2° < \theta < 25°$	R = 0.0357	$R_w = 0.0392$

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2)

2p-bromophenyl-1,3-oxathiolanesulphuroxide

$C_9H_8O_2SBr$	MW = 260.1	t = 18 °C
monoclinic	$P2_1$ (No. 4)	noncentrosymmetric
a = 5.903(2) Å	b = 7.418(3) Å	c = 11.240(3) Å
$\alpha = 90°$	$\beta = 97.87(3)°$	$\gamma = 90°$
F(000) = 258 e	$\mu = 43.40\ cm^{-1}$	$V = 487.6\ Å^3$
Z = 2	$d_c = 1.772\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 2126$	$N_{un} = 1064$	$N_{ob} = 911$
obs. if $I > 3\sigma(I)$	$N_v = 126$	$N_{ob}/N_v = 7.2$
$2° < \theta < 25°$	R = 0.0429	$R_w = 0.0468$

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3)

$C_{72}H_{132}Br_4P_2Pt_2$

$C_{72}H_{132}Br_4P_2Pt_2$	MW = 1769.4	t = 18 °C
orthorhombic	Pbca (No. 61)	centrosymmetric
a = 9.532(2) Å	b = 16.042(3) Å	c = 26.537(4) Å
α = 90°	β = 90°	γ = 90°
F(000) = 3560 e	μ = 110.03 cm^{-1}	V = 4057.8 $Å^3$
Z = 4	d_c = 2.896 g/cm^3	λ = 0.70926 Å
N_{me} = 3927	N_{un} = 2815	N_{ob} = 1563
obs. if I> 3σ(I)	N_v = 196	N_{ob}/N_v = 8.0
$2^\circ<\theta<23^\circ$	R = 0.0489	R_w = 0.0545

4)

$C_{27}H_{30}N_3OPPt$

$C_{27}H_{30}N_3OPPt$	MW = 638.5	t = 18 °C
monoclinic	$P2_1/c$ (No. 14)	centrosymmetric
a = 12.601(1) Å	b = 10.274(1) Å	c = 20.066(2) Å
α = 90°	β = 106.55(1)°	γ = 90°
F(000) = 1256 e	μ = 60.15 cm^{-1}	V = 2490.2 $Å^3$
Z = 4	d_c = 1.703 g/cm^3	λ = 0.70926 Å
N_{me} = 4452	N_{un} = 4368	N_{ob} = 2896
obs. if I> 3σ(I)	N_v = 331	N_{ob}/N_v = 8.7
$2^\circ<\theta<25^\circ$	R = 0.0374	R_w = 0.0387

5)

$C_{12}H_{17}NO_3$

$C_{12}H_{17}NO_3$	MW = 221.3	t = 18 °C
monoclinic	$P2_1/c$ (No. 14)	centrosymmetric
a = 7.013(2) Å	b = 18.976(3) Å	c = 9.779(4) Å
α = 90°	β = 108.8(2)°	γ = 90°
F(000) = 472 e	μ = 0.92 cm^{-1}	V = 1232.0 $Å^3$
Z = 4	d_c = 1.194 g/cm^3	λ = 0.70926 Å
N_{me} = 2016	N_{un} = 1704	N_{ob} = 911
obs. if I> 3σ(I)	N_v = 166	N_{ob}/N_v = 5.5
$2°<\theta<23°$	R = 0.0635	R_w = 0.0690

6)

2-methyl-1-phenylsulfonyl-4-penten-1-one

$C_{18}H_{18}O_3S$	MW = 314.4	t = 18 °C
monoclinic	$P2_1/c$ (No. 14)	centrosymmetric
a = 10.528(2) Å	b = 13.721(3) Å	c = 12.256(2) Å
α = 90°	β = 112.42(1)°	γ = 90°
F(000) = 664 e	μ = 2.07 cm^{-1}	V = 1636.6 $Å^3$
Z = 4	d_c = 1.276 g/cm^3	λ = 0.70926 Å
N_{me} = 3029	N_{un} = 2272	N_{ob} = 882
obs. if I> 2σ(I)	N_v = 243(disorder)	N_{ob}/N_v = 3.6
$2°<\theta<23°$	R = 0.0432	R_w = 0.0440

7) 2-(4-methylphenyl)sulfonyl-1-phenyl-1-(allyloxy)-1,4-pentadiene

$C_{21}H_{22}O_3S$	MW = 354.5	t = 18 °C
monoclinic	C2/c (No. 15)	centrosymmetric
a = 18.759(3) Å	b = 8.036(3) Å	c = 25.533(3) Å
α = 90°	β = 95.25(1)°	γ = 90°
F(000) = 1504 e	μ = 1.75 cm^{-1}	V = 3848.2 $Å^3$
Z = 4	d_c = 1.224 g/cm^3	λ = 0.70926 Å
N_{me} = 3597	N_{un} = 2667	N_{ob} = 1485
obs. if I> 3σ(I)	N_v = 326(disorder)	N_{ob}/N_v = 4.6
$2° < \theta < 23°$	R = 0.0508	R_w = 0.0545

8)

2-(4-methylphenyl)sulfonyl-1-phenyl-4-penten-1-one

$C_{18}H_{18}O_3S$	MW = 314.4	t = 18 °C
monoclinic	Pn (No. 7)	noncentrosymmetric
a = 5.357(3) Å	b = 8.824(3) Å	c = 17.349(3) Å
α = 90°	β = 91.47(3)°	γ = 90°
F(000) = 332 e	μ = 1.97 cm^{-1}	V = 819.8 $Å^3$
Z = 2	d_c = 1.274 g/cm^3	λ = 0.70926 Å
N_{me} = 1449	N_{un} = 1182	N_{ob} = 644
obs. if I> 2σ(I)	N_v = 234(disorder)	N_{ob}/N_v = 2.8
$2° < \theta < 23°$	R = 0.0645	R_w = 0.0651

9) R,S(4l,5n)-5-acetoxy-4-methyl-5-phenyl-4-phenylsulfonyl-1-hexene

$C_{21}H_{24}O_4S$	MW = 372.5	t = 18 °C
orthorhombic	$P2_12_12_1$ (No. 19)	noncentrosymmetric
a = 9.18[illegible](2) Å	b = 12.320(4) Å	c = 17.144(3) Å
$\alpha = 90^\circ$	$\beta = 90^\circ$	$\gamma = 90^\circ$
F(000) = 792 e	$\mu = 1.80\ cm^{-1}$	$V = 1939.2\ Å^3$
Z = 4	$d_c = 1.276\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 1969$	$N_{un} = 1855$	$N_{ob} = 1282$
obs. if $I > 2\sigma(I)$	$N_v = 294$ (disorder)	$N_{ob}/N_v = 4.4$
$2^\circ < \theta < 23^\circ$	R = 0.0531	$R_w = 0.0571$

10) 2,2'-bis[2N-(1,1,3,3-tetramethylguanidino)]biphenyl dipicrate

$C_{21}H_{34}N_6 \cdot 2C_6H_2N_3O_7$	MW = 354.5	t = 18 °C
tetragonal	$P4_12_12$ (No. 92)	noncentrosymmetric
a = 12.372([illegible]) Å	b = 12.372(6) Å	c = 25.370(3) Å
$\alpha = 90^\circ$	$\beta = 90^\circ$	$\gamma = 90^\circ$
F(000) = 1752 e	$\mu = 1.06\ cm^{-1}$	$V = 3882.9\ Å^3$
Z = 4	$d_c = 1.435\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 3123$	$N_{un} = 2694$	$N_{ob} = 1083$
obs. if $I > 3\sigma(I)$	$N_v = 306$ (disorder)	$N_{ob}/N_v = 3.5$
$2^\circ < \theta < 23^\circ$	R = 0.0684	$R_w = 0.0684$

11)

$C_{13}H_{21}N_3$

$C_{13}H_{21}N_3$	MW = 219.3	t = 18 °C
monoclinic	$P2_1/c$ (No. 14)	centrosymmetric
a = 11.912(2) Å	b = 8.927(1) Å	c = 13.506(3) Å
α = 90°	β = 112.71(1)°	γ = 90°
F(000) = 480 e	μ = 0.72 cm^{-1}	V = 1324.9 $Å^3$
Z = 4	d_c = 1.099 g/cm^3	λ = 0.70926 Å
N_{me} = 2733	N_{un} = 1843	N_{ob} = 756
obs. if I> $3\sigma(I)$	N_v = 185(disorder)	N_{ob}/N_v = 4.1
$2° < \theta < 23°$	R = 0.0684	R_w = 0.0715

12)

$C_{28}H_{29}Cl_2N_3O_9$

$C_{28}H_{29}Cl_2N_3O_9$	MW = 622.4	t = 18 °C
monoclinic	$P2_1/c$ (No. 14)	centrosymmetric
a = 14.539(3) Å	b = 13.685(3) Å	c = 23.579(7) Å
α = 90°	β = 140.38(2)°	γ = 90°
F(000) = 1296 e	μ = 2.69 cm^{-1}	V = 2991.0 $Å^3$
Z = 4	d_c = 1.382 g/cm^3	λ = 0.70926 Å
N_{me} = 3016	N_{un} = 2774	N_{ob} = 1595
obs. if I> $3\sigma(I)$	N_v = 526(disorder)	N_{ob}/N_v = 3.0
$2° < \theta < 23°$	R = 0.0636	R_w = 0.0671

13)

triphenylantimony dichloride

$C_{18}H_{15}SbCl_2$	MW = 423.9	t = 18 °C
orthorhombic	$P2_12_12_1$ (No. 19)	noncentrosymmetric
a = 9.163(8) Å	b = 17.085(8) Å	c = 22.173(9) Å
$\alpha = 90°$	$\beta = 90°$	$\gamma = 90°$
F(000) = 1664 e	$\mu = 19.09\ cm^{-1}$	V = 3470.9 $Å^3$
Z = 8	$d_c = 1.622\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 3574$	$N_{un} = 3334$	$N_{ob} = 2481$
obs. if $I > 3\sigma(I)$	$N_v = 342$	$N_{ob}/N_v = 7.3$
$2° < \theta < 23°$	R = 0.0371	$R_w = 0.0384$

14)

bis(di-isopropylaminc)thiophosphoryl chloride

$C_{12}H_{28}ClN_2PS$	MW = 298.8	t = 18 °C
monoclinic	$P2_1/n$ (No. 14)	centrosymmetric
a = 9.740(1) Å	b = 14.206(1) Å	c = 12.693(1) Å
$\alpha = 90°$	$\beta = 100.33(2)°$	$\gamma = 90°$
F(000) = 648 e	$\mu = 4.16\ cm^{-1}$	V = 1727.8 $Å^3$
Z = 4	$d_c = 1.149\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 3197$	$N_{un} = 2747$	$N_{ob} = 1365$
obs. if $I > 3\sigma(I)$	$N_v = 207$	$N_{ob}/N_v = 6.6$
$2° < \theta < 23°$	R = 0.0537	$R_w = 0.0595$

15)

bis(di-isopropylamino)selenophosphoryl chloride

$C_{12}H_{28}ClN_2PSe$	MW = 345.7	t = 18 °C
monoclinic	$P2_1/n$ (No. 14)	centrosymmetric
a = 9.723(2) Å	b = 14.203(2) Å	c = 12.826(2) Å
$\alpha = 90°$	$\beta = 99.73(2)°$	$\gamma = 90°$
F(000) = 720 e	$\mu = 23.57\ cm^{-1}$	V = 1745.7 $Å^3$
Z = 4	$d_c = 1.315\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 3228$	$N_{un} = 3004$	$N_{ob} = 1640$
obs. if $I > 3\sigma(I)$	$N_v = 179$(disorder)	$N_{ob}/N_v = 9.2$
$2° < \theta < 23°$	R = 0.0633	$R_w = 0.0703$

16)

bis(di-isopropylamino)phospholiumheptachloro-dialuminate

$C_{12}H_{28}N_2P.Al_2Cl_7$	MW = 533.5	t = 18 °C
monoclinic	$P2_1/n$ (No. 14)	centrosymmetric
a = 12.732(7) Å	b = 12.285(9) Å	c = 17.492(7) Å
$\alpha = 90°$	$\beta = 103.92(4)°$	$\gamma = 90°$
F(000) = 1096 e	$\mu = 8.79\ cm^{-1}$	V = 2655.6 $Å^3$
Z = 4	$d_c = 1.334\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 4032$	$N_{un} = 3685$	$N_{ob} = 1427$
obs. if $I > 3\sigma(I)$	$N_v = 291$	$N_{ob}/N_v = 4.9$
$2° < \theta < 23°$	R = 0.0530	$R_w = 0.0562$

17)

diphenylamine-trichloroaluminium

$C_{12}H_{11}AlCl_3N$	MW = 302.6	t = 18 °C
monoclinic	C2/c (No. 15)	centrosymmetric
a = 15.072(3) Å	b = 13.398(3) Å	c = 14.603(3) Å
$\alpha = 90°$	$\beta = 102.95(2)°$	$\gamma = 90°$
F(000) = 1232 e	$\mu = 6.78\ cm^{-1}$	V = 2873.7 $Å^3$
Z = 8	$d_c = 1.399\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 2181$	$N_{un} = 1985$	$N_{ob} = 1104$
obs. if I> 3σ(I)	$N_v = 166$	$N_{ob}/N_v = 6.7$
$2° < \theta < 23°$	R = 0.0455	$R_w = 0.0468$

18)

N-methylpropane-1,3-diammonium hexachlorostannate(IV)

$C_4N_2H_{12}SnCl_6$	MW = 419.5	t = 18 °C
monoclinic	$P2_1/n$ (No. 14)	centrosymmetric
a = 7.205(2) Å	b = 25.806(6) Å	c = 14.880(3) Å
$\alpha = 90°$	$\beta = 89.47(2)°$	$\gamma = 90°$
F(000) = 1616 e	$\mu = 29.89\ cm^{-1}$	V = 2766.5 $Å^3$
Z = 8	$d_c = 2.014\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 6071$	$N_{un} = 4880$	$N_{ob} = 3114$
obs. if I> 2σ(I)	$N_v = 278$	$N_{ob}/N_v = 11.2$
$2° < \theta < 25°$	R = 0.0545	$R_w = 0.0555$

19)

N,N'-dimethyl-1,2-ethane-diammonium hexachlorostannate(IV)

$C_4N_2H_{14}SnCl_6$	MW = 421.5	t = 18 °C
monoclinic	$P2_1$ (No. 4)	noncentrosymmetric
a = 6.865(3) Å	b = 13.191(5) Å	c = 8.002(2) Å
$\alpha = 90°$	$\beta = 100.78(3)°$	$\gamma = 90°$
F(000) = 408 e	$\mu = 29.05\ cm^{-1}$	V = 711.8 Å
Z = 2	$d_c = 1.966\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 1760$	$N_{un} = 1434$	$N_{ob} = 1001$
obs. if $I > 2\sigma(I)$	$N_v = 138$	$N_{ob}/N_v = 7.3$
$2° < \theta < 25°$	R = 0.0444	$R_w = 0.0458$

20) N,N,N'-trimethylpropane-1,3-diammonium hexachlorostannate(IV)

$C_6N_2H_{18}SnCl_6$	MW = 449.5	t = 18 °C
orthorhombic	Pbcn (No. 60)	centrosymmetric
a = 7.884(2) Å	b = 14.994(2) Å	c = 25.548(4) Å
$\alpha = 90°$	$\beta = 90°$	$\gamma = 90°$
F(000) = 1760 e	$\mu = 25.46\ cm^{-1}$	V = 3256.4 Å^3
Z = 8	$d_c = 1.834\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 3422$	$N_{un} = 2270$	$N_{ob} = 1848$
obs. if $I > 2\sigma(I)$	$N_v = 167$	$N_{ob}/N_v = 11.1$
$2° < \theta < 23°$	R = 0.0280	$R_w = 0.0291$

21)

sodium tetraphenylborate

$C_{24}H_{20}BNa$	MW = 324.2	t = 18 °C
tetragonal	$I\bar{4}2m$ (No. 121)	noncentrosymmetric
a = 11.461(2) Å	b = 11.461(2) Å	c = 7.423(1) Å
α = 90°	β = 90°	γ = 90°
F(000) = 360 e	μ = 0.79 cm^{-1}	V = 975.0 $Å^3$
Z = 2	d_c = 1.656 g/cm^3	λ = 0.70926 Å
N_{me} = 1658	N_{un} = 446	N_{ob} = 244
obs. if I> 3σ(I)	N_v = 45	N_{ob}/N_v = 5.4
$2° < \theta < 30°$	R = 0.0513	R_w = 0.0542

22)

rubidium tetraphenylborate

$C_{24}H_{20}BRb$	MW = 404.7	t = 18 °C
tetragonal	$I\bar{4}2m$ (No. 121)	noncentrosymmetric
a = 11.218(2) Å	b = 11.218(2) Å	c = 8.092(1) Å
α = 90°	β = 90°	γ = 90°
F(000) = 412 e	μ = 23.67 cm^{-1}	V = 1018.3 $Å^3$
Z = 2	d_c = 1.320 g/cm^3	λ = 0.70926 Å
N_{me} = 1291	N_{un} = 679	N_{ob} = 380
obs. if I> 3σ(I)	N_v = 45	N_{ob}/N_v = 8.4
$2° < \theta < 25°$	R = 0.0362	R_w = 0.0362

23)

cesium tetraphenylborate

$C_{24}H_{20}BCs$	MW = 452.1	t = 18 °C
tetragonal	$I\bar{4}2m$ (No. 121)	noncentrosymmetric
a = 11.263(4) Å	b = 11.263(4) Å	c = 8.385(4) Å
α = 90°	β = 90°	γ = 90°
F(000) = 448 e	μ = 17.29 cm^{-1}	V = 1063.8 $Å^3$
Z = 2	d_c = 1.411 g/cm^3	λ = 0.70926 Å
N_{me} = 443	N_{un} = 240	N_{ob} = 229
obs. if I> 3σ(I)	N_v = 45	N_{ob}/N_v = 5.1
$2° < \theta < 23°$	R = 0.0396	R_w = 0.0415

24)

2-chlorocyclohexyltellurium(IV) trichloride

$C_6H_{10}TeCl_3$	MW = 351.6	t = 18 °C
monoclinic	$P2_1/n$ (No. 14)	centrosymmetric
a = 8.825(2) Å	b = 11.832(3) Å	c = 10.990(2) Å
α = 90°	β = 105.85°	γ = 90°
F(000) = 664 e	μ = 36.89 cm^{-1}	V = 1103.9 $Å^3$
Z = 4	d_c = 2.115 g/cm^3	λ = 0.70926 Å
N_{me} = 1904	N_{un} = 1532	N_{ob} = 805
obs. if I> 2σ(I)	N_v = 103	N_{ob}/N_v = 7.8
$2° < \theta < 23°$	R = 0.0666	R_w = 0.0669

25)

2-methoxycyclohexyltellurium(IV) tribromide

$C_7H_{13}Br_3OTe$	MW = 480.5	t = 18 °C
monoclinic	$P2_1/a$ (No. 14)	centrosymmetric
a = 8.488(1) Å	b = 11.294(8) Å	c = 13.073(3) Å
$\alpha = 90^\circ$	$\beta = 97.61(8)^\circ$	$\gamma = 90^\circ$
F(000) = 880 e	$\mu = 119.24\ cm^{-1}$	V = 1242.0 $Å^3$
Z = 4	$d_c = 2.569\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 1891$	$N_{un} = 1695$	$N_{ob} = 1285$
obs. if $I > 3\sigma(I)$	$N_v = 126$	$N_{ob}/N_v = 10.2$
$2^\circ < \theta < 23^\circ$	R = 0.0461	$R_w = 0.0520$

26)

2-ethoxycyclohexyltellurium(IV) trichloride

$C_8H_{16}Cl_3OTe$	MW = 362.2	t = 18 °C
monoclinic	$P2_1/c$ (No. 14)	centrosymmetric
a = 12.304(3) Å	b = 8.626(2) Å	c = 24.624(4) Å
$\alpha = 90^\circ$	$\beta = 91.28(2)^\circ$	$\gamma = 90^\circ$
F(000) = 1400 e	$\mu = 28.68\ cm^{-1}$	V = 2612.8 $Å^3$
Z = 8	$d_c = 1.841\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 4017$	$N_{un} = 3634$	$N_{ob} = 2769$
obs. if $I > 3\sigma(I)$	$N_v = 274$	$N_{ob}/N_v = 10.1$
$2^\circ < \theta < 23^\circ$	R = 0.0675	$R_w = 0.0765$

27)

2-m-propanoxycyclohexyltellurium(IV) trichloride

$C_9H_{17}Cl_3OTe$	MW = 375.2	t = 18 °C
monoclinic	$P2_1/n$ (No. 14)	centrosymmetric
a = 8.375(1) Å	b = 11.891(6) Å	c = 14.345(9) Å
$\alpha = 90^\circ$	$\beta = 94.57(2)^\circ$	$\gamma = 90^\circ$
F(000) = 728 e	$\mu = 26.35\ cm^{-1}$	V = 1424.0 $Å^3$
Z = 4	$d_c = 1.750\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 2175$	$N_{un} = 1968$	$N_{ob} = 1306$
obs. if $I > 3\sigma(I)$	$N_v = 251$(disorder)	$N_{ob}/N_v = 5.2$
$2^\circ < \theta < 23^\circ$	R = 0.0377	$R_w = 0.0413$

28)

2-isopropanoxycyclohexyltellurium(IV) tribromide

$C_9H_{17}Br_3OTe$	MW = 508.5	t = 18 °C
monoclinic	$P2_1/n$ (No. 14)	centrosymmetric
a = 8.924(2) Å	b = 14.763(7) Å	c = 11.868(4) Å
$\alpha = 90^\circ$	$\beta = 106.29(2)^\circ$	$\gamma = 90^\circ$
F(000) = 944 e	$\mu = 98.75\ cm^{-1}$	V = 1500.7 $Å^3$
Z = 4	$d_c = 2.251\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 2150$	$N_{un} = 1835$	$N_{ob} = 1239$
obs. if $I > 3\sigma(I)$	$N_v = 212$(disorder)	$N_{ob}/N_v = 5.8$
$2^\circ < \theta < 23^\circ$	R = 0.0602	$R_w = 0.0602$

29)

2-isopropanolcycloheptyltellurium(IV) trichloride

$C_{10}H_{12}Cl_3OTe$	MW = 382.2	t = 18 °C
monoclinic	$P2_1/n$ (No. 14)	centrosymmetric
a = 12.740(1) Å	b = 9.045(3) Å	c = 13.961(3) Å
$\alpha = 90^\circ$	$\beta = 112.41(3)^\circ$	$\gamma = 90^\circ$
F(000) = 708 e	$\mu = 25.81\ cm^{-1}$	$V = 1487.3\ Å^3$
Z = 4	$d_c = 1.707\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 3605$	$N_{un} = 2616$	$N_{ob} = 1611$
obs. if $I > 3\sigma(I)$	$N_v = 215$	$N_{ob}/N_v = 7.5$
$2^\circ < \theta < 23^\circ$	R = 0.0393	$R_w = 0.0414$

30)

p-anisyl-2-chlorocyclohexyltellurium(IV) dichloride

$C_{13}H_{17}Cl_3OTe$	MW = 423.2	t = 18 °C
triclinic	$P\bar{1}$ (No. 2)	centrosymmetric
a = 11.780(3) Å	b = 11.847(2) Å	c = 12.062(2) Å
$\alpha = 95.03(1)^\circ$	$\beta = 108.48(2)^\circ$	$\gamma = 90.61(2)^\circ$
F(000) = 824 e	$\mu = 24.26\ cm^{-1}$	$V = 1589.1\ Å^3$
Z = 4	$d_c = 1.769\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 5148$	$N_{un} = 4408$	$N_{ob} = 3234$
obs. if $I > 2\sigma(I)$	$N_v = 368$	$N_{ob}/N_v = 8.8$
$2^\circ < \theta < 23^\circ$	R = 0.0486	$R_w = 0.0514$

31)

p-phenoxyphenyl-2-chlorocyclohexyltellurium(IV) dichloride

$C_{18}H_{19}Cl_3OTe$	MW = 485.3	t = 18 °C
orthorhombic	Pbca (No. 61)	centrosymmetric
a = 42.176(13) Å	b = 10.885(2) Å	c = 8.349(6) Å
$\alpha = 90^\circ$	$\beta = 90^\circ$	$\gamma = 90^\circ$
F(000) = 1904 e	$\mu = 19.78\ cm^{-1}$	$V = 3832.9\ Å^3$
Z = 8	$d_c = 1.682\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 2110$	$N_{un} = 1777$	$N_{ob} = 912$
obs. if $I > 3\sigma(I)$	$N_v = 230$	$N_{ob}/N_v = 4.0$
$2^\circ < \theta < 23^\circ$	R = 0.0486	$R_w = 0.0510$

32)

p-anisyl-2-chloro-3-methylcyclohexyltellurium(IV) dichloride

$C_{14}H_{19}Cl_3OTe$	MW = 437.3	t = 18 °C
triclinic	$P\bar{1}$ (No. 2)	centrosymmetric
a = 10.419(2) Å	b = 10.906(3) Å	c = 8.285(3) Å
$\alpha = 92.40(3)^\circ$	$\beta = 95.85(2)^\circ$	$\gamma = 61.71(3)^\circ$
F(000) = 428 e	$\mu = 23.41\ cm^{-1}$	$V = 824.6\ Å^3$
Z = 2	$d_c = 1.761\ g/cm^3$	$\lambda = 0.70926$ Å
$N_{me} = 3107$	$N_{un} = 2885$	$N_{ob} = 2213$
obs. if $I > 2\sigma(I)$	$N_v = 199$	$N_{ob}/N_v = 11.1$
$2^\circ < \theta < 25^\circ$	R = 0.0444	$R_w = 0.0458$

33)

p-anisyl-2-chloro-4-methylcyclohexyltellurium(IV) dichloride

$C_{14}H_{19}Cl_3OTe$	MW = 437.3	t = 18 °C
triclinic	$P\bar{1}$ (No. 2)	centrosymmetric
a = 11.573(5) Å	b = 12.208(9) Å	c = 12.659(5) Å
α = 99.28(5)°	β = 106.62(3)°	γ = 90.47(5)°
F(000) = 856 e	μ = 22.35 cm^{-1}	V = 1688.5 $Å^3$
Z = 4	d_c = 1.720 g/cm^3	λ = 0.70926 Å
N_{me} = 3318	N_{un} = 3119	N_{ob} = 1938
obs. if I> 3σ(I)	N_v = 433(disorder)	N_{ob}/N_v = 4.5
$2° < \theta < 20°$	R = 0.0690	R_w = 0.0753

34) 2',4'-dimethoxyphenyl(trans-6-oxabicyclo[3.2.1]oct-4-yl)tellurium(IV) dichloride

$C_{15}H_{19}Cl_2O_3Te$	MW = 445.8	t = 18 °C
monoclinic	$P2_1/c$ (No. 14)	centrosymmetric
a = 9.626(2) Å	b = 15.768(5) Å	c = 11.176(3) Å
α = 90°	β = 92.08(2)°	γ = 90°
F(000) = 876 e	μ = 20.81 cm^{-1}	V = 1695.2 $Å^3$
Z = 4	d_c = 1.747 g/cm^3	λ = 0.70926 Å
N_{me} = 2558	N_{un} = 2347	N_{ob} = 1548
obs. if I> 3σ(I)	N_v = 216	N_{ob}/N_v = 7.2
$2° < \theta < 23°$	R = 0.0472	R_w = 0.0487

Appendix 4

Tables on Microfiches

1) Fractional Atomic Positional Parameters and Anisotropic Temperature Factors ($Å^2$) from Multipole Refinement of $2N_3P_3Az_6 \cdot C_6H_6$ (Data Set II).
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Appendix 4

Tables on Microfiches

Fractional Atomic Positional Parameters and Anisotropic Temperature Factors ($Å^2$) from multipole refinement of $2N_3P_3Az_6 \cdot C_6H_6$

lb2TX molly

	fractional co-ordinates			beta					
	xf	yf	zf						
P(1	0.7842	-0.4463	-0.2511	0.00271	0.00297	0.00312	-0.00001	-0.00069	0.00020
N(1	0.6430	-0.3921	-0.1684	0.00348	0.00352	0.00343	0.00059	0.00035	0.00059
N(2	0.7818	-0.6053	-0.2687	0.00513	0.00304	0.00528	-0.00042	0.00011	-0.00083
N(3	0.9019	-0.4755	-0.1502	0.00362	0.00742	0.00492	-0.00107	-0.00323	0.00106
C(1	1.0452	-0.4966	-0.2118	0.00315	0.01410	0.00794	0.00005	-0.00286	0.00098
C(2	0.9854	-0.3705	-0.1591	0.00722	0.01204	0.00918	-0.00780	-0.00792	-0.00088
C(3	0.8723	-0.6627	-0.3811	0.00657	0.00460	0.00778	0.00061	0.00163	-0.00431
C(4	0.7255	-0.6275	-0.3830	0.00726	0.00621	0.00931	-0.00133	-0.00428	-0.00680
C(9	0.9280	-0.8777	-0.0504	0.00699	0.00636	0.00733	0.00263	0.00010	0.00219
H(1	1.0708	-0.4894	-0.3182	5.01297	0.00000	0.00000	0.00000	0.00000	0.00000
H(2	1.1145	-0.5698	-0.1611	5.69516	0.00000	0.00000	0.00000	0.00000	0.00000
H(3	0.9717	-0.2851	-0.2349	3.95416	0.00000	0.00000	0.00000	0.00000	0.00000
H(4	1.0098	-0.3589	-0.0662	4.93164	0.00000	0.00000	0.00000	0.00000	0.00000
H(5	0.9355	-0.5987	-0.4466	3.99206	0.00000	0.00000	0.00000	0.00000	0.00000
H(6	0.9156	-0.7650	-0.3570	4.47448	0.00000	0.00000	0.00000	0.00000	0.00000
H(7	0.6891	-0.5440	-0.4524	4.64029	0.00000	0.00000	0.00000	0.00000	0.00000
H(8	0.6678	-0.7071	-0.3548	3.91310	0.00000	0.00000	0.00000	0.00000	0.00000
H(9	0.8801	-0.7794	-0.0921	4.42395	0.00000	0.00000	0.00000	0.00000	0.00000

bond		length	z:2(A,B)	z:2(B,A)	delta(A,B) (Angstrom:2)
P(1	- N(1	1.595	0.0128	0.0133	0.0006
P(1	- N(2	1.673	0.0160	0.0161	0.0002
P(1	- N(3	1.689	0.0059	0.0063	0.0004
N(2	- C(3	1.489	0.0116	0.0126	0.0010
N(2	- C(4	1.483	0.0072	0.0072	0.0000
N(3	- C(1	1.478	0.0254	0.0241	0.0013
N(3	- C(2	1.471	0.0024	0.0038	0.0014
C(1	- C(2	1.474	0.0768	0.0756	0.0012
C(3	- C(4	1.478	0.0324	0.0318	0.0005

Intermolecular Distances Involving the Hydrogen Atoms for $2N_3P_3Az_6 \cdot C_6H_6$

(Data Set I)

C(111)-H(1)	1.027(1)
C(111)-H(2)	1.020(1)
C(112)-H(3)	0.986(1)
C(112)-H(4)	0.937(1)
C(121)-H(5)	0.915(1)
C(121)-H(6)	1.000(1)
C(122)-H(7)	0.955(1)
C(122)-H(8)	1.017(1)
C(9) -H(9)	0.948(1)

Intramolecular Distances Involving the Hydrogen Atoms for $2N_3P_3Az_6 \cdot C_6H_6$

(Data Set II)

atom	atom	distance	atom	atom	distance
C(111)	H(1)	1.00(2)	C(121)	H(5)	0.98(2)
C(111)	H(2)	0.91(3)	C(121)	H(6)	0.98(2)
C(112)	H(3)	0.93(2)	C(122)	H(7)	0.92(2)
C(112)	H(4)	0.93(3)	C(122)	H(8)	0.94(2)
C(9)	H(9)	0.95(2)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table Torsional Angles (degrees) for $2N_3P_3Az_6.C_6H_6$ (Data Set I)

N(1)	-P	-N(1)'	-P'	-3.9 (1)
N(1)'	-P	-N(1)	-P''	3.9 (1)
N(1)	-P	-N(11)	-C(111)	-156.4 (1)
N(1)	-P	-N(11)	-C(112)	-86.7 (1)
N(11)	-P	-N(1)	-P''	130.4 (1)
N(1)	-P	-N(12)	-C(121)	97.6 (1)
N(1)	-P	-N(12)	-C(122)	166.4 (1)
N(12)	-P	-N(1)	-P''	-123.0 (1)
N(1)'	-P	-N(11)	-C(111)	-27.0 (1)
N(1)'	-P	-N(11)	-C(112)	42.7 (1)
N(11)	-P	-N(1)'	-P'	-128.4 (1)
N(1)'	-P	-N(12)	-C(121)	-32.3 (1)
N(1)'	-P	-N(12)	-C(122)	36.5 (1)
N(12)	-P	-N(1)'	-P'	121.6 (1)
N(11)	-P	-N(12)	-C(121)	-150.2 (1)
N(11)	-P	-N(12)	-C(122)	-81.4 (1)
N(12)	-P	-N(11)	-C(111)	90.5 (1)
N(12)	-P	-N(11)	-C(112)	160.2 (1)
P	-N(11)	-C(111)	-C(112)	107.9 (1)
P	-N(11)	-C(112)	-C(111)	-109.1 (1)
P	-N(12)	-C(121)	-C(122)	108.2 (1)
P	-N(12)	-C(122)	-C(121)	-107.9 (1)
C(9)'''	-C(9)	-C(9)''''	-C(9)'	0.9 (2)
C(9)''''	-C(9)	-C(9)'''	-C(9)'	-0.9 (2)

primed atoms have symmetry:

' -	Y,	Z,	X,
'' -	Z,	X,	Y,
''' -	-Y + 1.000,	-Z + 1.000,	-X + 1.000,
''''-	-Z + 1.000	-X + 1.000	-Y + 1.000

Torsion or Conformation Angles (degrees) for $2N_3P_3Az_6.C_6H_6$ (Data Set II)

(1)	(2)	(3)	(4)	angle	(1)	(2)	(3)	(4)	angle
P(1)	N(1)	P(1)	N(1)	4.0(1)	N(1)	P(1)	N(1)	P(1)	4.0(1)
P(1)	N(1)	P(1)	N(2)	128.52(7)	N(1)	P(1)	N(2)	C(4)	86.5(1)
P(1)	N(1)	P(1)	N(3)	-121.66(7)	N(1)	P(1)	N(2)	C(3)	156.29(9)
P(1)	N(1)	P(1)	N(1)	-4.0(1)	N(1)	P(1)	N(3)	C(2)	-97.4(1)
P(1)	N(1)	P(1)	N(2)	-130.46(7)	N(1)	P(1)	N(3)	C(1)	-166.3(1)
P(1)	N(1)	P(1)	N(3)	122.93(7)	N(1)	P(1)	N(1)	P(1)	-4.0(1)
P(1)	N(2)	C(4)	C(3)	109.33(9)	N(2)	P(1)	N(3)	C(2)	150.2(1)
P(1)	N(2)	C(3)	C(4)	-107.8(1)	N(2)	P(1)	N(3)	C(1)	81.3(1)
P(1)	N(3)	C(2)	C(1)	-108.3(1)	N(3)	P(1)	N(2)	C(4)	-160.37(9)
P(1)	N(3)	C(1)	C(2)	107.8(1)	N(3)	P(1)	N(2)	C(3)	-90.5(1)

The sign is positive if when looking from atom 2 to atom 3 a clockwise motion of atom 1 would superimpose it on atom 4.

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

An * indicates weak reflections not used in the final refinements.

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	2	11	96	108	0	3	11	97	-104	0	4	11	75	-83
0	5	11	120	133	0	6	11	129	-141	0	7	10	148	-159
0	6	10	192	205	0	5	10	159	171	0	2	10	227	237
0	0	10	129	-141	0	-1	10	107	115	0	-2	10	87	89
0	-4	10	110	-118	0	-5	9	31	35	0	-4	9	51	-57
0	-3	9	64	-66	0	-2	9	192	-196	0	0	9	60	-65
0	1	9	331	-350	0	2	9	65	63	0	3	9	104	114
0	4	9	126	-137	0	6	9	236	257	0	7	9	130	142
0	9	9	48	60	8	0	9	84	-87	0	8	8	68	-76
0	7	8	45	48	0	6	8	137	-149	0	5	8	300	-333
0	4	8	212	-229	0	3	8	77	88	0	2	8	222	-239
0	1	8	35	-41	0	0	8	156	159	0	-1	8	34	-28
0	-3	8	42	48	0	-4	8	63	68	0	-6	8	194	215
0	-7	8	97	107	-7	0	8	157	-172	-7	0	7	184	-200
0	-5	7	29	-32	0	-4	7	292	-330	0	-3	7	169	183
0	-2	7	349	373	0	-1	7	172	177	0	0	7	151	151
0	1	7	163	168	0	2	7	122	125	0	3	7	67	79
0	4	7	120	133	0	5	7	45	-51	0	6	7	37	-41
7	0	9	75	-81	7	0	10	81	-85	6	0	11	93	-101
6	0	10	40	39	6	0	8	69	80	6	0	7	166	184
0	6	6	209	226	0	5	6	52	-57	0	4	6	245	-258
0	2	6	252	283	0	1	6	56	-61	0	0	6	234	-236
0	-1	6	49	52	0	-2	6	100	104	0	-3	6	431	-496
0	-4	6	297	-331	0	-5	6	105	112	-6	0	7	212	-228
-6	0	9	117	132	-5	0	8	157	172	-5	0	7	129	139
-5	0	5	301	356	0	-4	5	165	175	0	-3	5	261	-291
0	-2	5	57	-62	0	-1	5	161	168	0	0	5	284	-282
0	1	5	418	-452	0	3	5	396	448	0	4	5	108	-125
0	5	5	259	-277	5	0	6	194	221	5	0	7	181	195
5	0	8	117	-130	5	0	9	65	-80	5	0	10	163	176
5	0	11	159	179	4	0	11	175	196	4	0	9	334	-367
4	0	8	140	-158	4	0	7	218	236	4	0	6	224	-266
4	0	5	275	-325	0	4	4	152	162	0	3	4	178	214
0	2	4	169	-208	0	1	4	183	-190	0	0	4	78	-56*
0	-1	4	402	423	0	-2	4	95	-99	0	-3	4	168	182
-4	0	4	295	325	-4	0	5	164	-185	-4	0	7	66	73
-4	0	6	45	-44	-4	0	9	34	-38	-3	0	10	35	40
-3	0	8	255	-279	-3	0	7	140	-157	-3	0	5	98	-113
-3	0	3	144	153	0	-2	3	49	50	0	-1	3	132	-143
0	0	3	154	160	0	1	3	287	-296	0	2	3	186	208
0	3	3	167	-180	3	0	4	374	461	3	0	5	193	215
3	0	6	73	-89	3	0	7	81	98	3	0	8	166	183
3	0	9	286	-306	3	0	10	299	-325	3	0	11	37	51
2	0	11	54	59	2	0	9	154	171	2	0	8	306	341
2	0	7	82	-90	2	0	6	122	130	2	0	5	455	498
2	0	4	35	43	2	0	3	339	413	0	2	2	268	306

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	1	2	553	-596	0	0	2	261	-250	0	-1	2	142	158
-2	0	2	550	-622	-2	0	3	86	-116*	-2	0	4	85	85
-2	0	5	244	261	-2	0	7	159	-174	-2	0	9	204	231
-2	0	10	95	-108	-2	0	11	56	-61	-1	0	10	158	-174
-1	0	9	99	112	-1	0	8	334	373	-1	0	7	75	-86
-1	0	6	29	-42	-1	0	5	45	72*	-1	0	4	507	563
-1	0	3	22	-32	-1	0	2	1162	-1362	-1	0	1	454	463
1	0	2	503	-553	1	0	3	401	440	1	0	4	372	-398
1	0	5	410	-462	1	0	6	220	-247	1	0	7	231	-253
1	0	8	108	-114	1	0	9	121	135	1	0	10	28	34
0	0	10	122	-141	0	0	9	55	-65	0	0	8	140	159
0	0	7	138	151	0	0	6	222	-236	0	0	5	266	-282
0	0	4	72	-56*	0	0	3	142	160	0	0	2	244	-250
0	0	2	245	-250	0	0	3	147	160	0	0	4	75	-56*
0	0	5	259	-282	0	0	6	218	-236	0	0	7	141	151
0	0	8	144	159	0	0	9	60	-65	0	0	10	123	-141
1	0	10	33	34	1	0	9	125	135	1	0	8	110	-114
1	0	7	231	-253	1	0	6	217	-247	1	0	5	425	-462
1	0	4	365	-398	1	0	3	404	440	1	0	2	514	-553
-1	0	1	459	463	-1	0	2	1156	-1362	-1	0	3	23	-32
-1	0	4	506	563	-1	0	5	44	72*	-1	0	6	30	-42
-1	0	7	75	-86	-1	0	8	336	373	-1	0	9	96	112
-1	0	10	156	-174	-2	0	11	50	-61	-2	0	10	97	-108
-2	0	9	204	231	-2	0	8	31	26	-2	0	7	158	-174
-2	0	5	241	261	-2	0	4	80	85	-2	0	3	84	-116*
-2	0	2	559	-622	0	-1	2	147	158	0	0	2	260	-250
0	1	2	552	-596	0	2	2	282	306	2	0	3	363	413
2	0	4	36	43	2	0	5	457	498	2	0	6	123	130
2	0	7	85	-90	2	0	8	313	341	2	0	9	155	171
2	0	11	53	59	3	0	11	40	51	3	0	10	299	-325
3	0	9	284	-306	3	0	8	167	183	3	0	7	86	98
3	0	6	72	-89	3	0	5	200	215	3	0	4	381	461
0	3	3	169	-180	0	2	3	190	208	0	1	3	288	-296
0	0	3	156	160	0	-1	3	132	-143	0	-2	3	49	50
-3	0	3	142	153	-3	0	5	101	-113	-3	0	7	139	-157
-3	0	8	250	-279	-3	0	10	37	40	-4	0	9	44	-38
-4	0	8	44	-44	-4	0	7	64	73	-4	0	5	165	-185
-4	0	4	298	325	0	3	4	167	182	0	-2	4	94	-99
0	-1	4	400	423	0	0	4	80	-56*	0	1	4	183	-190
0	2	4	174	-208	0	3	4	184	214	0	4	4	154	162
4	0	5	281	-325	4	0	6	248	-266	4	0	7	219	236
4	0	8	142	-158	4	0	9	339	-367	4	0	11	179	196
5	0	11	163	179	5	0	10	167	176	5	0	9	72	-80
5	0	8	119	-130	5	0	7	178	195	5	0	6	196	221
0	5	5	263	-277	0	4	5	111	-125	0	3	5	414	448
0	1	5	426	-452	0	0	5	287	-282	0	-1	5	162	168
0	-2	5	58	-62	0	-3	5	262	-291	0	-4	5	166	175

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-5	0	5	317	356	-5	0	7	130	139	-5	0	8	158	172
-6	0	9	117	132	-6	0	7	209	-228	-6	0	6	38	33
0	-5	6	104	112	0	-4	6	294	-331	0	-3	6	443	-496
0	-2	6	98	104	0	-1	6	52	52	0	0	6	240	-236
0	1	6	57	-61	0	2	6	251	283	0	4	6	248	-258
0	5	6	48	-57	0	6	6	216	226	6	0	7	166	184
6	0	8	74	80	6	0	10	35	39	6	0	11	95	-101
7	0	10	77	-85	7	0	9	75	-81	0	6	7	37	-41
0	5	7	48	-51	0	4	7	121	133	0	3	7	71	79
0	2	7	123	125	0	1	7	164	168	0	0	7	153	151
0	-1	7	173	177	0	-2	7	359	373	0	-3	7	174	183
0	-4	7	299	-330	-7	0	7	181	-200	-7	0	8	156	-172
0	-7	8	96	107	0	-6	8	199	215	0	-4	8	59	68
0	-3	8	40	48	0	-1	8	32	-28	0	0	8	159	159
0	1	8	41	-41	0	2	8	233	-239	0	3	8	80	88
0	4	8	222	-229	0	5	8	304	-333	0	6	8	138	-149
0	7	8	47	48	0	8	8	66	-76	8	0	9	82	-87
0	9	9	51	60	0	7	9	130	142	0	6	9	243	257
0	4	9	127	-137	0	3	9	103	114	0	2	9	69	63
0	1	9	340	-350	0	0	9	64	-65	0	-2	9	194	-196
0	-3	9	67	-66	0	-4	9	56	-57	0	-5	9	30	35
0	-6	9	37	41	0	-4	10	113	-118	0	-2	10	90	89
0	-1	10	107	115	0	0	10	133	-141	0	1	10	28	19
0	2	10	222	237	0	3	10	31	36	0	5	10	152	171
0	6	10	192	205	0	7	10	149	-159	0	6	11	127	-141
0	5	11	120	133	0	4	11	74	-83	0	3	11	94	-104
0	2	11	97	108	0	1	11	113	115	0	-1	11	84	-88
0	-2	11	138	146	1	2	12	112	-122	1	1	12	35	-34
1	-2	11	104	-106	1	-1	11	206	-218	1	1	11	74	79
1	2	11	100	-107	1	3	11	88	-94	1	4	11	55	64
1	6	11	208	-223	1	8	10	59	-71	1	7	10	276	-296
1	6	10	168	-185	1	5	10	55	52	1	4	10	27	-32
1	3	10	104	-114	1	2	10	59	67	1	1	10	145	152
1	-1	10	63	66	1	-2	10	64	67	1	-3	10	52	55
1	-6	9	124	-141	1	-5	9	72	-81	1	-4	9	28	-33
1	-3	9	48	-50	1	1	9	128	134	1	2	9	169	186
1	3	9	101	117	1	4	9	38	37	1	5	9	74	84
1	6	9	159	173	1	7	9	31	-33	1	9	9	106	120
8	1	10	82	89	8	1	9	43	47	1	8	8	64	70
1	7	8	146	159	1	6	8	156	176	1	5	8	48	48
1	4	8	68	-86	1	3	8	144	-160	1	2	8	265	-272
1	1	8	54	-56	1	-1	8	349	-357	1	-2	8	169	-176
1	-3	8	68	70	1	-4	8	57	-61	1	-5	8	126	-139
1	-6	8	29	23	1	-7	8	153	170	-7	-1	8	87	-95
-7	-1	7	151	168	1	-6	7	203	216	1	-5	7	90	-105
1	-4	7	96	109	1	-3	7	357	383	1	-2	7	462	483
1	-1	7	165	-168	1	1	7	311	320	1	2	7	120	-133

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	3	7	265	-296	1	5	7	86	90	1	6	7	60	-64
1	7	7	101	-106	7	1	8	155	-180	7	1	9	37	32
7	1	10	45	-45	6	1	11	193	-208	6	1	8	128	-141
6	1	7	148	-158	1	6	6	283	298	1	5	6	202	212
1	4	6	70	-77	1	3	6	337	-373	1	2	6	432	475
1	1	6	153	166	1	-2	6	443	450	1	-3	6	181	204
1	-4	6	294	-321	1	-5	6	35	-38	-6	-1	6	120	-134
-6	-1	7	160	-171	-6	-1	8	157	-178	-6	-1	9	80	-94
-5	-1	9	73	-76	-5	-1	7	42	55	-5	-1	6	35	37
-5	-1	5	32	-37	1	-3	5	290	-330	1	-2	5	41	-44
1	-1	5	86	-92	1	1	5	233	243	1	2	5	317	378
1	3	5	139	162	1	4	5	194	-218	1	5	5	100	114
5	1	6	256	293	5	1	7	104	113	5	1	8	146	-145
5	1	9	89	96	5	1	10	249	270	5	1	11	119	-132
4	1	11	211	232	4	1	10	222	243	4	1	9	32	37
4	1	8	212	-243	4	1	7	67	79	4	1	6	149	-171
4	1	5	168	-204	1	4	4	123	111	1	2	4	27	-31
1	1	4	71	-94*	1	-1	4	65	-70	1	-2	4	25	-25
1	-3	4	39	50	-4	-1	4	40	45	-4	-1	5	62	-75
-4	-1	6	174	191	-4	-1	7	212	239	-4	-1	8	63	81
-4	-1	10	110	123	-3	-1	10	69	75	-3	-1	9	54	64
-3	-1	8	161	-190	-3	-1	7	53	67	-3	-1	6	214	231
-3	-1	5	131	134	-3	-1	4	421	-456	-3	-1	3	53	-45*
1	-2	3	173	211	1	-1	3	111	118	1	1	3	370	412
1	2	3	759	876	1	3	3	498	-539	3	1	4	27	-31
3	1	5	142	-164	3	1	6	409	-453	3	1	7	69	-73
3	1	9	178	-197	3	1	10	29	30	3	1	11	39	41
2	1	12	71	-81	2	1	11	91	-99	2	1	10	80	-89
2	1	9	61	-67	2	1	8	97	105	2	1	7	124	-132
2	1	6	119	137	2	1	5	235	273	2	1	4	119	-139
2	1	3	74	82	1	2	2	78	85	1	1	2	295	321
1	-1	2	603	620	-2	-1	2	462	536	-2	-1	3	611	-722
-2	-1	4	149	-184	-2	-1	5	154	172	-2	-1	6	23	42
-2	-1	7	323	-360	-2	-1	8	134	-155	-2	-1	9	77	85
-2	-1	10	58	74	-2	-1	11	127	-145	-1	-1	11	44	41
-1	-1	10	42	48	-1	-1	9	126	146	-1	-1	8	73	81
-1	-1	7	171	-195	-1	-1	6	128	-136	-1	-1	5	368	429
-1	-1	4	176	188	-1	-1	3	347	-425	-1	-1	2	257	-294
-1	1	1	393	400	1	1	2	285	321	1	1	3	353	412
1	1	4	69	-94*	1	1	5	210	243	1	1	6	144	166
1	1	7	297	320	1	1	8	52	-56	1	1	9	118	134
1	1	10	133	152	1	1	11	66	79	1	1	12	32	-34
1	-1	11	192	-218	1	-1	10	59	66	1	-1	9	27	28
1	-1	8	325	-357	1	-1	7	150	-168	1	-1	5	84	-92
1	-1	4	59	-70	1	-1	3	104	118	1	-1	2	567	620
-1	1	1	371	400	-1	1	1	421	400	-1	1	2	171	177
-1	1	3	21	28	-1	1	4	62	75	-1	1	5	68	-75

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-1	1	6	92	-106	-1	1	7	86	93	-1	1	8	160	177
-1	1	9	188	-203	-1	1	10	182	-202	-1	1	11	103	118
-2	1	10	60	-74	-2	1	9	71	81	-2	1	8	95	105
-2	1	7	99	115	-2	1	6	112	125	-2	1	5	211	241
-2	1	4	87	101	-2	1	3	95	112	-2	1	2	246	253
-1	-1	2	286	-294	-1	1	2	174	177	-1	2	2	37	36
2	-1	3	35	-44	2	-1	4	129	-143	2	-1	6	92	-106
2	-1	7	396	-438	2	-1	8	122	-132	2	-1	9	280	305
3	-1	11	58	-64	3	-1	10	124	-137	3	-1	9	83	93
3	-1	8	382	421	3	-1	7	153	168	3	-1	6	108	118
3	-1	5	315	355	3	-1	4	86	107	-1	3	3	423	-505
-1	2	3	266	-313	-1	1	3	28	28	-1	-1	3	375	-425
-1	-2	3	106	114	-3	1	3	84	89	-3	1	4	278	-310
-3	1	5	227	-260	-3	1	6	40	47	-3	1	7	38	39
-3	1	8	64	-79	-3	1	10	80	92	-4	1	10	47	57
-4	1	9	104	-120	-4	1	8	61	-63	-4	1	7	50	55
-4	1	6	332	-375	-4	1	5	325	-348	-4	1	4	172	188
-1	-3	4	291	313	-1	-2	4	171	170	-1	-1	4	196	188
-1	1	4	66	75	-1	2	4	170	-185	-1	3	4	36	-34
-1	4	4	348	393	4	-1	5	159	-164	4	-1	6	28	-26
4	-1	7	171	189	4	-1	8	63	59	4	-1	9	45	-42
4	-1	10	234	-254	5	-1	8	60	-62	5	-1	7	109	-122
5	-1	6	179	-188	-1	5	5	173	-194	-1	4	5	210	-241
-1	3	5	165	171	-1	2	5	353	-371	-1	1	5	76	-75
-1	-1	5	403	429	-1	-2	5	139	-152	-1	-3	5	175	-193
-1	-4	5	342	380	-5	1	6	216	-241	-5	1	8	198	216
-5	1	9	95	-105	-6	1	9	48	53	-6	1	8	232	248
-1	-5	6	540	587	-1	-4	6	79	86	-1	-3	6	227	-238
-1	-2	6	131	-146	-1	-1	6	143	-136	-1	1	6	99	-106
-1	2	6	147	151	-1	3	6	55	-69	-1	4	6	61	67
-1	5	6	119	126	6	-1	7	106	-113	6	-1	8	180	198
6	-1	9	143	154	7	-1	10	186	-199	7	-1	8	167	173
-1	6	7	134	-146	-1	5	7	135	148	-1	4	7	393	434
-1	3	7	138	-148	-1	2	7	176	-182	-1	1	7	94	93
-1	-1	7	186	-195	-1	-2	7	91	-94	-1	-3	7	169	-185
-1	-4	7	89	-98	-1	-5	7	61	-72	-1	-6	7	94	-108
-7	1	7	208	-217	-1	-7	8	68	-76	-1	-6	8	91	-102
-1	-5	8	31	31	-1	-4	8	113	122	-1	-3	8	100	106
-1	-1	8	79	81	-1	1	8	169	177	-1	2	8	182	-197
-1	3	8	317	338	-1	4	8	234	256	-1	5	8	41	-53
-1	6	8	255	-272	-1	7	8	49	55	-1	8	8	36	-31
8	-1	9	191	-193	-1	8	9	64	-70	-1	7	9	82	85
-1	5	9	358	-400	-1	4	9	138	-151	-1	2	9	104	-112
-1	1	9	205	-203	-1	-1	9	142	146	-1	-2	9	138	-151
-1	-3	9	108	-114	-1	-4	9	89	94	-1	-5	9	187	207
-1	-4	10	115	-119	-1	-3	10	185	-192	-1	-2	10	49	48
-1	-1	10	53	48	-1	1	10	191	-202	-1	2	10	52	55

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-1	3	10	56	61	-1	4	10	47	-51	-1	6	10	180	196
-1	7	10	82	93	-1	3	11	100	104	-1	2	11	84	84
-1	1	11	112	118	-1	-1	11	39	41	-1	-2	11	152	158
-2	2	11	105	-112	-2	4	11	116	126	-2	5	10	102	-115
-2	3	10	123	-134	-2	-3	10	54	-55	-2	-4	10	74	81
-2	-4	9	189	200	-2	-3	9	35	34	-2	-2	9	107	-111
-2	2	9	60	67	-2	3	9	130	144	-2	5	9	85	-94
-2	6	9	148	-160	-2	8	9	86	-96	8	-2	9	76	-86
-2	8	8	70	74	-2	7	8	85	91	-2	6	8	64	-65
-2	5	8	177	193	-2	4	8	324	345	-2	2	8	193	-202
-2	-2	8	127	-139	-2	-3	8	153	156	-2	-4	8	41	39
-2	-5	8	288	-307	-2	-6	8	149	-163	-2	-7	8	59	69
-7	2	8	33	43	-7	2	7	112	121	-2	-6	7	121	130
-2	-5	7	52	-50	-2	-3	7	161	174	-2	-2	7	36	-31
-2	2	7	68	-68	-2	3	7	372	-396	-2	4	7	90	96
-2	5	7	265	288	-2	6	7	63	-68	-2	7	7	70	-81
7	-2	8	199	207	7	-2	9	121	126	6	-2	10	50	47
6	-2	9	137	149	6	-2	7	260	-271	-2	6	6	67	-70
-2	5	6	162	172	-2	4	6	267	-302	-2	3	6	378	-418
-2	2	6	171	184	-2	-3	6	72	80	-2	-4	6	83	88
-2	-5	6	44	46	-6	2	6	33	33	-6	2	7	59	71
-6	2	8	66	76	-6	2	9	81	-93	-5	2	9	107	-125
-5	2	7	121	134	-5	2	6	341	-384	-5	2	5	231	-253
-2	-4	5	118	122	-2	-3	5	139	153	-2	2	5	50	52
-2	3	5	122	139	-2	4	5	113	-123	-2	5	5	52	55
5	-2	6	51	59	5	-2	7	191	-210	5	-2	8	133	-144
5	-2	9	30	35	5	-2	10	77	84	4	-2	10	44	54
4	-2	9	28	27	4	-2	8	112	119	4	-2	7	177	191
4	-2	6	160	169	4	-2	5	213	238	-2	4	4	110	128
-2	3	4	177	-203	-2	2	4	147	-168	-2	-2	4	296	-316
-2	-3	4	156	168	-4	2	5	494	-562	-4	2	6	68	80
-4	2	7	88	101	-4	2	8	59	-63	-4	2	9	75	-89
-4	2	10	174	191	-3	2	10	111	129	-3	2	9	52	59
-3	2	8	163	-181	-3	2	7	344	376	-3	2	6	391	434
-3	2	5	116	128	-3	2	4	161	-178	-2	-2	3	58	-44*
-2	2	3	239	259	-2	3	3	322	-373	3	-2	4	82	-88
3	-2	6	157	-170	3	-2	7	179	-187	3	-2	9	137	146
3	-2	11	116	130	2	-2	11	84	-93	2	-2	10	50	55
2	-2	9	59	-64	2	-2	8	185	-200	2	-2	7	375	-409
2	-2	6	51	64	2	-2	5	69	-72	2	-2	4	291	-342
2	-2	3	319	336	-2	2	2	285	335	-2	2	2	322	335
-2	2	3	249	259	-2	2	4	150	-168	-2	2	5	49	52
-2	2	6	159	184	-2	2	7	64	-68	-2	2	8	185	-202
-2	2	9	56	67	-2	2	11	102	-112	-2	-2	9	95	-111
-2	-2	8	118	-139	-2	-2	7	35	-31	-2	-2	4	276	-316
-2	-2	3	55	-44*	-2	2	2	298	335	2	2	2	254	289
2	2	3	502	-577	2	2	4	361	-414	2	2	5	55	-35*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	2	7	352	-401	2	2	10	84	-99	2	2	11	94	-105
3	2	12	39	50	3	2	9	49	47	3	2	8	226	246
3	2	6	80	-92	3	2	5	92	104	3	2	4	100	-120
2	3	3	401	-444	2	2	3	504	-577	2	-2	3	337	336
-3	-2	3	263	313	-3	-2	4	145	-159	-3	-2	5	33	-34
-3	-2	6	97	107	-3	-2	7	183	212	-3	-2	8	87	110
-3	-2	10	149	162	-4	-2	9	62	-68	-4	-2	8	67	82
-4	-2	7	64	67	-4	-2	6	90	-113	-4	-2	5	180	-201
2	-3	4	86	86	2	-2	4	314	-342	2	2	4	364	-414
2	3	4	42	-43	2	4	4	295	312	4	2	6	74	-79
4	2	7	181	206	4	2	8	25	24	4	2	9	191	223
4	2	10	60	72	4	2	11	46	-60	5	2	11	239	-273
5	2	10	42	-49	5	2	9	79	98	5	2	8	27	48
5	2	7	97	-113	5	2	6	58	71	2	4	5	24	-28
2	3	5	98	113	2	2	5	55	-35*	2	-2	5	71	-72
2	-3	5	105	-117	-5	-2	5	51	-59	-5	-2	6	156	-173
-5	-2	7	133	-159	-5	-2	9	168	-183	-6	-2	8	84	97
-6	-2	7	56	66	-6	-2	6	84	91	2	-5	6	140	159
2	-4	6	138	158	2	-3	6	316	342	2	-2	6	56	64
2	4	6	166	186	2	5	6	34	39	2	6	6	238	-264
6	2	7	287	-327	6	2	8	90	-99	6	2	9	63	67
6	2	10	65	-72	6	2	11	78	-85	7	2	11	150	165
7	2	10	94	-100	7	2	9	81	87	7	2	8	39	38
2	7	7	56	-56	2	6	7	55	-53	2	5	7	25	31
2	4	7	203	236	2	3	7	113	-126	2	2	7	380	-401
2	-2	7	400	-409	2	-3	7	139	146	2	-4	7	35	36
2	-5	7	104	-115	2	-6	7	52	60	-7	-2	7	106	119
-7	-2	8	71	80	2	-7	8	38	39	2	-6	8	146	-160
2	-5	8	135	-147	2	-4	8	194	208	2	-3	8	59	-69
2	-2	8	190	-200	2	3	8	339	363	2	4	8	134	156
2	5	8	89	102	2	6	8	129	147	2	7	8	113	114
2	8	8	72	79	8	2	10	43	-40	2	9	9	42	-50
2	8	9	66	-68	2	7	9	151	-163	2	6	9	48	-51
2	5	9	94	-97	2	4	9	118	-135	2	3	9	39	-47
2	-2	9	60	-64	2	-3	9	78	86	2	-4	9	47	50
2	-6	9	151	-167	2	-4	10	80	87	2	-2	10	51	55
2	2	10	93	-99	2	3	10	56	-63	2	4	10	34	-32
2	6	10	61	-68	2	7	10	58	-60	2	8	10	122	129
2	7	11	211	229	2	6	11	36	-43	2	4	11	46	49
2	2	11	102	-105	2	-2	11	86	-93	2	3	12	170	184
3	3	11	47	52	3	4	11	53	56	3	5	11	53	54
3	6	11	96	105	3	7	11	112	124	3	7	10	65	74
3	6	10	122	133	3	5	10	109	122	3	4	10	97	116
3	3	10	77	-83	3	-3	10	53	-52	3	-4	10	30	-40
3	-5	9	183	199	3	-4	9	59	64	3	-3	9	89	-94
3	3	9	60	-64	3	4	9	100	-113	3	5	9	32	39
3	7	9	63	-66	3	8	9	157	-171	3	3	10	62	71

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
8	3	9	170	-179	3	8	8	39	-34	3	7	8	30	36
3	6	8	96	-104	3	5	8	292	-319	3	4	8	152	-174
3	3	8	101	114	3	-3	8	138	-148	3	-4	8	114	127
3	-5	8	51	56	3	-6	8	48	-56	-7	-3	7	60	-66
3	-6	7	50	-55	3	-5	7	161	-179	3	-3	7	248	-260
3	3	7	204	225	3	4	7	191	222	3	5	7	26	-41
3	6	7	57	-53	3	7	7	309	337	7	3	8	148	165
7	3	9	57	-65	7	3	10	56	-68	7	3	11	144	160
6	3	11	156	181	6	3	10	46	-51	6	3	8	257	271
6	3	7	77	87	3	6	6	243	-257	3	3	6	93	-101
3	-3	6	40	-41	3	-4	6	147	-157	3	-5	6	66	69
-6	-3	6	133	152	-6	-3	8	67	71	-5	-3	9	93	106
-5	-3	7	90	-97	-5	-3	6	70	87	-5	-3	5	255	298
3	-4	5	84	96	3	-3	5	63	-74	3	3	5	117	123
3	4	5	122	-136	3	5	5	222	-225	5	3	6	167	-197
5	3	7	167	-192	5	3	8	54	61	5	3	9	117	-136
5	3	10	102	-121	5	3	11	37	-44	4	3	10	111	-123
4	3	9	38	-35	4	3	7	134	152	4	3	5	46	47
3	4	4	121	130	3	3	4	512	576	3	-3	4	154	-167
-4	-3	4	142	161	-4	-3	5	59	-61	-4	-3	6	108	-117
-4	-3	7	208	-254	-4	-3	9	91	-104	-3	-3	9	50	60
-3	-3	8	38	45	-3	-3	6	132	-161	-3	-3	5	57	60
-3	-3	4	21	-19	-3	3	3	296	304	3	3	3	190	-208
3	3	4	505	576	3	3	5	114	123	3	3	6	92	-101
3	3	7	196	225	3	3	8	101	114	3	3	9	57	-64
3	3	10	72	-83	3	3	11	43	52	3	-3	10	49	-52
3	-3	9	83	-94	3	-3	8	132	-148	3	-3	7	232	-260
3	-3	6	38	-41	3	-3	5	59	-74	3	-3	4	148	-167
-3	3	3	262	304	-3	3	3	307	304	-3	3	4	125	-128
-3	3	5	434	453	-3	3	6	169	189	-3	3	7	221	-240
-3	3	9	51	52	-3	3	10	94	-103	-4	3	10	35	39
-4	3	9	66	78	-4	3	7	57	66	-4	3	6	322	340
-4	3	5	122	130	-4	3	4	80	-83	-3	3	4	121	-128
-3	4	4	144	-161	4	-3	5	213	-216	4	-3	6	113	123
4	-3	7	97	104	4	-3	8	64	-75	5	-3	10	131	148
5	-3	8	58	-63	5	-3	7	123	125	5	-3	6	334	375
-3	5	5	95	106	-3	4	5	66	-64	-3	3	5	394	453
-3	-3	5	61	60	-3	-4	5	75	-84	-5	3	5	163	-170
-5	3	7	89	-92	-5	3	9	66	72	-6	3	8	76	-79
-6	3	7	63	-63	-3	-5	6	50	50	-3	-4	6	243	-270
-3	-3	6	147	-161	-3	3	6	173	189	-3	4	6	391	-425
-3	5	6	65	-69	-3	6	6	45	50	6	-3	7	185	-197
6	-3	8	161	-165	7	-3	9	72	74	7	-3	8	45	-42
-3	7	7	96	-105	-3	5	7	55	-57	-3	4	7	128	-136
-3	3	7	224	-240	-3	-4	7	96	-105	-3	-5	7	81	90
-3	-6	7	300	316	-7	3	7	44	46	-3	-6	8	102	114
-3	-5	8	116	-122	-3	-4	8	51	-52	-3	-3	8	45	45

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-3	4	8	39	-42	-3	5	8	100	113	-3	7	8	59	62
-3	8	8	58	66	-3	7	9	116	129	-3	6	9	155	169
-3	5	9	58	65	-3	4	9	60	65	-3	3	9	51	52
-3	-3	9	56	60	-3	-4	9	54	-66	-3	-5	9	75	-78
-3	3	10	95	-103	-3	4	10	116	-131	-3	5	10	29	-27
-4	4	10	62	-71	-4	4	9	47	-52	-4	5	9	59	-63
-4	6	9	32	37	-4	6	8	111	-120	-4	5	8	116	-126
-4	4	8	44	47	-4	-4	8	42	40	-4	-5	8	81	89
-4	-6	8	92	102	-7	4	7	172	-179	-4	-6	7	72	69
-4	-5	7	80	86	-4	4	7	51	-60	-4	5	7	117	-130
-4	6	7	68	-79	6	-4	9	31	-32	6	-4	7	194	202
-4	6	6	108	117	-4	5	6	60	67	-4	4	6	229	250
-4	-4	6	29	29	-4	-5	6	137	146	-6	4	6	165	-168
-6	4	7	134	-136	-5	4	9	63	73	-5	4	5	51	54
-4	-4	5	196	218	-4	4	5	145	155	-4	5	5	178	-197
5	-4	7	167	182	5	-4	8	85	93	5	-4	9	125	-143
4	-4	10	121	-137	4	-4	9	106	-122	4	-4	6	344	-395
4	-4	5	140	-158	-4	4	4	170	180	-4	4	4	185	180
-4	4	5	152	155	-4	4	6	244	250	-4	4	7	53	-60
-4	4	8	44	47	-4	4	9	42	-52	-4	4	10	65	-71
-4	-4	8	37	40	-4	-4	6	26	29	-4	-4	5	185	218
-4	4	4	177	180	4	4	4	176	-196	4	4	5	458	-506
4	4	6	137	149	4	4	7	90	-102	4	4	8	361	-400
4	4	10	92	106	4	4	11	46	47	5	4	10	135	151
5	4	9	48	53	5	4	7	74	-85	5	4	6	145	150
4	4	5	468	-506	4	-4	5	142	-158	-5	-4	5	213	232
-5	-4	6	163	199	-5	-4	8	71	85	-6	-4	8	165	-186
-6	-4	7	104	-113	4	-5	6	113	-129	4	-4	6	370	-395
4	4	6	140	149	4	5	6	209	231	4	6	6	258	260
6	4	7	210	234	6	4	8	30	38	6	4	10	33	-41
6	4	11	36	39	7	4	9	117	-132	7	4	8	86	-95
4	7	7	131	137	4	6	7	55	64	4	5	7	248	-271
4	4	7	92	-102	4	-5	7	83	-92	4	-6	7	102	112
4	-6	8	34	39	4	-5	8	64	71	4	4	8	363	-400
4	5	8	157	-175	4	6	8	73	81	4	7	8	33	-42
4	8	8	175	-186	8	4	10	169	171	4	9	9	170	182
4	8	9	50	-53	4	7	9	72	-78	4	6	9	137	148
4	5	9	205	227	4	-4	9	113	-122	4	-5	9	74	75
4	-4	10	126	-137	4	4	10	96	106	4	5	10	109	114
4	7	10	80	-92	4	6	11	98	-108	4	5	11	55	-62
4	4	11	44	47	5	5	11	147	-159	5	6	11	146	-156
5	8	10	156	165	5	6	10	177	-197	5	5	10	101	-106
5	5	9	203	222	5	6	9	47	-43	5	8	9	48	51
5	9	9	52	58	8	5	10	153	169	8	5	9	71	80
5	8	8	32	22	5	6	8	31	26	5	5	8	194	204
5	-6	8	42	-48	5	-6	7	44	48	5	-5	7	73	-82
5	5	7	184	-205	5	6	7	171	-179	5	7	7	121	-124

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
7	5	8	58	64	7	5	9	40	-45	7	5	10	36	33
6	5	11	36	-40	6	5	10	170	-188	6	5	8	49	55
6	5	7	197	-210	5	6	6	241	-248	5	5	6	399	430
5	-5	6	205	-219	-6	-5	6	37	38	-5	-5	8	51	-65
-5	-5	7	41	-42	-5	-5	6	65	-80	-5	5	5	104	-113
5	5	5	617	657	5	5	6	404	430	5	5	7	186	-205
5	5	8	189	204	5	5	9	200	222	5	5	10	95	-106
5	5	11	147	-159	5	-5	7	75	-82	5	-5	6	190	-219
-5	5	5	104	-113	-5	5	5	111	-113	-5	5	6	43	41
-5	5	7	111	117	-6	5	8	155	164	-6	5	7	60	68
-6	5	6	205	-213	-5	-5	6	72	-80	-5	5	6	33	41
-5	6	6	102	113	6	-5	7	36	38	6	-5	8	86	95
-5	6	7	58	62	-5	5	7	111	117	-5	-5	7	38	-42
-5	-6	7	124	-137	-5	-5	8	60	-65	-5	6	8	114	-128
-6	-6	7	75	82	-6	6	7	180	196	6	-6	7	99	-114
-6	6	7	187	196	-6	-6	7	70	82	6	6	6	416	-430
6	6	7	70	-79	6	6	8	129	134	6	6	9	33	-36
6	6	10	88	-92	7	6	10	82	90	7	6	8	97	110
6	7	7	210	214	6	6	7	75	-79	6	-6	7	110	-114
6	6	8	124	134	6	7	8	112	108	6	7	9	39	-38
6	6	9	37	-36	6	6	10	88	-92	6	7	10	80	85
7	7	10	45	50	7	7	9	111	-119	8	7	9	69	-77
7	8	8	253	-260	7	7	8	38	-33	7	7	7	136	148
7	7	9	110	-119	7	7	10	47	50	8	8	8	139	-146
0	4	16	57	62	0	3	16	34	-36	0	2	16	103	-115
0	-3	15	77	83	0	-2	15	66	67	0	1	15	82	90
0	2	15	34	-26	0	3	15	104	-121	0	6	15	65	-72
0	7	15	35	-39	0	9	14	42	55	0	7	14	91	-99
0	5	14	37	44	0	4	14	82	-90	0	3	14	44	-43
0	2	14	124	134	0	1	14	111	122	0	-2	14	59	62
0	-7	13	82	87	0	-6	13	65	-71	0	-5	13	106	-110
0	0	13	43	-46	0	2	13	59	63	0	5	13	79	86
0	6	13	143	156	0	8	13	54	-55	0	11	12	40	35
0	10	12	90	102	0	4	12	38	-37	0	3	12	101	-110
0	2	12	42	-43	0	0	12	72	-75	0	-1	12	117	-125
0	-2	12	108	-115	0	-3	12	88	92	0	-5	12	87	-93
0	-6	12	67	73	0	-7	12	138	150	0	-8	11	123	-132
0	-7	11	38	39	0	-6	11	145	160	0	-4	11	40	41
0	-3	11	145	150	0	6	11	126	-141	0	7	11	132	-143
0	8	11	67	-75	0	10	11	47	-50	10	0	14	40	-44
10	0	12	60	-67	10	0	11	77	-84	0	10	10	49	-55
0	9	10	62	70	0	8	10	69	-78	0	-5	10	30	-37
0	-7	10	97	-111	0	-8	10	101	-113	-9	0	11	47	48
-9	0	10	42	41	0	-6	9	37	41	0	9	9	56	60
9	0	10	180	185	9	0	11	66	-73	9	0	13	38	41
9	0	14	63	70	8	0	15	40	37	8	0	14	75	81
8	0	12	70	-73	8	0	11	127	135	8	0	10	101	104

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-8	0	8	52	-56	-8	0	10	83	86	-8	0	12	69	-79
-7	0	12	110	-114	-7	0	11	82	-94	-7	0	10	64	64
-7	0	9	85	88	7	0	11	113	124	7	0	13	111	-118
6	0	14	60	-76	6	0	13	83	-91	6	0	11	94	-101
-6	0	9	121	132	-6	0	12	62	74	-6	0	13	71	79
-5	0	12	36	33	5	0	12	33	-37	5	0	13	47	58
5	0	14	39	49	4	0	15	57	63	4	0	14	120	140
4	0	13	54	-66	-4	0	11	44	-40	-4	0	12	157	-172
-4	0	13	41	-50	-3	0	13	157	179	-3	0	12	48	54
-3	0	11	91	-104	3	0	13	132	-155	3	0	14	36	-48
3	0	15	64	78	2	0	16	38	43	2	0	14	104	-119
2	0	12	96	110	-2	0	12	217	243	-2	0	13	83	98
-2	0	15	39	-52	-1	0	14	102	-126	-1	0	13	81	-98
1	0	12	98	113	1	0	13	42	54	1	0	14	39	44
1	0	15	43	-48	1	0	16	46	48	0	0	13	40	-46
0	0	12	66	-75	0	0	12	61	-75	0	0	13	39	-46
1	0	16	34	48	1	0	14	43	44	1	0	13	43	54
1	0	12	97	113	-1	0	13	81	-98	-1	0	14	105	-126
-2	0	15	48	-52	-2	0	13	84	98	-2	0	12	214	243
2	0	12	101	110	2	0	14	103	-119	3	0	15	63	78
3	0	14	46	-48	3	0	13	134	-155	-3	0	11	93	-104
-3	0	12	49	54	-3	0	13	154	179	-4	0	13	46	-50
-4	0	12	151	-172	-4	0	11	41	-40	4	0	13	62	-66
4	0	14	122	140	4	0	15	52	63	5	0	14	37	49
5	0	13	53	58	5	0	12	38	-37	-5	0	12	35	33
-5	0	13	45	-40	-6	0	13	71	79	-6	0	12	66	74
-6	0	9	120	132	6	0	11	96	-101	6	0	13	81	-91
6	0	14	72	-76	7	0	13	105	-118	7	0	12	37	-38
7	0	11	120	124	-7	0	9	81	88	-7	0	10	61	64
-7	0	11	90	-94	-7	0	12	105	-114	-8	0	12	72	-79
-8	0	10	81	86	-8	0	8	51	-56	8	0	10	100	104
8	0	11	128	135	8	0	12	73	-73	8	0	14	74	81
8	0	15	38	37	9	0	14	66	70	9	0	11	71	-73
9	0	10	177	185	0	9	9	54	60	0	-6	9	33	41
0	-8	9	36	36	-9	0	10	38	41	-9	0	11	46	48
0	-8	10	106	-113	0	-7	10	102	-111	0	-5	10	30	-37
0	8	10	73	-78	0	9	10	68	70	0	10	10	47	-55
10	0	11	81	-84	10	0	12	68	-67	10	0	14	38	-44
0	10	11	52	-50	0	9	11	41	-39	0	8	11	71	-75
0	7	11	127	-143	0	6	11	133	-141	0	-3	11	146	150
0	-4	11	44	41	0	-6	11	147	160	0	-8	11	123	-132
0	-7	12	140	150	0	-6	12	63	73	0	-5	12	87	-93
0	-3	12	88	92	0	-2	12	109	-115	0	-1	12	120	-125
0	0	12	71	-75	0	2	12	36	-43	0	3	12	101	-110
0	4	12	34	-37	0	10	12	94	102	0	10	13	53	53
0	8	13	50	-55	0	6	13	148	156	0	5	13	81	86
0	2	13	52	63	0	0	13	44	-46	0	-5	13	104	-110

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	-6	13	63	-71	0	-7	13	79	87	0	-2	14	56	62
0	1	14	113	122	0	2	14	122	134	0	4	14	83	-90
0	5	14	43	44	0	7	14	87	-99	0	9	14	51	55
0	6	15	75	-72	0	3	15	106	-121	0	1	15	78	90
0	-2	15	66	67	0	-3	15	79	83	0	1	16	37	-33
0	2	16	105	-115	0	3	16	34	-36	0	4	16	56	62
1	4	16	81	88	1	3	16	100	108	1	-2	15	64	-60
1	-1	15	84	-92	1	1	15	39	-43	1	2	15	109	-122
1	3	15	55	-63	1	4	15	52	60	1	6	15	37	-39
1	7	15	41	52	1	8	14	40	37	1	7	14	39	-32
1	6	14	71	-72	1	3	14	65	-70	1	1	14	36	43
1	-2	14	63	69	1	-4	14	95	95	1	-5	14	99	108
1	-7	13	73	-74	1	-6	13	139	-154	1	-4	13	54	62
1	-2	13	46	-46	1	-1	13	100	108	1	2	13	47	-49
1	4	13	45	54	1	7	13	44	-50	1	10	13	38	-50
1	11	13	52	-58	1	11	12	43	-47	1	8	12	80	87
1	7	12	123	134	1	5	12	84	87	1	4	12	173	186
1	2	12	118	-122	1	1	12	38	-34	1	-2	12	129	-136
1	-4	12	47	52	1	-5	12	94	-101	1	-6	12	91	-96
1	-7	12	39	42	1	-8	12	58	63	1	-7	11	75	87
1	-6	11	65	67	1	-5	11	40	41	1	-4	11	50	51
1	7	11	101	-114	1	8	11	157	171	1	9	11	58	67
1	11	11	68	86	11	1	12	103	104	11	1	13	51	54
10	1	14	62	-70	10	1	13	43	54	10	1	12	70	76
1	10	10	103	-112	1	9	10	87	97	1	8	10	64	-71
-10	-1	10	59	-62	-9	-1	10	39	-39	-9	-1	9	87	-90
1	-7	9	37	33	1	-6	9	125	-141	9	1	10	35	38
9	1	11	188	-201	9	1	12	50	-45	8	1	14	59	68
8	1	13	58	61	8	1	12	60	-69	8	1	10	88	89
-8	-1	9	117	-131	-8	-1	10	80	89	-8	-1	11	84	91
-7	-1	12	64	-74	-7	-1	10	62	67	7	1	11	54	62
7	1	14	51	65	7	1	15	48	58	-6	-1	9	76	-94
-5	-1	14	76	78	-5	-1	12	120	135	-5	-1	11	112	123
5	1	12	113	-129	5	1	15	69	-87	4	1	16	48	-51
4	1	14	101	116	4	1	13	47	49	4	1	12	65	-78
-4	-1	11	63	64	-4	-1	12	166	-188	-4	-1	13	52	-51
-3	-1	15	62	-68	-3	-1	12	190	-215	-3	-1	11	148	-166
3	1	14	55	60	3	1	15	72	89	3	1	16	44	-48
2	1	14	75	-91	2	1	13	63	-73	2	1	12	65	-81
-2	-1	11	126	-145	-2	-1	12	56	65	-2	-1	13	124	141
-1	-1	13	56	69	1	1	15	34	-43	1	-1	15	77	-92
1	-1	13	94	108	-1	1	12	62	-74	-1	1	13	157	-180
-1	1	14	44	-50	-1	1	15	83	103	-2	1	14	102	-120
-2	1	13	105	-121	-2	1	12	93	110	2	-1	12	181	203
2	-1	13	104	125	2	-1	14	63	-70	3	-1	15	54	63
3	-1	14	96	-115	3	-1	13	34	-43	3	-1	12	114	129
-3	1	11	57	67	-3	1	12	104	123	-3	1	13	78	90

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-4	1	11	87	99	4	-1	12	61	-72	4	-1	13	116	-133
5	-1	13	67	76	-5	1	10	150	-166	-5	1	13	83	-95
-6	1	13	57	68	-6	1	12	115	123	-6	1	11	52	-52
-6	1	10	74	-82	-6	1	9	47	53	6	-1	12	137	152
6	-1	13	87	96	6	-1	14	54	-62	7	-1	14	78	-86
7	-1	13	71	-76	7	-1	12	50	60	-7	1	9	104	113
-7	1	13	111	123	-8	1	12	50	-53	-8	1	10	38	-37
-8	1	9	49	-52	8	-1	11	96	98	8	-1	13	43	-41
9	-1	14	44	43	9	-1	13	50	50	9	-1	10	101	103
-1	9	9	30	-37	-1	-8	9	162	179	-9	1	9	36	43
-9	1	10	46	-50	-1	-9	10	141	159	-1	-8	10	55	64
-1	-7	10	127	-142	-1	-5	10	44	52	-1	7	10	85	93
-1	9	10	103	113	10	-1	12	41	46	11	-1	13	108	-115
-1	10	11	86	-99	-1	7	11	34	26	-1	6	11	30	32
-1	-2	11	155	158	-1	-4	11	134	-141	-1	-6	11	36	37
-1	-7	11	118	-129	-1	-8	11	120	-137	-1	-8	12	81	-86
-1	-6	12	90	103	-1	-3	12	76	86	-1	-2	12	32	39
-1	1	12	70	-74	-1	3	12	45	47	-1	4	12	50	-52
-1	5	12	154	-169	-1	6	12	68	-76	-1	7	12	46	51
-1	8	12	73	-77	-1	9	12	125	-138	-1	11	12	49	62
-1	11	13	57	64	-1	10	13	54	67	-1	8	13	39	-50
-1	7	13	69	78	-1	6	13	162	174	-1	5	13	55	-63
-1	4	13	62	-68	-1	3	13	78	85	-1	1	13	170	-180
-1	-1	13	67	69	-1	-3	13	44	-44	-1	-5	13	40	38
-1	-7	13	45	49	-1	-4	14	60	-67	-1	-3	14	99	-104
-1	-2	14	42	40	-1	1	14	47	-50	-1	2	14	106	116
-1	3	14	48	56	-1	4	14	55	-67	-1	5	14	67	69
-1	6	14	90	101	-1	6	15	47	-56	-1	4	15	33	-29
-1	2	15	106	117	-1	1	15	89	103	-1	-2	15	80	87
-2	-2	15	40	-39	-2	2	15	53	50	-2	4	15	34	39
-2	6	15	34	-37	-2	8	14	45	39	-2	6	14	42	49
-2	5	14	38	45	-2	4	14	44	-45	-2	3	14	38	34
-2	-3	14	82	-86	-2	-4	14	52	50	-2	-5	14	90	94
-2	-6	13	54	-66	-2	-4	13	97	101	-2	-2	13	71	-76
-2	2	13	116	-126	-2	5	13	177	-192	-2	9	13	37	-47
-2	10	12	70	-82	-2	9	12	61	-67	-2	8	12	67	80
-2	7	12	98	110	-2	6	12	96	-106	-2	5	12	53	-61
-2	4	12	129	138	-2	3	12	84	92	-2	2	12	63	-69
-2	-2	12	42	-38	-2	-3	12	56	58	-2	-4	12	39	44
-2	-5	12	33	-36	-2	-6	12	56	-58	-2	-8	12	35	-34
-2	-9	11	69	77	-2	-7	11	42	-50	-2	-5	11	52	-49
-2	-4	11	70	-70	-2	-3	11	93	-93	-2	-2	11	39	-32
-2	4	11	112	126	-2	5	11	123	135	-2	6	11	66	-70
-2	7	11	32	41	-2	8	11	129	140	-2	10	11	57	-62
-2	11	11	36	41	11	-2	12	81	81	10	-2	13	95	101
10	-2	12	110	112	-2	10	10	33	-30	-2	9	10	61	67
-2	7	10	73	-82	-2	-4	10	75	81	-2	-5	10	123	132

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-2	-7	10	77	78	-2	-8	10	133	146	-2	-9	10	65	74
-10	2	10	65	-61	-9	2	10	101	-106	-9	2	9	157	-162
-2	-8	9	53	54	-2	-7	9	42	52	-2	-6	9	62	-74
-2	8	9	86	-96	-2	9	9	89	-99	9	-2	11	73	-76
9	-2	13	43	52	8	-2	12	67	-69	8	-2	10	48	-48
8	-2	9	82	-86	-2	-7	8	59	69	-8	2	8	83	-90
-8	2	9	96	-103	-8	2	11	70	76	-7	2	13	46	44
-7	2	11	44	53	-7	2	10	39	44	7	-2	10	57	-59
7	-2	12	55	58	6	-2	13	140	155	6	-2	11	113	-126
-6	2	9	79	-93	-6	2	10	94	-110	-6	2	13	55	-61
-5	2	13	82	-88	-5	2	11	57	70	-5	2	10	38	32
5	-2	11	97	-108	5	-2	12	168	-191	5	-2	15	101	-117
4	-2	15	54	-59	4	-2	14	66	74	4	-2	13	33	-37
4	-2	12	73	-77	-4	2	11	112	126	-4	2	12	49	-64
-4	2	14	40	44	-3	2	11	104	-118	3	-2	12	87	97
3	-2	13	45	53	3	-2	15	53	63	2	-2	13	40	44
-2	2	12	59	-69	-2	2	13	106	-126	-2	-2	13	68	-76
-2	-2	12	31	-38	-2	-2	11	32	-32	2	2	13	55	66
3	2	14	76	90	3	2	13	78	89	3	2	12	41	50
-3	-2	11	74	88	-3	-2	12	153	-172	-3	-2	13	49	-60
-4	-2	14	91	97	-4	-2	12	40	47	-4	-2	11	212	235
4	2	12	113	-129	4	2	15	104	-117	5	2	16	64	70
5	2	15	64	-74	5	2	14	80	-91	5	2	13	72	83
5	2	12	39	-46	-5	-2	10	180	-196	-5	-2	11	50	54
-5	-2	12	71	85	-5	-2	13	40	-45	-6	-2	13	59	-69
-6	-2	11	63	-75	-6	-2	10	109	-120	-6	-2	9	53	61
6	2	12	239	256	6	2	13	59	69	6	2	14	35	-29
7	2	12	97	104	7	2	11	152	165	-7	-2	8	73	80
-7	-2	9	34	44	-7	-2	11	38	35	-8	-2	12	78	84
-8	-2	10	54	-58	-8	-2	9	68	-78	8	2	11	50	-58
8	2	12	40	-41	8	2	13	58	-57	9	2	12	38	37
9	2	11	86	-94	9	2	10	85	-86	2	-6	9	148	-167
2	-7	9	53	-64	2	-8	9	100	107	-9	-2	10	75	-79
-9	-2	11	52	-53	2	-9	10	82	90	2	-5	10	105	116
2	9	10	58	64	2	10	10	71	-75	10	2	11	158	169
10	2	12	88	95	11	2	13	92	-99	2	10	11	41	-48
2	9	11	60	-62	2	8	11	215	232	2	7	11	222	229
2	-3	11	102	-106	2	-7	11	33	-34	2	-7	12	84	-89
2	-6	12	77	-86	2	-3	12	34	-44	2	-2	12	30	-26
2	3	12	170	184	2	4	12	70	76	2	5	12	79	-84
2	7	12	109	115	2	9	12	127	-141	2	11	13	43	49
2	8	13	63	-72	2	6	13	45	-56	2	5	13	135	-150
2	4	13	49	-52	2	3	13	77	87	2	2	13	63	66
2	-2	13	42	44	2	-3	13	72	-77	2	-4	13	54	57
2	-5	13	139	149	2	-6	13	38	38	2	-5	14	96	100
2	-4	14	40	-34	2	-3	14	57	-63	2	7	15	90	95
2	6	15	56	56	2	5	15	37	31	2	4	15	72	84

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	3	15	52	53	2	3	16	51	58	2	4	16	44	-43
2	5	16	54	-63	3	5	16	68	-71	3	4	16	59	-63
3	-3	15	104	114	3	8	15	47	-55	3	9	15	47	-46
3	9	14	57	59	3	8	14	64	61	3	5	14	58	59
3	3	14	34	-41	3	-3	14	33	-39	3	-4	14	154	-163
3	-5	14	70	-80	3	-6	13	102	108	3	-5	13	68	76
3	-4	13	61	-63	3	3	13	39	-36	3	4	13	138	-155
3	6	13	76	86	3	7	13	48	-59	3	9	13	92	100
3	10	13	90	97	3	12	12	52	-55	3	10	12	98	105
3	8	12	173	-192	3	5	12	115	-127	3	4	12	142	-156
3	-9	11	56	-66	3	-8	11	82	-91	3	-6	11	42	-51
3	-5	11	56	-57	3	-4	11	72	-74	3	7	11	117	124
3	8	11	50	-50	3	9	11	160	-178	3	11	11	45	-39
11	3	12	118	-131	11	3	13	44	-54	11	3	14	69	73
10	3	11	75	77	3	-5	10	65	69	3	-6	10	81	91
3	-8	10	64	-70	-10	-3	10	72	72	-9	-3	11	68	-72
-9	-3	9	69	70	9	3	10	95	101	9	3	11	79	89
9	3	12	105	109	9	3	13	50	51	9	3	14	46	43
8	3	13	57	-58	8	3	12	109	-122	8	3	11	48	-46
3	-7	8	36	-38	-8	-3	11	60	-68	-7	-3	10	61	70
-7	-3	9	58	55	-7	-3	8	128	-141	7	3	11	144	160
7	3	12	84	-91	7	3	13	140	-159	7	3	14	38	-46
6	3	15	68	79	6	3	14	60	-66	6	3	13	34	-39
6	3	12	171	189	-6	-3	9	260	279	-6	-3	10	68	79
-6	-3	11	74	-75	-6	-3	13	50	53	-5	-3	13	54	-60
-5	-3	12	45	51	-5	-3	11	149	-164	-5	-3	10	90	-102
5	3	12	161	179	5	3	13	48	55	5	3	16	67	86
4	3	16	56	71	4	3	15	42	-46	4	3	14	56	-72
4	3	12	76	-81	-4	-3	10	158	-166	-4	-3	11	37	34
-4	-3	12	47	50	-4	-3	13	33	39	-3	-3	13	47	55
-3	-3	12	53	68	-3	-3	11	62	74	3	-3	15	97	114
3	-3	14	32	-39	3	-3	12	28	31	-3	3	11	146	-170
-3	3	13	50	54	-3	3	15	51	-58	-4	3	13	48	53
-4	3	12	53	-56	-4	3	11	42	-47	4	-3	11	129	151
4	-3	12	42	54	4	-3	13	31	-26	4	-3	14	121	137
4	-3	15	70	85	5	-3	15	36	-42	5	-3	14	33	40
5	-3	13	52	-55	5	-3	12	104	-114	5	-3	11	50	50
-5	3	10	80	89	-5	3	11	71	79	-5	3	14	66	78
-6	3	11	42	-52	-6	3	9	34	-38	6	-3	10	64	67
6	-3	11	78	-84	6	-3	12	73	-81	6	-3	13	36	-42
7	-3	14	55	47	7	-3	12	60	64	7	-3	11	72	79
7	-3	9	71	74	-7	3	8	89	-93	-7	3	9	42	49
-7	3	11	46	-46	-7	3	12	82	-98	-8	3	11	76	81
-8	3	10	140	157	-8	3	8	59	-65	-3	-7	8	71	75
8	-3	9	39	-43	8	-3	10	61	60	8	-3	11	83	84
9	-3	12	102	-107	9	-3	11	85	-87	9	-3	10	42	44
-3	8	9	64	-64	-3	7	9	115	129	-3	-6	9	129	-134

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-3	-8	9	83	-99	-9	3	9	126	-135	-9	3	10	38	51
-9	3	11	91	96	-10	3	10	77	-87	-3	-9	10	41	-44
-3	6	10	65	67	-3	7	10	106	-120	-3	8	10	80	-87
-3	9	10	51	57	10	-3	11	120	-123	11	-3	12	69	70
-3	9	11	79	96	-3	7	11	119	-133	-3	5	11	108	121
-3	4	11	47	-50	-3	3	11	154	-170	-3	-3	11	71	74
-3	-5	11	35	28	-3	-6	11	79	86	-3	-7	11	68	77
-3	-8	11	58	58	-3	-9	11	39	45	-3	-5	12	87	-94
-3	-4	12	63	-63	-3	-3	12	69	68	-3	4	12	91	103
-3	5	12	80	88	-3	6	12	35	-42	-3	8	12	77	88
-3	9	12	66	71	-3	10	12	38	33	-3	7	13	56	-62
-3	4	13	40	39	-3	3	13	55	54	-3	-3	13	56	55
-3	-4	13	55	58	-3	-5	13	78	-86	-3	-6	13	61	-59
-3	-4	14	48	52	-3	-3	14	38	35	-3	4	14	64	-66
-3	7	14	106	-119	-3	8	14	38	-40	-3	5	15	82	89
-3	3	15	58	-58	-4	6	14	65	66	-4	4	14	57	-57
-4	-4	13	40	-52	-4	4	13	71	69	-4	6	13	127	140
-4	7	13	82	91	-4	10	12	50	59	-4	8	12	51	-59
-4	5	12	34	33	-4	-4	12	37	-41	-4	-5	12	37	42
-4	-6	12	104	110	-4	-6	11	53	50	-4	-5	11	66	74
-4	-4	11	53	-54	-4	4	11	83	-94	-4	7	11	87	-102
-4	8	11	66	-73	10	-4	12	100	-104	-4	10	10	45	50
-4	8	10	55	-66	-4	7	10	56	65	-4	6	10	107	117
-4	5	10	73	-80	-4	4	10	70	-71	-4	-4	10	74	-76
-4	-6	10	98	-102	-4	-7	10	84	-86	-9	4	10	115	120
-4	-7	9	37	40	-4	6	9	33	37	-4	7	9	157	168
-4	8	9	44	43	9	-4	10	119	123	9	-4	11	69	71
9	-4	12	64	-65	8	-4	12	69	75	8	-4	11	134	140
8	-4	9	75	-81	-4	6	8	46	38	-4	-6	8	93	102
-4	-7	8	55	59	-8	4	8	38	-39	-8	4	9	114	116
-8	4	10	60	70	-8	4	11	111	-132	-8	4	12	76	-87
-7	4	11	114	-135	-7	4	9	32	36	-7	4	8	67	-75
7	-4	9	53	-62	7	-4	10	164	-173	7	-4	11	38	-37
7	-4	12	45	38	7	-4	13	36	-43	6	-4	14	80	-92
6	-4	9	34	-32	-6	4	9	70	82	-6	4	12	74	89
-6	4	13	52	65	-5	4	10	38	48	5	-4	10	34	36
5	-4	11	74	86	5	-4	12	80	90	5	-4	14	46	46
4	-4	12	57	65	4	-4	11	56	68	4	-4	10	122	-137
-4	4	10	60	-71	-4	4	11	80	-94	-4	4	13	58	69
-4	4	14	49	-57	-4	-4	13	47	-52	-4	-4	12	39	-41
-4	-4	11	52	-54	-4	-4	10	68	-76	4	4	12	69	-78
4	4	14	37	47	5	4	13	38	49	5	4	12	94	110
-5	-4	9	141	153	-5	-4	10	69	81	-6	-4	13	64	65
-6	-4	10	157	176	-6	-4	8	169	-186	6	4	13	125	-140
6	4	15	54	61	6	4	16	60	-72	7	4	14	48	61
7	4	13	69	-81	7	4	12	197	-220	-7	-4	8	157	-175
-7	-4	9	115	-126	-7	-4	11	76	84	-7	-4	12	84	-86

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-8	-4	9	68	-68	-8	-4	8	42	41	4	-7	8	78	87
8	4	11	40	-38	8	4	13	89	100	8	4	14	100	116
9	4	15	41	-52	9	4	14	47	-50	9	4	13	57	54
9	4	12	68	76	9	4	10	92	99	4	-6	9	109	122
4	-8	9	39	41	-9	-4	9	40	47	-9	-4	11	40	39
4	-9	10	39	-49	4	-8	10	100	-117	4	-5	10	103	-118
4	-4	10	127	-137	4	10	10	103	-111	10	4	12	49	-59
11	4	14	61	68	4	10	11	68	73	4	8	11	65	-72
4	7	11	75	-82	4	-4	11	61	68	4	-5	11	82	-85
4	-7	11	86	99	4	-9	11	64	-76	4	-8	12	105	119
4	-7	12	61	72	4	-4	12	58	65	4	4	12	64	-78
4	6	12	42	49	4	7	12	50	-56	4	8	12	103	-109
4	9	12	106	116	4	10	12	74	82	4	11	12	49	-39
12	4	13	91	101	4	11	13	84	-98	4	9	13	143	154
4	8	13	63	72	4	7	13	80	-84	4	6	13	114	123
4	5	13	126	142	4	-6	13	51	-56	4	-5	14	62	-64
4	4	14	37	47	4	5	14	111	123	4	8	14	69	70
4	9	14	38	-27	4	10	14	112	-122	4	11	14	69	-80
4	6	15	91	-106	4	5	15	77	-82	5	6	16	62	69
5	5	15	45	-41	5	7	15	98	110	5	8	15	53	50
5	11	14	69	77	5	10	14	71	-77	5	9	14	79	-83
5	7	14	48	-56	5	6	14	124	-135	5	-5	14	42	50
5	-5	13	60	64	5	5	13	38	39	5	7	13	93	-97
5	8	13	51	50	5	10	13	110	-121	5	11	13	54	-69
5	9	12	60	69	5	7	12	53	64	5	6	12	76	85
5	-6	12	72	-79	5	-7	12	58	-60	5	-8	11	72	82
5	-7	11	98	108	5	-5	11	35	-22	5	6	11	141	-156
5	7	11	111	126	5	8	11	38	48	5	9	11	39	-37
5	11	11	60	66	11	5	12	37	38	5	10	10	101	-112
5	9	10	52	-56	5	8	10	158	165	5	-5	10	72	-76
5	-6	10	31	31	5	-8	10	67	-72	5	-7	9	109	-126
5	-6	9	75	-85	5	-5	9	53	-60	9	5	10	130	-140
9	5	11	103	-113	9	5	14	128	-140	8	5	15	102	-115
8	5	13	116	132	8	5	12	39	44	8	5	10	156	169
5	-6	8	47	-48	5	-7	8	105	119	-8	-5	8	155	166
-8	-5	10	46	-52	-8	-5	11	80	82	-7	-5	12	55	-58
-7	-5	9	136	-156	-7	-5	8	44	57	-7	-5	7	221	244
7	5	11	65	74	7	5	12	55	-61	7	5	13	81	96
7	5	14	120	139	6	5	13	64	-74	6	5	12	74	-77
6	5	11	36	-40	-6	-5	8	139	-155	-6	-5	9	91	-107
-6	-5	12	43	-44	-5	-5	13	34	38	-5	-5	12	72	89
-5	-5	10	57	62	-5	-5	9	45	48	5	5	13	38	39
5	5	15	36	-41	5	-5	14	35	50	5	-5	13	53	64
5	-5	10	72	-76	5	-5	9	52	-60	-5	5	9	36	-34
-5	5	10	36	-31	-5	5	13	103	-115	-6	5	13	66	-70
-6	5	12	86	95	-6	5	11	70	82	-6	5	8	158	164
6	-5	9	99	109	6	-5	10	72	82	6	-5	11	53	-59

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
6	-5	13	66	75	7	-5	11	106	-117	7	-5	10	100	-109
7	-5	9	168	182	7	-5	8	87	89	-7	5	7	76	-81
-7	5	8	35	38	-7	5	9	37	29	-7	5	10	104	-115
-7	5	11	35	31	-7	5	12	142	157	-8	5	11	89	-100
-8	5	10	74	-76	-5	7	8	140	-153	-5	8	8	64	72
8	-5	9	38	-39	8	-5	10	143	-147	8	-5	12	43	40
9	-5	12	79	83	9	-5	11	111	113	9	-5	10	56	50
-5	9	9	84	-90	-5	7	9	34	-41	-5	6	9	153	-168
-5	5	9	29	-34	-5	-5	9	47	48	-5	-7	9	112	119
-5	-8	9	41	50	-5	-8	10	64	71	-5	-6	10	47	-53
-5	-5	10	54	62	-5	6	10	70	76	-5	7	10	75	83
10	-5	11	42	50	-5	10	11	47	-53	-5	9	11	35	-44
-5	5	11	36	36	-5	-6	11	91	-93	-5	-7	11	104	-109
-5	-7	12	41	-36	-5	-5	12	85	89	-5	6	12	91	-104
-5	9	12	70	-81	-5	7	13	100	113	-5	5	13	110	-115
-6	6	13	129	-144	-6	8	12	51	54	-6	7	12	57	-61
-6	6	12	91	-101	-6	-6	12	52	-54	-6	-8	11	58	61
-6	-6	11	73	-73	-6	6	11	52	62	-6	8	11	73	79
-6	9	11	67	75	-6	9	10	34	41	-6	-6	10	34	26
-6	-7	10	78	85	-6	-9	10	62	-67	-9	6	9	86	-88
-6	-8	9	60	-66	-6	-7	9	61	66	-6	6	9	57	-65
-6	7	9	78	-88	-6	9	9	65	-79	9	-6	10	50	-54
8	-6	11	73	-78	8	-6	10	71	-74	8	-6	9	59	63
-6	8	8	63	74	-6	7	8	50	-54	-6	6	8	63	70
-6	-6	8	58	60	-6	-7	8	39	-43	-8	6	8	85	-91
-7	6	12	53	50	-7	6	11	82	92	-7	6	8	78	83
-6	-6	7	77	82	-6	7	7	36	-38	7	-6	8	60	-70
7	-6	9	207	225	7	-6	10	70	83	6	-6	13	66	72
6	-6	10	147	169	6	-6	9	28	-28	6	-6	8	211	-237
-6	6	8	63	70	-6	6	9	56	-65	-6	6	11	44	62
-6	6	12	87	-101	-6	6	13	128	-144	-6	-6	12	47	-54
-6	-6	11	69	-73	-6	-6	8	52	60	-6	-6	7	72	82
6	6	11	87	101	6	6	12	91	105	6	6	15	55	67
7	6	13	37	42	7	6	11	71	76	-7	-6	7	76	84
-7	-6	8	126	147	-7	-6	11	58	59	-8	-6	8	131	144
6	-7	8	146	-162	6	-6	8	216	-237	8	6	11	104	-111
8	6	14	92	-106	8	6	15	47	-54	9	6	15	65	79
9	6	14	51	-64	9	6	12	65	72	9	6	11	51	-55
9	6	10	119	-130	6	-7	9	180	-205	6	-8	9	52	-59
-9	-6	10	75	-82	6	-9	10	58	67	6	-7	10	44	48
6	-6	10	152	169	6	8	10	109	118	6	9	10	71	-74
10	6	11	103	117	10	6	12	44	41	10	6	13	49	-55
6	11	11	89	102	6	10	11	79	88	6	9	11	100	-107
6	8	11	53	-61	6	7	11	207	214	6	6	11	92	101
6	-7	12	63	-72	6	6	12	95	105	6	7	12	45	52
6	8	12	116	-130	6	10	12	44	35	6	12	12	59	-62
12	6	13	44	-51	6	8	13	44	-56	6	7	13	102	-111

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
6	-6	13	68	72	6	7	14	50	56	6	8	14	41	35
6	7	15	61	68	6	6	15	66	67	7	7	14	50	47
7	7	13	59	-66	7	8	13	48	53	7	9	13	82	93
7	11	12	61	-68	7	8	12	102	-111	7	7	12	131	-147
7	8	11	86	-96	7	10	11	59	72	11	7	12	107	-119
10	7	14	50	52	10	7	12	38	-36	10	7	11	47	44
7	8	10	67	72	7	7	10	50	50	7	-7	10	56	66
7	-8	10	47	-49	-9	-7	9	53	56	7	9	9	54	52
9	7	12	72	69	9	7	14	60	57	8	7	13	46	52
8	7	11	55	-64	8	7	9	69	-77	7	-7	8	149	-166
-8	-7	8	77	-85	-8	-7	10	40	-46	-7	-7	8	42	-44
-7	7	7	45	-47	7	7	10	48	50	7	7	11	38	38
7	7	12	128	-147	7	7	13	61	-66	7	-7	10	61	66
7	-7	8	147	-166	-7	7	7	45	-47	-7	7	7	39	-47
-7	7	9	51	57	-7	7	10	43	-42	-8	7	10	60	63
-8	7	9	86	96	-8	7	8	57	-59	-7	-7	8	39	-44
-7	7	8	46	51	-7	8	8	63	69	8	-7	9	78	83
8	-7	11	33	28	9	-7	10	41	37	-7	9	9	47	-55
-7	8	9	35	38	-7	7	9	51	57	-7	-8	9	69	-81
-7	-8	10	49	-50	-7	-7	10	43	42	-7	7	10	41	-42
-7	8	10	114	-125	-8	8	10	64	-73	-9	8	9	66	67
-8	8	9	71	82	8	-8	10	32	-50	-8	8	8	47	51
-8	8	8	53	51	-8	8	9	74	82	-8	8	10	71	-73
-8	8	8	39	51	8	8	9	125	137	8	8	10	90	93
8	8	12	78	83	8	8	13	104	123	9	8	12	69	80
9	8	10	39	-37	8	9	9	152	166	8	8	9	129	137
-9	-8	9	38	40	8	-8	10	49	-50	8	8	10	85	93
8	10	10	72	-78	11	8	13	62	63	8	11	11	54	-62
8	10	11	45	-53	8	8	12	79	83	8	9	12	75	78
8	12	12	71	81	8	10	13	62	-72	8	8	13	106	123
9	9	13	103	-119	9	10	13	98	-106	9	10	12	55	-51
9	11	11	60	71	11	9	12	86	91	10	9	11	60	72
9	10	10	53	-62	9	9	10	85	-96	9	9	10	85	-96
9	9	13	106	-119	10	10	10	109	118	10	10	11	118	131
11	10	12	52	-50	10	10	11	122	131	10	10	12	43	-39
10	11	12	61	-59	11	11	11	184	-199	0	-2	19	36	-30
0	2	19	49	-55	0	6	18	41	-44	0	-1	18	35	36
0	-6	17	55	-55	0	0	17	43	47	0	3	17	56	60
0	11	17	46	-51	0	7	16	36	43	0	4	16	52	62
0	3	16	39	-36	0	2	16	104	-115	0	1	16	37	-33
0	-1	16	72	-75	0	-2	16	53	-51	0	-7	15	55	51
0	-6	15	53	49	0	12	15	38	50	0	14	14	39	-45
0	11	14	42	-55	0	-6	14	36	-47	0	-9	14	53	-54
0	-11	13	54	63	0	12	13	58	-71	13	0	15	62	-72
12	0	16	44	-49	12	0	14	101	104	0	-9	12	50	-59
0	-10	12	50	60	-12	0	12	42	-42	11	0	18	40	45
10	0	14	37	-44	-9	0	14	49	50	9	0	16	41	-38

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
8	0	18	45	48	-8	0	15	42	-36	-8	0	16	71	-76
-7	0	15	41	-41	7	0	18	49	57	7	0	19	53	64
-4	0	17	53	58	-3	0	17	47	52	3	0	19	39	36
2	0	18	51	-57	-2	0	18	55	-63	1	0	16	43	48
0	0	18	45	45	0	0	17	43	47	0	0	17	37	47
1	0	16	42	48	-2	0	18	56	-63	-2	0	16	41	47
2	0	18	49	-57	-3	0	17	41	52	-4	0	17	53	58
5	0	18	42	-50	6	0	17	36	-37	7	0	19	50	64
7	0	18	39	57	-7	0	17	39	45	-8	0	16	66	-76
8	0	18	46	48	9	0	16	42	-38	-9	0	14	48	50
10	0	14	52	-44	-11	0	11	40	-36	-11	0	12	39	-31
-12	0	12	41	-42	0	-10	12	53	60	0	-9	12	51	-59
12	0	14	88	104	13	0	15	58	-72	0	12	13	63	-71
0	-11	13	49	63	0	-9	14	51	-54	0	-6	14	44	-47
0	11	14	38	-55	0	12	15	46	50	0	-6	15	48	49
0	-7	15	45	51	0	-2	16	48	-51	0	-1	16	64	-75
0	1	16	35	-33	0	2	16	106	-115	0	3	16	40	-36
0	4	16	60	62	0	11	17	38	-51	0	3	17	60	60
0	0	17	41	47	0	-6	17	49	-55	0	-1	18	36	36
0	0	18	44	45	0	7	18	46	-45	0	2	19	38	-55
1	7	18	45	7*	1	4	18	52	-45	1	-5	17	39	42
1	3	17	54	60	1	4	17	44	-40	1	5	17	78	-86
1	8	17	48	-52	1	7	16	72	76	1	6	16	51	55
1	-6	16	44	-46	1	-8	15	45	45	1	12	15	44	50
14	1	15	44	44	1	-10	14	39	-45	1	-10	13	47	-54
12	1	15	46	-56	1	-11	12	44	48	-10	-1	11	36	-31
-9	-1	15	71	75	9	1	15	65	-75	9	1	17	47	43
8	1	19	54	-66	-8	-1	14	38	36	-8	-1	16	34	-29
6	1	19	47	48	-5	-1	16	36	-36	-5	-1	15	37	50
-4	-1	16	48	-59	-3	-1	17	50	55	-3	-1	15	50	-68
3	1	18	38	56	3	1	19	38	43	-1	-1	17	43	-44
-1	1	18	38	38	-2	1	17	50	-59	2	-1	16	58	72
-3	1	18	36	-45	4	-1	18	33	31	5	-1	17	60	73
5	-1	16	56	75	-6	1	15	40	-26	-6	1	14	39	-43
6	-1	16	37	37	6	-1	18	80	-92	7	-1	17	46	-60
-7	1	16	51	55	-7	1	17	39	40	-8	1	15	53	-52
-9	1	13	47	-48	10	-1	14	51	-55	11	-1	15	53	56
11	-1	14	68	-72	11	-1	13	107	-115	-11	1	11	55	-51
-11	1	13	42	48	-12	1	12	51	-52	12	-1	13	57	-59
12	-1	14	67	78	12	-1	15	68	70	13	-1	14	54	67
-1	11	13	56	64	-1	-7	13	55	49	-1	-8	14	41	-37
-1	-7	14	43	-48	-1	-4	15	67	-75	-1	-6	15	41	45
-1	-8	15	38	-43	-1	-7	16	38	49	-1	-6	16	42	44
-1	1	16	44	35	-1	2	16	59	-65	-1	3	16	44	-51
-1	10	17	63	66	-1	-1	17	37	-44	-1	1	18	48	38
-1	2	18	41	47	-1	7	19	49	-49	-1	3	19	38	-45
-1	1	19	43	46	-2	6	19	39	28	-2	6	18	50	52

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-2	-5	17	40	35	-2	3	17	34	36	-2	5	17	54	-48
-2	8	17	52	-58	-2	10	17	48	51	-2	9	16	74	-81
-2	4	16	47	51	-2	-7	15	62	-65	-2	-3	15	51	-54
-2	13	15	42	-57	-2	9	14	52	59	-2	-5	14	90	94
-2	-8	14	46	47	-2	-9	14	46	58	-2	-11	13	32	-25
-2	-10	13	37	-35	-2	-8	13	40	45	12	-2	13	95	-94
-11	2	12	44	44	11	-2	14	102	-105	11	-2	17	49	-44
-9	2	13	66	-68	9	-2	17	45	53	6	-2	17	59	65
-6	2	14	74	-85	-6	2	17	46	-43	-5	2	15	42	56
5	-2	17	58	75	5	-2	18	43	45	4	-2	16	82	-97
-2	-2	15	34	-39	-4	-2	15	33	38	4	2	17	49	58
4	2	19	48	-59	-5	-2	15	46	54	-6	-2	14	61	-67
9	2	16	43	46	-9	-2	13	40	-35	-9	-2	14	55	-50
-10	-2	15	47	-49	-10	-2	14	56	-60	10	2	15	41	50
11	2	17	44	-40	2	-10	11	50	51	-11	-2	13	52	54
12	2	13	59	-65	2	-10	13	36	-45	2	-9	14	52	62
2	-6	14	97	104	2	12	14	57	66	2	13	15	47	-53
2	-4	15	76	-81	2	-5	15	43	-49	2	-8	15	37	-41
2	8	16	78	-84	2	9	16	48	-45	2	12	16	57	-59
2	10	17	42	57	2	6	17	42	38	2	4	17	114	-126
2	3	18	40	-43	2	5	18	51	64	2	6	18	54	59
3	10	18	58	-63	3	5	18	74	79	3	4	18	40	48
3	-3	18	34	20	3	5	17	98	105	3	6	17	62	69
3	9	17	57	56	3	13	17	41	41	3	13	16	53	53
3	10	16	50	43	3	7	16	42	-58	3	-4	16	47	51
3	-7	16	39	40	3	-8	15	36	-38	3	-5	15	65	-73
3	14	14	43	-45	3	-8	14	64	-66	3	-9	13	36	43
3	-8	13	33	29	3	13	13	48	58	12	3	14	71	76
3	-9	12	41	-40	-12	-3	12	54	-60	-12	-3	13	39	-51
-11	-3	12	39	-38	11	3	14	72	73	10	3	17	57	-67
10	3	15	41	40	-10	-3	12	35	27	-10	-3	13	70	69
-7	-3	13	73	78	6	3	17	56	-63	-5	-3	14	57	-69
3	-3	19	41	35	-4	3	16	43	-43	-4	3	15	52	-54
4	-3	15	75	85	4	-3	16	41	-53	4	-3	17	48	-58
5	-3	16	47	-64	5	-3	15	41	-42	6	-3	17	38	45
7	-3	15	42	47	-8	3	14	57	55	8	-3	16	38	-40
9	-3	17	52	56	10	-3	13	81	84	11	-3	13	61	64
11	-3	12	72	70	-3	-11	12	42	42	-3	-10	13	41	-48
-3	-8	14	50	55	-3	8	14	46	-40	-3	9	14	34	35
-3	13	14	49	68	-3	12	15	42	48	-3	9	15	54	53
-3	8	15	52	66	-3	5	15	85	89	-3	-5	16	58	-61
-3	4	16	62	71	-3	7	16	47	41	-3	8	16	53	66
-3	10	16	49	-61	-3	9	17	55	-59	-3	-4	18	37	40
-3	5	18	38	-29	-4	7	18	39	-40	-4	-5	17	48	-55
-4	8	16	63	65	-4	-5	16	40	-39	-4	-6	15	65	65
-4	4	15	67	-67	-4	9	15	49	58	-4	11	14	38	-55
-4	8	14	93	-104	-4	7	14	43	-49	-4	-11	13	42	48

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-4	-9	13	44	-48	-4	12	13	52	-61	-4	10	12	50	59
-11	4	12	51	-58	10	-4	13	38	-36	10	-4	12	99	-104
-9	4	13	52	60	9	-4	13	52	-58	9	-4	16	51	-50
8	-4	15	43	54	8	-4	14	54	49	-8	4	12	76	-87
-8	4	15	43	-53	-7	4	13	64	73	4	-4	16	43	51
4	-4	15	56	65	-4	4	15	59	-67	-4	-4	14	35	-33
5	4	17	68	-84	-6	-4	14	49	51	-6	-4	13	60	65
6	4	16	65	-72	7	4	18	59	70	7	4	17	40	45
-7	-4	14	64	66	-8	-4	13	67	-72	-8	-4	12	65	-67
9	4	15	50	-52	-10	-4	14	38	34	11	4	14	66	68
-11	-4	12	55	-54	-11	-4	13	56	-57	-12	-4	13	38	-44
4	-11	12	49	60	4	-8	12	103	119	12	4	15	58	-62
13	4	14	46	-55	4	-7	13	48	-54	4	-12	13	47	66
4	11	14	72	-80	4	11	15	53	55	4	-4	15	56	65
4	-7	15	48	53	4	-7	16	33	25	4	-4	16	51	51
4	8	16	64	63	4	9	16	40	37	4	14	17	44	-54
4	4	18	37	39	4	6	18	73	-75	4	10	18	46	-49
4	6	19	39	-41	4	7	20	50	54	5	7	19	48	54
5	11	18	53	58	5	-5	18	34	23	5	12	16	56	-69
5	7	16	38	44	5	6	16	61	69	5	-6	16	37	-45
5	11	15	67	79	5	12	14	70	81	5	11	14	70	77
5	-5	14	47	50	5	-6	14	40	44	5	-11	14	47	-58
5	-11	13	50	-57	5	-10	13	51	-59	5	-7	13	84	-91
12	5	15	50	-47	12	5	14	54	-48	-12	-5	12	65	68
10	5	16	55	63	10	5	15	55	63	-9	-5	12	71	73
8	5	19	48	-48	-8	-5	13	49	-56	-7	-5	13	61	-68
-7	-5	12	55	-58	7	5	17	47	51	6	5	17	61	64
-5	-5	15	47	47	5	-5	14	41	50	-6	5	14	43	-46
6	-5	17	37	41	7	-5	14	77	-87	-8	5	16	41	46
-8	5	14	54	-49	8	-5	13	35	-29	9	-5	12	77	83
-9	5	11	44	-51	-10	5	12	49	53	-10	5	11	49	53
-5	-9	11	40	43	-11	5	11	39	-41	-5	-11	12	41	-52
-5	9	12	75	-81	12	-5	15	40	38	-5	11	13	42	48
-5	-5	13	42	38	-5	6	14	83	84	-5	7	14	72	89
-5	12	14	35	-43	-5	8	15	55	-61	-5	7	15	41	-42
-5	-5	15	45	47	-5	-7	15	42	-46	-5	-6	16	65	66
-5	6	17	38	43	-6	-7	15	59	-59	-6	-6	15	52	-63
-6	-8	14	50	59	-6	6	13	129	-144	-6	11	13	34	37
12	-6	14	39	-41	-6	10	12	46	-52	-6	8	12	46	54
-6	-6	12	50	-54	-11	6	12	58	52	-6	-8	11	55	61
-6	10	11	43	-51	-6	11	11	53	-56	10	-6	14	41	40
10	-6	13	45	49	-10	6	11	65	62	-9	6	12	50	-54
8	-6	13	43	-45	-8	6	12	43	43	7	-6	13	44	48
6	-6	16	32	-25	6	-6	14	35	44	6	-6	13	60	72
-6	6	13	119	-144	-6	-6	15	50	-63	-6	-6	14	39	-47
-6	-6	12	50	-54	-8	-6	12	66	72	9	6	19	46	64
9	6	16	61	65	9	6	15	67	79	-9	-6	11	49	-55

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-9	-6	14	37	-36	10	6	15	86	101	10	6	17	67	-71
11	6	16	45	-60	6	-10	11	34	35	6	-8	12	46	-49
12	6	13	49	-51	6	-6	13	63	72	6	-9	13	37	39
6	-11	13	39	-48	6	-10	14	57	62	6	-9	14	33	35
6	-6	14	44	44	6	11	14	78	87	6	12	15	69	-80
6	7	16	54	-56	6	8	16	56	-62	6	11	16	52	-64
7	13	16	57	75	7	7	16	46	-46	7	-9	15	49	-56
7	8	15	46	-46	7	11	15	48	-37	7	-7	13	59	61
7	-9	12	31	-30	7	-9	11	50	-59	7	-8	11	33	-44
11	7	15	46	-38	10	7	16	57	-59	7	-9	10	45	52
-10	-7	10	52	56	-9	-7	14	33	-18	-9	-7	11	37	-42
9	7	15	51	50	-7	-7	14	73	78	-7	-7	13	42	41
7	-7	13	50	61	-8	7	13	41	44	9	-7	13	55	-65
-9	7	10	89	97	-9	7	12	43	-48	-7	-9	10	55	-58
-7	10	10	48	54	10	-7	12	46	-49	11	-7	13	58	58
-7	10	11	33	42	-7	9	11	81	89	-7	-7	11	38	40
-7	11	12	31	-40	-7	-7	13	48	41	-7	-8	13	61	-59
-7	-9	13	51	-62	-7	-9	14	35	-52	-7	-7	14	75	78
-7	9	15	33	35	-8	8	15	46	-45	-8	-8	14	50	-50
-8	-10	13	45	57	-8	-8	13	62	-58	-8	11	13	37	34
-8	-9	12	72	75	-8	8	11	59	-70	10	-8	12	39	-37
-8	9	10	52	-60	-9	8	11	40	-37	-9	8	9	68	67
9	-8	11	52	55	8	-8	12	56	65	-8	8	11	60	-70
-8	-8	14	47	-50	-8	-8	13	53	-58	-9	-8	9	37	40
-9	-8	10	43	48	8	-9	10	49	-57	10	8	15	45	-43
11	8	17	70	76	8	-9	11	40	-50	8	-8	12	55	65
12	8	13	79	75	13	8	14	47	-53	8	12	16	52	46
8	9	18	51	-44	9	10	15	59	59	9	10	14	42	52
11	9	13	43	58	-9	-9	13	42	45	-10	9	11	43	43
-9	-10	11	55	-62	-11	9	12	35	35	-11	10	11	43	55
10	10	14	51	66	11	10	12	49	-50	10	11	12	46	-59
10	11	13	60	62	10	10	14	58	66	10	11	16	47	-54
11	12	16	49	58	11	11	13	50	28	11	11	12	56	-62
12	12	12	71	80	0	0	11	25	-22*	1	0	11	25	21*
0	-5	7	26	-32	1	-1	9	23	28	2	-1	11	25	-34*
5	-1	10	28	28*	-5	1	5	25	36*	-1	6	9	22	-8*
-1	5	10	25	33*	-1	4	11	23	8*	-2	-4	7	27	39*
3	2	7	23	29*	-4	-2	10	24	26*	2	3	6	19	-23*
-6	-3	7	21	-22*	-3	-3	4	23	-19	-3	-3	7	25	35*
-4	-4	9	26	-28*	-6	6	6	22	-27*	6	8	8	27	-23*
6	9	9	29	-33*	7	7	8	28	-33	0	10	13	31	53
0	11	13	28	-34*	0	-5	11	29	-25*	0	9	11	30	-39
0	11	11	30	18*	-8	0	9	29	27*	7	0	12	31	-38
-5	0	13	32	-40	3	0	16	29	-34*	-1	0	12	25	31*
2	0	16	29	43	3	0	16	30	-34*	9	0	13	33	41
9	0	12	29	-38*	0	-9	10	25	31*	0	-5	11	25	-25*
0	9	13	31	36*	0	-5	14	30	-29*	0	7	15	35	-39

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	5	15	28	16*	0	2	15	31	-26	-7	-1	9	24	18*
5	1	13	27	22*	2	1	15	27	-8*	-4	1	12	31	-29*
6	-1	11	25	-34*	-8	1	11	32	-40*	-8	1	8	31	26*
8	-1	12	32	-12*	-1	8	11	28	26*	-1	-4	12	32	31*
-1	-6	13	29	33*	-1	8	14	27	-29*	-2	6	13	26	-32*
9	-2	10	32	44*	8	-2	13	33	-33*	-4	2	13	31	45*
2	-2	12	26	-26	-4	-2	13	30	-35*	-8	-2	8	23	13*
8	2	15	30	-37*	9	2	14	31	-16*	2	-8	10	29	39*
2	-6	10	26	13*	2	11	11	33	44*	2	-5	11	27	-24*
2	9	15	32	-41*	2	6	16	30	25*	3	6	12	29	33*
3	-3	12	29	31	3	-7	10	28	-34*	-8	-3	8	27	-23*
5	3	15	28	30*	-3	-3	14	27	35	-3	-3	10	23	23*
3	3	13	31	-36	3	3	14	28	-41	-4	3	14	29	31*
-6	3	13	29	-31*	-3	-7	10	31	-28*	-3	-3	10	27	23*
10	-3	12	31	-37*	-3	6	11	25	-26*	-3	-4	11	30	-30*
-3	3	14	30	-33*	-4	6	12	26	-32*	-4	10	11	26	22*
-4	-8	10	30	-36*	-9	4	11	31	35*	4	-4	13	25	-23*
6	4	12	29	-40*	9	4	11	29	-13*	5	10	11	34	26*
10	5	14	34	-37*	9	5	15	38	-47*	7	5	15	31	-36*
-5	5	11	29	36	-5	8	10	25	26*	-5	-6	12	32	38*
7	6	15	33	-42*	10	6	14	35	36*	6	11	12	32	-28*
6	6	14	29	-20*	7	11	13	33	32*	8	7	10	31	-28*
-7	8	11	26	-24*	-7	7	11	25	-32*	-8	9	9	28	-35*
8	8	11	32	-27*	8	9	11	31	-32*	8	8	11	30	-27*
8	11	13	33	-32*	9	9	14	37	-34*	10	10	12	40	-39
0	-7	17	31	-27*	0	-2	17	31	-29*	14	0	16	32	28*
0	-7	14	34	-25*	-11	0	12	34	-31	11	0	15	33	47*
10	0	15	30	-39*	-7	0	17	33	45	6	0	19	31	42*
5	0	18	33	-50	-2	0	16	32	47	1	0	17	31	43*
1	0	17	32	43*	-2	0	17	31	-34*	2	0	17	32	-28*
3	0	17	30	-41*	-6	0	14	30	28*	-7	0	15	34	-41
-8	0	15	30	-36	-9	0	16	29	-37*	-10	0	11	28	-25*
10	0	15	37	-39*	11	0	18	31	45	12	0	16	38	-49
0	14	14	36	-45	0	-5	16	32	-42*	0	8	16	36	38*
0	-4	17	30	28*	0	10	18	32	-37*	0	6	19	35	-37*
1	11	18	36	28*	1	1	18	31	-37*	1	2	17	29	41*
1	9	16	36	-41*	1	13	15	31	-29*	13	1	14	37	-43*
10	1	16	34	42*	-10	-1	14	35	-41*	-8	-1	15	29	26*
-7	-1	14	30	-35*	-5	-1	17	28	-24*	5	1	16	34	-29*
2	1	19	33	39*	1	1	18	33	-37*	4	-1	17	28	30*
6	-1	17	27	-11*	-7	1	14	33	19*	-1	-11	12	28	-26*
-1	12	14	35	-38*	-1	13	15	29	-32*	-1	-3	15	32	6*
-1	-3	16	34	40*	-1	5	16	34	-43*	-1	11	16	33	41*
-1	6	17	36	38*	-1	6	18	35	37*	-2	9	18	33	21*
-2	4	18	33	-35*	-2	2	18	35	42*	-2	-3	18	36	-49*
-2	-4	18	32	-36*	-2	9	17	30	-46*	-2	8	16	30	-16*
-2	3	16	28	25*	-2	-4	15	33	-32*	-2	-2	15	31	-39

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-2	8	15	30	42*	-2	-9	12	32	-34*	-10	2	11	35	-29*
-10	2	13	37	-43*	-10	2	14	33	-42*	8	-2	15	29	-37*
7	-2	18	29	-33*	-5	2	18	35	41*	-3	2	17	30	-34*
-3	2	16	29	-38*	-2	2	18	31	42*	2	2	19	31	29*
5	2	17	36	53*	7	2	16	35	-35*	2	-9	13	28	32*
2	-11	14	25	-19*	2	13	17	33	20*	2	9	17	40	46*
2	-4	18	32	-45*	3	7	18	38	-39*	3	3	18	36	-40*
3	11	17	40	-48*	3	8	16	36	-39*	3	9	15	36	-46
3	-6	14	28	22*	3	-11	13	29	31*	3	-10	11	28	29*
-9	-3	14	31	-38*	-6	-3	14	34	-41*	-6	-3	15	33	-32*
5	3	18	35	-29*	-3	-3	16	29	16*	6	-3	16	31	-17*
9	-3	15	31	-38*	-9	3	16	36	-31*	-10	3	12	34	-38*
-3	-9	12	32	-42*	-3	11	13	27	-40*	-3	-7	13	35	33*
-3	-11	13	26	19*	-3	-10	14	33	-42*	-3	3	17	34	28*
-3	-4	17	36	44*	-3	-6	17	33	-40*	-4	9	16	34	44*
-4	7	15	31	-47*	-4	11	12	33	46*	-4	-10	12	33	51*
-11	4	11	35	-39*	7	-4	14	28	-28*	-4	-4	16	28	-33*
-4	-4	15	30	-22*	-7	-4	16	26	-24*	8	4	17	35	30*
9	4	18	37	-46*	-9	-4	11	32	39	11	4	17	35	32*
12	4	14	38	30*	4	-11	14	26	-15*	4	14	14	32	-21*
4	10	17	36	-38*	4	7	17	34	-32*	4	5	19	35	-46*
5	9	16	32	-32*	5	8	16	33	-3*	5	9	15	31	-20*
5	14	15	36	39*	14	5	15	42	52*	5	-9	14	30	37*
13	5	14	40	-50*	5	-10	12	28	-21*	-10	-5	13	29	-23*
9	5	19	34	39*	8	5	18	35	-53*	-8	-5	12	33	36*
-6	-5	13	30	30*	9	-5	14	27	33*	-5	-10	11	29	-37*
-5	11	12	30	38*	-5	12	13	29	-17*	-5	-6	14	36	-34*
-5	10	14	26	23*	-5	11	14	29	-19*	-5	-8	15	32	-24*
-6	7	17	30	28*	-6	-8	15	33	27*	-6	6	15	29	31*
-6	8	14	29	31*	-6	7	14	31	36*	-6	-6	14	33	-47
-6	-7	13	34	33*	-6	12	13	29	22*	11	-6	13	35	35*
11	-6	15	30	-32*	-7	6	14	35	-30*	6	6	16	32	23*
-8	-6	15	31	26*	-10	-6	12	29	-24*	-10	-6	11	34	-36*
6	-10	12	27	-25*	13	6	17	34	-27*	13	6	15	40	37*
6	-7	14	31	30*	14	6	16	37	-47*	15	6	16	36	-36*
6	13	17	39	54*	7	7	19	33	-14*	7	10	18	41	-44*
7	7	17	34	-25*	7	12	17	42	50*	7	12	14	37	-46*
7	-10	14	27	29*	7	13	13	35	34*	11	7	18	36	44*
10	7	17	36	-44*	-10	-7	12	29	-21*	-9	-7	10	27	31*
7	7	16	37	-46	-10	7	13	29	-38*	-7	7	12	26	-37*
-7	8	14	26	-35*	-8	12	12	27	29*	-8	-10	12	30	36*
-8	-10	11	33	-36*	10	-8	13	29	-42*	8	-8	15	30	39*
8	13	17	36	-44*	9	10	16	35	0*	14	9	15	42	40*
12	9	17	42	-53*	12	9	13	37	-26*	9	12	12	40	55*
9	-9	12	30	34*	11	9	18	39	-36*	10	9	14	36	-10*
9	-9	10	28	-28*	-9	9	9	35	-30*	-9	-9	13	31	45
-10	10	10	26	25*	10	10	16	39	-50*	14	10	16	41	-30*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
11	11	12	41	-62	0	1	10	19	19	0	5	9	17	19*
-4	0	6	18	14*	1	-2	9	16	-26*	3	1	8	21	27*
1	-1	6	15	21*	2	-1	10	17	25*	-6	1	6	22	-19*
-2	3	8	16	-23*	-2	-2	6	15	11*	3	-2	8	20	-13*
3	-2	10	21	28*	6	3	9	18	-30*	-3	-3	10	21	23*
-3	6	7	17	-25*	-3	6	8	19	21*	-6	4	8	25	-20*
-5	4	8	22	26*	4	-4	7	16	26*	4	4	9	21	21*
6	5	9	23	-34*	0	8	15	24	29*	0	6	14	20	-32*
0	-4	14	27	-29*	0	-1	13	22	21*	0	1	12	23	2*
0	-9	10	22	31*	9	0	12	20	-38*	5	0	15	19	-9*
4	0	16	24	0*	-1	0	15	20	23*	-5	0	14	24	11*
-10	0	10	20	-23*	0	6	12	19	6*	0	7	12	20	20*
0	11	13	28	-34*	0	-3	13	21	-21*	0	-1	15	24	-28*
1	-3	15	18	-12*	1	3	13	21	30*	10	1	11	28	-28*
-9	-1	11	28	41*	8	1	15	28	3*	-7	-1	13	27	-36*
6	1	15	24	20*	6	1	13	24	23*	5	1	16	21	-29*
-4	-1	14	21	26*	1	1	12	24	-34	-1	5	11	20	25*
-1	-5	14	20	36*	-2	-3	13	19	-19*	-2	-7	12	26	-41*
6	-2	12	18	18*	-6	2	11	26	-14*	2	2	16	25	24*
-7	-2	10	24	-32*	-7	-2	12	25	42*	-8	-2	11	24	29*
9	2	13	28	-31*	2	-4	11	22	-23*	2	-9	11	21	28*
2	11	12	25	-3*	2	-2	14	20	-17*	2	5	14	21	-7*
3	11	14	24	-25*	3	9	10	23	-13*	3	-7	9	20	-13*
-7	-3	12	25	20*	-7	-3	11	24	-32*	-6	-3	12	19	-18*
8	-3	13	25	-38*	8	-3	14	27	38*	-3	9	9	18	-27*
-3	-7	9	25	-22*	-3	-4	10	21	20*	-3	10	10	23	-32*
-3	4	15	23	5*	-4	7	12	23	18*	-4	-8	9	22	25*
6	-4	12	20	2*	-7	-4	10	18	25*	4	-7	9	18	22*
-9	-4	10	26	34*	4	10	13	29	-35*	4	4	13	24	32*
4	-5	13	20	-28*	4	-4	14	20	-16*	4	6	14	21	-25*
-9	-5	10	22	-30*	9	5	12	24	29*	6	5	16	23	-33*
5	-5	12	17	21*	-5	5	12	24	-36*	7	-5	13	22	-33*
8	-5	11	24	14*	-5	5	10	23	-31	-7	6	7	22	30*
-6	-6	9	21	-25*	-7	-6	9	23	31*	-8	-6	10	24	-31*
8	6	12	25	-41*	6	-7	11	21	24*	6	-8	11	21	-13*
6	9	13	28	-32*	7	7	15	22	-41*	7	10	14	31	-27*
7	9	10	20	2*	9	7	13	30	30*	8	7	12	28	-34*
-7	-7	11	22	40	-7	-7	9	20	-20*	-7	-7	11	24	40
10	8	12	29	-44*	0	8	19	29	33*	0	11	18	27	-34*
0	7	18	29	-45	0	5	18	27	-14*	0	-3	16	25	26*
0	-5	16	29	-42*	0	-6	16	24	-16*	0	-7	16	27	29*
0	12	14	27	-35*	-10	0	15	30	33*	-9	0	15	22	32*
9	0	15	22	-35*	6	0	18	27	-48*	-6	0	14	25	28*
-6	0	16	25	13*	-3	0	16	22	34*	0	0	18	28	45
-4	0	16	24	-9*	5	0	17	27	-16*	6	0	19	22	42*
7	0	17	23	-26*	8	0	15	24	37	-10	0	14	21	15*
11	0	14	30	34*	0	13	13	22	20*	0	8	15	22	29*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET 1)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	6	18	30	-44	0	8	19	29	33*	0	1	19	21	-9*
1	8	19	24	32*	1	5	18	25	-29*	1	11	15	29	31*
1	-8	14	25	33*	1	13	13	25	28*	13	1	15	30	-37*
-11	-1	14	25	-33*	-7	-1	13	27	-36*	-6	-1	14	26	-26*
-6	-1	17	23	-19*	4	1	20	25	-35*	3	1	20	20	-3*
2	1	17	23	-30*	-2	-1	16	24	31*	1	-1	17	25	42*
-2	1	18	23	-34*	-3	1	16	24	27*	-4	1	16	26	35*
-6	1	16	30	35*	7	-1	19	23	30*	10	-1	18	28	-27*
11	-1	17	28	-33*	-11	1	12	30	27*	-1	-10	13	23	29*
14	-1	15	25	-14*	-1	-7	15	29	-29*	-1	-6	17	26	-22*
-1	-5	18	20	-18*	-1	-2	18	24	18*	-1	5	19	22	24*
-2	7	18	25	39*	-2	12	16	24	-6*	-2	10	16	25	-14*
-2	-8	15	27	-30*	12	-2	14	29	-21*	-2	-11	12	21	-18*
-10	2	15	27	21*	-7	2	16	27	26*	-4	2	17	22	-9*
2	-2	16	23	35*	-2	2	17	26	-12*	-2	2	19	22	34*
2	2	17	21	30*	3	2	17	27	19*	5	2	20	24	31*
6	2	16	23	25*	6	2	18	28	-19*	7	2	17	23	-31*
-8	-2	15	24	36*	8	2	16	22	-23*	10	2	16	31	39*
13	2	16	29	38*	2	12	13	28	20*	2	11	15	27	20*
2	-6	15	20	-5*	2	-7	15	22	-33*	2	5	17	30	-34*
2	-4	17	23	-10*	2	-7	17	21	20*	2	-5	18	22	-28*
2	2	18	22	30*	2	2	19	22	29*	2	-3	19	25	33*
3	-3	16	25	20*	13	3	14	23	-20*	-11	-3	13	26	32*
11	3	18	28	42*	10	3	16	31	-39*	8	3	18	26	38*
-7	-3	15	21	-23*	6	3	18	30	-39*	-3	3	17	25	28*
-9	3	13	29	-22*	-10	3	11	26	19*	12	-3	16	29	-33*
-3	-8	13	26	28*	-3	-6	14	29	-20*	-3	10	15	23	-35*
-3	-10	15	19	6*	-3	6	17	28	-22*	-3	-3	18	22	-30*
-4	4	18	21	-9*	-4	4	17	23	21*	-4	-6	16	25	27*
-4	12	15	21	45*	-4	9	14	23	-26*	-4	10	13	20	42*
12	-4	15	27	28*	12	-4	14	30	38*	-4	-11	12	25	20*
11	-4	13	22	25*	9	-4	15	24	-7*	8	-4	17	27	-38*
-7	4	16	30	33*	7	-4	16	22	28*	-5	4	18	29	-24*
-5	4	15	23	-25*	4	-9	14	23	-22*	4	12	14	23	14*
4	14	15	24	29*	4	6	16	24	34*	4	7	16	25	43*
4	10	16	33	41*	4	11	16	28	16*	4	5	17	21	27*
4	9	18	32	-25*	4	11	18	26	38*	4	12	18	25	42*
4	4	19	27	24*	5	5	20	26	1*	15	5	16	30	-29*
5	-8	13	25	-42*	13	5	16	25	45*	-9	-5	14	26	-20*
-9	-5	11	22	31*	9	5	15	26	-47*	-8	-5	15	25	40*
-7	-5	14	21	-6*	7	5	19	28	-35*	5	5	17	23	-22*
-6	5	15	29	44*	-7	5	17	27	-25*	8	-5	16	25	29*
-10	5	10	21	-14*	10	-5	15	27	-25*	11	-5	14	28	-38*
-5	12	12	22	35*	-5	-6	13	24	36*	-5	-8	14	24	-6*
-5	-5	16	27	27*	-5	8	16	21	-13*	-5	-5	17	21	-22*
-5	5	18	23	9*	-6	7	15	23	30*	-6	11	15	23	-32*
-6	7	13	26	-33*	-6	11	12	23	-23*	9	-6	14	20	24*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
8	-6	14	27	-44*	7	-6	15	22	-26*	7	-6	17	18	3*
-6	-6	13	19	16*	12	6	16	30	1*	6	12	16	32	-46*
6	12	17	26	34*	6	7	17	31	-35*	6	-6	17	21	31*
7	8	18	33	46*	7	-7	16	22	28*	7	-7	14	20	17*
-11	-7	11	27	26*	7	-10	11	22	10*	-7	-7	15	20	25*
-9	7	15	26	10*	-11	7	12	22	19*	-7	-10	12	28	42*
-7	-8	14	25	24*	-7	10	15	21	30*	-7	-7	15	28	25*
-7	8	16	21	20*	-10	-8	12	20	-12*	11	8	15	32	-28*
13	8	17	29	-32*	8	13	13	31	-7*	8	-8	13	22	26*
8	10	14	32	-27*	8	13	14	30	-29*	8	13	16	28	15*
8	10	17	34	-41*	8	10	18	32	-22*	9	11	14	29	53*
9	9	14	31	-34*	9	13	13	25	-46*	12	9	14	26	-27*
9	9	14	30	-34*	-9	9	9	20	-30*	-9	-9	12	21	22*
-9	9	12	20	-4*	-9	10	12	22	-31*	-9	10	13	17	-23*
-10	10	12	20	-33*	11	10	15	32	-47*	11	10	13	25	4*
10	10	13	27	28*	10	15	15	33	-37*	10	11	15	33	-53*
10	11	17	26	12*	12	12	14	27	-28*	13	12	14	33	-25*
12	12	14	29	-28*	12	13	14	29	-28*	0	4	10	3	-11*
0	3	10	14	36	0	-3	10	3	-11*	0	-6	9	16	41
0	-1	9	3	13*	0	8	9	4	-7*	0	-2	8	3	13*
0	-5	8	15	20*	0	-6	7	4	32*	0	7	7	6	-16*
7	0	8	13	-26*	6	0	9	9	9*	0	3	6	9	-12*
-6	0	6	16	33	-6	0	8	14	-16*	-5	0	9	7	14*
-5	0	6	3	-4*	0	2	5	8	-23*	4	0	10	19	-7*
-4	0	6	22	14*	-4	0	10	4	-21*	-3	0	9	22	-30*
-3	0	6	3	4*	-3	0	4	14	-29*	2	0	10	12	-22*
-2	0	6	14	23*	-2	0	8	4	26	-1	0	11	4	-12*
1	0	11	4	21*	0	0	11	4	-22*	-1	0	11	15	-12*
-2	0	6	14	23*	2	0	10	11	-22*	-3	0	4	14	-29*
-3	0	6	3	4*	-3	0	9	17	-30*	-4	0	10	12	-21*
4	0	10	4	-7*	0	2	5	2	-23*	-5	0	6	4	-4*
-5	0	9	15	14*	-6	0	8	4	-16*	0	3	6	11	-12*
6	0	9	4	9*	7	0	8	18	-26*	0	7	7	3	-16*
0	-6	7	3	32*	0	-5	8	10	20*	0	-2	8	3	13*
0	8	9	14	-7*	0	5	9	3	19*	0	-1	9	3	13*
0	-3	10	14	-11*	0	4	10	3	-11*	0	0	11	4	-22*
1	3	12	4	-20*	1	5	11	4	16*	1	-4	10	11	3*
1	8	9	15	4*	1	4	7	3	-11*	6	1	10	21	-29*
6	1	9	3	-10*	1	-1	6	14	21*	-5	-1	8	11	-14*
1	-4	5	2	-10*	1	3	4	13	7*	-4	-1	9	11	9*
3	1	12	36	12*	-2	1	11	4	-5*	2	-1	5	2	4*
-3	1	9	18	-12*	4	-1	11	4	-23*	5	-1	11	18	-29*
5	-1	9	21	-15*	-5	1	7	12	25*	-6	1	7	3	28*
-1	6	6	15	-4*	6	-1	10	16	-29*	7	-1	9	12	-2*
-1	7	7	3	8*	-7	1	8	4	-3*	-1	-2	8	3	1*
-1	3	9	5	8*	-1	-6	9	3	-16*	-1	5	11	15	25*
-2	3	11	16	-4*	-2	6	10	21	5*	-2	4	10	3	10*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-2	2	10	3	-27*	-2	-2	10	14	-25*	-2	-5	9	3	2*
-2	4	9	4	4*	-2	7	9	8	7*	6	-2	8	21	-32*
-5	2	8	24	-18*	-2	-2	5	2	-3*	4	-2	11	14	22*
-4	2	4	2	-19*	-3	2	3	2	17*	3	-2	5	3	12*
-2	2	10	15	-27*	-2	-2	10	4	-25*	-2	-2	6	3	11*
-2	-2	5	2	-3*	2	2	6	11	-25*	2	2	8	3	-20*
2	2	9	19	1*	2	2	12	4	-4*	3	2	11	16	16*
3	2	10	11	38*	-3	-2	9	3	8*	-4	-2	4	10	7*
4	2	5	14	8*	2	5	5	3	-10*	2	-4	5	30	4*
-5	-2	8	17	31*	2	2	6	3	-25*	2	2	8	14	-20*
8	2	9	4	4*	2	2	9	13	1*	2	-5	9	3	-6*
2	-3	10	14	-14*	2	5	10	13	-1*	2	5	11	4	-24*
2	3	11	20	8*	2	2	12	18	-4*	3	3	12	4	7*
3	8	10	23	37*	3	6	9	3	-16*	3	9	9	4	-1*
3	-4	7	20	-8*	3	5	6	6	-15*	3	4	6	3	22*
-5	-3	8	20	23*	4	3	11	4	-8*	4	3	8	10	4*
4	3	6	4	1*	-4	-3	8	13	2*	-3	-3	7	19	35*
3	3	12	4	7*	-3	3	8	3	8*	-4	3	8	3	-26*
4	-3	9	4	-8*	4	-3	10	17	-4*	5	-3	9	13	-22*
-5	3	6	3	-15*	-5	3	8	21	5*	-6	3	6	3	3*
6	-3	9	16	-6*	-3	3	8	3	8*	-3	-3	10	19	23*
-4	-4	9	16	-28*	-4	7	8	4	18*	-4	-4	7	10	-25*
-4	7	7	18	-16*	7	-4	8	22	-16*	6	-4	8	13	-4*
-5	4	7	12	23*	-5	4	6	3	-16*	5	-4	6	3	-19*
4	-4	8	9	3*	4	-4	7	13	26*	-4	-4	7	19	-25*
4	4	9	3	21*	5	4	11	21	-2*	5	4	8	3	4*
4	5	5	3	2*	-5	-4	7	3	-16*	-6	-4	6	3	-26*
6	4	9	15	-13*	7	4	10	4	-13*	-7	-4	7	4	11*
4	-4	8	3	3*	8	4	9	13	4*	4	6	10	33	-9*
4	8	10	24	22*	5	7	10	9	-32*	5	7	9	21	-26*
5	7	8	4	-9*	5	-5	8	15	-4*	-6	-5	7	19	18*
5	-5	8	17	-4*	-5	5	8	7	16*	-5	7	7	10	22*
-5	5	8	15	16*	-6	6	6	10	-27*	-6	6	6	7	-27*
7	6	9	9	3*	8	6	9	4	8*	6	8	9	4	-20*
7	8	9	4	15*	0	1	16	4	-33	0	-1	15	4	-28*
0	0	15	4	-2*	0	4	15	32	3*	0	5	15	5	16*
0	10	14	5	-3*	0	8	14	5	-20*	0	0	14	4	-12*
0	-1	14	4	-15*	0	-3	14	22	-14*	0	-5	14	17	-29*
0	-4	13	4	7*	0	-3	13	4	-21*	0	-2	13	19	-21*
0	1	13	4	11*	0	3	13	4	-6*	0	4	13	4	5*
0	7	13	4	24*	0	9	13	23	36*	0	12	12	5	1*
0	9	12	13	-6*	0	8	12	17	18*	0	7	12	11	20*
0	6	12	13	6*	0	5	12	4	-14*	0	-4	12	4	1*
0	-8	12	26	16*	0	-9	11	24	-14*	11	0	12	36	8*
11	0	13	5	26*	10	0	13	5	-1*	0	-6	10	4	-16*
-10	0	10	57	-23*	-9	0	9	4	10*	0	-8	9	23	36
0	-7	9	23	-29*	8	0	13	5	-2*	-8	0	11	4	-3*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-7	0	13	5	15*	7	0	14	18	-19*	7	0	15	15	36*
6	0	15	5	14*	6	0	12	23	-12*	-6	0	10	22	13*
-6	0	11	4	-19*	-5	0	14	5	11*	-5	0	11	18	6*
-5	0	10	4	1*	4	0	12	11	-6*	-4	0	14	21	12*
-3	0	15	27	-33*	-3	0	14	4	11*	3	0	12	4	1*
2	0	15	16	10*	2	0	13	18	-15*	-2	0	14	4	-15*
-1	0	12	22	31*	0	0	15	4	-2*	0	0	14	10	-12*
0	0	14	4	-12*	0	0	15	4	-2*	1	0	15	26	-48
-1	0	15	6	23*	-2	0	14	4	-15*	2	0	13	4	-15*
2	0	15	4	10*	3	0	12	4	1*	-3	0	14	36	11*
-3	0	15	21	-33*	-4	0	14	4	12*	4	0	12	16	-6*
4	0	16	5	0*	5	0	15	5	-9*	-5	0	10	4	1*
-5	0	11	4	6*	-6	0	11	23	-19*	-6	0	10	7	13*
6	0	12	15	-12*	6	0	15	5	14*	7	0	15	11	36*
7	0	14	5	-19*	-7	0	13	5	15*	-8	0	11	18	-3*
-8	0	9	10	27*	8	0	13	15	-2*	0	-7	9	16	-29*
-9	0	9	23	10*	0	-6	10	4	-16*	10	0	13	25	-1*
11	0	13	5	26*	11	0	12	5	8*	0	11	11	16	18*
0	-7	11	4	39	0	-9	11	4	-14*	0	-8	12	4	16*
0	-4	12	4	1*	0	1	12	12	2*	0	5	12	14	-14*
0	8	12	23	18*	0	9	12	4	-6*	0	11	12	22	35
0	12	12	14	1*	0	7	13	13	24*	0	4	13	21	5*
0	3	13	4	-6*	0	1	13	4	11*	0	-1	13	19	21*
0	-2	13	4	-21*	0	-4	13	4	7*	0	-4	14	6	-29*
0	-3	14	5	-14*	0	-1	14	23	-15*	0	0	14	4	-12*
0	3	14	23	-43	0	6	14	8	-32*	0	8	14	5	-20*
0	10	14	5	-3*	0	8	15	11	29*	0	4	15	7	3*
0	0	15	4	-2*	1	5	16	5	-9*	1	2	16	22	-29*
1	1	16	5	19*	1	5	15	24	3*	1	8	15	9	41*
1	10	14	23	-38*	1	9	14	24	28*	1	5	14	4	-6*
1	4	14	23	-3*	1	2	14	17	-5*	1	-1	14	12	14*
1	-3	14	19	18*	1	-5	13	17	-28*	1	-3	13	21	-22*
1	1	13	4	27*	1	5	13	32	-3*	1	6	13	4	-9*
1	8	13	14	-22*	1	9	13	23	-12*	1	12	12	46	10*
1	10	12	5	-16*	1	9	12	5	-5*	1	6	12	4	-19*
1	3	12	15	-20*	1	-1	12	20	-16*	1	-3	12	19	1*
1	-9	11	9	-5*	1	-8	11	21	29*	1	-3	11	8	27*
1	10	11	5	-8*	1	-5	10	12	17*	1	-6	10	4	14*
1	-7	10	4	-9*	1	-8	10	4	19*	1	-9	10	4	-3*
1	-8	9	8	31*	9	1	13	27	-8*	9	1	14	18	-34*
8	1	11	4	-29*	-8	-1	8	4	7*	-8	-1	12	24	21*
-7	-1	11	4	20*	7	1	12	12	30*	7	1	13	16	25*
6	1	14	18	-25*	6	1	12	11	-36*	-6	-1	10	4	-21*
-6	-1	11	4	-20*	-6	-1	12	45	8*	-6	-1	13	19	-19*
-5	-1	13	4	-13*	-5	-1	10	13	22*	5	1	14	25	-25*
4	1	15	17	-40*	-3	-1	14	18	29*	-3	-1	13	35	2*
3	1	12	13	12*	3	1	13	4	-10*	2	1	16	12	8*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-2	-1	14	24	44*	-2	-1	15	4	-16*	-1	-1	15	15	9*
-1	-1	14	8	17*	-1	-1	12	12	7*	1	1	13	4	27*
1	1	14	4	43	1	1	16	14	19*	1	-1	14	4	14*
1	-1	12	8	-16*	-2	1	15	17	21*	2	-1	15	19	-3*
-3	1	14	4	-24*	-3	1	15	24	-25*	-4	1	14	4	-3*
-4	1	13	4	15*	4	-1	14	8	5*	4	-1	15	17	-30*
5	-1	15	4	-18*	5	-1	14	10	16*	5	-1	12	4	28*
5	-1	11	10	-29*	-5	1	11	9	-23*	-5	1	12	18	-10*
-5	1	14	18	-59*	6	-1	15	23	-1*	7	-1	15	5	-3*
7	-1	11	16	24*	-7	1	10	17	-42*	-7	1	11	4	-26*
-7	1	12	4	9*	8	-1	10	4	-17*	8	-1	14	5	-4*
9	-1	12	17	17*	9	-1	11	21	-17*	-1	-6	9	16	-16*
-1	-7	9	20	23*	-9	1	11	14	-5*	-10	1	10	28	-42*
-1	-6	10	4	-5*	-1	8	10	4	17*	-1	10	10	22	-33*
10	-1	11	5	-1*	10	-1	13	12	-19*	11	-1	12	27	-28*
-1	11	11	24	28*	-1	9	11	4	-43*	-1	-3	11	18	15*
-1	-5	11	23	6*	-1	-9	11	18	26*	-1	-7	12	4	20*
-1	-5	12	4	13*	-1	-1	12	4	7*	-1	2	12	4	-3*
-1	10	12	5	6*	-1	12	12	21	9*	-1	9	13	5	-19*
-1	2	13	4	-21*	-1	-2	13	4	-8*	-1	-4	13	25	13*
-1	-1	14	4	17*	-1	7	14	19	-17*	-1	9	14	5	17*
-1	7	15	25	-33*	-1	5	15	5	19*	-1	3	15	15	-35*
-1	-1	15	4	9*	-1	-3	15	18	6*	-2	3	15	16	11*
-2	5	15	6	41*	-2	7	14	19	28*	-2	2	14	4	-15*
-2	-2	14	25	-3*	-2	-7	13	26	5*	-2	-5	13	13	14*
-2	3	13	4	11*	-2	4	13	15	-23*	-2	7	13	22	-2*
-2	8	13	14	-19*	-2	10	13	5	3*	-2	11	12	37	-16*
-2	-8	11	4	-18*	-2	-6	11	23	-25*	-2	9	11	20	45*
10	-2	11	5	-14*	-2	8	10	4	-13*	-2	-6	10	22	17*
-9	2	11	4	28*	9	-2	12	19	-10*	8	-2	14	23	-27*
8	-2	11	12	21*	-8	2	10	4	21*	-8	2	12	4	31*
-7	2	12	10	27*	-7	2	9	4	23*	-7	2	8	8	43
7	-2	11	4	-10*	7	-2	13	18	31*	7	-2	14	5	9*
6	-2	15	9	3*	6	-2	14	23	13*	-6	2	12	14	16*
-5	2	14	24	12*	-5	2	12	4	-1*	5	-2	13	37	2*
5	-2	14	17	28*	4	-2	11	4	22*	-3	2	15	4	-13*
-3	2	14	4	-17*	-3	2	13	5	20*	-3	2	12	4	-27*
3	-2	14	4	26*	2	-2	15	17	-12*	2	-2	14	16	-17*
-2	2	14	34	-15*	-2	2	15	4	50	-2	-2	15	25	-39
-2	-2	14	8	-3*	2	2	12	11	-4*	2	2	14	16	4*
2	2	15	21	-1*	3	2	16	10	-32*	3	2	15	21	16*
-3	-2	14	4	-22*	-4	-2	10	18	26*	4	2	13	4	12*
4	2	14	17	-39*	4	2	16	5	-1*	-5	-2	14	31	6*
-6	-2	12	4	20*	6	2	15	15	29*	6	2	16	11	25*
7	2	15	6	22*	7	2	14	18	-12*	7	2	13	6	41*
-7	-2	13	24	15*	2	-7	8	21	39	8	2	14	18	-2*
9	2	15	5	-4*	-9	-2	9	13	-7*	-10	-2	10	4	-4*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	-7	10	23	7*	10	2	13	9	13*	10	2	14	24	-27*
11	2	12	22	-45*	2	-6	11	4	-14*	2	-8	11	4	-3*
2	-8	12	4	3*	2	-5	12	4	6*	2	-4	12	4	-22*
2	2	12	4	-4*	2	6	12	5	-15*	2	8	12	4	-14*
2	10	12	15	0*	2	12	12	27	-47*	12	2	13	25	-65
2	12	13	5	20*	2	10	13	6	9*	2	9	13	5	-14*
2	7	13	13	-28*	2	-7	13	19	-46*	2	2	14	4	4*
2	3	14	17	31*	2	4	14	4	1*	2	6	14	24	-28*
2	7	14	42	-6*	2	8	14	38	26*	2	9	14	5	-19*
2	10	14	15	22*	2	8	15	5	-7*	2	2	15	24	-1*
2	-2	15	5	-12*	2	-3	15	12	-23*	2	2	16	5	24*
3	6	16	5	-17*	3	3	16	17	-25*	3	3	15	25	18*
3	4	15	25	35*	3	5	15	5	16*	3	6	15	13	-27*
3	7	15	5	2*	3	10	14	5	13*	3	7	14	18	8*
3	6	14	17	21*	3	4	14	4	-8*	3	-7	13	19	30*
3	-3	13	21	-26*	3	5	13	8	-29*	3	8	13	33	-16*
3	11	13	5	6*	3	12	13	5	-3*	12	3	13	6	27*
3	11	12	5	-12*	3	9	12	5	-19*	3	7	12	4	18*
3	3	12	22	7*	3	-4	12	9	-21*	3	-5	12	4	9*
3	-6	12	4	25*	3	-7	12	4	23*	3	-8	12	15	22*
3	-7	11	19	-17*	3	-3	11	4	20*	3	10	11	5	1*
10	3	14	5	1*	10	3	13	11	-22*	10	3	12	13	-36*
3	10	10	5	-17*	3	-9	10	4	36*	-9	-3	10	4	11*
3	-8	9	23	27*	3	-6	9	8	6*	9	3	15	17	15*
8	3	15	5	5*	8	3	14	23	17*	-8	-3	9	3	-12*
-8	-3	10	4	-15*	-8	-3	12	15	-15*	7	3	15	17	7*
6	3	16	5	0*	5	3	14	19	-39*	4	3	13	23	-36*
-4	-3	14	4	6*	3	3	12	4	7*	3	3	15	4	18*
3	3	16	15	-25*	3	-3	13	11	-26*	3	-3	11	4	20*
-3	3	12	12	-18*	-3	3	14	22	-33*	-5	3	12	4	-25*
-5	3	13	4	-6*	-6	3	12	4	-15*	-6	3	10	4	-18*
6	-3	14	21	-34*	7	-3	13	12	34*	7	-3	10	23	-24*
-7	3	10	18	18*	-7	3	13	4	-30*	-8	3	12	29	-49*
-8	3	9	4	8*	8	-3	12	13	-21*	9	-3	13	5	-10*
-3	-8	10	5	19*	-3	-6	10	10	9*	-3	-5	10	15	28*
-3	11	11	4	-5*	-3	10	11	7	-15*	-3	8	11	16	17*
-3	-8	12	45	-13*	-3	-7	12	17	21*	-3	-6	12	14	6*
-3	3	12	4	-18*	-3	7	12	4	10*	-3	11	12	5	-4*
-3	9	13	4	4*	-3	8	13	27	-55*	-3	6	13	4	-11*
-3	5	13	17	-29*	-3	5	14	24	9*	-3	6	14	4	-14*
-4	5	14	4	8*	-4	-6	13	14	24*	-4	-5	13	26	-40*
-4	5	13	4	6*	-4	8	13	23	-21*	-4	9	12	18	-27*
-4	4	12	22	-33*	-4	-7	12	18	34*	-4	-9	11	17	18*
-4	-8	11	4	-2*	-4	-7	11	7	-13*	-4	5	11	14	-1*
-4	6	11	4	14*	-4	9	11	16	-24*	-4	11	11	8	9*
10	-4	11	13	-45*	-4	9	10	24	32*	-4	-5	10	4	-20*
-4	-9	10	4	-32*	-10	4	10	15	11*	-9	4	9	4	20*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-4	-6	9	4	-30*	-4	-5	9	3	8*	-4	9	9	4	-32*
8	-4	13	5	-19*	8	-4	10	4	-12*	-7	4	12	4	-18*
-7	4	10	27	-49*	6	-4	13	15	-22*	6	-4	11	4	-28*
6	-4	10	4	0*	-6	4	10	4	-10*	-6	4	11	4	2*
-5	4	14	5	13*	-5	4	13	4	1*	-5	4	12	40	5*
-5	4	11	21	-16*	5	-4	13	4	23*	4	-4	14	4	-16*
-4	4	12	19	-33*	4	4	13	12	32*	4	4	15	19	-4*
4	4	16	26	5*	5	4	16	14	-3*	5	4	15	5	35*
5	4	14	19	36*	-5	-4	11	10	-18*	-5	-4	12	4	-17*
-5	-4	13	8	21*	-6	-4	12	4	-22*	-6	-4	11	4	8*
-6	-4	9	4	4*	6	4	14	16	-23*	7	4	15	6	35*
7	4	11	4	-7*	-8	-4	11	12	5*	-8	-4	10	4	7*
8	4	12	8	-2*	8	4	15	5	-24*	-10	-4	10	23	9*
4	-7	10	4	-14*	4	-6	10	10	-3*	4	9	10	17	18*
10	4	11	23	-53*	10	4	13	26	-29*	10	4	14	17	-25*
11	4	13	18	34*	11	4	12	20	-19*	4	11	11	5	-19*
4	9	11	5	-19*	4	-6	11	4	-7*	4	-8	11	17	27*
4	-6	12	22	-32*	4	-5	12	14	24*	4	5	12	9	13*
4	12	12	28	21*	4	12	13	5	-1*	4	-4	13	21	-23*
4	7	14	5	-34*	4	9	15	49	-15*	4	8	15	21	-4*
4	7	15	12	-10*	4	4	15	5	-4*	4	4	16	37	5*
4	5	16	5	-19*	4	6	16	23	34*	5	5	16	5	-20*
5	6	15	5	-17*	5	9	15	6	-20*	5	8	14	5	15*
5	5	14	5	9*	5	-6	13	21	-43*	5	6	13	5	-5*
5	9	13	7	-12*	5	12	13	18	21*	12	5	13	6	5*
5	12	12	21	30*	5	11	12	5	-5*	5	10	12	14	16*
5	8	12	13	-4*	5	5	12	23	19*	5	-5	12	4	21*
5	-6	11	7	-10*	11	5	13	5	6*	11	5	14	6	11*
10	5	13	24	-35*	10	5	12	28	48*	10	5	11	5	10*
5	-7	10	11	-12*	5	-9	10	31	-1*	-9	-5	9	16	-3*
5	-8	9	13	8*	9	5	13	5	-13*	8	5	14	5	-24*
8	5	11	4	-13*	-8	-5	9	15	10*	-7	-5	11	24	33*
-7	-5	10	19	-23*	6	5	15	5	9*	6	5	14	5	0*
-6	-5	10	20	6*	-6	-5	11	4	8*	-5	-5	11	18	-28*
5	5	12	18	19*	5	5	14	12	9*	5	5	16	26	-20*
5	-5	11	4	-22	-5	5	14	12	-14*	-6	5	10	22	-11*
-6	5	9	15	35*	6	-5	12	18	40*	7	-5	12	4	-13*
-8	5	9	4	-1*	-8	5	8	15	1*	-5	-7	8	4	-19*
-5	-6	8	3	-1*	-5	8	9	4	-4*	-5	-6	9	4	10*
-9	5	9	15	-16*	-9	5	10	16	-20*	-5	-9	10	15	5*
-5	-7	10	4	11*	-5	9	10	4	1*	-5	10	10	4	3*
-5	8	11	4	18*	-5	7	11	4	7*	-5	6	11	21	4*
-5	-5	11	4	-28*	-5	-8	11	20	-1*	-5	5	12	21	-36*
-5	7	12	4	14*	-5	8	12	21	27*	-5	6	13	6	-25*
-5	-5	13	4	38	-5	5	14	4	-14*	-6	-7	11	4	-5*
-6	7	11	4	-19*	-6	10	10	4	17*	-6	8	10	4	-10*
-6	7	10	10	14*	-6	6	10	4	-5*	-6	-8	10	26	39*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-9	6	10	24	23*	-6	-6	9	24	-25*	-6	8	9	38	-26*
9	-6	11	5	0*	8	-6	12	15	-9*	-8	6	9	26	-14*
-8	6	10	25	23*	-8	6	11	21	30*	-7	6	10	4	-8*
-7	6	9	4	-7*	7	-6	11	4	-15*	7	-6	12	21	24*
6	-6	12	33	-27*	6	-6	11	4	-11*	-6	6	10	25	-5*
-6	-6	10	15	26	6	6	13	38	0*	6	6	14	5	-20*
7	6	14	5	33*	7	6	12	19	22*	-7	-6	10	18	-23*
-8	-6	11	3	23*	-8	-6	9	4	15*	8	6	10	4	-12*
8	6	13	5	-2*	9	6	13	5	-33*	6	9	9	25	-33*
6	-6	9	4	-28	-9	-6	9	4	33*	6	-8	10	4	11*
6	10	10	18	-18*	11	6	13	31	-49*	11	6	12	5	-25*
6	-6	11	4	-11*	6	-6	12	4	-27*	6	9	12	18	-17*
6	12	13	21	42*	6	11	13	5	18*	6	10	13	5	-5*
6	6	13	17	0*	6	9	14	5	19*	6	10	14	19	46*
6	9	15	7	-12*	6	8	15	40	-20*	7	8	15	21	-46
7	9	14	10	-10*	7	8	14	5	34*	7	10	13	21	45*
7	12	12	5	-26*	7	10	12	12	38*	7	9	12	17	39*
7	-7	11	18	1*	7	7	11	16	38	7	9	11	25	6*
7	11	11	24	-11*	11	7	13	6	-27*	10	7	13	20	-29*
7	10	10	11	19*	7	-8	9	9	9*	7	-7	9	18	-31*
7	8	9	4	15*	9	7	10	5	5*	9	7	11	22	7*
8	7	15	42	4*	8	7	14	29	11*	-8	-7	9	4	-6*
-7	-7	10	40	42	-7	-7	9	9	-20*	7	7	14	29	47
7	7	15	25	-41*	7	-7	11	4	1*	7	-7	9	20	-31*
-7	7	8	26	51	-7	7	11	5	-32*	8	-7	10	4	-7*
-9	7	9	14	24*	-7	9	10	11	-2*	-8	-8	9	4	-12*
8	-8	9	4	-3*	-8	-8	9	21	-12*	8	8	14	5	-23*
9	8	14	20	2*	9	8	13	5	2*	9	8	11	25	-42*
8	-8	9	9	-3*	8	9	10	5	-14*	10	8	11	5	-15*
10	8	13	5	-14*	11	8	12	5	-19*	8	10	12	5	3*
8	11	12	5	-27*	8	9	13	5	-1*	8	8	14	5	-23*
8	9	14	55	-61*	9	9	14	26	-34*	9	11	12	6	1*
9	9	12	25	7*	9	9	11	5	-33*	9	10	11	29	43*
10	9	13	29	-30*	10	9	12	7	-20*	9	9	9	48	-8*
9	9	11	17	-33*	9	9	12	5	7*	10	11	11	6	2*
0	-1	19	12	-30*	0	0	19	19	-5*	0	1	19	18	-9*
0	3	19	18	-22*	0	4	19	22	17*	0	5	19	5	5*
0	6	19	27	-37*	0	7	19	41	-21*	0	10	18	43	-37*
0	9	18	5	18*	0	8	18	6	-7*	0	4	18	5	0*
0	3	18	5	-18*	0	2	18	12	10*	0	1	18	5	14*
0	0	18	24	45	0	-2	18	7	1*	0	-3	18	29	7*
0	-4	18	12	21*	0	-5	18	4	30*	0	-5	17	5	-11*
0	-4	17	9	28*	0	-3	17	25	-5*	0	-1	17	10	6*
0	1	17	16	1*	0	2	17	5	-10*	0	4	17	20	45*
0	5	17	19	23*	0	6	17	5	21*	0	7	17	5	22*
0	8	17	5	12*	0	9	17	25	4*	0	10	17	33	-9*
0	12	17	26	-23*	0	14	16	5	4*	0	13	16	9	13*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	12	16	5	-1*	0	11	16	5	22*	0	10	16	5	2*
0	9	16	11	-3*	0	8	16	38	38*	0	6	16	24	1*
0	5	16	10	13*	0	0	16	5	-11*	0	-4	16	5	5*
0	-8	16	4	12*	0	-9	16	14	-7*	0	-10	15	4	5*
0	-9	15	16	-8*	0	-8	15	4	15*	0	-5	15	5	6*
0	-4	15	5	10*	0	8	15	5	29*	0	9	15	38	11*
0	10	15	18	-15*	0	11	15	5	1*	0	13	15	5	6*
0	14	15	11	17*	0	15	15	23	13*	14	0	15	6	-10*
0	13	14	7	17*	0	10	14	5	-3*	0	-8	14	4	-21*
0	-10	14	15	-20*	0	-11	14	33	11*	0	-12	13	12	14*
0	-10	13	4	10*	0	-9	13	4	-15*	0	-8	13	4	20*
0	13	13	15	20*	13	0	14	20	1*	13	0	16	5	-24*
12	0	17	5	4*	12	0	15	22	-1*	12	0	13	6	18*
0	-11	12	4	7*	-12	0	13	12	-19*	-11	0	14	38	-13*
-11	0	13	3	-3*	-11	0	11	18	-36	0	-10	11	4	18*
11	0	14	5	34*	11	0	16	25	-12*	11	0	17	21	-3*
10	0	18	5	11*	10	0	17	5	3*	10	0	16	5	-2*
-10	0	11	26	-25*	-10	0	12	19	23*	-10	0	13	5	22*
-10	0	14	10	15*	-9	0	16	22	-37*	-9	0	13	5	0*
-9	0	12	15	27*	9	0	17	5	9*	9	0	18	5	-25*
8	0	19	15	-17*	8	0	17	42	5*	8	0	16	26	-29*
8	0	15	26	37	-8	0	13	18	-33*	-8	0	14	5	21*
-7	0	16	5	1*	-7	0	14	21	15*	7	0	16	5	11*
7	0	17	5	-26*	6	0	17	18	-37	6	0	16	9	-5*
-6	0	15	19	19*	-6	0	17	13	10*	-5	0	18	22	-2*
-5	0	17	25	-11*	-5	0	16	5	-42*	-5	0	15	5	-11*
5	0	16	5	17*	5	0	17	11	-16*	5	0	19	18	-24*
4	0	19	5	9*	4	0	18	5	21*	4	0	17	5	3*
4	0	16	5	0*	-4	0	15	26	-38*	-4	0	16	5	-9*
-4	0	18	13	12*	-3	0	18	5	-17*	3	0	16	5	-34*
3	0	17	26	-41*	3	0	18	5	0*	2	0	19	5	-4*
2	0	17	23	-28*	2	0	16	25	43	-2	0	17	21	-34*
-2	0	19	24	-4*	-1	0	19	4	0*	-1	0	18	5	-6*
-1	0	17	5	-11*	-1	0	16	5	-6*	1	0	18	5	-20*
1	0	19	22	-19*	0	0	19	5	-5*	0	0	16	8	-11*
0	0	16	19	-11*	0	0	19	31	-5*	1	0	19	8	-19*
1	0	18	18	-20*	-1	0	16	5	-6*	-1	0	17	5	-11*
-1	0	18	5	-6*	-1	0	19	10	0*	-2	0	19	4	-4*
2	0	16	25	43	2	0	19	18	-4*	3	0	19	15	36
3	0	18	21	0*	3	0	16	5	-34*	-3	0	16	20	34*
-3	0	18	5	-17*	-4	0	18	4	12*	-4	0	15	18	-38*
4	0	16	5	0*	4	0	17	12	3*	4	0	18	17	21*
4	0	19	16	9*	5	0	19	19	-24*	5	0	16	5	17*
-5	0	15	5	-11*	-5	0	16	25	-42*	-5	0	17	5	-11*
-5	0	18	4	-2*	-6	0	17	5	10*	-6	0	16	17	13*
-6	0	15	5	19*	6	0	16	16	-5*	6	0	18	6	-48*
7	0	16	22	11*	-7	0	14	5	15*	-7	0	16	26	1*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-8	0	14	46	21*	-8	0	13	21	-33*	8	0	16	5	-29*
8	0	17	49	5*	8	0	19	5	-17*	9	0	18	16	-25*
9	0	17	5	9*	9	0	15	15	-35*	-9	0	12	5	27*
-9	0	13	19	0*	-9	0	15	5	32*	-10	0	15	24	33*
-10	0	13	5	22*	-10	0	12	12	23*	10	0	16	5	-2*
10	0	17	5	3*	10	0	18	13	11*	11	0	17	5	-3*
11	0	16	12	-12*	11	0	15	30	47*	0	-10	11	4	18*
-11	0	13	16	-3*	-11	0	14	5	-13*	-12	0	13	16	-19*
0	-11	12	4	7*	12	0	13	5	18*	12	0	15	29	-1*
12	0	17	26	4*	13	0	16	18	-24*	13	0	14	6	1*
0	-8	13	4	20*	0	-9	13	4	-15*	0	-10	13	24	10*
0	-12	13	8	14*	0	-11	14	21	11*	0	-10	14	4	-20*
0	-8	14	17	-21*	0	-7	14	22	-25*	0	10	14	5	-3*
0	12	14	5	-35*	0	13	14	7	17*	14	0	15	6	-10*
14	0	16	25	28*	0	15	15	17	13*	0	14	15	22	17*
0	13	15	5	6*	0	11	15	50	1*	0	10	15	15	-15*
0	9	15	17	11*	0	-4	15	8	10*	0	-5	15	18	6*
0	-8	15	24	15*	0	-9	15	33	-8*	0	-10	15	20	5*
0	-9	16	19	-7*	0	-8	16	4	12*	0	-7	16	13	29*
0	-6	16	5	-16*	0	-4	16	22	5*	0	-3	16	5	26*
0	0	16	38	-11*	0	5	16	5	13*	0	6	16	19	1*
0	7	16	5	43	0	9	16	5	-3*	0	10	16	7	2*
0	11	16	5	22*	0	12	16	5	-1*	0	13	16	24	13*
0	14	16	18	4*	0	12	17	16	-23*	0	10	17	25	-9*
0	9	17	23	4*	0	8	17	7	12*	0	7	17	5	22*
0	6	17	5	21*	0	5	17	19	23*	0	4	17	27	45*
0	2	17	5	-10*	0	1	17	25	1*	0	-1	17	27	6*
0	-2	17	5	-29*	0	-3	17	37	-5*	0	-5	17	5	-11*
0	-7	17	18	-27*	0	-5	18	13	30*	0	-4	18	16	21*
0	-3	18	5	7*	0	-2	18	5	1*	0	1	18	5	14*
0	2	18	16	10*	0	3	18	15	-18*	0	4	18	5	0*
0	5	18	5	-14*	0	8	18	5	-7*	0	9	18	40	18*
0	11	18	20	-34*	0	7	19	5	-21*	0	5	19	24	5*
0	4	19	5	17*	0	3	19	5	-22*	0	0	19	5	-5*
0	-1	19	17	-30*	0	-2	19	24	-30	1	5	20	22	-25*
1	4	20	5	-5*	1	3	20	25	32*	1	2	20	6	14*
1	-3	19	13	-16*	1	-2	19	20	-5*	1	-1	19	5	0*
1	1	19	26	-24*	1	2	19	5	-4*	1	3	19	5	29*
1	4	19	5	24*	1	5	19	27	5*	1	6	19	11	13*
1	7	19	11	31*	1	9	19	40	-11*	1	10	18	43	-2*
1	9	18	5	15*	1	8	18	5	11*	1	6	18	5	0*
1	3	18	21	-6*	1	2	18	5	-6*	1	-1	18	5	23*
1	-2	18	5	11*	1	-3	18	5	-30*	1	-4	18	4	-20*
1	-5	18	4	31*	1	-7	17	4	-18*	1	-6	17	4	-4*
1	-4	17	25	16*	1	-3	17	5	-17*	1	-2	17	5	6*
1	-1	17	21	42*	1	1	17	14	-27*	1	6	17	21	-28*
1	7	17	5	-25*	1	9	17	18	-25*	1	10	17	19	5*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	11	17	10	-7*	1	12	17	42	-6*	1	13	17	5	-2*
1	14	16	22	-9*	1	13	16	5	-29*	1	12	16	16	-28*
1	11	16	5	19*	1	10	16	5	-6*	1	8	16	26	7*
1	5	16	37	-9*	1	-1	16	4	12*	1	-2	16	18	-27*
1	-3	16	13	-10*	1	-4	16	5	5*	1	-5	16	14	-18*
1	-7	16	12	-23*	1	-8	16	4	-8*	1	-9	16	15	-8*
1	-10	15	11	-5*	1	-9	15	4	21*	1	-7	15	5	0*
1	-6	15	5	17*	1	-5	15	20	2*	1	-4	15	4	-15*
1	9	15	44	-15*	1	10	15	5	-19*	1	14	15	5	5*
1	15	15	5	18*	14	1	16	10	44*	1	14	14	49	-22*
1	13	14	46	37*	1	12	14	27	48*	1	11	14	5	-22*
1	-6	14	4	-9*	1	-7	14	4	1*	1	-9	14	15	17*
1	-11	14	4	-18*	1	-12	13	4	22*	1	-11	13	4	16*
1	-9	13	44	-43*	1	-8	13	18	29*	1	12	13	5	-32*
13	1	16	21	38*	13	1	17	5	39*	12	1	17	5	9*
12	1	16	26	-25*	12	1	14	6	9*	12	1	13	43	-23*
1	-9	12	4	-3*	1	-10	12	21	16*	-12	-1	12	5	17*
-12	-1	13	5	17*	-11	-1	13	11	1*	-11	-1	12	5	-11*
-11	-1	11	5	-6*	1	-10	11	18	29*	11	1	14	7	-15*
11	1	15	5	14*	11	1	16	5	-9*	11	1	17	7	-10*
11	1	18	5	1*	10	1	18	8	13*	10	1	17	21	30*
10	1	15	26	-28*	-10	-1	12	41	-18*	-10	-1	13	18	-33*
-10	-1	15	16	4*	-9	-1	16	16	26*	-9	-1	14	17	15*
-9	-1	13	5	-11*	-9	-1	12	12	17*	9	1	16	5	-3*
9	1	18	23	-19*	9	1	19	5	-14*	8	1	18	5	3*
8	1	17	25	-5*	8	1	16	5	-32*	-8	-1	13	16	-18*
-7	-1	17	5	-10*	-7	-1	16	6	-16*	-7	-1	15	12	-14*
7	1	16	5	0*	7	1	17	5	-8*	7	1	18	27	38*
7	1	19	19	0*	6	1	18	5	19*	6	1	17	31	2*
6	1	16	11	8*	-6	-1	15	5	29*	-6	-1	16	32	21*
-5	-1	18	15	10*	5	1	17	5	6*	5	1	18	16	-2*
5	1	19	5	-12*	5	1	20	5	-10*	4	1	19	5	-29*
4	1	18	9	29*	4	1	17	5	-7*	-4	-1	15	14	-12*
-4	-1	17	14	4*	-4	-1	18	5	17*	-3	-1	18	5	24*
-3	-1	16	9	10*	3	1	17	5	-13*	2	1	20	5	-6*
2	1	18	5	-1*	-2	-1	17	5	12*	-2	-1	18	14	3*
-2	-1	19	18	23*	-1	-1	19	5	-12*	-1	-1	18	5	-4*
-1	-1	16	5	-11*	1	1	17	22	-27*	1	1	19	12	-24*
1	-1	19	17	0*	1	-1	18	5	23*	1	-1	16	5	12*
-1	1	16	22	35	-1	1	17	17	-27*	-1	1	19	5	46
-2	1	19	23	42*	-2	1	16	29	31*	2	-1	17	5	8*
2	-1	18	25	-25*	2	-1	19	12	-12*	3	-1	19	21	-18*
3	-1	18	23	-25*	3	-1	17	5	-26*	3	-1	16	5	-27*
-3	1	17	27	-36*	-3	1	19	8	-1*	-4	1	18	23	7*
-4	1	17	5	23*	-4	1	15	5	29*	4	-1	16	18	1*
4	-1	19	5	-9*	5	-1	19	5	-28*	5	-1	18	5	-9*
-5	1	15	15	-3*	-5	1	16	5	5*	-5	1	17	5	-8*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-5	1	18	6	-5*	-6	1	17	26	-35*	6	-1	19	5	-9*
7	-1	18	5	-11*	7	-1	16	5	6*	7	-1	15	29	-3*
-7	1	15	5	-19*	-8	1	16	45	-4*	-8	1	14	5	6*
-8	1	13	5	-11*	8	-1	15	19	15*	8	-1	16	5	3*
8	-1	17	38	-5*	8	-1	18	28	51*	8	-1	19	5	17*
9	-1	18	23	-28*	9	-1	17	7	12*	9	-1	16	13	-2*
9	-1	15	5	31*	-9	1	12	5	9*	-9	1	14	5	-22*
-9	1	15	5	-19*	-9	1	16	40	-24*	-10	1	15	6	3*
-10	1	14	23	-2*	-10	1	13	17	31*	-10	1	12	21	49*
-10	1	11	5	6*	10	-1	15	24	-1*	10	-1	16	5	22*
10	-1	17	5	-40*	11	-1	16	6	3*	-1	-10	11	4	37*
-11	1	14	5	1*	-12	1	13	5	1*	-1	-10	12	19	26*
-1	-9	12	18	-24*	-1	12	12	5	9*	12	-1	16	33	-24*
12	-1	17	5	2*	13	-1	16	5	-20*	13	-1	15	46	-10*
-1	13	13	21	27*	-1	12	13	5	-11*	-1	-8	13	4	30*
-1	-9	13	22	7*	-1	-11	13	4	5*	-1	-12	13	13	-26*
-1	-11	14	4	8*	-1	-10	14	4	20*	-1	-9	14	24	17*
-1	-6	14	23	-7*	-1	10	14	16	1*	-1	11	14	21	-29*
-1	13	14	20	-1*	-1	14	14	26	-37*	-1	14	15	5	12*
-1	12	15	9	-6*	-1	11	15	22	-13*	-1	10	15	5	-23*
-1	9	15	25	12*	-1	8	15	5	10*	-1	7	15	5	-33*
-1	-5	15	23	7*	-1	-9	15	16	-11*	-1	-10	15	4	9*
-1	-9	16	4	0*	-1	-8	16	15	9*	-1	-5	16	21	-18*
-1	-4	16	16	-7*	-1	-2	16	18	18*	-1	-1	16	5	-11*
-1	4	16	21	-13*	-1	6	16	27	-35*	-1	7	16	26	-26*
-1	8	16	5	-10*	-1	9	16	5	-23*	-1	10	16	28	34*
-1	12	16	38	-4*	-1	13	16	17	13*	-1	12	17	22	-36*
-1	11	17	5	-10*	-1	9	17	27	39*	-1	8	17	5	-9*
-1	7	17	18	23*	-1	5	17	5	12*	-1	4	17	5	-12*
-1	3	17	5	6*	-1	2	17	21	2*	-1	1	17	17	-27*
-1	-2	17	26	-30*	-1	-3	17	5	-2*	-1	-4	17	25	-4*
-1	-5	17	10	-9*	-1	-7	17	16	13*	-1	-4	18	9	-20*
-1	-3	18	5	-1*	-1	-1	18	5	-4*	-1	3	18	7	-9*
-1	4	18	5	-10*	-1	5	18	28	44*	-1	7	18	25	-24*
-1	8	18	5	-28*	-1	9	18	13	38*	-1	10	18	5	-3*
-1	8	19	5	-14*	-1	6	19	5	-8*	-1	4	19	5	-9*
-1	2	19	15	-7*	-1	-1	19	6	-12*	-1	-2	19	5	38*
-2	2	19	5	34*	-2	3	19	46	-6*	-2	4	19	34	-8*
-2	5	19	5	8*	-2	8	18	5	-14*	-2	5	18	5	0*
-2	3	18	21	6*	-2	-2	18	5	6*	-2	-7	17	15	25*
-2	-6	17	5	9*	-2	-4	17	46	38*	-2	-3	17	15	-13*
-2	-2	17	5	0*	-2	2	17	5	-12*	-2	4	17	5	-22*
-2	6	17	5	3*	-2	7	17	20	17*	-2	11	17	26	42*
-2	13	16	11	-20*	-2	11	16	39	46*	-2	7	16	5	6*
-2	6	16	19	-36*	-2	5	16	27	-30*	-2	2	16	12	11*
-2	-2	16	5	17*	-2	-3	16	5	14*	-2	-4	16	21	6*
-2	-5	16	12	-2*	-2	-6	16	5	8*	-2	-7	16	19	10*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-2	-8	16	4	-23*	-2	-10	15	4	9*	-2	-9	15	4	11*
-2	-6	15	12	3*	-2	-5	15	5	17*	-2	6	15	5	-37
-2	7	15	16	-1*	-2	9	15	28	-1*	-2	10	15	19	-38*
-2	11	15	5	-8*	-2	12	15	16	4*	-2	14	15	5	-29*
14	-2	15	16	-2*	-2	14	14	5	-26*	-2	13	14	18	28*
-2	12	14	5	24*	-2	11	14	5	15*	-2	10	14	24	13*
-2	-6	14	22	-25*	-2	-7	14	4	-22*	-2	-10	14	4	-3*
-2	-11	14	20	-12*	-2	-12	13	33	-15*	-2	-9	13	20	18*
-2	-7	13	4	5*	-2	11	13	5	14*	-2	12	13	5	1*
-2	13	13	14	18*	13	-2	14	29	31*	13	-2	15	5	9*
13	-2	16	5	17*	12	-2	16	5	-2*	12	-2	15	5	23*
-2	12	12	11	-12*	-2	-10	12	18	30*	-12	2	12	5	14*
-12	2	13	15	26*	-11	2	14	5	-18*	-11	2	13	24	40*
-11	2	11	5	-7*	-2	-10	11	12	1*	11	-2	13	5	-24*
11	-2	15	22	6*	11	-2	16	35	22*	10	-2	17	25	-12*
10	-2	16	20	52*	10	-2	15	15	-13*	10	-2	14	22	-21*
-10	2	12	28	31*	-9	2	16	5	3*	-9	2	15	18	21*
-9	2	14	28	-26*	-9	2	12	5	-2*	9	-2	14	5	8*
9	-2	15	5	-22*	9	-2	16	5	17*	9	-2	18	5	-15*
8	-2	18	16	30*	8	-2	17	19	0*	8	-2	16	9	-11*
-8	2	13	15	6*	-8	2	14	12	44*	-8	2	15	5	26*
-8	2	16	25	10*	-7	2	17	10	-32*	-7	2	15	5	-3*
-7	2	14	5	-13*	7	-2	15	5	-13*	7	-2	16	5	10*
7	-2	17	10	-32*	6	-2	19	12	-7*	6	-2	18	5	-20*
6	-2	16	21	36*	6	-2	15	5	3*	-6	2	15	5	-4*
-6	2	16	5	3*	-5	2	17	15	-5*	-5	2	16	5	11*
5	-2	16	39	-11*	5	-2	19	16	-11*	4	-2	19	5	-26*
4	-2	18	19	28*	4	-2	17	5	-19*	-4	2	15	23	31*
-4	2	16	21	-23*	-4	2	18	26	9*	-3	2	19	5	-7*
-3	2	18	5	8*	3	-2	16	6	-33*	3	-2	17	5	-13*
3	-2	18	23	4*	3	-2	19	22	-8*	2	-2	19	10	26*
2	-2	18	32	14*	2	-2	17	5	21*	-2	2	16	5	11*
-2	-2	18	12	6*	-2	-2	17	12	0*	-2	-2	16	13	17*
2	2	18	12	30*	2	2	20	5	11*	3	2	20	5	-21*
3	2	19	5	-32*	3	2	18	5	-1*	-3	-2	15	13	-26*
-3	-2	16	13	-31*	-3	-2	17	5	-7*	-3	-2	18	5	-11*
-4	-2	18	5	-4*	-4	-2	17	7	-14*	-4	-2	16	16	-31*
4	2	18	19	-5*	4	2	20	30	-20*	5	2	19	25	-4*
5	2	18	5	4*	-5	-2	14	5	6*	-5	-2	16	5	4*
-5	-2	17	5	-14*	-6	-2	17	10	-6*	-6	-2	16	14	25*
-6	-2	15	21	7*	6	2	17	5	6*	6	2	19	5	13*
6	2	20	37	12*	7	2	19	5	-34*	7	2	18	5	-15*
-7	-2	13	5	15*	-7	-2	14	5	-15*	-7	-2	15	5	-12*
-7	-2	16	14	14*	-7	-2	17	17	2*	-8	-2	16	15	11*
-8	-2	14	5	0*	-8	-2	13	30	18*	8	2	17	5	3*
8	2	18	5	-7*	8	2	19	5	-31*	9	2	19	24	28*
9	2	18	36	-17*	9	2	17	5	41*	9	2	15	5	-4*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-9	-2	12	11	17*	-9	-2	15	5	7*	-10	-2	13	37	10*
-10	-2	12	5	8*	-10	-2	11	5	-17*	10	2	17	5	-14*
10	2	18	25	-27*	10	2	19	11	23*	11	2	18	5	-10*
11	2	16	22	-7*	11	2	15	6	32*	11	2	14	43	-13*
-11	-2	11	25	15*	-11	-2	12	5	26*	-11	-2	14	5	23*
-12	-2	13	6	17*	-12	-2	12	5	-20*	2	-11	12	4	-8*
2	-10	12	4	-18*	2	-9	12	19	-27*	12	2	14	6	5*
12	2	15	6	-20*	12	2	16	6	12*	12	2	17	14	26*
12	2	18	35	5*	13	2	17	6	8*	13	2	15	6	8*
13	2	14	23	-15*	2	13	13	7	45*	2	-8	13	39	-5*
2	-11	13	11	-31*	2	-12	13	15	-14*	2	-10	14	4	14*
2	-8	14	4	16*	2	-7	14	4	-24*	2	11	14	28	45*
2	13	14	5	13*	2	14	14	22	-19*	14	2	15	24	29*
14	2	16	6	-8*	2	15	15	5	3*	2	14	15	27	18*
2	12	15	12	-7*	2	10	15	21	-14*	2	9	15	43	-41*
2	-9	15	18	20*	2	-10	15	20	16*	2	-9	16	15	2*
2	-8	16	4	-24*	2	-7	16	10	-17*	2	-6	16	5	2*
2	-5	16	5	-13*	2	-4	16	12	27*	2	-3	16	23	32*
2	-2	16	5	35*	2	6	16	5	25*	2	7	16	5	-14*
2	10	16	6	15*	2	11	16	35	-1*	2	13	16	6	-4*
2	14	16	28	24*	2	12	17	22	-8*	2	11	17	6	-14*
2	8	17	32	-14*	2	7	17	20	-22*	2	3	17	27	-38*
2	2	17	5	30*	2	-2	17	5	21*	2	-3	17	26	-10*
2	-5	17	25	23*	2	-6	17	10	25*	2	-3	18	5	-2*
2	-2	18	23	14*	2	4	18	23	-18*	2	7	18	5	8*
2	8	18	15	8*	2	9	18	15	35*	2	10	18	6	1*
2	11	18	6	3*	2	12	18	20	-2*	2	10	19	23	-5*
2	9	19	6	-22*	2	8	19	6	-5*	2	7	19	6	-9*
2	6	19	23	4*	2	5	19	24	24*	2	4	19	5	4*
2	3	19	5	14*	2	-2	19	5	26*	2	2	20	5	11*
2	3	20	5	-10*	2	4	20	5	-25*	2	5	20	22	-19*
2	6	20	5	-6*	3	6	20	5	-10*	3	5	20	5	-13*
3	4	20	7	-8*	3	3	20	5	-12*	3	-3	19	5	35
3	3	19	5	-25*	3	4	19	14	26*	3	5	19	25	-9*
3	6	19	30	-48*	3	7	19	29	-26*	3	8	19	6	10*
3	9	19	8	-13*	3	10	19	6	-9*	3	12	18	6	3*
3	11	18	20	-34*	3	9	18	6	6*	3	8	18	20	7*
3	6	18	5	-18*	3	-4	18	5	-6*	3	-5	18	5	-28*
3	-7	17	22	16*	3	-6	17	5	-1*	3	-5	17	11	2*
3	-4	17	19	8*	3	-3	17	5	-19*	3	3	17	5	-29*
3	4	17	13	12*	3	7	17	6	-7*	3	8	17	6	25*
3	10	17	6	2*	3	12	17	47	25*	3	15	16	7	-12*
3	14	16	6	27*	3	12	16	25	-6*	3	11	16	6	3*
3	9	16	6	27*	3	6	16	22	-17*	3	-5	16	15	8*
3	-6	16	5	-1*	3	-8	16	19	-3*	3	-9	16	15	-18*
3	-10	15	24	19*	3	-9	15	18	-29*	3	-7	15	5	9*
3	-6	15	20	28*	3	-4	15	5	4*	3	10	15	25	-20*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	11	15	18	-5*	3	12	15	6	-13*	3	13	15	22	-24*
3	14	15	21	15*	3	15	15	6	-10*	15	3	16	6	-20*
14	3	16	6	-13*	14	3	15	6	0*	3	13	14	22	-44*
3	12	14	10	-10*	3	11	14	22	-25*	3	-7	14	6	-11*
3	-9	14	21	0*	3	-10	14	18	27*	3	-11	14	20	3*
3	-12	13	12	4*	3	-10	13	4	28*	3	-7	13	4	30*
3	12	13	18	-3*	13	3	15	6	-12*	13	3	16	6	3*
13	3	17	6	-9*	12	3	18	8	19*	12	3	17	29	34*
12	3	16	6	-2*	12	3	15	6	-10*	12	3	13	30	27*
3	-10	12	4	-9*	3	-11	12	4	-12*	-11	-3	14	25	49*
-11	-3	11	12	2*	11	3	15	30	35*	11	3	16	6	-35*
11	3	17	6	-24*	10	3	19	12	15*	10	3	18	6	-17*
-10	-3	11	5	4*	-10	-3	14	5	25*	-10	-3	15	5	-28*
-9	-3	15	24	-29*	-9	-3	13	5	15*	-9	-3	12	24	-25*
9	3	15	5	15*	9	3	16	6	13*	9	3	17	19	-4*
9	3	18	17	-24*	9	3	19	5	28*	8	3	19	5	7*
8	3	17	5	25*	8	3	16	5	21*	-8	-3	12	5	-15*
-8	-3	13	5	10*	-8	-3	14	5	4*	-8	-3	15	5	-9*
-8	-3	16	19	-9*	-7	-3	16	5	-4*	-7	-3	14	17	24*
7	3	16	41	-31*	7	3	17	5	-17*	7	3	18	5	19*
7	3	19	5	7*	6	3	20	5	-13*	6	3	19	19	16*
6	3	16	5	0*	-6	-3	16	23	26*	-6	-3	17	8	4*
-5	-3	17	5	2*	-5	-3	16	5	6*	-5	-3	15	19	-12*
5	3	17	5	-33*	5	3	19	5	27*	5	3	20	20	38*
4	3	20	22	22*	4	3	19	14	10*	4	3	18	5	-7*
4	3	17	13	33*	-4	-3	15	40	39*	-4	-3	16	12	12*
-4	-3	17	5	6*	-4	-3	18	20	21*	-3	-3	18	24	-30*
-3	-3	17	5	7*	-3	-3	15	5	20*	3	3	17	6	-29*
3	3	18	20	-40*	3	3	19	5	-25*	3	3	20	15	-12*
3	-3	18	5	20	3	-3	17	14	-19*	3	-3	16	5	20*
-3	3	16	5	-6*	-3	3	18	5	12*	-3	3	19	6	0*
-4	3	18	5	-4*	-4	3	17	5	8*	4	-3	18	14	8*
4	-3	19	5	-7*	5	-3	18	23	25*	5	-3	17	14	-29*
-5	3	15	29	37*	-5	3	16	5	-18*	-5	3	17	5	16*
-5	3	18	6	11*	-6	3	17	21	1*	-6	3	16	5	5*
-6	3	15	5	24*	-6	3	14	17	11*	6	-3	15	24	-6*
6	-3	18	26	13*	7	-3	18	11	7*	7	-3	17	5	-14*
7	-3	16	5	2*	-7	3	13	16	-30*	-7	3	14	7	-13*
-7	3	15	5	-28*	-7	3	16	5	-11*	-7	3	17	5	-11*
-8	3	16	25	-35*	-8	3	15	5	-1*	-8	3	13	21	13*
8	-3	14	5	38*	8	-3	15	5	-19*	8	-3	17	25	-24*
8	-3	18	5	22*	9	-3	16	18	-33*	9	-3	14	5	21*
-9	3	12	21	31*	-9	3	14	15	59*	-9	3	15	16	22*
-10	3	15	19	22*	-10	3	14	29	-7*	-10	3	13	30	-55*
10	-3	14	4	28*	10	-3	15	15	-19*	10	-3	16	15	36*
10	-3	17	23	36*	11	-3	17	5	-19*	11	-3	16	5	21*
11	-3	15	6	-4*	11	-3	14	14	-3*	-3	-10	11	4	1*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-11	3	11	5	-14*	-11	3	12	5	6*	-11	3	13	5	-23*
-11	3	14	5	-8*	-12	3	13	19	6*	-12	3	12	5	27*
-3	-10	12	23	3*	-3	-8	12	4	-13*	-3	11	12	5	-4*
-3	12	12	9	-5*	12	-3	13	47	-30*	12	-3	14	6	-20*
12	-3	15	27	-13*	13	-3	15	6	-41*	13	-3	14	18	10*
-3	13	13	5	2*	-3	12	13	20	-40*	-3	10	13	5	-6*
-3	-9	13	29	-40*	-3	-12	13	4	5*	-3	-11	14	20	-9*
-3	-9	14	23	13*	-3	-7	14	19	23*	-3	-5	14	37	1*
-3	10	14	5	15*	-3	11	14	5	-6*	-3	12	14	25	43*
-3	14	14	5	-12*	-3	13	15	5	-8*	-3	11	15	5	-3*
-3	7	15	17	1*	-3	6	15	5	-15*	-3	4	15	15	5*
-3	-3	15	9	20*	-3	-4	15	5	11*	-3	-5	15	5	5*
-3	-6	15	25	8*	-3	-7	15	5	-1*	-3	-8	15	5	6*
-3	-9	15	6	22*	-3	-8	16	4	-19*	-3	-7	16	5	-4*
-3	-6	16	25	-23*	-3	-4	16	5	9*	-3	-3	16	5	16*
-3	3	16	5	-6*	-3	5	16	21	18*	-3	6	16	11	-6*
-3	9	16	23	-33*	-3	11	16	5	0*	-3	12	16	5	-13*
-3	11	17	5	8*	-3	10	17	20	-13*	-3	8	17	5	-4*
-3	7	17	4	18*	-3	5	17	9	-33*	-3	4	17	26	11*
-3	-3	17	5	7*	-3	-5	17	5	1*	-3	3	18	23	12*
-3	4	18	5	-11*	-3	6	18	39	-21*	-3	7	18	22	10*
-3	8	18	16	0*	-3	4	19	5	15*	-3	3	19	5	0*
-4	6	18	5	-20*	-4	5	18	5	10*	-4	-4	17	16	2*
-4	5	17	13	13*	-4	6	17	5	1*	-4	7	17	6	1*
-4	8	17	5	9*	-4	9	17	5	1*	-4	10	17	5	-1*
-4	11	16	16	8*	-4	10	16	6	-4*	-4	7	16	5	0*
-4	6	16	29	-2*	-4	5	16	5	6*	-4	4	16	5	7*
-4	-4	16	21	-33*	-4	-7	16	4	34*	-4	-8	16	4	-9*
-4	-9	15	4	4*	-4	-8	15	23	-1*	-4	-7	15	19	14*
-4	-5	15	25	15*	-4	-4	15	5	-22*	-4	5	15	5	10*
-4	6	15	5	-24*	-4	8	15	38	-14*	-4	10	15	8	6*
-4	11	15	17	-13*	-4	13	15	33	19*	-4	14	14	4	-2*
-4	13	14	5	33*	-4	12	14	24	-27*	-4	10	14	23	-6*
-4	-4	14	41	-33	-4	-5	14	19	-28*	-4	-6	14	5	-13*
-4	-7	14	5	4*	-4	-8	14	4	-20*	-4	-9	14	27	-16*
-4	-10	14	25	-19*	-4	-11	14	37	4*	-4	-12	13	4	-1*
-4	-10	13	16	20*	-4	-8	13	28	-40*	-4	-7	13	14	-1*
-4	-6	13	20	24*	-4	9	13	10	-10*	-4	11	13	6	-13*
-4	13	13	16	-3*	13	-4	14	21	30*	13	-4	15	5	-7*
12	-4	13	18	-6*	-4	12	12	5	27*	-4	-8	12	10	-33*
-4	-9	12	4	-19*	-12	4	12	5	-17*	-12	4	13	15	12*
-11	4	14	5	-1*	-11	4	13	23	-11*	-4	-10	11	8	-8*
-4	-9	11	18	18*	11	-4	12	6	-17*	11	-4	14	28	4*
11	-4	15	13	19*	11	-4	16	16	20*	10	-4	17	5	19*
10	-4	16	5	-5*	10	-4	15	5	-28*	10	-4	14	5	2*
-10	4	11	5	14*	-10	4	12	5	-1*	-10	4	13	5	17*
-10	4	14	5	23*	-10	4	15	5	-6*	-9	4	15	22	-30*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-9	4	14	5	23*	-9	4	12	19	-18*	9	-4	14	16	15*
9	-4	17	5	6*	8	-4	16	11	-4*	-8	4	13	13	9*
-8	4	14	5	-8*	-8	4	16	28	2*	-7	4	17	5	19*
-7	4	15	5	-16*	-7	4	14	19	-34*	7	-4	15	26	46*
7	-4	17	13	-14*	7	-4	18	16	-7*	6	-4	18	24	-26*
6	-4	17	15	-5*	6	-4	16	10	-3*	6	-4	15	5	-5*
-6	4	14	45	25*	-6	4	15	26	16*	-6	4	16	5	7*
-6	4	17	30	-6*	-5	4	17	11	1*	-5	4	16	5	-19*
5	-4	15	19	27*	5	-4	16	5	5*	5	-4	17	23	-32*
5	-4	18	20	-14*	4	-4	18	5	15*	4	-4	17	5	-25*
-4	4	16	5	7*	-4	4	17	5	21*	-4	4	18	9	-9*
-4	-4	17	20	2*	4	4	17	5	19*	4	4	18	5	39
4	4	19	5	24*	4	4	20	5	11*	5	4	20	5	-4*
5	4	19	5	5*	5	4	18	5	-10*	-5	-4	14	5	-25*
-5	-4	15	5	-18*	-5	-4	16	5	-3*	-5	-4	17	21	-21*
-6	-4	17	11	4*	-6	-4	16	5	2*	-6	-4	15	25	-12*
6	4	17	5	-28*	6	4	18	5	18*	6	4	19	5	17*
6	4	20	20	-38*	7	4	20	4	-15*	7	4	19	5	-6*
7	4	16	23	-28*	-7	-4	13	5	1*	-7	-4	15	5	-14*
-8	-4	16	14	-33*	-8	-4	15	5	20*	-8	-4	14	3	10*
8	4	16	5	13*	8	4	18	5	10*	8	4	19	7	-43*
9	4	19	5	-4*	9	4	17	5	0*	9	4	16	13	-33*
-9	-4	12	41	16*	-9	-4	13	5	-4*	-9	-4	14	37	22*
-9	-4	15	18	15*	-10	-4	13	5	20*	-10	-4	12	5	-11*
-10	-4	11	10	23*	10	4	15	7	-10*	10	4	16	5	-22*
10	4	17	6	-12*	10	4	18	5	22*	10	4	19	27	17*
11	4	18	29	53*	11	4	16	6	-20*	11	4	15	15	-10*
4	-10	11	19	-15*	-11	-4	11	5	-7*	-11	-4	14	16	2*
-12	-4	12	5	17*	4	-10	12	8	-14*	4	-9	12	4	3*
12	4	16	6	-18*	12	4	17	20	37*	12	4	18	10	-22*
13	4	17	29	-2*	13	4	16	6	23*	13	4	15	26	-29*
4	13	13	6	29*	4	-8	13	13	1*	4	-9	13	8	-3*
4	-10	13	23	-25*	4	-11	13	17	32*	4	-10	14	23	-25*
4	-8	14	24	-27*	4	-7	14	4	-18*	4	-6	14	10	-15*
4	13	14	24	-30*	14	4	15	23	35*	14	4	16	6	18*
14	4	17	5	-1*	15	4	16	20	2*	4	15	15	14	14*
4	13	15	18	-3*	4	12	15	6	24*	4	10	15	29	-27*
4	9	15	21	-15*	4	-5	15	24	-25*	4	-6	15	5	4*
4	-8	15	20	19*	4	-9	15	4	-19*	4	-10	15	14	-1*
4	-8	16	23	37*	4	-6	16	17	-11*	4	-5	16	5	4*
4	12	16	6	5*	4	13	16	13	15*	4	14	16	6	-9*
4	15	16	5	-21*	4	13	17	22	-17*	4	12	17	6	22*
4	11	17	8	-23*	4	9	17	23	-10*	4	8	17	6	7*
4	6	17	19	-21*	4	4	17	9	19*	4	-4	17	5	-25*
4	-5	17	13	14*	4	-6	17	4	-30*	4	-7	17	4	-23*
4	-5	18	4	12*	4	-4	18	5	15*	4	5	18	26	-11*
4	7	18	21	-16*	4	8	18	6	13*	4	10	19	6	12*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	9	19	7	-28*	4	8	19	29	27*	4	7	19	12	26*
4	4	20	13	11*	4	5	20	5	-6*	4	6	20	24	37*
5	7	20	5	9*	5	6	20	15	37*	5	5	19	23	-26*
5	6	19	10	28*	5	8	19	22	4*	5	9	19	10	-21*
5	10	19	27	33*	5	12	18	6	15*	5	10	18	11	20*
5	9	18	39	-6*	5	8	18	6	2*	5	7	18	22	18*
5	6	18	5	-20*	5	5	18	17	-25*	5	-7	17	22	-35*
5	-6	17	34	-5*	5	-5	17	8	15*	5	5	17	15	-22*
5	6	17	5	-12*	5	7	17	6	-3*	5	8	17	6	-24*
5	9	17	21	-15*	5	10	17	25	-1*	5	11	17	6	-14*
5	12	17	6	-4*	5	13	17	6	-11*	5	14	17	25	-12*
5	15	16	16	-21*	5	14	16	6	-10*	5	13	16	25	-24*
5	11	16	30	-23*	5	10	16	6	24*	5	-5	16	5	16*
5	-7	16	4	-17*	5	-8	16	4	10*	5	-9	15	21	13*
5	-8	15	24	17*	5	-7	15	5	16*	5	-6	15	5	-8*
5	-5	15	12	-14*	5	10	15	27	34*	5	12	15	6	-9*
5	13	15	6	-18*	5	15	15	6	6*	14	5	17	25	-25*
14	5	16	6	-4*	5	14	14	30	19*	5	13	14	6	1*
5	-7	14	15	21*	5	-8	14	4	10*	5	-10	14	29	11*
5	-12	13	4	31*	5	-9	13	8	19*	5	12	13	6	21*
5	13	13	6	-18*	13	5	15	6	14*	13	5	17	10	-16*
12	5	18	29	-42*	12	5	17	26	17*	12	5	16	6	3*
12	5	13	6	5*	5	-8	12	4	40*	5	-9	12	4	12*
5	-11	12	4	17*	-11	-5	13	5	-22*	-11	-5	12	12	-5*
-11	-5	11	5	11*	5	-10	11	4	7*	5	-9	11	15	34*
11	5	14	20	11*	11	5	15	6	13*	11	5	16	42	5*
11	5	17	20	-2*	11	5	18	20	0*	10	5	19	28	24*
10	5	18	5	18*	10	5	17	15	-4*	-10	-5	10	17	-35*
-10	-5	11	5	-30*	-10	-5	12	23	-5*	-10	-5	14	5	-22*
-9	-5	15	12	20*	-9	-5	13	5	11*	9	5	16	29	48*
9	5	17	6	12*	9	5	18	30	-45*	8	5	17	5	5*
8	5	16	5	6*	-8	-5	14	27	-5*	-7	-5	16	16	-16*
-7	-5	15	5	1*	7	5	16	5	4*	7	5	18	5	15*
7	5	20	5	-2*	6	5	20	5	-20*	6	5	19	43	17*
6	5	18	5	33*	6	5	16	16	-33*	-6	-5	14	5	12*
-6	-5	15	19	-5*	-6	-5	16	5	31*	-5	-5	17	18	-22*
-5	-5	16	17	27*	-5	-5	14	20	-1*	-5	-5	13	18	38
5	5	18	23	-25*	5	5	19	23	-26*	5	5	20	13	1*
5	-5	18	22	23	5	-5	17	5	15*	5	-5	16	5	16*
5	-5	15	5	-14*	-5	5	14	12	-14*	-5	5	15	14	-7*
-5	5	16	5	-22*	-5	5	17	20	15*	-5	5	18	5	9*
-6	5	17	5	-35*	-6	5	16	17	-26*	6	-5	14	13	-9*
6	-5	15	5	-21*	6	-5	16	5	10*	7	-5	17	8	8*
7	-5	16	5	30*	7	-5	15	18	-24*	-7	5	13	27	39*
-7	5	14	28	-35*	-7	5	15	23	25*	-7	5	16	24	34*
-8	5	15	17	9*	-8	5	13	5	19*	-8	5	12	4	6*
8	-5	14	21	-10*	8	-5	15	5	27*	8	-5	17	25	-17*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
9	-5	16	12	-20*	9	-5	15	5	23*	9	-5	13	13	-4*
-9	5	12	15	-7*	-9	5	13	5	-12*	-9	5	14	5	-23*
-9	5	15	11	-21*	-10	5	14	5	-3*	-10	5	13	26	33*
10	-5	12	5	-24*	10	-5	13	5	4*	10	-5	14	6	-6*
10	-5	16	5	-9*	11	-5	15	48	-7*	11	-5	13	5	-18*
11	-5	12	25	0*	-5	11	11	19	-14*	-11	5	12	5	9*
-11	5	13	5	9*	-11	5	14	4	-12*	-12	5	13	4	2*
-12	5	12	5	-26*	-5	-10	12	26	17*	-5	-9	12	25	41*
-5	-8	12	24	3*	-5	-7	12	23	-36	-5	10	12	18	-28*
12	-5	13	19	-26*	12	-5	14	37	-7*	13	-5	14	5	22*
-5	13	13	4	-21*	-5	10	13	21	24*	-5	9	13	5	-18*
-5	8	13	18	47*	-5	-7	13	17	-7*	-5	-8	13	21	-19*
-5	-9	13	13	29*	-5	-10	13	4	29*	-5	-11	13	4	13*
-5	-10	14	4	4*	-5	-9	14	4	18*	-5	-7	14	5	-48*
-5	-5	14	5	-1*	-5	5	14	4	-14*	-5	8	14	17	6*
-5	9	14	5	-11*	-5	13	14	4	-3*	-5	12	15	4	10*
-5	11	15	11	-22*	-5	10	15	5	-5*	-5	9	15	29	-14*
-5	6	15	17	-5*	-5	5	15	5	-7*	-5	-6	15	5	9*
-5	-9	15	14	12*	-5	-7	16	4	8*	-5	5	16	5	-22*
-5	6	16	14	-20*	-5	7	16	7	-22*	-5	9	16	5	10*
-5	10	16	8	4*	-5	8	17	5	2*	-5	7	17	12	17*
-5	5	17	5	15*	-6	6	17	5	-8*	-6	9	16	32	-13*
-6	8	16	4	4*	-6	7	16	35	-20*	-6	6	16	16	-21*
-6	-6	16	4	9*	-6	8	15	5	-6*	-6	9	15	4	9*
-6	10	15	16	-8*	-6	12	14	4	-5*	-6	11	14	4	18*
-6	10	14	16	29*	-6	9	14	5	12*	-6	6	14	5	9*
-6	-7	14	27	28*	-6	-9	14	19	12*	-6	-10	14	24	-16*
-6	-11	13	4	-8*	-6	-10	13	14	-16*	-6	-9	13	14	-18*
-6	-8	13	17	31*	-6	-6	13	10	16*	-6	8	13	5	15*
-6	9	13	23	-21*	-6	10	13	12	-18*	-6	13	13	4	-2*
12	-6	13	5	-21*	-6	12	12	25	45*	-6	9	12	23	8*
-6	-7	12	47	-34*	-6	-8	12	10	8*	-6	-9	12	4	7*
-6	-10	12	13	-31*	-6	-11	12	9	-35*	-12	6	12	16	-4*
-11	6	13	10	8*	-11	6	11	23	28*	-6	-10	11	4	-21*
-6	-9	11	10	12*	11	-6	12	5	-1*	11	-6	14	19	-31*
10	-6	15	18	-6*	10	-6	12	5	17*	10	-6	11	23	-10*
-10	6	10	43	-29*	-10	6	12	19	7*	-10	6	13	4	-30*
-10	6	14	13	-10*	-9	6	15	13	11*	-9	6	14	12	0*
-9	6	13	25	-30*	-9	6	11	20	0*	9	-6	12	14	8*
9	-6	13	5	-4*	9	-6	15	32	21*	9	-6	16	5	-10*
8	-6	16	6	-3*	8	-6	15	25	-6*	8	-6	12	33	-9*
-8	6	13	20	12*	-8	6	14	17	14*	-8	6	15	5	16*
-8	6	16	4	22*	-7	6	16	5	-16*	-7	6	15	29	31*
-7	6	13	4	-19*	7	-6	14	10	-17*	7	-6	16	5	6*
6	-6	17	16	31*	6	-6	15	12	-16*	-6	6	14	5	9*
-6	6	15	5	31*	-6	6	16	30	-21*	-6	6	17	5	-8*
-6	-6	16	4	9*	6	6	17	5	29*	6	6	18	5	3*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
6	6	19	5	30*	6	6	20	5	-13*	7	6	19	17	-37*
7	6	18	8	-21*	7	6	17	18	-32*	7	6	16	7	-5*
-7	-6	12	21	-13*	-7	-6	13	5	0*	-7	-6	14	5	10*
-7	-6	15	8	-28*	-8	-6	14	5	1*	-8	-6	13	12	28*
-8	-6	11	17	23*	8	6	16	24	34*	8	6	17	31	-1*
8	6	18	9	-21*	8	6	19	22	6*	9	6	18	24	-7*
9	6	17	6	0*	-9	-6	12	5	24*	-9	-6	13	23	12*
-10	-6	14	6	-1*	-10	-6	13	5	22*	-10	-6	10	5	20*
10	6	16	17	18*	10	6	18	6	11*	10	6	19	19	-1*
11	6	18	6	6*	11	6	17	6	-26*	11	6	15	7	17*
11	6	14	27	8*	6	-9	11	10	6*	-11	-6	11	12	10*
-11	-6	12	5	4*	-11	-6	13	5	17*	-12	-6	12	5	3*
6	-11	12	10	-6*	6	-9	12	15	-24*	12	6	14	23	-16*
12	6	5	11	-8*	12	6	17	6	14*	12	6	18	13	-2*
13	6	16	6	19*	13	6	14	6	15*	6	13	13	13	3*
6	12	13	6	42*	6	-7	13	4	-1*	6	-8	13	4	-13*
6	-10	13	22	15*	6	-8	14	23	-17*	6	12	14	6	24*
6	13	14	27	-15*	6	14	14	15	18*	14	6	15	9	27*
14	6	17	28	-22*	6	15	15	8	-30*	6	14	15	17	25*
6	13	15	21	-33*	6	11	15	6	-8*	6	10	15	6	23*
6	9	15	16	-12*	6	-6	15	5	-16*	6	-7	15	5	-7*
6	-8	15	16	-23*	6	-9	15	20	-26*	6	-8	16	4	-13*
6	-7	16	35	-19*	6	-6	16	13	-25	6	6	16	16	23*
6	9	16	6	-4*	6	10	16	6	22*	6	13	16	54	27*
6	14	16	15	21*	6	15	16	6	-17*	6	14	17	27	11*
6	11	17	14	-11*	6	10	17	28	6*	6	9	17	23	33*
6	8	17	6	-21*	6	6	17	17	29*	6	6	18	5	3*
6	7	18	6	-3*	6	8	18	6	14*	6	9	18	54	28*
6	10	18	6	3*	6	11	18	6	-4*	6	12	18	27	-12*
6	10	19	6	7*	6	9	19	22	-9*	6	8	19	32	-8*
6	7	19	25	10*	6	6	19	15	30*	6	6	20	14	-13*
7	8	19	24	-3*	7	9	19	6	-17*	7	10	19	6	-11*
7	12	18	16	-3*	7	11	18	6	-16*	7	9	18	19	-3*
7	7	18	26	13*	7	8	17	23	31*	7	9	17	27	37*
7	10	17	25	-23*	7	11	17	19	-2*	7	13	17	6	17*
7	15	16	6	-18*	7	14	16	6	5*	7	12	16	6	41*
7	11	16	30	-16*	7	10	16	6	8*	7	9	16	6	26*
7	8	16	6	-1*	7	-8	15	11	-22*	7	-7	15	10	13*
7	9	15	6	-14*	7	10	15	47	3*	7	12	15	28	-44*
7	13	15	6	1*	7	14	15	6	22*	7	15	15	18	-27*
15	7	16	6	17*	14	7	16	47	-39*	14	7	15	6	-9*
7	14	14	23	-6*	7	13	14	11	-25*	7	11	14	6	-13*
7	-8	14	19	-30*	7	-9	14	10	-31*	7	-11	13	4	12*
7	-10	13	4	15*	7	-9	13	16	24*	7	-8	13	4	7*
7	12	13	18	36*	13	7	14	6	14*	13	7	15	6	0*
13	7	16	8	0*	13	7	17	26	-21*	12	7	18	25	5*
12	7	17	28	43*	12	7	16	17	16*	12	7	15	6	-21*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
12	7	14	19	42*	12	7	13	6	24*	7	-7	12	40	23*
7	-8	12	24	-4*	7	-10	12	4	-11*	7	-11	12	13	13*
-12	-7	12	13	-3*	-11	-7	12	5	-22*	11	7	14	6	1*
11	7	16	23	-55*	11	7	17	19	50*	10	7	19	5	-29*
10	7	18	6	23*	10	7	15	6	8*	-10	-7	11	5	-3*
-10	-7	13	13	19*	-9	-7	13	5	5*	-9	-7	12	15	-26*
9	7	16	6	0*	9	7	17	17	-25*	9	7	18	30	-9*
9	7	19	6	14*	8	7	19	6	25*	8	7	18	28	18*
8	7	17	6	30*	8	7	16	15	8*	8	7	15	6	4*
-8	-7	11	19	-36*	-8	-7	12	5	-11*	-8	-7	13	9	-21*
-8	-7	14	18	7*	-7	-7	12	5	0*	-7	-7	11	17	40
7	7	17	23	-25*	7	7	18	6	13*	7	7	19	6	-14*
7	-7	16	33	28*	7	-7	15	19	13*	7	-7	14	5	17*
7	-7	12	8	23*	-7	7	12	24	-37*	-7	7	13	5	-25*
-7	7	14	5	-16*	-7	7	15	5	-2*	-7	7	16	15	-14*
-8	7	15	6	-16*	-8	7	14	5	13*	-8	7	12	17	8*
-8	7	11	4	-33*	8	-7	12	6	12*	8	-7	13	5	0*
8	-7	14	5	-10*	8	-7	15	5	14*	8	-7	16	4	8*
9	-7	15	5	2*	9	-7	14	20	-15*	9	-7	12	5	-43*
9	-7	11	20	-19*	-9	7	11	25	-12*	-9	7	13	5	12*
-9	7	14	22	45*	-10	7	14	4	4*	-10	7	12	28	-41*
-10	7	11	16	10*	-10	7	10	20	6*	10	-7	11	5	4*
10	-7	13	9	10*	10	-7	14	5	36*	10	-7	15	21	-12*
11	-7	14	36	23*	11	-7	12	5	-10*	-7	11	11	6	-33*
-7	-8	11	4	9*	-7	-9	11	4	8*	-7	-10	11	4	-1*
-11	7	11	19	22*	-11	7	13	4	-14*	-12	7	12	15	17*
-7	-11	12	4	-1*	-7	-9	12	9	1*	-7	-8	12	13	-23*
-7	-7	12	5	0*	-7	8	12	4	22*	-7	9	12	15	27*
-7	10	12	4	-14*	-7	12	12	18	9*	12	-7	13	24	-7*
-7	12	13	21	-22*	-7	11	13	15	7*	-7	10	13	4	-20*
-7	9	13	18	-19*	-7	8	13	13	-9*	-7	7	13	5	-25*
-7	-10	13	4	10*	-7	7	14	5	-16*	-7	9	14	4	-18*
-7	10	14	21	23*	-7	11	14	4	3*	-7	8	15	4	0*
-7	7	15	4	-2*	-7	7	16	4	-14*	-8	10	14	4	8*
-8	9	14	10	-37*	-8	8	14	35	-23*	-8	-9	13	23	12*
-8	8	13	30	31*	-8	9	13	15	-18*	-8	10	13	21	-2*
-8	11	12	4	17*	-8	10	12	19	0*	-8	9	12	9	22*
-8	8	12	4	30*	-8	-8	12	21	-7*	-8	-11	12	4	-32*
-11	8	12	4	4*	-11	8	11	6	-34*	-8	-9	11	4	15*
-8	-8	11	24	-8*	-8	9	11	10	2*	-8	10	11	4	15*
-8	11	11	4	4*	11	-8	12	5	-7*	11	-8	13	12	12*
10	-8	14	4	-3*	10	-8	11	5	19*	-8	10	10	11	24*
-8	-8	10	4	-1*	-8	-9	10	25	13*	-10	8	10	4	-13*
-10	8	11	4	8*	-10	8	12	18	-8*	-10	8	13	18	5*
-9	8	14	23	28*	-9	8	13	8	35*	-9	8	12	20	9*
-9	8	10	4	31*	9	-8	10	12	-2*	9	-8	12	22	28*
9	-8	13	22	-30*	9	-8	14	33	1*	8	-8	15	11	39*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
8	-8	14	20	-5*	8	-8	13	18	26*	8	-8	11	22	10*
-8	8	12	4	30*	-8	8	13	19	31*	-8	8	14	4	-23*
-8	8	15	20	-45	-8	-8	12	13	-7*	-8	-8	11	36	-8*
-8	-8	10	4	-1*	8	8	15	6	-21*	8	8	16	6	-1*
8	8	17	6	27*	8	8	18	6	-4*	8	8	19	6	0*
9	8	19	23	-17*	9	8	18	27	-24*	9	8	17	22	-27*
9	8	16	19	-14*	9	8	15	44	-23*	-9	-8	11	25	15*
-9	-8	12	10	28*	-9	-8	13	30	14*	-10	-8	13	4	12*
-10	-8	11	5	10*	-10	-8	10	5	14*	10	8	14	25	-26*
10	8	16	6	-14*	10	8	17	17	25*	10	8	18	27	30*
11	8	18	21	1*	11	8	16	16	22*	11	8	14	6	-1*
8	-8	11	19	10*	8	-10	11	4	-6*	-11	-8	11	16	17*
-11	-8	12	5	-3*	8	-11	12	5	16*	8	-10	12	14	-23*
8	-9	12	4	6*	12	8	14	6	6*	12	8	15	6	-24*
12	8	16	60	53*	12	8	17	44	-1*	13	8	16	6	14*
13	8	15	6	-1*	8	12	13	6	8*	8	-9	13	16	8*
8	-10	13	4	-13*	8	-9	14	8	-25*	8	-8	14	5	-5*
8	11	14	46	0*	8	12	14	19	-19*	8	14	14	6	-27*
14	8	15	6	17*	14	8	16	6	3*	8	15	15	6	-2*
8	14	15	6	17*	8	13	15	22	13*	8	12	15	44	21*
8	11	15	31	18*	8	10	15	6	50*	8	9	15	6	11*
8	8	15	6	-21*	8	8	16	6	-1*	8	9	16	14	19*
8	10	16	46	14*	8	11	16	14	22*	8	14	16	41	-38*
8	12	17	26	5*	8	11	17	6	-2*	8	9	17	6	-13*
8	8	17	19	27*	8	8	18	6	-4*	8	11	18	6	21*
8	9	19	20	-12*	8	8	19	7	0*	9	11	18	34	32*
9	10	18	27	37*	9	9	18	6	-2*	9	9	17	19	-20*
9	10	17	35	-11*	9	11	17	8	1*	9	12	17	6	-10*
9	13	17	18	-25*	9	14	16	23	-24*	9	13	16	6	-17*
9	12	16	26	-28*	9	11	16	40	-25*	9	9	16	24	18*
9	9	15	10	23*	9	11	15	6	12*	9	12	15	6	-14*
9	13	15	6	-1*	9	14	15	6	20*	9	15	15	23	-18*
14	9	16	6	-1*	9	14	14	6	31*	9	13	14	6	-29*
9	12	14	6	-15*	9	-9	14	4	9*	9	-10	13	4	-4*
9	-9	13	16	19*	9	11	13	6	24*	9	12	13	6	-7*
13	9	14	20	-31*	13	9	15	31	43*	13	9	16	6	4*
13	9	17	6	-18*	12	9	16	6	20*	12	9	15	12	-8*
9	-10	12	6	-3*	9	-11	12	4	-9*	-11	-9	11	33	7*
9	-10	11	10	-10*	9	-9	11	10	-1*	11	9	14	33	8*
11	9	15	6	-1*	11	9	16	6	2*	11	9	17	6	2*
10	9	18	6	28*	10	9	17	6	29*	10	9	16	29	7*
10	9	15	6	20*	-10	-9	10	5	-14*	-10	-9	11	5	-22*
-10	-9	12	19	-18*	-9	-9	12	14	22*	-9	-9	11	4	-17*
-9	-9	10	19	-19*	-9	9	9	4	-30*	9	9	15	6	23*
9	9	16	6	18*	9	9	17	25	-20*	9	9	18	6	-2*
9	-9	14	22	9*	9	-9	13	10	19*	9	-9	12	9	34*
9	-9	11	18	-1*	9	-9	10	32	-28*	-9	9	10	15	1*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR PHOSPHAZENE CLATHRATE (DATA SET I)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-9	9	11	4	4*	-9	9	12	8	-4*	-9	9	13	4	-6*
-9	9	14	27	-13*	-10	9	13	4	1*	-10	9	12	4	19*
-10	9	10	4	1*	-9	-9	10	23	-19*	-9	9	10	4	1*
-9	10	10	4	20*	10	-9	11	5	12*	10	-9	12	5	4*
10	-9	13	4	-12*	11	-9	12	5	-10*	-9	11	11	12	-26*
-9	10	11	4	-24*	-9	9	11	4	4*	-9	-9	11	4	-17*
-11	9	11	11	10*	-9	-10	12	16	-33*	-9	11	12	4	-6*
-9	9	13	11	-6*	-9	9	14	16	-13*	-10	10	12	18	-33*
-10	-10	11	4	-2*	-10	10	11	35	29*	-10	11	11	4	-28*
10	-10	12	4	1*	10	-10	11	21	20*	-10	10	10	21	25*
-10	10	11	18	29*	-10	-10	11	4	-2*	-10	10	10	10	25*
10	10	13	22	28*	10	10	15	23	8*	10	10	17	20	10*
10	10	18	6	21*	11	10	17	6	-12*	11	10	16	6	-28*
11	10	14	6	13*	10	-10	11	21	20*	-11	-10	11	11	15*
10	-10	12	4	1*	10	12	12	21	-43*	12	10	13	6	-28*
12	10	14	19	-10*	12	10	15	6	-9*	12	10	16	18	16*
12	10	17	6	-15*	13	10	16	6	-6*	13	10	15	19	34*
13	10	14	31	12*	10	13	13	6	7*	10	12	13	6	-5*
10	11	14	6	14*	10	12	14	43	-16*	10	13	14	17	17*
10	14	14	30	39*	14	10	15	7	-11*	10	14	15	12	2*
10	13	15	6	25*	10	12	15	6	-25*	10	10	15	6	8*
10	10	16	6	-50*	10	12	16	6	2*	10	13	16	7	25*
10	14	16	6	-10*	10	12	17	6	19*	10	10	17	8	10*
10	10	18	32	21*	11	11	17	18	24*	11	13	16	58	16*
11	11	16	22	20*	11	11	15	6	-33*	11	12	15	19	11*
11	13	15	20	26*	11	14	15	6	-14*	14	11	15	54	-39*
11	14	14	7	-3*	11	13	14	6	-8*	11	12	14	7	-1*
11	11	14	24	-7*	11	12	13	32	37*	11	13	13	9	8*
13	11	14	26	-7*	13	11	15	12	7*	13	11	16	30	-24*
12	11	16	10	36*	12	11	15	24	16*	12	11	14	7	-10*
12	11	13	23	37*	11	12	12	20	39*	11	11	13	6	28
11	11	14	6	-7*	11	11	15	33	-33*	11	11	16	7	20*
11	11	17	14	24*	12	12	13	6	7*	12	12	15	26	17*
12	12	16	34	17*	13	12	15	31	0*	12	13	13	33	-43*
12	12	13	33	7*	12	14	14	33	8*	12	13	15	22	20*
12	12	15	35	17*	12	12	16	7	17*	13	13	15	7	24*
13	14	14	6	47*	13	13	14	7	18*	13	13	13	27	-52*
13	13	14	7	18*	13	13	15	7	24*					

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II) page 1

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
^^^^^^^ h = 0 ^^^^^^^					-1	-9	139	121	5	-2	-10	369	338	12
					-1	6	279	245	9	-2	-7	101	100	10
0	6	886	875	13	-1	9	375	352	11	-2	-4	957	913	20
0	9	671	633	17	-1	12	172	164	7	-2	5	1362	1252	18
0	12	615	584	29	-1	15	457	450	5	-2	8	107	92	6
0	15	1861	1955	19	-1	18	612	619	8	-2	11	37	29	4
0	18	1262	1240	14	-1	21	301	303	8	-2	14	586	604	20
0	21	419	422	7	-1	24	225	219	7	-2	17	668	689	11
0	24	421	410	8	-1	27	114	118	11	-2	20	195	193	7
0	30	335	346	8	-1	30	209	209	5	-2	23	34	25	7*
0	33	579	570	10	-1	33	124	141	14	-2	26	50	18	13*
0	36	188	221	10	-1	36	94	100	9	-2	29	60	42	10*
					0	-37	85	18	19*	-2	32	261	267	13
^^^^^^^ h = 1 ^^^^^^^					0	-34	110	121	12	-2	35	82	79	19*
					0	-31	206	201	6	-1	-29	150	156	6
0	-38	123	115	12	0	-28	227	224	8	-1	-26	64	5	18*
0	-35	107	111	9	0	-25	158	151	8	-1	-23	62	60	11*
0	-32	72	3	12*	0	-22	81	73	12	-1	-20	34	22	8*
0	-29	171	177	11	0	-19	358	366	8	-1	-17	181	201	3
0	-26	462	476	7	0	-16	778	782	11	-1	-14	96	39	31*
0	-23	747	760	15	0	-13	682	662	23	-1	-11	82	73	7
0	-20	607	632	10	0	-10	1014	946	32	-1	-8	42	36	9*
0	-17	751	755	14	0	-7	1810	1630	18	-1	-5	665	660	22
0	-14	60	17	17*	0	-4	956	919	13	-1	-2	565	550	11
0	-11	399	367	13	0	-1	1271	1197	13	-1	1	453	479	7
0	-8	1335	1321	38	0	2	764	759	9	-1	4	1385	1345	34
0	-5	259	254	7	0	5	1291	1236	27	-1	7	446	417	12
0	1	640	643	9	0	8	1359	1233	35	-1	10	342	314	13
0	4	994	972	25	0	11	393	355	15	-1	13	30	6	5*
0	10	1865	1728	21	0	14	451	459	8	-1	16	225	250	5
0	13	1475	1523	15	0	17	589	607	12	-1	19	164	168	6
0	16	1228	1270	17	0	20	391	402	8	-1	22	35	16	9*
0	19	227	231	4	0	23	340	349	7	-1	25	66	80	9
0	22	101	91	15	0	26	281	274	7	-1	28	117	120	10
0	25	394	391	7	0	29	82	93	8	-1	31	71	61	14*
0	28	271	268	9	0	32	110	113	12	-1	37	108	28	13
0	31	375	367	7	0	35	80	76	9	0	-36	75	23	17*
0	34	183	165	13	0	38	49	78	24*	0	-33	144	154	11
										0	-30	194	181	8
^^^^^^^ h = 2 ^^^^^^^					^^^^^^^ h = 3 ^^^^^^^					0	-27	60	53	12*
										0	-24	82	98	9
-1	-36	104	101	15	-2	-37	57	2	18*	0	-21	77	74	9
-1	-33	156	166	8	-2	-34	179	178	8	0	-18	413	406	8
-1	-30	118	124	11	-2	-31	154	156	10	0	-15	730	769	14
-1	-27	61	39	11*	-2	-28	84	92	12	0	-12	20	30	5*
-1	-24	82	58	8	-2	-25	203	204	7	0	-9	436	332	12
-1	-21	304	306	8	-2	-22	116	112	8	0	-6	623	567	17
-1	-18	523	524	6	-2	-19	65	67	11*	0	-3	119	102	6
-1	-15	649	662	8	-2	-16	785	810	12	0	0	917	882	18
-1	-12	414	418	14	-2	-13	64	80	7	0	3	489	473	9

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II) page 2

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
0	6	257	302	10	-2	9	514	490	18	0	19	644	657	11
0	9	205	123	9	-2	12	286	252	12	0	22	268	268	4
0	12	337	312	15	-2	15	554	579	8	0	25	109	115	7
0	15	307	322	4	-2	18	103	100	6	0	28	251	251	7
0	18	617	623	9	-2	21	133	134	6	0	31	342	343	6
0	21	98	98	11	-2	27	51	22	17*	0	34	185	186	11
0	24	132	138	6	-2	30	129	129	8	0	37	124	88	12
0	27	76	79	19*	-2	33	174	160	7					
0	30	52	16	16*	-2	36	98	28	13	^^^^^^^ h = 5 ^^^^^^^				
0	33	89	85	17*	-1	-34	71	24	18*					
					-1	-31	91	71	12	-4	-36	85	152	15*
^^^^^^^ h = 4 ^^^^^^^					-1	-28	209	208	6	-4	-33	149	154	8
					-1	-25	209	217	6	-4	-27	320	317	6
-3	-35	78	34	15*	-1	-22	157	146	6	-4	-24	637	631	12
-3	-32	292	302	7	-1	-19	135	130	7	-4	-21	586	583	9
-3	-29	226	228	9	-1	-16	177	160	4	-4	-18	656	678	9
-3	-26	281	280	10	-1	-13	92	102	5	-4	-15	522	529	7
-3	-23	259	255	6	-1	-10	666	670	17	-4	-12	380	374	12
-3	-20	136	138	7	-1	-7	651	659	19	-4	-9	1465	1460	40
-3	-17	496	513	7	-1	-4	982	966	24	-4	-6	1398	1367	37
-3	-14	636	677	9	-1	-1	777	769	12	-4	-3	1801	1706	23
-3	-11	41	61	10*	-1	2	444	440	7	-4	3	1162	1032	36
-3	-8	1154	1151	27	-1	5	1269	1225	27	-4	6	309	341	12
-3	-5	612	592	15	-1	8	849	828	20	-4	9	994	997	12
-3	-2	87	104	9	-1	11	276	275	12	-4	12	883	890	22
-3	1	1620	1630	17	-1	14	449	457	6	-4	15	1004	968	30
-3	4	115	132	3	-1	17	44	22	10*	-4	18	488	485	7
-3	7	1415	1421	41	-1	20	89	108	8	-4	24	438	422	8
-3	10	592	607	18	-1	23	270	261	5	-4	27	344	348	6
-3	13	216	217	9	-1	26	187	188	5	-4	30	335	340	9
-3	16	255	266	4	-1	29	231	234	5	-4	33	206	214	9
-3	19	272	284	6	-1	32	123	87	12	-4	36	119	86	12
-3	22	237	230	5	0	-35	132	129	8	-3	-34	150	148	11
-3	25	371	372	8	0	-32	221	233	10	-3	-31	212	205	9
-3	28	123	125	13	0	-29	70	34	12*	-3	-28	107	112	17
-3	31	72	47	14*	0	-26	62	53	15*	-3	-25	182	188	8
-3	34	70	81	20*	0	-23	148	156	5	-3	-22	57	82	7
-3	37	55	34	20*	0	-20	547	557	8	-3	-19	440	446	8
-2	-33	69	72	16*	0	-17	980	1013	12	-3	-16	967	960	17
-2	-30	66	13	12*	0	-14	799	798	26	-3	-13	707	712	23
-2	-24	345	341	8	0	-11	353	354	9	-3	-10	1171	1140	27
-2	-21	71	78	12	0	-8	509	490	8	-3	-7	35	68	13*
-2	-18	229	233	5	0	-5	1629	1515	43	-3	-4	228	247	8
-2	-15	115	115	7	0	-2	1031	1030	22	-3	-1	295	347	8
-2	-12	589	571	17	0	1	1275	1284	27	-3	2	607	634	12
-2	-9	485	472	19	0	4	268	196	8	-3	5	454	416	13
-2	-6	624	641	18	0	7	804	737	27	-3	8	698	647	19
-2	-3	78	79	4	0	10	64	73	8	-3	11	543	521	20
-2	3	372	355	8	0	13	659	673	9	-3	14	341	345	13
-2	6	140	153	6	0	16	1154	1208	16	-3	17	801	813	11

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-3	20	374	387	5	-1	27	93	95	6	-5	26	49	35	7
-3	23	507	503	6	-1	30	66	5	13*	-5	29	62	70	10
-3	26	135	156	10	-1	36	119	136	10	-5	32	67	63	14*
-3	29	110	112	7	0	-31	66	70	9	-5	35	165	156	9
-3	32	181	178	11	0	-28	297	296	8	-4	-35	76	36	16*
-3	35	84	71	14	0	-25	333	322	9	-4	-32	65	71	15*
-2	-32	71	94	25*	0	-22	548	544	9	-4	-29	259	270	7
-2	-29	98	111	11	0	-19	109	98	7	-4	-26	386	383	6
-2	-26	309	312	6	0	-16	185	176	7	-4	-23	379	378	6
-2	-23	514	501	10	0	-13	947	907	29	-4	-20	68	30	10
-2	-20	246	240	4	0	-10	886	865	21	-4	-17	113	123	5
-2	-17	313	318	5	0	-7	1183	1176	12	-4	-14	445	451	6
-2	-14	67	81	9	0	-4	1138	1158	29	-4	-11	905	901	20
-2	-11	228	228	12	0	-1	216	137	7	-4	-8	829	848	18
-2	-8	1370	1366	23	0	2	664	567	17	-4	-5	244	224	9
-2	-5	576	575	15	0	5	923	868	25	-4	-2	291	246	5
-2	-2	358	342	12	0	8	516	516	17	-4	1	189	146	5
-2	1	164	152	5	0	11	1195	1216	16	-4	4	1078	1047	28
-2	4	209	211	7	0	14	316	324	9	-4	7	1068	1075	11
-2	7	1593	1527	40	0	17	69	81	9	-4	10	824	810	18
-2	10	1448	1379	34	0	20	330	332	6	-4	13	358	334	12
-2	13	616	617	22	0	23	305	303	5	-4	16	309	303	13
-2	16	177	190	4	0	26	443	446	8	-4	19	189	198	7
-2	19	47	43	6	0	29	350	349	9	-4	22	513	508	8
-2	22	99	95	7	0	32	71	92	14*	-4	25	335	331	7
-2	25	347	331	5	0	35	85	18	17*	-4	28	105	110	9
-2	28	192	198	9						-4	31	94	78	19*
-2	31	67	33	17*	^^^^^^^	h =	6	^^^^^^^		-4	34	79	16	16*
-2	34	69	22	16*						-3	-36	53	42	21*
-1	-36	89	81	8	-5	-37	137	151	12	-3	-30	123	131	12
-1	-33	48	18	15*	-5	-34	154	169	15	-3	-27	57	51	10*
-1	-30	185	197	9	-5	-31	165	169	5	-3	-24	128	130	9
-1	-27	267	265	7	-5	-28	159	156	7	-3	-21	264	274	4
-1	-24	156	167	8	-5	-25	155	158	6	-3	-18	68	52	10
-1	-21	149	152	7	-5	-22	489	480	8	-3	-15	299	308	7
-1	-18	107	109	7	-5	-19	344	342	7	-3	-12	46	34	8*
-1	-15	162	147	7	-5	-16	316	324	7	-3	-9	40	37	6
-1	-12	657	631	21	-5	-13	1135	1129	12	-3	-6	1188	1144	31
-1	-9	366	371	9	-5	-10	424	414	13	-3	-3	299	313	10
-1	-6	106	74	7	-5	-7	184	174	6	-3	0	537	498	12
-1	-3	829	806	24	-5	-4	156	212	6	-3	3	88	79	7
-1	0	375	364	7	-5	-1	551	584	12	-3	6	41	4	11*
-1	3	1332	1307	34	-5	2	968	971	24	-3	9	253	279	8
-1	6	1463	1417	36	-5	5	253	270	4	-3	12	226	232	8
-1	9	420	422	8	-5	8	548	517	9	-3	15	133	152	6
-1	12	102	97	7	-5	11	682	683	14	-3	18	85	97	9
-1	15	35	27	8*	-5	14	490	478	11	-3	21	51	35	7
-1	18	156	158	4	-5	17	128	109	5	-3	24	58	39	8
-1	21	565	558	10	-5	20	543	538	7	-3	27	221	217	6
-1	24	219	219	5	-5	23	290	289	8	-3	30	66	75	13*

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k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-3	36	66	19	19*	0	-30	189	182	7	-5	-27	170	163	4
-2	-34	85	52	9	0	-27	194	196	9	-5	-24	179	185	5
-2	-31	98	101	7	0	-24	338	338	6	-5	-21	317	322	6
-2	-28	102	101	16	0	-21	60	9	12*	-5	-18	350	361	5
-2	-25	102	108	8	0	-18	254	246	11	-5	-15	399	413	6
-2	-22	55	65	10*	0	-15	336	328	9	-5	-12	490	496	6
-2	-19	196	199	4	0	-12	703	699	18	-5	-9	398	377	12
-2	-16	430	455	14	0	-9	582	594	7	-5	-6	301	319	9
-2	-13	282	268	8	0	-6	380	387	5	-5	-3	853	811	21
-2	-10	833	788	20	0	-3	1003	960	16	-5	0	1511	1417	36
-2	-7	561	529	13	0	0	1047	958	31	-5	3	306	253	8
-2	-4	528	507	15	0	3	1369	1333	28	-5	6	27	48	12*
-2	-1	289	280	7	0	6	751	736	23	-5	9	74	67	9
-2	2	335	299	10	0	9	1010	999	21	-5	12	610	592	12
-2	5	287	283	8	0	12	54	57	5	-5	15	438	428	12
-2	8	421	381	12	0	15	188	195	6	-5	18	264	260	11
-2	11	230	217	10	0	18	316	314	6	-5	21	220	220	7
-2	14	73	72	4	0	21	474	472	8	-5	24	61	39	6
-2	17	399	423	6	0	24	318	315	7	-5	27	139	142	10
-2	20	128	126	6	0	27	179	189	5	-5	30	153	144	6
-2	23	234	230	6	0	30	112	74	22*	-5	33	150	126	8
-2	26	108	122	17	0	33	63	70	14*	-4	-34	86	50	9
-2	29	94	91	9						-4	-31	84	85	6
-2	32	92	80	25*	^^^^^^^	h =	7	^^^^^^^		-4	-28	83	90	6
-2	35	74	5	15*						-4	-22	242	246	6
-1	-35	65	80	19*	-6	-35	83	1	16*	-4	-19	419	414	6
-1	-32	85	101	16*	-6	-32	94	33	11	-4	-16	318	302	6
-1	-29	74	88	7	-6	-29	107	95	11	-4	-13	238	261	7
-1	-26	79	72	9	-6	-26	328	333	5	-4	-10	266	276	8
-1	-23	63	52	10	-6	-23	261	260	4	-4	-7	515	480	12
-1	-20	516	517	9	-6	-20	182	190	5	-4	-4	764	772	26
-1	-17	370	350	12	-6	-17	335	364	7	-4	-1	41	72	8*
-1	-14	207	197	6	-6	-14	133	150	5	-4	2	141	159	3
-1	-11	182	185	4	-6	-11	836	834	12	-4	5	233	224	5
-1	-8	734	762	9	-6	-8	523	515	9	-4	8	389	369	11
-1	-5	635	623	11	-6	-5	101	116	5	-4	11	751	740	12
-1	-2	36	58	16*	-6	-2	573	533	13	-4	14	489	443	16
-1	1	618	519	13	-6	1	554	490	13	-4	17	224	207	7
-1	4	529	511	15	-6	4	519	535	7	-4	20	197	202	5
-1	7	777	784	19	-6	7	741	745	9	-4	23	124	122	8
-1	10	440	425	16	-6	10	595	582	8	-4	26	87	89	9
-1	13	761	754	9	-6	13	563	571	14	-4	29	163	159	4
-1	16	125	112	4	-6	16	533	554	15	-4	35	98	68	22*
-1	19	460	463	8	-6	22	312	315	9	-3	-35	65	63	16*
-1	22	107	114	5	-6	25	144	159	9	-3	-32	54	39	12*
-1	25	82	66	7	-6	28	107	113	9	-3	-26	204	207	4
-1	28	149	150	7	-6	31	155	151	6	-3	-23	218	216	6
-1	31	111	10	12	-6	34	56	39	14*	-3	-20	221	226	5
-1	34	53	57	14*	-5	-33	124	148	19	-3	-17	150	163	5
0	-33	113	102	18	-5	-30	83	35	15*	-3	-14	161	151	12

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k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-3	-11	409	397	11	-1	2	486	464	14	-7	15	51	81	10*
-3	-8	202	238	9	-1	5	151	154	6	-7	18	140	136	9
-3	-5	163	146	7	-1	8	814	795	26	-7	21	276	269	12
-3	-2	1006	965	26	-1	11	319	330	5	-7	24	232	231	6
-3	1	590	570	15	-1	14	167	150	7	-6	-31	49	38	15*
-3	4	132	126	4	-1	17	376	375	5	-6	-28	88	93	15*
-3	7	322	331	8	-1	20	49	11	9*	-6	-25	298	299	13
-3	10	293	322	12	-1	23	239	236	10	-6	-22	155	154	4
-3	13	723	755	14	-1	26	121	128	15	-6	-19	173	167	6
-3	16	269	289	6	-1	29	75	41	10	-6	-16	104	102	5
-3	19	150	150	5	-1	32	52	70	17*	-6	-13	340	356	6
-3	22	64	32	12*	0	-32	86	10	14	-6	-10	744	750	9
-3	25	133	133	7	0	-29	95	96	12	-6	-7	294	293	9
-3	28	75	100	14*	0	-26	80	60	6	-6	-4	79	84	25*
-3	31	152	149	7	0	-23	49	47	10*	-6	-1	485	433	14
-3	34	97	82	21*	0	-20	166	156	9	-6	2	70	19	49*
-2	-33	170	132	16	0	-17	221	220	7	-6	5	215	229	5
-2	-30	93	54	12	0	-14	98	53	11	-6	8	526	535	6
-2	-27	78	43	13*	0	-8	181	179	4	-6	11	372	392	9
-2	-24	39	45	10*	0	-5	499	535	6	-6	14	238	243	9
-2	-21	93	101	11	0	-2	88	69	5	-6	17	115	107	9
-2	-18	507	504	14	0	1	47	14	7	-6	20	128	126	9
-2	-15	525	543	14	0	4	493	446	14	-6	23	279	280	10
-2	-12	156	156	7	0	7	507	490	8	-6	26	175	184	8
-2	-9	210	204	5	0	10	177	172	5	-6	29	72	13	9
-2	-6	410	425	13	0	16	261	271	5	-6	35	66	2	18*
-2	-3	546	537	14	0	19	139	144	6	-5	-35	77	65	15*
-2	0	1025	965	17	0	22	59	54	11*	-5	-32	83	6	13
-2	3	195	183	9	0	25	60	2	11*	-5	-26	167	160	9
-2	6	72	78	10	0	28	146	141	5	-5	-23	178	179	7
-2	9	289	274	10	0	31	80	66	6	-5	-20	321	327	7
-2	12	93	83	8	0	34	68	49	14*	-5	-17	40	2	19*
-2	15	658	686	9						-5	-14	130	121	5
-2	18	338	366	7	^^^^^^^	h =	8	^^^^^^^		-5	-11	280	276	13
-2	21	108	115	10						-5	-8	600	585	17
-2	24	190	186	5	-7	-30	122	128	12	-5	-5	398	390	12
-2	27	77	11	9	-7	-27	170	176	9	-5	-2	368	374	10
-2	30	167	171	16	-7	-24	50	22	10*	-5	1	137	121	8
-2	33	130	124	7	-7	-21	58	52	8	-5	4	367	379	5
-1	-34	83	71	14*	-7	-18	153	160	3	-5	7	559	547	15
-1	-31	130	120	11	-7	-15	166	182	5	-5	10	595	596	11
-1	-25	240	225	9	-7	-12	555	571	8	-5	13	413	404	10
-1	-22	60	49	8	-7	-9	142	138	10	-5	16	49	21	9*
-1	-19	211	204	10	-7	-6	262	276	4	-5	19	331	311	15
-1	-16	507	484	12	-7	-3	97	125	5	-5	22	153	153	8
-1	-13	118	121	7	-7	0	123	118	4	-5	25	240	233	7
-1	-10	384	395	5	-7	3	522	505	10	-5	28	97	101	9
-1	-7	377	383	5	-7	6	683	678	14	-5	31	107	25	12
-1	-4	416	390	7	-7	9	160	177	3	-5	34	79	64	11
-1	-1	541	540	14	-7	12	351	355	6	-4	-33	92	111	21*

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k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-4	-30	146	135	12	-2	-14	466	454	9	0	2	28	43	6*
-4	-27	60	43	12*	-2	-11	451	460	6	0	5	617	615	11
-4	-24	337	330	7	-2	-8	884	922	9	0	8	507	520	8
-4	-21	380	377	6	-2	-5	1416	1429	23	0	11	425	434	7
-4	-18	206	205	7	-2	-2	84	49	27*	0	14	308	312	4
-4	-15	251	253	7	-2	1	634	624	16	0	17	168	164	8
-4	-12	748	726	22	-2	4	339	307	11	0	20	247	241	5
-4	-9	475	463	14	-2	7	525	532	19	0	23	127	122	15
-4	-6	569	581	16	-2	10	1046	1063	18	0	26	80	61	8
-4	-3	831	826	22	-2	13	588	591	11	0	29	125	120	7
-4	0	1051	1014	22	-2	16	226	223	7	0	32	71	7	10
-4	3	1034	1046	30	-2	19	132	129	9					
-4	6	182	198	5	-2	22	128	125	9	^^^^^^^	h =	9	^^^^^^^	
-4	9	544	533	15	-2	25	296	297	9					
-4	12	488	486	15	-2	28	309	316	10	-8	-28	194	198	5
-4	15	290	291	10	-2	31	142	137	8	-8	-25	426	418	6
-4	18	215	216	5	-2	34	73	36	19*	-8	-22	430	432	10
-4	21	495	484	6	-1	-33	63	41	16*	-8	-19	483	491	10
-4	27	33	47	14*	-1	-27	140	120	9	-8	-16	49	30	6
-4	30	105	106	12	-1	-21	191	186	11	-8	-13	194	200	4
-4	33	64	111	20*	-1	-18	38	23	9*	-8	-10	1101	1124	25
-3	-34	174	128	11	-1	-15	142	132	5	-8	-7	1132	1186	16
-3	-31	256	253	6	-1	-12	436	463	7	-8	-4	1165	1146	14
-3	-28	365	360	8	-1	-9	529	536	9	-8	-1	359	328	7
-3	-25	348	350	5	-1	-6	228	214	4	-8	2	220	192	5
-3	-22	163	155	9	-1	-3	259	255	5	-8	5	484	497	9
-3	-19	184	182	8	-1	0	490	475	9	-8	8	1141	1198	16
-3	-16	538	530	14	-1	3	455	457	11	-8	11	833	857	9
-3	-13	1030	1019	26	-1	6	549	542	8	-8	14	532	538	6
-3	-10	1303	1352	16	-1	9	374	359	6	-8	17	277	274	5
-3	-7	1280	1318	22	-1	12	227	214	8	-8	20	119	111	5
-3	-4	404	414	10	-1	15	118	112	6	-8	23	554	544	11
-3	-1	609	598	14	-1	18	37	20	7*	-8	26	416	404	10
-3	2	942	909	22	-1	21	336	339	9	-8	29	306	308	9
-3	5	1446	1402	26	-1	24	233	229	6	-8	32	137	149	11
-3	8	1369	1372	19	-1	27	86	98	14	-7	-35	128	122	11
-3	11	552	550	23	-1	30	61	8	16*	-7	-32	90	78	10
-3	14	125	124	7	-1	33	70	42	13*	-7	-29	69	59	10
-3	17	147	152	11	0	-34	61	52	11*	-7	-26	168	165	5
-3	20	551	564	12	0	-31	48	56	19*	-7	-23	383	380	7
-3	23	676	667	9	0	-28	60	69	14*	-7	-20	395	391	6
-3	26	402	396	9	0	-25	125	130	6	-7	-17	150	150	7
-3	29	191	185	7	0	-22	185	225	19	-7	-14	359	359	6
-3	32	78	25	15*	0	-19	372	378	6	-7	-11	230	213	6
-3	35	104	68	12	0	-16	239	244	5	-7	-8	550	560	7
-2	-32	96	72	13	0	-13	57	30	8	-7	-5	540	539	7
-2	-29	207	203	9	0	-10	227	231	5	-7	-2	774	741	23
-2	-23	545	532	8	0	-7	345	356	6	-7	1	655	627	12
-2	-20	423	399	16	0	-4	611	593	12	-7	4	301	301	7
-2	-17	109	103	8	0	-1	214	208	7	-7	7	384	399	6

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-7	10	644	672	9	-5	20	518	514	9	-2	-34	107	95	11
-7	13	609	625	9	-5	23	378	380	7	-2	-31	230	236	9
-7	16	238	242	8	-5	26	153	159	5	-2	-28	290	294	6
-7	19	271	274	4	-5	29	121	113	12	-2	-25	290	316	30
-7	22	285	282	9	-4	-32	92	32	24*	-2	-22	199	201	6
-7	25	132	119	13	-4	-29	220	228	9	-2	-19	221	223	7
-7	28	87	105	17*	-4	-26	457	466	11	-2	-16	437	437	6
-7	31	131	137	16	-4	-23	583	590	8	-2	-13	836	845	13
-7	34	108	112	15	-4	-20	725	716	11	-2	-10	859	894	10
-6	-33	98	24	11	-4	-17	594	590	20	-2	-7	1324	1340	17
-6	-30	64	28	11*	-4	-14	72	74	14*	-2	-4	400	411	9
-6	-27	50	40	13*	-4	-11	788	797	14	-2	-1	406	374	7
-6	-24	263	259	7	-4	-8	1210	1229	12	-2	2	796	747	17
-6	-21	102	106	16	-4	-5	1338	1381	19	-2	5	1155	1166	12
-6	-18	81	79	7	-4	-2	1108	1092	21	-2	8	1116	1116	22
-6	-15	72	85	4	-4	1	598	562	14	-2	11	516	530	7
-6	-12	350	348	7	-4	4	645	658	12	-2	14	98	107	12
-6	-9	613	616	19	-4	7	1303	1295	27	-2	17	181	189	7
-6	-6	343	366	9	-4	10	1312	1322	21	-2	20	548	555	8
-6	-3	34	15	7*	-4	13	1143	1147	18	-2	23	421	425	9
-6	0	220	223	4	-4	16	836	843	13	-2	26	440	425	10
-6	3	35	6	5	-4	19	261	260	7	-2	29	143	156	15
-6	6	134	123	6	-4	22	278	278	7	-2	35	60	75	19*
-6	9	589	605	7	-4	25	318	302	8	-1	-26	59	40	13*
-6	12	184	187	5	-4	28	423	419	8	-1	-23	140	145	7
-6	15	41	26	5	-4	31	305	298	10	-1	-20	304	302	6
-6	18	146	140	7	-4	34	139	155	18	-1	-17	62	9	11*
-6	21	186	184	3	-3	-33	229	235	8	-1	-14	189	179	4
-6	24	350	336	7	-3	-30	250	238	10	-1	-11	224	225	6
-6	27	84	86	10	-3	-27	108	113	15	-1	-8	200	204	4
-6	30	78	29	12	-3	-24	46	47	8*	-1	-5	490	492	6
-6	33	74	24	14*	-3	-21	691	706	10	-1	-2	248	255	7
-5	-34	68	42	11	-3	-18	929	915	25	-1	1	250	261	8
-5	-31	80	67	14*	-3	-15	802	797	19	-1	4	308	304	5
-5	-28	249	249	7	-3	-12	152	155	5	-1	7	96	94	22*
-5	-25	220	227	5	-3	-9	309	304	6	-1	10	431	415	8
-5	-22	58	51	10*	-3	-6	584	581	13	-1	13	288	279	4
-5	-19	142	138	9	-3	-3	1779	1792	37	-1	16	56	43	4
-5	-16	178	170	10	-3	0	1168	1198	25	-1	19	267	252	6
-5	-13	437	436	9	-3	3	1553	1565	34	-1	22	151	158	5
-5	-10	1082	1068	29	-3	6	1526	1525	38	-1	25	48	1	17*
-5	-7	231	226	7	-3	9	424	413	13	-1	28	157	125	12
-5	-4	121	138	8	-3	12	975	970	14	-1	31	75	24	8
-5	-1	601	599	17	-3	15	753	751	14	0	-33	97	58	13
-5	2	30	34	6*	-3	18	832	842	10	0	-30	88	88	14
-5	5	1110	1110	18	-3	21	567	566	8	0	-27	180	164	9
-5	8	611	580	15	-3	24	244	235	7	0	-24	130	127	9
-5	11	206	187	8	-3	27	101	83	12	0	-21	344	354	6
-5	14	237	252	8	-3	30	230	236	6	0	-18	191	196	4
-5	17	115	105	7	-3	33	175	176	13	0	-15	105	107	6

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
0	-12	249	251	5	-8	-3	183	217	4	-6	19	195	197	8
0	-9	139	143	7	-8	0	328	363	8	-6	22	126	118	6
0	-6	629	649	8	-8	3	915	956	17	-6	25	154	155	8
0	-3	693	701	10	-8	6	1248	1271	18	-6	28	77	69	11
0	0	533	540	12	-8	9	392	387	7	-6	31	65	40	12*
0	3	133	100	5	-8	12	96	99	6	-5	-33	177	196	16
0	6	272	255	8	-8	18	332	331	5	-5	-30	124	105	20
0	9	209	206	7	-8	21	638	635	8	-5	-27	78	83	11
0	12	498	490	8	-8	24	287	289	8	5	-24	83	33	11
0	15	339	330	6	-8	27	169	159	6	-5	-21	347	350	7
0	18	47	21	8*	-8	30	99	89	16	-5	-18	703	695	14
0	21	95	101	11	-8	33	74	46	15*	-5	-15	555	543	11
0	24	75	32	11	-7	-34	75	74	16*	-5	-12	467	475	9
0	27	207	210	11	-7	-28	160	149	6	-5	-9	56	59	8
0	30	143	142	11	-7	-25	113	99	6	-5	-6	1213	1211	27
0	33	105	80	11	-7	-22	256	262	6	-5	-3	1177	1203	37
					-7	-19	267	268	5	-5	0	1127	1144	29
^^^^^^^	h =	10	^^^^^^^		-7	-16	200	208	4	-5	3	1037	1037	14
					-7	-13	90	105	3	-5	6	489	477	15
-9	-29	178	179	6	-7	-10	340	344	5	-5	9	47	49	7
-9	-26	65	47	17*	-7	-7	308	320	7	-5	12	133	125	8
-9	-23	387	384	6	-7	-4	483	505	7	-5	15	587	558	17
-9	-20	488	490	6	-7	-1	627	616	16	-5	18	678	650	23
-9	-17	586	590	9	-7	2	193	200	5	-5	21	328	321	9
-9	-14	354	348	7	-7	5	528	516	13	-5	24	172	177	6
-9	-11	75	61	7	-7	8	316	320	7	-5	27	161	160	6
-9	-8	349	352	5	-7	11	445	444	7	-5	30	199	198	6
-9	-5	457	487	7	-7	14	477	485	10	-5	33	170	180	10
-9	-2	701	691	15	-7	17	255	261	6	-4	-34	148	133	11
-9	1	394	368	8	-7	20	94	100	12	-4	-31	236	233	8
-9	4	781	766	12	-7	23	104	107	8	-4	-28	358	364	11
-9	7	72	63	4	-7	26	57	64	16*	-4	-25	294	300	9
-9	10	631	643	10	-7	29	207	204	8	-4	-22	35	37	14*
-9	13	664	667	7	-7	32	154	142	12	-4	-19	366	354	11
-9	16	602	617	7	-6	-29	65	65	10	-4	-16	630	635	9
-9	19	577	585	13	-6	-26	209	215	6	-4	-13	1286	1281	26
-9	22	96	83	9	-6	-23	190	191	6	-4	-10	1102	1099	23
-9	25	129	144	14	-6	-20	52	45	7	-4	-7	781	769	14
-9	28	84	81	12	-6	-17	40	46	16*	-4	-4	245	245	9
-9	31	178	167	11	-6	-14	48	31	9*	-4	-1	93	103	8
-8	-33	101	107	12	-6	-11	19	13	8*	-4	2	1037	1061	11
-8	-30	154	186	17	-6	-8	663	651	18	-4	5	1225	1205	33
-8	-27	349	343	8	-6	-5	119	124	4	-4	8	645	623	18
-8	-24	84	82	10	-6	-2	30	37	6*	-4	11	291	284	12
-8	-21	88	89	5	-6	1	97	121	6	-4	14	49	6	13*
-8	-18	235	232	6	-6	4	498	506	7	-4	17	436	425	9
-8	-15	290	290	7	-6	7	854	830	13	-4	20	815	803	16
-8	-12	747	750	11	-6	10	376	381	5	-4	23	486	489	12
-8	-9	661	645	11	-6	13	72	46	7	-4	26	352	353	6
-8	-6	94	76	4	-6	16	111	122	6	-4	29	158	142	11

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-4	32	54	51	20*	-1	-13	296	299	5	-10	0	818	851	14
-3	-32	53	28	19*	-1	-10	65	84	11	-10	3	620	642	12
-3	-29	232	239	7	-1	-7	216	221	9	-10	6	692	718	11
-3	-26	290	294	11	-1	-4	156	159	5	-10	9	666	673	11
-3	-23	422	435	12	-1	-1	889	887	15	-10	12	135	131	4
-3	-20	532	537	12	-1	2	577	578	11	-10	15	276	276	6
-3	-17	504	508	8	-1	5	25	2	12*	-10	18	324	322	7
-3	-14	58	11	11*	-1	8	47	53	8*	-10	21	268	259	8
-3	-11	602	612	8	-1	11	124	109	7	-10	24	345	335	6
-3	-8	411	420	5	-1	14	340	323	10	-10	27	211	203	9
-3	-5	1103	1088	25	-1	17	165	158	7	-9	-31	72	63	14*
-3	-2	793	797	20	-1	20	116	124	10	-9	-28	110	131	8
-3	1	283	291	7	-1	23	113	114	9	-9	-25	333	331	8
-3	4	603	602	9	-1	26	43	21	13*	-9	-22	188	186	5
-3	7	544	549	8	-1	29	90	18	14	-9	-19	159	161	4
-3	10	991	978	12	0	-32	52	65	19*	-9	-16	65	66	9
-3	13	1054	1034	11	0	-29	164	182	9	-9	-13	351	353	6
-3	16	750	731	13	0	-26	131	146	8	-9	-10	636	650	10
-3	19	139	144	7	0	-23	264	265	8	-9	-7	729	750	15
-3	22	130	118	3	0	-20	177	181	6	-9	-4	595	612	7
-3	25	182	180	8	0	-17	111	119	12	-9	-1	254	231	7
-3	28	348	346	6	0	-14	231	233	5	-9	2	269	291	8
-3	34	55	128	19*	0	-11	332	328	6	-9	5	404	413	6
-2	-33	58	52	20*	0	-8	373	376	9	-9	8	585	589	8
-2	-30	73	44	14*	0	-5	366	370	6	-9	11	546	529	8
-2	-27	55	19	14*	0	-2	97	100	5	-9	14	393	402	6
-2	-24	55	4	13*	0	1	87	104	9	-9	17	48	37	10*
-2	-21	209	207	7	0	4	435	452	6	-9	20	217	240	7
-2	-18	221	237	5	0	7	473	481	7	-9	23	227	240	11
-2	-15	271	265	6	0	10	444	454	8	-9	26	297	309	8
-2	-12	206	209	4	0	13	255	254	6	-9	29	235	231	8
-2	-9	195	192	7	0	16	54	20	12*	-8	-32	102	105	10
-2	-6	819	817	9	0	19	120	114	8	-8	-23	65	54	8
-2	-3	530	538	10	0	22	154	147	5	-8	-20	477	473	7
-2	0	280	267	8	0	25	124	121	7	-8	-17	604	599	8
-2	3	583	591	12	0	28	70	71	11	-8	-14	335	337	6
-2	6	34	25	5	0	31	95	76	9	-8	-11	177	182	5
-2	9	99	93	5						-8	-8	246	256	4
-2	12	50	54	5	^^^^^^^	h =	11	^^^^^^^		-8	-5	894	906	11
-2	15	109	119	4						-8	-2	759	763	8
-2	18	400	400	12	-10	-30	113	108	13	-8	1	572	560	10
-2	21	157	161	6	-10	-27	214	215	4	-8	4	228	209	4
-2	24	72	67	8	-10	-24	267	270	5	-8	7	72	87	5
-2	27	120	117	5	-10	-21	49	15	9*	-8	10	184	194	6
-2	30	108	104	10	-10	-18	279	283	6	-8	13	467	476	7
-2	33	78	74	13	-10	-15	407	396	12	-8	16	636	638	8
-1	-31	118	96	7	-10	-12	371	369	6	-8	19	424	423	10
-1	-28	53	7	16*	-10	-9	590	576	10	-8	22	149	144	10
-1	-19	223	221	6	-10	-6	302	282	4	-8	25	87	48	10
-1	-16	229	226	7	-10	-3	329	362	6	-8	28	241	230	6

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-8	31	209	195	9	-5	-2	783	782	25	-3	26	80	104	14*
-7	-33	68	18	18*	-5	1	359	359	8	-3	32	78	3	23*
-7	-30	115	101	16	-5	4	361	367	6	-2	-32	71	8	15*
-7	-27	81	16	11	-5	7	200	211	5	-2	-29	59	32	9
-7	-24	53	31	11*	-5	10	491	477	13	-2	-26	155	159	7
-7	-21	173	177	5	-5	13	835	827	13	-2	-23	52	56	16*
-7	-18	281	277	7	-5	16	603	577	17	-2	-20	124	130	5
-7	-15	255	269	6	-5	19	110	120	9	-2	-17	50	57	11*
-7	-12	202	203	6	-5	22	132	134	6	-2	-14	69	31	9
-7	-9	220	230	5	-5	28	161	157	6	-2	-11	43	58	8*
7	-6	231	249	4	-5	31	199	193	7	-2	-8	429	433	7
-7	-3	237	243	4	-4	-33	218	215	10	-2	-5	85	69	6
-7	0	141	137	6	-4	-30	155	173	11	-2	-2	185	167	5
-7	3	520	521	11	-4	-27	58	37	17*	-2	1	116	128	5
-7	6	30	15	7*	-4	-21	272	268	8	-2	4	355	341	8
-7	9	246	251	5	-4	-18	430	435	9	-2	7	648	645	9
-7	12	107	116	4	-4	-15	626	620	9	-2	10	207	202	4
-7	15	74	96	13*	-4	-12	296	298	6	-2	13	210	211	6
-7	18	392	400	8	-4	-9	153	145	6	-2	16	65	44	17*
-7	21	209	205	7	-4	-6	203	208	6	-2	19	50	32	20*
-7	24	128	110	13	-4	-3	1253	1234	23	-2	22	128	122	9
-6	-31	76	76	15*	-4	0	1911	1915	36	-2	25	196	188	8
-6	-25	181	186	7	-4	3	1050	1064	13	-1	-30	144	139	11
-6	-22	71	81	11	-4	6	219	212	8	-1	-27	98	65	12
-6	-19	71	61	11	-4	9	222	220	9	-1	-24	175	157	8
-6	-16	433	428	9	-4	12	460	447	18	-1	-21	152	152	6
-6	-13	172	168	7	-4	15	630	615	14	-1	-18	370	366	8
-6	-10	456	461	13	-4	18	398	391	9	-1	-15	305	304	5
-6	-7	588	595	13	-4	21	205	206	4	-1	-12	189	198	4
-6	-4	184	185	4	-4	24	149	138	4	-1	-9	242	248	6
-6	-1	70	17	7	-4	27	94	74	7	-1	-6	145	139	7
-6	2	124	133	9	-4	30	135	154	6	-1	-3	479	490	5
-6	5	122	114	4	-4	33	210	220	9	-1	0	340	328	9
-6	8	476	488	11	-3	-31	52	74	10*	-1	3	536	519	6
-6	11	68	76	9	-3	-28	101	74	11	-1	6	477	486	7
-6	14	100	94	6	-3	-19	244	241	5	-1	9	372	381	7
-6	17	320	334	5	-3	-16	298	299	7	-1	12	69	73	8
-6	20	61	98	15*	-3	-13	516	515	8	-1	15	272	271	9
-6	23	182	188	8	-3	-10	352	362	5	-1	18	304	298	9
-6	26	140	136	6	-3	-7	187	198	4	-1	21	226	229	8
-5	-32	71	71	13*	-3	-4	57	54	3	-1	24	130	111	7
-5	-29	107	87	9	-3	-1	143	137	6	-1	27	102	101	10
-5	-26	179	183	7	-3	2	309	313	4	-1	30	88	111	12
-5	-23	208	223	13	-3	5	141	142	7	0	-31	140	136	12
-5	-20	415	422	6	-3	8	63	74	8	0	-28	136	144	7
-5	-17	466	462	8	-3	11	62	69	11*	0	-25	35	41	18*
-5	-14	92	104	12	-3	14	160	172	7	0	-22	73	56	10
-5	-11	28	7	19*	-3	17	242	244	6	0	-19	93	106	11
-5	-8	46	41	11*	-3	20	274	263	7	0	-16	319	328	10
-5	-5	312	316	8	-3	23	210	206	9	0	-13	210	210	6

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
0	-10	43	40	16*	10	16	147	154	7	-7	-2	461	459	7
0	-7	360	371	7	-10	19	99	63	9	-7	1	440	449	10
0	-4	252	271	4	-10	22	234	232	5	-7	4	394	389	7
0	-1	84	83	5	-10	25	182	178	11	-7	7	417	409	9
0	2	145	135	5	-9	-30	98	78	15	-7	10	41	18	15*
0	5	361	372	8	-9	-27	150	135	6	-7	13	274	277	5
0	8	154	150	5	-9	-24	95	92	15	-7	16	90	99	14
0	11	74	72	6	-9	-18	160	163	5	-7	19	136	134	5
0	14	118	116	6	-9	-15	356	355	7	-7	22	211	204	7
0	17	213	224	6	-9	-12	275	269	7	-7	25	59	48	12*
0	20	135	133	11	-9	-9	246	244	4	-7	28	137	123	7
0	23	50	22	13*	-9	-6	86	105	5	-7	31	84	62	21*
0	26	87	68	6	-9	-3	237	257	4	-6	-30	143	128	6
0	29	93	93	[illegible]	-9	0	491	525	10	-6	-27	142	145	8
					-9	3	490	499	8	-6	-24	70	81	13*
^^^^^^^	h =	12	^^^^^^^		-9	6	290	300	10	-6	-21	163	165	5
					-9	9	299	314	5	-6	-18	50	27	16*
-11	-28	65	41	9	-9	12	62	27	7	-6	-15	77	74	13*
-11	-25	65	59	8	-9	15	180	187	5	-6	-12	58	51	7
-11	-22	118	114	5	-9	18	308	316	6	-6	-9	165	157	9
-11	-19	97	102	12	-9	21	71	115	10	-6	-6	214	201	6
-11	-16	162	166	10	-9	24	175	174	12	-6	-3	92	82	8
-11	-13	72	7	13*	-9	30	65	36	19*	-6	0	119	109	12
-11	-10	56	33	10*	-8	-31	114	48	13	-6	3	341	348	8
-11	-7	240	249	5	-8	-28	205	204	9	-6	6	703	693	22
-11	-4	49	32	8*	-8	-25	46	10	17*	-6	9	305	303	7
-11	-1	31	17	6*	-8	-22	112	95	13	-6	12	179	177	5
-11	2	73	62	8	-8	-19	40	10	8*	-6	15	69	99	16*
-11	5	155	156	5	-8	-16	115	115	8	-6	18	56	43	6
-11	8	120	124	7	-8	-13	361	350	7	-6	21	82	76	7
-11	11	49	49	12*	-8	-10	80	85	7	-6	30	87	66	9
-11	14	146	147	6	-8	-7	46	39	15*	-5	-31	74	48	18*
-11	17	135	140	11	-8	-4	150	147	5	-5	-28	58	58	17*
-11	20	45	5	13*	-8	-1	165	175	5	-5	-25	66	67	15*
-11	26	86	80	16*	-8	2	308	301	10	-5	-22	93	62	10
-11	29	57	51	10*	-8	5	612	596	17	-5	-19	77	61	11
-10	-26	117	112	10	-8	11	67	66	6	-5	-16	106	109	6
-10	-23	68	55	7	-8	14	149	151	6	-5	-13	374	386	5
-10	-20	65	7	10	-8	17	74	79	17*	-5	-10	216	213	8
-10	-17	75	90	5	-8	20	249	235	6	-5	-7	85	80	13
-10	-14	140	132	9	-8	23	46	33	13*	-5	-4	454	455	15
-10	-11	404	397	8	-8	26	76	80	14*	-5	-1	54	61	6
-10	-8	367	365	7	-8	29	118	108	14	-5	2	101	99	7
-10	-5	210	218	4	-7	-32	73	5	16*	-5	5	215	203	6
-10	-2	257	267	6	-7	-29	129	112	6	-5	8	302	291	9
-10	1	337	332	7	-7	-26	190	176	9	-5	11	112	97	6
-10	4	96	107	5	-7	-17	58	53	18*	-5	14	71	74	8
-10	7	278	278	6	-7	-11	443	439	6	-5	17	124	124	8
-10	10	52	18	11*	-7	-8	193	190	4	-5	20	76	79	7
-10	13	237	245	5	-7	-5	201	198	5	-5	26	85	23	10

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-5	29	111	109	6	-2	-1	300	302	8	0	27	67	72	19*
-5	32	48	15	20*	-2	2	145	130	5					
-4	-29	45	17	18*	-2	5	386	383	5	^^^^^^^	h =	13	^^^^^^^	
-4	-26	72	73	11	-2	8	297	290	5					
-4	-23	48	40	16*	-2	11	753	736	12	-12	-29	111	65	15
-4	-20	53	58	13*	-2	14	362	354	6	-12	-26	104	83	29*
-4	-17	89	91	7	-2	17	50	31	14*	-12	-23	211	206	5
-4	-14	55	13	9*	-2	20	137	134	9	-12	-20	192	179	6
-4	-11	199	214	6	-2	23	100	99	6	-12	-14	50	41	8
-4	-8	160	154	4	-2	26	223	232	6	-12	-11	99	97	8
-4	-5	338	320	12	-2	29	154	156	11	-12	-8	494	495	9
-4	-2	134	123	6	-2	32	54	63	18*	-12	-5	571	564	12
-4	1	243	241	5	-1	-29	55	39	16*	-12	-2	357	355	5
-4	4	232	231	4	-1	-26	108	102	8	-12	1	288	287	7
-4	7	178	176	6	-1	-23	117	109	13	-12	4	75	71	5
-4	10	175	175	4	-1	-20	320	325	6	-12	7	404	400	7
-4	13	206	209	4	-1	-17	235	217	10	-12	10	283	296	8
-4	16	36	26	11*	-1	-14	215	218	4	-12	13	266	271	8
-4	19	70	66	8	-1	-11	70	62	8	-12	16	138	141	7
-4	22	105	92	12	-1	-8	200	204	5	-12	19	68	39	9
-4	25	36	12	18*	-1	-5	724	726	10	-12	22	83	94	8
-4	28	100	43	10	-1	-2	272	269	7	-12	28	148	150	16
-4	31	70	36	19*	-1	1	187	168	5	-11	-27	85	73	14*
-3	-30	73	39	16*	-1	4	105	107	5	-11	-24	247	231	5
-3	-27	148	139	10	-1	7	165	170	4	-11	-21	275	276	5
-3	-24	176	165	9	-1	10	307	292	5	-11	-18	231	234	4
-3	-18	76	80	6	-1	13	360	369	8	-11	-15	215	211	7
-3	-15	262	266	5	-1	16	232	237	6	-11	-12	265	263	5
-3	-12	561	571	7	-1	19	293	300	11	-11	-9	206	204	6
-3	-9	415	416	5	-1	22	153	145	8	-11	-6	260	242	5
-3	-6	71	69	8	-1	25	69	16	11	-11	-3	239	234	5
-3	-3	41	19	12*	-1	28	215	211	6	-11	0	100	76	8
-3	0	181	166	6	0	-27	81	89	20*	-11	3	411	393	10
-3	3	425	414	6	0	-24	48	3	20*	-11	6	166	171	4
-3	6	214	202	6	0	-21	102	99	8	-11	9	325	329	7
-3	9	218	218	5	0	-18	112	114	11	-11	12	209	215	4
-3	12	95	98	5	0	-15	94	77	10	-11	15	197	211	7
-3	15	47	3	9*	0	-12	133	118	8	-11	18	263	261	8
-3	18	167	161	7	0	-9	74	86	13*	-11	21	161	156	9
-3	21	309	301	8	0	-6	90	90	6	-11	24	81	89	17*
-3	24	261	257	9	0	-3	160	148	5	-10	-28	77	105	18*
-3	27	82	81	22*	0	0	144	146	3	-10	-25	69	53	8
-2	-28	216	204	14	0	3	198	199	6	-10	-22	121	107	11
-2	-25	174	178	12	0	6	59	73	12*	-10	-19	36	6	16*
-2	-22	332	334	6	0	9	147	138	5	-10	-10	39	17	6
-2	-19	138	143	8	0	12	264	262	8	-10	-7	145	150	12
-2	-13	423	427	6	0	15	96	97	11	-10	-4	53	34	5
-2	-10	395	399	7	0	18	69	9	12*	-10	-1	103	109	4
-2	-7	387	383	9	0	21	58	63	19*	-10	2	72	70	6
-2	-4	570	563	8	0	24	55	20	10*	-10	5	385	391	9

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-10	8	40	4	7*	-7	-7	286	297	4	-5	30	62	5	20*
-10	11	101	106	7	-7	-4	725	723	8	-4	-28	89	65	17*
-10	14	83	84	10	-7	-1	759	764	8	-4	-25	115	120	8
-10	20	91	59	9	-7	2	723	716	9	-4	-22	113	114	9
-10	26	33	52	12*	-7	5	502	488	15	-4	-19	256	256	7
-9	-26	182	190	6	-7	8	219	216	6	-4	-16	136	151	5
-9	-23	195	194	5	-7	14	369	359	10	-4	-13	242	228	5
-9	-20	82	25	11	-7	17	491	500	9	-4	-10	211	199	5
-9	-14	166	160	6	-7	20	405	380	8	-4	-7	87	77	6
-9	-11	381	381	6	-7	23	218	218	8	-4	-4	222	213	8
-9	-8	310	316	6	-7	29	129	131	7	-4	-1	465	449	11
-9	-5	122	121	5	-6	-29	146	133	7	-4	2	121	113	6
-9	-2	54	58	5	-6	-26	120	126	6	-4	5	194	189	3
-9	1	223	236	5	-6	-23	140	121	9	-4	8	178	177	7
-9	4	176	180	6	-6	-20	101	78	9	-4	11	317	314	8
-9	7	234	238	8	-6	-17	237	242	4	-4	14	451	441	9
-9	10	487	488	8	-6	-14	436	448	10	-4	17	221	217	4
-9	13	218	215	5	-6	-11	436	440	10	-4	20	98	86	5
-9	16	49	34	15*	-6	-8	263	255	8	-4	23	95	95	17*
-9	19	74	33	12	-6	-5	71	56	8	-4	26	79	93	15*
-9	22	130	137	8	-6	-2	84	97	6	-4	29	102	95	10
-9	25	231	230	8	-6	1	93	98	10	-3	-26	103	68	12
-9	28	116	96	8	-6	4	457	459	6	-3	-23	167	168	8
-8	-27	135	120	11	-6	7	158	153	4	-3	-20	456	453	9
-8	-24	325	310	9	-6	10	177	161	9	-3	-17	470	459	8
-8	-21	230	234	6	-6	13	78	59	10	-3	-14	398	405	6
-8	-18	277	284	6	-6	16	91	96	6	-3	-11	129	130	5
-8	-15	176	180	6	-6	19	296	301	6	-3	-8	40	45	7*
-8	-12	47	9	8*	-6	22	193	205	6	-3	-5	469	457	6
-8	-9	427	429	8	-6	25	102	116	6	-3	-2	1088	1064	22
-8	-6	390	390	5	-6	28	85	37	11	-3	1	1041	1045	12
-8	-3	581	573	11	-5	-27	69	44	15*	-3	4	310	305	7
-8	0	592	580	9	-5	-24	98	94	7	-3	7	37	28	10*
-8	3	204	196	8	-5	-21	183	184	8	-3	10	378	362	6
-8	6	187	187	4	-5	-18	168	166	5	-3	13	698	687	11
-8	9	408	401	7	-5	-15	242	245	6	-3	16	520	507	14
-8	12	488	489	6	-5	-12	83	91	8	-3	19	380	378	12
-8	15	408	408	10	-5	-9	183	180	5	-3	22	238	235	4
-8	18	196	181	9	-5	-6	28	24	9*	-3	25	57	4	19*
-8	24	124	112	6	-5	-3	231	225	7	-3	28	154	149	10
-8	27	147	153	9	-5	0	358	371	7	-3	31	84	173	15*
-8	30	112	109	11	-5	3	73	66	10	-2	-27	153	156	7
-7	-31	159	128	11	-5	6	130	117	12	-2	-24	102	110	13
-7	-28	67	86	14*	-5	9	68	53	7	-2	-21	49	23	14*
-7	-25	53	32	15*	-5	12	462	448	22	-2	-18	134	138	5
-7	-22	91	94	7	-5	15	242	236	7	-2	-15	277	279	7
-7	-19	503	510	12	-5	18	195	197	9	-2	-12	556	559	9
-7	-16	567	563	8	-5	21	56	79	17*	-2	-9	415	426	7
-7	-13	424	415	9	-5	24	56	70	8	-2	-6	230	237	6
-7	-10	353	347	8	-5	27	82	68	9	-2	-3	245	237	8

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-2	0	419	401	10						-11	13	602	595	9
-2	3	695	681	10	-13	-24	64	52	10	-11	16	269	267	5
-2	6	662	646	11	-13	-21	179	190	5	-11	19	54	22	10*
-2	9	494	487	8	-13	-18	416	422	8	-11	22	97	69	12
-2	12	46	40	10*	-13	-15	431	426	11	-11	25	127	114	11
-2	15	49	48	5	-13	-12	342	337	11	-11	28	176	182	11
-2	18	201	193	7	-13	-9	221	234	7	-10	-30	61	41	18*
-2	21	384	386	6	-13	-6	309	310	7	-10	-27	61	20	17*
-2	24	275	273	7	-13	-3	596	591	8	-10	-24	97	87	13
-2	27	115	83	13	-13	0	553	534	9	-10	-21	45	6	18*
-1	-28	88	113	9	-13	3	555	541	9	-10	-18	304	302	6
-1	-25	253	233	7	-13	6	286	285	5	-10	-15	284	286	7
-1	-22	193	197	5	-13	9	257	251	4	-10	-12	229	234	4
-1	-19	203	202	6	-13	12	143	141	7	-10	-9	229	227	6
-1	-16	202	201	6	-13	15	418	427	8	-10	-6	86	80	8
-1	-13	144	135	7	-13	18	418	423	9	-10	-3	259	257	5
-1	-10	514	513	9	-13	21	270	274	9	-10	0	324	324	7
-1	-7	680	673	13	-13	24	212	201	8	-10	3	184	212	27
-1	-4	468	461	7	-13	27	67	6	14*	-10	6	123	114	8
-1	-1	293	299	9	-12	-28	244	247	8	-10	9	198	206	6
-1	2	217	230	6	-12	-25	353	355	9	-10	12	44	2	16*
-1	5	194	183	5	-12	-22	154	159	7	-10	15	240	271	11
-1	8	545	537	7	-12	-19	206	209	4	-10	18	229	228	7
-1	11	424	411	9	-12	-16	469	460	8	-10	21	163	166	6
-1	14	182	173	7	-12	-13	629	616	9	-10	24	140	151	9
-1	17	316	315	6	-12	-10	860	840	12	-10	27	50	45	22*
-1	20	45	48	11*	-12	-7	582	579	8	-9	-28	77	83	14*
-1	23	237	244	6	-12	-4	100	88	7	-9	-25	69	53	14*
-1	26	264	274	11	-12	-1	372	376	6	-9	-22	125	127	10
-1	29	105	103	9	-12	2	654	646	8	-9	-19	147	143	10
0	-26	82	69	8	-12	5	833	843	13	-9	-16	231	229	4
0	-23	60	32	13*	-12	8	815	820	11	-9	-13	314	309	7
0	-20	141	146	8	-12	14	39	26	18*	-9	-10	429	409	7
0	-17	120	118	7	-12	20	369	377	10	-9	-7	201	202	3
0	-14	93	111	8	-12	23	397	390	13	-9	-4	54	37	5
0	-11	260	256	7	-12	26	349	346	10	-9	-1	609	615	9
0	-8	144	138	7	-11	-29	75	45	14*	-9	2	403	404	8
0	-5	285	294	8	-11	-26	220	223	5	-9	5	188	187	5
0	-2	226	232	9	-11	-23	213	211	5	-9	8	258	259	5
0	1	96	101	8	-11	-20	206	198	4	-9	11	123	124	7
0	4	75	76	15*	-11	-17	145	147	7	-9	14	292	285	9
0	7	121	116	9	-11	-14	79	70	12	-9	17	185	193	9
0	10	51	23	11*	-11	-11	386	380	8	-9	20	135	134	8
0	13	172	169	7	-11	-8	357	348	5	-9	23	247	242	8
0	16	163	154	5	-11	-5	406	406	6	-9	26	82	94	16*
0	19	61	11	14*	-11	-2	646	640	10	-8	-29	168	180	8
0	22	79	88	16*	-11	1	254	243	4	-8	-26	280	271	11
0	25	88	64	8	-11	4	51	41	9*	-8	-23	175	170	6
					-11	7	160	158	6	-8	-20	113	113	9
^^^^^^^	h =	14	^^^^^^^		-11	10	379	364	7	-8	-17	188	198	4

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-8	-14	461	460	10	-6	26	101	73	12	-3	8	517	509	12
-8	-11	569	565	11	-5	-29	46	8	21*	-3	11	463	453	9
-8	-8	663	652	8	-5	-23	189	182	9	-3	14	423	419	9
-8	-5	364	361	5	-5	-20	171	162	8	-3	17	169	159	6
-8	-2	47	44	6	-5	-17	369	375	7	-3	20	140	138	6
-8	1	564	579	8	-5	-14	61	91	7	-3	23	242	236	7
-8	4	559	540	15	-5	-11	266	272	4	-3	26	184	202	6
-8	7	686	681	9	-5	-8	244	248	4	-3	29	218	232	9
-8	10	448	454	6	-5	-5	273	263	6	-2	-26	122	116	6
-8	13	174	164	5	-5	-2	398	408	6	-2	-23	232	218	5
-8	19	259	255	7	-5	1	347	346	5	-2	-20	285	271	8
-8	22	261	263	5	-5	4	121	116	5	-2	-17	319	325	7
-8	25	239	238	8	-5	7	38	2	14*	-2	-14	229	229	7
-8	28	130	122	10	-5	10	369	361	7	-2	-11	146	148	4
-7	-30	48	6	21*	-5	13	330	320	7	-2	-8	239	237	4
-7	-27	156	142	11	-5	16	468	451	11	-2	-5	271	264	6
-7	-24	111	121	11	-5	19	135	160	10	-2	-2	341	341	5
-7	-18	607	591	9	-5	22	79	70	9	-2	1	263	262	6
-7	-15	187	210	18	-5	25	127	110	13	-2	4	282	287	7
-7	-12	183	173	6	-5	28	94	75	15	-2	7	50	49	7
-7	-9	118	118	8	-4	-27	121	102	12	-2	10	405	396	8
-7	-6	416	417	6	-4	-24	61	12	16*	-2	13	380	368	7
-7	-3	842	842	11	-4	-21	66	57	11	-2	16	414	409	13
-7	0	668	673	8	-4	-18	260	264	9	-2	19	300	302	10
-7	3	61	61	10	-4	-15	455	453	7	-2	22	55	11	8
-7	6	38	27	13*	-4	-12	387	397	5	-2	25	114	111	6
-7	9	128	126	6	-4	-9	108	113	4	-2	28	78	53	12
-7	12	501	503	8	-4	-6	76	75	8	-1	-27	74	56	14*
-7	15	636	641	10	-4	-3	151	146	8	-1	-18	67	51	10
-7	18	325	315	9	-4	0	557	551	9	-1	-15	106	110	8
-7	27	153	145	8	-4	3	710	708	14	-1	-9	197	189	6
-7	30	218	219	9	-4	6	406	399	7	-1	-6	102	100	5
-6	-28	70	50	16*	-4	9	76	88	9	-1	-3	48	5	11*
-6	-25	78	55	11	-4	12	103	102	9	-1	0	44	29	8*
-6	-22	64	64	14*	-4	15	148	144	5	-1	3	67	60	7
-6	-19	261	247	8	-4	18	485	479	12	-1	6	335	326	6
-6	-16	364	346	8	-4	21	285	283	9	-1	9	138	130	7
-6	-13	413	410	5	-4	24	77	76	21*	-1	12	78	76	9
-6	-10	213	237	18	-4	30	73	29	14*	-1	15	162	160	5
-6	-7	265	253	7	-3	-28	153	162	9	-1	21	105	105	11
-6	-4	261	256	5	-3	-25	163	178	15	-1	24	116	108	8
-6	-1	720	733	11	-3	-22	227	220	5	-1	27	99	30	14
-6	2	723	737	8	-3	-19	216	223	8	0	-25	84	92	16*
-6	5	252	255	7	-3	-13	222	221	7	0	-16	176	172	6
-6	8	309	294	12	-3	-10	553	572	11	0	-13	315	319	6
-6	11	81	79	8	-3	-7	563	560	10	0	-10	282	275	7
-6	14	248	257	10	-3	-4	616	612	13	0	-7	171	167	7
-6	17	251	247	7	-3	-1	389	384	7	0	-4	228	227	4
-6	20	233	241	5	-3	2	32	2	7*	0	-1	143	186	24
-6	23	187	181	7	-3	5	429	413	9	0	2	267	271	8

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
0	5	265	269	5	-12	-6	232	217	6	-9	-18	235	238	8
0	8	138	135	7	-12	-3	688	680	9	-9	-15	90	73	10
0	11	252	248	5	-12	0	984	984	12	-9	-12	63	60	9
0	14	49	35	10*	-12	3	606	597	7	-9	-9	438	437	7
0	17	148	149	9	-12	6	387	411	16	-9	-6	607	583	7
0	20	94	87	8	-12	9	82	93	10	-9	-3	460	459	7
0	23	114	109	12	-12	12	377	388	9	-9	0	348	333	5
					-12	15	473	480	9	-9	3	143	137	5
^^^^^^^ h = 15 ^^^^^^^					-12	21	323	341	10	-9	9	412	410	8
					-12	24	243	245	7	-9	12	274	279	8
-14	-25	135	161	13	-12	27	59	8	9	-9	15	268	280	9
-14	-22	141	135	10	-11	-28	185	127	9	-9	18	118	102	11
-14	-19	104	105	9	-11	-25	150	129	11	-9	21	80	19	14*
-14	-16	308	313	9	-11	-19	45	19	11*	-9	24	131	116	7
-14	-13	443	443	8	-11	-16	185	178	9	-9	27	132	142	7
-14	-10	510	498	8	-11	-13	436	429	9	-8	-28	140	154	9
-14	-7	640	631	8	-11	-10	435	425	6	-8	-22	144	133	10
-14	-4	129	125	4	-11	-7	134	132	4	-8	-19	345	335	11
-14	-1	295	288	4	-11	-4	73	79	10	-8	-16	672	653	10
-14	2	364	375	8	-11	-1	210	205	4	-8	-13	326	339	4
-14	5	521	516	6	-11	2	502	490	6	-8	-10	167	159	8
-14	8	601	599	11	-11	5	292	290	6	-8	-7	115	110	5
-14	11	243	219	18	-11	8	284	292	8	-8	-4	169	166	6
-14	14	185	189	7	-11	11	283	279	3	-8	-1	577	583	9
-14	17	156	153	8	-11	14	126	130	11	-8	2	578	572	6
-14	20	237	244	6	-11	20	177	175	7	-8	5	587	576	23
-14	23	332	327	9	-11	23	170	183	14	-8	8	239	238	7
-13	-23	419	434	10	-11	26	155	148	13	-8	11	235	241	6
-13	-20	370	378	7	-10	-29	59	20	18*	-8	14	401	386	10
-13	-17	100	96	10	-10	-26	98	77	17*	-8	17	543	532	8
-13	-14	167	171	11	-10	-23	201	196	5	-8	20	285	282	7
-13	-11	343	339	10	-10	-17	234	236	6	-8	23	133	117	8
-13	-8	762	756	12	-10	-14	49	29	12*	-8	26	40	10	18*
-13	-5	840	831	11	-10	-11	75	83	14*	-7	-29	204	189	10
-13	-2	357	351	5	-10	-8	356	347	7	-7	-26	126	135	7
-13	1	51	9	7	-10	-5	51	5	8	-7	-23	100	96	17
-13	4	191	194	9	-10	-2	305	319	5	-7	-20	77	56	12
-13	7	568	567	9	-10	1	274	271	8	-7	-17	115	108	13
-13	10	782	797	11	-10	4	119	118	5	-7	-14	299	302	7
-13	16	252	248	5	-10	7	441	433	9	-7	-11	313	314	6
-13	19	127	131	7	-10	10	272	272	6	-7	-8	300	297	7
-13	22	77	86	8	-10	13	97	85	10	-7	-5	319	323	6
-13	25	269	272	7	-10	16	217	215	6	-7	1	360	371	6
-12	-27	93	63	20*	-10	19	110	104	8	-7	4	487	484	9
-12	-24	110	111	9	-10	22	145	142	8	-7	7	404	393	13
-12	-21	292	294	8	-10	25	130	135	9	-7	10	243	252	11
-12	-18	398	404	7	-10	28	55	30	15*	-7	13	183	187	7
-12	-15	394	391	6	-9	-27	69	42	15*	-7	16	58	6	15*
-12	-12	428	413	9	-9	-24	268	253	10	-7	19	199	210	5
-12	-9	206	196	6	-9	-21	221	240	9	-7	22	106	114	22*

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-7	25	99	103	13	-3	-18	253	245	8	0	6	248	248	8
-7	28	102	135	11	-3	-15	252	251	6	0	9	282	277	5
-6	-27	54	19	18*	-3	-12	292	287	7	0	12	70	56	11
-6	-15	132	132	15	-3	-9	224	230	6	0	15	58	6	6
-6	-9	165	161	7	-3	-6	134	135	9	0	18	67	72	9
-6	-6	125	127	6	-3	-3	226	216	5	0	21	92	114	11
-6	-3	131	135	6	-3	0	503	484	8	0	24	102	[illegible]	9
-6	0	258	261	5	-3	3	457	455	10					
-6	3	137	141	4	-3	6	508	497	8	^^^^^^^	h =	16	^^^^^^^	
-6	6	80	67	7	-3	9	328	318	8					
-6	9	80	75	6	-3	12	161	161	14	-15	-23	106	153	15
-6	12	99	95	7	-3	15	262	253	8	-15	-20	148	156	10
-6	15	113	116	6	-3	18	272	259	5	-15	-17	130	125	8
-5	-28	88	63	15*	-3	21	168	170	7	-15	-14	110	97	9
-5	-25	62	47	8	-3	24	171	178	6	-15	-11	157	153	7
-5	-22	83	56	8	-3	27	137	131	10	-15	-8	221	217	6
-5	-19	58	65	13*	-2	-25	150	131	10	-15	-5	182	185	8
-5	-16	74	30	12	-2	-22	93	48	11	-15	-2	82	64	8
-5	-10	100	107	13	-2	-19	130	116	10	-15	1	43	24	12*
-5	-7	278	290	8	-2	-16	79	85	10	-15	4	105	111	5
-5	-4	330	329	8	-2	-13	85	92	8	-15	7	330	316	6
-5	-1	238	241	7	-2	-10	318	317	7	-15	10	297	299	9
-5	2	59	55	5	-2	-7	296	290	7	-15	16	203	190	27
-5	5	133	134	8	-2	-4	47	54	6	-15	19	72	70	21*
-5	8	176	179	6	-2	-1	110	109	3	-15	22	116	102	10
-5	11	151	154	4	-2	2	101	99	6	-14	-24	75	61	12
-5	14	170	180	8	-2	5	249	237	6	-14	-21	193	208	12
-5	17	19	28	9*	-2	8	297	297	6	-14	-18	395	409	11
-5	26	118	108	9	-2	11	50	59	5	-14	-15	367	368	10
-5	29	112	126	11	-2	14	45	42	9*	-14	-12	54	41	9*
-4	-26	45	1	23*	-2	20	163	163	8	-14	-9	57	3	6
-4	-20	168	160	12	-2	23	197	197	11	-14	-6	168	166	9
-4	-17	310	302	8	-1	-17	82	86	11	-14	-3	603	595	9
-4	-14	345	348	8	-1	-11	90	89	8	-14	0	661	641	9
-4	-11	267	273	7	-1	-8	196	185	8	-14	3	561	563	8
-4	-8	129	127	11	-1	-5	165	157	6	-14	6	544	528	7
-4	-5	254	260	6	-1	-2	35	33	13*	-14	9	129	112	9
-4	-2	263	256	7	-1	1	81	75	8	-14	12	270	265	7
-4	1	244	242	7	-1	4	115	112	4	-14	15	410	402	8
-4	4	170	181	7	-1	7	208	201	7	-14	18	368	368	6
-4	7	161	153	8	-1	10	73	12	10	-14	21	220	217	6
-4	10	46	14	13*	-1	13	77	66	7	-14	24	90	68	12
-4	13	140	147	8	-1	16	181	176	6	-13	-25	219	220	10
-4	16	369	396	6	-1	22	56	62	13*	-13	-22	113	137	12
-4	19	216	216	10	0	-18	70	35	13*	-13	-19	117	125	10
-4	22	107	103	10	0	-12	273	282	9	-13	-16	405	412	7
-4	28	61	63	14*	0	-6	173	162	4	-13	-13	424	415	11
-3	-27	153	171	8	0	-3	106	99	9	-13	-10	638	630	10
-3	-24	112	101	11	0	0	230	236	6	-13	-7	675	671	11
-3	-21	75	16	11	0	3	212	201	5	-13	-4	192	195	4

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-13	-1	273	277	5	-10	17	102	128	11	-7	17	80	90	9
-13	2	449	441	9	-10	23	98	113	14	-7	20	46	1	13*
-13	5	561	575	9	-10	26	83	7	17*	-7	23	83	42	12
-13	8	719	727	10	-9	-26	155	176	17	-7	26	97	21	15
-13	11	264	280	8	-9	-23	144	144	11	-6	-26	47	4	20*
-13	17	248	227	9	-9	-20	210	194	6	-6	-23	89	51	6
-13	20	289	289	8	-9	-17	199	169	9	-6	-20	110	129	16
-13	23	371	364	7	-9	-14	117	131	10	-6	-17	239	232	8
-12	-26	196	199	12	-9	-11	197	193	6	-6	-14	80	113	11
-12	-23	295	299	10	-9	-8	235	242	4	-6	-11	125	132	4
-12	-20	219	212	9	-9	-5	285	282	5	-6	-8	36	36	17*
-12	-17	127	123	5	-9	-2	318	314	5	-6	-5	179	179	4
-12	-14	74	53	6	-9	1	33	30	6*	-6	-2	332	330	7
-12	-11	315	305	8	-9	4	225	229	6	-6	1	77	77	6
-12	-8	607	615	14	-9	7	327	323	5	-6	4	50	51	9*
-12	-5	441	425	7	-9	10	300	298	7	-6	7	152	149	7
-12	-2	419	423	6	-9	13	314	323	9	-6	10	79	81	10
-12	1	192	192	5	-9	16	136	150	8	-6	13	87	98	10
-12	4	153	146	7	-9	19	64	36	16*	-6	16	281	268	7
-12	7	465	451	8	-9	22	79	45	23*	-6	19	91	54	12
-12	13	398	397	9	-9	25	124	132	17	-6	25	70	28	18*
-12	16	256	260	9	-8	-27	93	84	17*	-5	-24	81	71	8
-12	22	72	70	16*	-8	-24	127	129	11	-5	-21	213	205	9
-12	25	198	189	11	-8	-21	107	110	11	-5	-18	191	186	8
-11	-24	54	99	17*	-8	-18	160	161	5	-5	-15	67	69	11
-11	-21	83	47	27*	-8	-12	116	122	9	-5	-9	89	31	10
-11	-18	103	97	6	-8	-9	285	283	6	-5	-6	126	128	5
-11	-15	97	114	12	-8	-6	377	385	9	-5	-3	231	232	6
-11	-12	81	80	7	-8	-3	402	395	6	-5	0	179	184	5
-11	-9	106	102	8	-8	0	190	183	5	-5	3	48	16	10*
-11	-3	68	57	11	-8	3	127	113	8	-5	6	100	102	8
-11	0	135	133	7	-8	6	52	45	4	-5	9	191	189	8
-11	3	56	64	18*	-8	9	203	201	7	-5	12	282	279	6
-11	6	68	79	15*	-8	12	231	225	7	-5	15	95	92	9
-11	9	116	111	8	-8	15	187	180	9	-5	18	108	106	12
-11	12	200	200	8	-8	18	47	35	21*	-5	21	73	57	15*
-11	15	107	124	11	-8	24	109	104	14	-4	-22	50	44	18*
-11	18	137	127	8	-8	27	170	148	9	-4	-19	48	18	15*
-10	-25	93	85	14	-7	-25	55	9	17*	-4	-16	224	222	8
-10	-19	96	67	10	-7	-19	100	105	10	-4	-13	59	29	31*
-10	-16	155	156	7	-7	-16	87	32	11	-4	-10	51	23	10*
-10	-13	195	193	7	-7	-13	129	113	8	-4	-7	108	103	5
-10	-10	231	239	5	-7	-7	94	71	13	-4	-4	151	150	6
-10	-7	82	89	10	-7	-4	77	87	13*	-4	-1	98	90	3
-10	-4	51	49	14*	-7	-1	97	103	7	-4	2	58	58	10*
-10	-1	88	73	7	-7	2	118	119	5	-4	5	46	26	6
-10	2	55	45	7	-7	5	83	65	5	-4	8	31	8	15*
-10	5	56	50	10*	-7	8	99	95	8	-4	11	89	79	8
-10	8	66	14	11*	-7	11	64	84	11*	-4	14	54	64	11*
-10	11	79	86	10	-7	14	84	89	12	-4	17	231	229	8

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-4	23	59	25	12*	0	4	150	150	6	-13	-3	260	261	4
-4	26	100	70	12	0	7	204	203	6	-13	0	232	248	12
-3	-23	56	58	16*	0	13	50	28	16*	-13	3	243	245	8
-3	-17	77	97	12	0	16	53	35	10*	-13	6	70	23	11
-3	-14	54	68	18*	0	19	76	102	8	-13	9	168	183	22
-3	-11	69	48	9						-13	15	196	135	11
-3	-8	45	24	11*	^^^^^^^	h =	17	^^^^^^^		-13	18	194	205	10
-3	-2	165	162	6						-13	21	77	94	15*
-3	1	42	27	10*	-16	-18	63	2	11*	-12	-22	60	85	18*
-3	4	186	179	5	-16	-15	56	22	17*	-12	-16	51	37	7
-3	7	129	118	3	-16	-12	80	66	8	-12	-13	70	53	9
-3	10	93	76	16*	-16	-9	85	89	7	-12	-10	57	49	6
-3	13	262	257	10	-16	-6	159	150	6	-12	-7	132	130	7
-3	16	66	3	7	-16	-3	74	70	7	-12	-4	78	78	10
-3	19	105	123	14	-16	0	56	30	7	-12	-1	124	127	3
-3	25	77	21	11	-16	3	77	94	15*	-12	2	37	37	14*
-2	-24	85	83	20*	-16	15	44	35	20*	-12	5	152	143	5
-2	-21	137	143	9	-15	-19	95	38	13	-12	8	61	33	10
-2	-18	219	215	8	-15	-16	141	130	14	-12	11	68	48	7
-2	-15	173	161	9	-15	-13	196	196	7	-12	14	58	52	7
-2	-12	75	35	9	-15	-10	115	107	9	-12	17	74	70	10
-2	-9	191	204	7	-15	-7	134	126	9	-12	20	64	65	12*
-2	-6	331	327	7	-15	-4	201	197	6	-11	-20	152	152	13
-2	0	357	375	11	-15	-1	66	26	10	-11	-17	144	139	10
-2	3	102	99	8	-15	2	98	82	8	-11	-14	116	119	10
-2	6	161	162	4	-15	8	49	45	16*	-11	-11	162	165	5
-2	9	167	156	6	-15	11	58	26	15*	-11	-8	36	37	10*
-2	12	224	221	7	-15	17	90	92	10	-11	-5	79	68	13
-2	15	319	330	18	-15	20	96	92	10	-11	-2	256	251	5
-2	18	156	151	10	-14	-23	141	157	20	-11	1	278	289	5
-2	21	67	42	18*	-14	-20	202	211	10	-11	4	86	88	14*
-1	-22	131	145	8	-14	-17	225	237	8	-11	13	158	154	9
-1	-19	160	156	9	-14	-14	87	82	14	-11	16	162	159	8
-1	-13	142	153	10	-14	-11	49	31	23*	-11	19	125	131	20
-1	-10	135	143	10	-14	-8	180	177	7	-11	22	78	77	20*
-1	-4	233	234	8	-14	-5	302	298	8	-11	25	94	76	11
-1	-1	176	190	8	-14	-2	270	273	7	-10	-21	131	116	14
-1	2	273	275	12	-14	1	84	90	9	-10	-18	136	134	14
-1	5	233	236	5	-14	7	211	218	10	-10	-15	238	230	14
-1	8	70	74	17*	-14	10	235	240	8	-10	-12	168	185	5
-1	11	145	148	15	-14	13	291	288	7	-10	-6	187	188	7
-1	14	97	102	17*	-14	16	309	307	8	-10	-3	226	225	5
-1	17	177	171	7	-14	19	132	131	10	-10	0	474	475	6
-1	20	96	104	13	-14	22	47	6	18*	-10	3	397	388	8
0	-20	52	101	17*	-13	-24	110	100	14	-10	6	136	131	6
0	-17	137	54	11	-13	-21	124	155	11	-10	9	62	25	12*
0	-8	200	189	9	-13	-15	176	176	6	-10	12	94	77	8
0	-5	64	69	10	-13	-12	84	89	11	-10	18	171	176	10
0	-2	123	102	11	-13	-9	183	181	4	-10	21	111	129	12
0	1	116	110	9	-13	-6	504	508	8	-10	24	51	11	22*

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-9	-22	108	105	11	-6	-4	27	31	15*	-3	20	140	150	13
-9	-19	111	134	11	-6	-1	176	184	5	-3	23	124	102	13
-9	-13	262	251	7	-6	2	510	515	12	-2	-20	69	51	13*
-9	-10	83	86	5	-6	5	579	580	10	-2	-17	103	96	10
-9	-7	34	55	10*	-6	8	368	364	6	-2	-8	342	353	7
-9	-4	158	155	5	-6	11	205	206	9	-2	-5	256	248	7
-9	-1	83	96	9	-6	14	98	144	20*	-2	-2	45	36	12*
-9	2	111	117	10	-6	17	211	218	7	-2	1	196	189	5
-9	5	48	27	12*	-6	20	269	265	10	-2	4	342	347	7
-9	8	188	194	5	-6	23	110	125	9	-2	7	374	370	6
-9	11	103	94	6	-5	-23	145	129	8	-2	10	403	383	7
-9	14	70	87	13*	-5	-20	114	118	10	-2	13	240	244	14
-9	17	123	126	6	-5	-17	65	63	11*	-2	16	50	47	14*
-9	20	64	54	11*	-5	-14	79	53	11	-2	19	124	99	11
-8	-23	65	41	9	-5	-11	206	214	7	-2	22	177	206	8
-8	-11	55	21	14*	-5	-8	410	410	6	-1	-21	220	222	7
-8	-8	187	200	8	-5	-5	429	415	7	-1	-18	131	138	5
-8	-5	161	164	4	-5	-2	342	353	7	-1	-6	275	288	8
-8	-2	203	199	4	-5	1	290	295	7	-1	0	350	347	6
-8	1	132	131	5	-5	4	134	139	8	-1	3	163	164	6
-8	4	24	29	9*	-5	7	340	338	7	-1	6	223	221	5
-8	7	60	54	9	-5	10	221	212	5	-1	9	324	319	5
-8	10	59	30	13*	-5	13	226	216	7	-1	12	292	314	12
-8	13	90	81	10	-5	16	224	217	9	-1	15	246	271	19
-8	16	137	143	11	-5	19	120	9	12	-1	18	152	155	11
-8	25	68	20	14*	-5	22	65	60	17*	0	-19	127	128	10
-7	-24	47	83	21*	-5	25	102	64	10	0	-13	210	199	10
-7	-21	146	144	10	-4	-24	52	31	18*	0	-10	138	131	10
-7	-18	427	419	6	-4	-21	62	50	15*	0	-7	69	50	12*
-7	-15	519	506	7	-4	-15	95	93	14	0	-1	283	278	6
-7	-12	119	125	11	-4	-12	79	69	9	0	2	326	335	5
-7	-9	52	12	13*	-4	0	118	111	5	0	5	194	193	5
-7	-6	57	57	4	-4	3	83	95	7	0	8	120	132	5
-7	-3	364	361	6	-4	6	62	46	13*	0	11	157	156	11
-7	0	664	654	10	-4	9	70	25	9	0	14	56	40	7
-7	3	398	393	6	-4	12	66	64	11*	0	17	149	180	11
-7	6	244	247	5	-4	15	75	42	14*	0	20	80	136	10
-7	9	48	23	8*	-4	24	71	5	12*					
-7	12	226	229	6	-3	-19	159	149	9	^^^^^^^ h = 18 ^^^^^^^				
-7	15	514	496	13	-3	-16	289	298	8					
-7	18	412	412	14	-3	-13	303	294	9	-17	-16	60	39	11*
-7	21	144	121	11	-3	-10	156	162	7	-17	-13	106	118	24*
-7	24	53	90	22*	-3	-4	173	180	6	-17	-10	88	96	8
-6	-25	115	122	14	-3	-1	319	310	7	-17	-4	83	92	11
-6	-22	65	6	16*	-3	2	306	313	6	-17	-1	174	175	10
-6	-19	145	137	9	-3	5	136	133	7	-17	2	235	231	7
-6	-16	329	322	8	-3	8	50	44	9*	-17	8	133	152	10
-6	-13	379	369	5	-3	11	59	56	14*	-17	11	48	3	13*
-6	-10	295	295	6	-3	14	224	219	5	-17	17	63	7	17*
-6	-7	176	172	6	-3	17	257	261	8	-16	-17	79	103	8

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-16	-14	168	172	8	-12	-3	68	78	15*	-9	18	61	20	16*
-16	-11	258	254	9	-12	0	206	215	5	-9	21	70	38	18*
-16	-8	364	382	12	-12	3	269	253	7	-8	-22	108	61	12
-16	-5	245	235	12	-12	6	444	432	10	-8	-19	71	13	13*
-16	-2	104	90	8	-12	9	413	400	9	-8	-16	242	231	6
-16	1	120	117	8	-12	12	92	93	17*	-8	-13	438	428	7
-16	4	111	111	7	-12	15	131	128	10	-8	-10	347	336	8
-16	7	204	213	8	-12	18	188	186	9	-8	-7	179	172	7
-16	10	189	189	9	-12	21	140	136	10	-8	-4	82	85	8
-16	16	86	69	13	-11	-22	147	132	11	-8	-1	155	156	6
-16	19	92	72	13	-11	-19	50	107	18*	-8	2	431	425	7
-15	-21	72	74	28*	-11	-13	119	113	9	-8	5	306	312	5
-15	-18	75	16	16*	-11	-10	310	319	6	-8	8	317	319	8
-15	-15	108	106	10	-11	-7	455	459	13	-8	11	280	281	8
-15	-12	129	120	6	-11	-4	346	342	7	-8	14	81	63	13
-15	-9	98	97	4	-11	-1	352	334	6	-8	17	167	153	8
-15	-6	180	179	6	-11	5	263	268	5	-8	20	129	126	9
-15	-3	76	70	13*	-11	8	353	372	8	-8	23	219	218	8
-15	0	348	327	8	-11	11	277	282	12	-7	-23	308	289	7
-15	3	204	199	7	-11	14	256	270	5	-7	-20	251	238	8
-15	6	111	124	9	-11	17	84	92	10	-7	-17	191	180	9
-15	9	202	190	6	-11	20	94	78	13	-7	-14	89	93	11
-15	12	92	107	9	-11	23	110	62	13	-7	-11	343	348	9
-15	15	46	31	17*	-10	-23	67	79	18*	-7	-8	501	495	8
-14	-22	49	6	23*	-10	-20	133	122	7	-7	-5	555	573	7
-14	-16	63	43	13*	-10	-17	319	321	9	-7	-2	592	598	9
-14	-13	85	96	7	-10	-14	201	203	8	-7	1	234	229	8
-14	-10	62	44	5	-10	-8	37	48	18*	-7	4	148	146	6
-14	-7	53	40	11*	-10	-5	101	83	8	-7	7	351	351	8
-14	-4	46	72	17*	-10	-2	302	304	5	-7	10	567	551	12
-14	-1	122	128	6	-10	1	321	323	7	-7	13	597	596	9
-14	20	43	13	17*	-10	4	135	135	10	-7	16	301	296	11
-13	-20	56	47	18*	-10	7	35	68	18*	-6	-21	187	185	7
-13	-17	107	97	7	-10	10	89	118	7	-6	-18	377	373	9
-13	-11	49	23	8	-10	13	214	230	9	-6	-15	379	403	8
-13	-8	133	143	10	-10	16	337	337	9	-6	-12	369	371	6
-13	-5	43	25	13*	-10	19	167	159	11	-6	-9	112	117	7
-13	-2	134	141	6	-10	22	72	32	18*	-6	-6	253	258	7
-13	1	64	62	10	-9	-18	81	60	13	-6	-3	489	492	7
-13	4	171	171	8	-9	-15	49	36	15*	-6	0	525	525	10
-13	7	260	263	6	-9	-12	67	2	11	-6	3	459	468	7
-13	13	90	97	11	-9	-9	36	52	15*	-6	6	260	263	7
-13	16	92	108	12	-9	-6	178	198	12	-6	9	104	104	8
-13	19	65	48	16*	-9	-3	133	141	5	-6	12	104	117	9
-13	22	67	65	19*	-9	0	71	42	13*	-6	15	426	414	7
-12	-18	175	187	10	-9	3	66	70	5	-6	18	342	346	12
-12	-15	206	210	9	-9	6	118	123	5	-6	21	264	264	8
-12	-12	148	152	4	-9	9	93	93	7	-5	-22	109	130	20*
-12	-9	351	348	5	-9	12	104	102	5	-5	-19	79	94	16*
-12	-6	265	269	6	-9	15	176	169	6	-5	-13	203	214	7

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-5	-10	333	334	6	-1	-8	260	256	9	-16	5	317	319	8
-5	-7	278	274	7	-1	-5	185	195	7	-16	8	208	203	8
-5	-4	66	69	8	-1	-2	67	27	18*	-16	14	163	166	8
-5	-1	80	77	7	-1	1	143	150	4	-16	17	181	189	10
-5	2	176	179	6	-1	4	154	151	5	-15	-20	55	36	22*
-5	5	381	377	7	-1	7	184	194	6	-15	-17	72	41	10
-5	8	409	399	10	-1	10	207	203	5	-15	-14	102	96	7
-5	11	356	350	7	-1	13	48	60	11*	-15	-11	136	143	9
-5	14	92	74	12	-1	16	48	29	13*	-15	-8	277	304	21
-5	17	110	121	9	-1	19	61	77	12*	-15	-5	264	271	6
-5	20	73	101	17*	0	-15	136	128	11	-15	-2	107	83	19*
-5	23	168	179	9	0	-9	133	123	10	-15	4	78	106	14*
-4	-17	58	61	16*	0	-3	143	154	8	-15	7	258	257	10
-4	-14	205	201	10	0	0	194	205	6	-15	16	107	15	13
-4	-11	127	114	10	0	3	136	141	6	-14	-21	55	35	18*
-4	-8	89	95	7	0	6	131	128	6	-14	-18	139	137	17
-4	-2	137	129	7	0	9	65	82	5	-14	-15	149	145	7
-4	1	295	289	5	0	12	77	63	6	-14	-12	98	118	10
-4	4	234	225	6	0	15	147	173	6	-14	-9	41	42	15*
-4	7	156	152	5	0	18	142	175	11	-14	-6	71	74	6
-4	10	129	117	10						-14	-3	155	161	7
-4	13	53	39	11*	^^^^^^^	h =	19	^^^^^^^		-14	0	286	265	8
-4	16	110	122	17						-14	3	120	125	8
-4	19	110	92	12	-18	-14	48	50	15*	-14	6	49	8	9*
-4	22	126	75	9	-18	-11	90	118	15	-14	12	90	83	9
-3	-18	88	85	12	-18	-8	154	147	8	-14	15	152	171	10
-3	-15	43	31	17*	-18	-5	107	94	17	-14	18	118	119	10
-3	-9	243	233	6	-18	-2	117	121	8	-13	-19	70	82	13*
-3	-6	328	331	7	-18	1	55	57	14*	-13	-16	60	21	15*
-3	0	47	44	14*	-18	7	205	189	8	-13	-13	100	112	10
-3	3	45	34	11*	-18	10	109	108	11	-13	-10	218	226	7
-3	6	39	47	11*	-17	-18	103	149	15	-13	-7	279	299	20
-3	9	243	251	5	-17	-15	102	138	16	-13	-4	274	276	4
-3	12	312	313	7	-17	-12	66	49	15*	-13	-1	121	116	7
-3	15	83	97	5	-17	-9	129	139	4	-13	2	60	35	11*
-3	21	62	2	12*	-17	-6	238	274	23	-13	5	185	184	7
-2	-19	166	178	9	-17	-3	259	252	9	-13	8	302	314	10
-2	-16	198	186	5	-17	0	225	234	7	-13	11	283	274	8
-2	-10	287	280	9	-17	3	118	94	9	-13	17	59	34	9
-2	-7	111	96	19*	-17	6	151	128	15	-13	20	90	22	14
-2	-1	419	426	6	-17	9	213	224	7	-12	-20	185	175	10
-2	2	423	418	6	-17	12	205	211	10	-12	-17	251	263	9
-2	5	317	324	13	-16	-19	178	178	11	-12	-14	200	202	8
-2	8	174	183	9	-16	-16	227	225	7	-12	-11	67	50	6
-2	11	41	20	8*	-16	-13	116	128	13	-12	-8	260	261	7
-2	14	193	197	11	-16	-10	75	40	16*	-12	-5	435	435	8
-2	17	151	153	8	-16	-7	67	25	11	-12	-2	319	335	6
-2	20	143	213	10	-16	-4	184	208	5	-12	1	293	294	7
-1	-17	72	89	16*	-16	-1	341	335	9	-12	4	127	129	6
-1	-11	218	224	9	-16	2	319	319	8	-12	7	118	109	9

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-12	10	237	228	5	-8	6	163	159	8	-4	-4	76	21	8
-12	13	257	260	5	-8	9	151	147	6	-4	-1	37	5	13*
-12	16	313	324	10	-8	12	300	298	8	-4	2	88	79	8
-12	19	198	196	13	-8	15	221	230	9	-4	5	258	264	7
-11	-15	241	245	9	-8	18	221	231	12	-4	8	144	142	10
-11	-12	279	283	6	-8	21	208	239	11	-4	11	57	43	13*
-11	-9	222	227	7	-7	-19	110	50	12	-4	14	60	40	16*
-11	-6	58	28	11*	-7	-16	331	330	8	-4	17	76	80	21*
-11	-3	56	16	12*	-7	-13	541	529	8	-4	20	102	98	10
-11	0	133	144	13	-7	-7	503	499	8	-3	-17	108	73	10
-11	3	345	335	6	-7	-4	199	199	7	-3	-14	73	97	18*
-11	6	340	337	8	-7	-1	279	283	5	-3	-11	270	264	9
-11	9	269	267	9	-7	2	505	509	6	-3	-8	381	371	8
-11	12	138	160	8	-7	5	561	559	9	-3	-5	239	255	7
-11	15	88	34	11	-7	8	567	577	12	-3	1	131	126	9
-11	18	161	169	11	-7	11	362	373	6	-3	4	229	223	4
-11	21	125	143	12	-7	14	51	22	13*	-3	7	368	365	12
-10	-22	65	63	17*	-7	17	196	197	10	-3	10	297	294	14
-10	-13	38	50	18*	-6	-20	225	216	9	-3	13	111	101	7
-10	-10	114	114	9	-6	-17	78	26	24*	-3	19	90	90	17*
-10	-7	100	92	9	-6	-14	114	123	9	-2	-15	60	45	14*
-10	-4	136	142	6	-6	-11	184	179	6	-2	-12	47	7	20*
-10	-1	148	149	6	-6	-8	365	372	7	-2	-9	115	119	12
-10	2	41	8	13*	-6	-5	454	458	8	-2	-6	232	226	7
-10	5	63	1	12*	-6	-2	157	156	4	-2	-3	232	240	7
-10	8	91	83	7	-6	1	91	82	8	-2	0	137	137	6
-10	11	206	212	6	-6	4	62	65	11*	-2	3	106	95	9
-10	14	177	184	9	-6	7	261	263	7	-2	9	116	117	13
-9	-20	160	150	6	-6	10	402	399	9	-2	12	156	155	5
-9	-17	86	94	21*	-6	13	287	295	6	-2	15	134	110	11
-9	-11	238	242	8	-6	16	52	62	12*	-2	18	116	85	19
-9	-8	359	367	7	-6	19	106	73	14	-1	-13	58	52	17*
-9	-5	288	288	7	-5	-15	57	48	14*	-1	-10	48	15	19*
-9	-2	187	190	5	-5	-12	147	136	9	-1	-7	71	56	11
-9	1	117	119	8	-5	-9	107	111	8	-1	-1	125	129	9
-9	4	115	103	7	-5	-6	80	87	8	-1	2	137	137	5
-9	7	333	333	7	-5	-3	125	118	5	-1	5	105	107	7
-9	10	406	413	7	-5	0	214	220	8	-1	8	46	46	12*
-9	13	238	241	6	-5	3	141	146	5	-1	14	102	119	9
-9	16	111	107	5	-5	6	113	116	17	-1	17	113	142	10
-9	19	90	67	7	-5	9	114	108	7	0	-11	133	83	10
-9	22	122	123	13	-5	12	67	56	24*	0	-8	74	80	11
-8	-21	253	244	10	-5	15	134	120	6	0	1	59	69	10*
-8	-18	156	163	10	-5	18	74	39	24*	0	7	102	93	8
-8	-15	311	307	7	-5	21	105	112	11	0	10	108	63	19*
-8	-12	266	269	8	-4	-19	95	88	13	0	13	42	6	17*
-8	-9	82	67	9	-4	-16	52	79	16*					
-8	-3	399	393	6	-4	-13	75	85	11	^^^^^^^	h =	20	^^^^^^^	
-8	0	603	603	7	-4	-10	131	129	10					
-8	3	502	502	8	-4	-7	82	93	9	-19	-12	50	28	15*

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-19	-9	38	47	17*	-14	13	218	236	5	-9	-13	190	182	9
-19	-6	97	73	9	-14	16	176	163	11	-9	-10	283	279	7
-19	-3	94	50	7	-13	-18	67	37	15*	-9	-7	187	184	8
-19	0	52	3	13*	-13	-15	143	158	6	-9	-4	107	101	6
-19	3	68	45	11	-13	-12	201	212	8	-9	-1	171	171	5
-18	-13	189	225	8	-13	-9	154	167	11	-9	2	55	52	9*
-18	-10	114	123	6	-13	-6	48	54	8	-9	5	250	247	7
-18	-7	46	48	15*	-13	-3	71	82	8	-9	8	172	172	12
-18	-4	207	203	5	-13	0	222	202	8	-9	11	70	83	9
-18	-1	273	273	5	-13	3	287	280	7	-9	14	76	96	12
-18	2	278	292	9	-13	6	299	296	5	-9	20	181	181	11
-18	8	84	56	11	-13	9	154	149	12	-8	-17	163	159	7
-17	-14	122	208	10	-13	12	82	3	13	-8	-14	79	40	20*
-17	-11	163	231	20	-13	15	57	61	13*	-8	-11	146	138	8
-17	-8	185	211	7	-13	18	98	98	14	-8	-8	331	326	8
-17	-5	163	164	5	-12	-19	130	121	11	-8	-5	368	371	7
-17	1	148	144	10	-12	-16	101	32	12	-8	-2	224	228	4
-17	4	204	217	8	-12	-13	142	138	8	-8	1	97	97	11
-17	7	214	217	8	-12	-10	313	319	8	-8	4	59	62	9
-17	10	173	195	8	-12	-7	483	476	8	-8	7	300	287	8
-17	13	120	110	14	-12	-4	293	300	8	-8	10	386	400	7
-16	-18	147	161	17	-12	-1	147	152	7	-8	13	266	275	7
-16	-15	136	145	18	-12	5	246	246	7	-8	16	175	193	10
-16	-9	165	197	6	-12	8	455	456	11	-8	19	121	114	13
-16	-6	202	255	18	-12	11	348	343	8	-7	-18	239	232	10
-16	-3	308	296	6	-12	14	132	158	14	-7	-15	128	130	10
-16	0	269	265	7	-12	17	106	92	20*	-7	-12	70	59	12*
-16	3	122	126	9	-11	-14	63	94	11*	-7	-6	119	135	8
-16	6	66	79	16*	-11	-11	51	46	13*	-7	-3	339	339	6
-16	12	251	253	9	-11	-8	145	170	13	-7	0	296	286	5
-16	15	250	252	10	-11	-5	195	202	4	-7	3	325	330	6
-15	-16	106	131	22*	-11	-2	182	180	9	-7	6	336	344	11
-15	-13	119	136	19	-11	4	119	111	6	-7	9	93	31	10
-15	-10	70	47	11	-11	7	80	88	8	-7	12	182	190	5
-15	-7	81	114	17*	-11	10	213	212	10	-7	15	193	193	9
-15	-4	42	56	13*	-11	13	150	160	13	-7	18	205	213	6
-15	-1	52	53	12*	-11	16	81	66	15*	-6	-16	127	120	18
-15	2	155	150	8	-11	19	88	101	13	-6	-13	106	89	10
-15	5	128	132	14	-10	-18	58	5	17*	-6	-10	155	159	8
-15	8	99	14	11	-10	-15	55	22	16*	-6	-7	188	192	6
-15	17	127	88	13	-10	-12	94	92	10	-6	-4	61	44	10
-14	-17	105	108	15	-10	-9	117	113	8	-6	-1	182	175	5
-14	-14	76	91	7	-10	-6	120	119	5	-6	2	114	119	8
-14	-8	111	106	8	-10	3	58	33	9	-6	5	193	180	7
-14	-5	126	129	7	-10	6	41	23	9*	-6	8	176	174	5
-14	-2	320	329	10	-10	9	100	113	8	-6	14	122	108	7
-14	1	285	284	8	-10	12	61	58	13*	-6	17	52	66	15*
-14	4	54	37	14*	-10	15	103	58	12	-5	-14	70	33	12*
-14	7	140	134	8	-10	18	71	19	16*	-5	-2	62	70	9
-14	10	198	184	5	-9	-19	80	7	14*	-5	1	48	46	16*

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II)

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-5	4	39	20	9*	-17	-13	159	234	9	-11	-16	104	87	16
-4	-15	80	72	23*	-17	-4	82	90	11	-11	-13	84	59	8
-4	-12	116	122	11	-17	-1	290	298	7	-11	-4	63	36	13*
-4	-6	124	118	11	-17	2	285	296	10	-11	-1	107	97	9
-4	-3	182	178	7	-17	5	150	141	9	-11	2	89	108	11
-4	0	140	137	5	-17	8	60	38	15*	-11	5	98	105	8
-4	3	143	133	4	-16	-14	107	91	10	-11	8	126	115	8
-4	6	110	101	9	-16	-11	167	173	9	-11	11	84	69	11
-4	9	63	24	12*	-16	-8	108	114	10	-11	14	46	32	17*
-4	15	89	68	13	-16	-5	69	48	10	-10	-17	81	73	13
-4	18	91	54	15*	-16	-2	61	36	11*	-10	-14	165	175	7
-3	-13	77	79	18*	-16	1	94	70	7	-10	-11	138	137	7
-3	-4	41	56	12*	-16	4	132	121	8	-10	-8	55	56	11*
-3	-1	67	15	10	-16	7	113	136	14	-10	-5	79	13	10
-3	2	42	12	18*	-16	10	121	111	9	-10	1	120	77	15
-3	5	50	72	9*	-16	13	109	102	12	-10	7	61	20	6
-3	8	56	63	7	-15	-9	103	75	10	-10	13	60	16	15*
-3	14	50	22	15*	-15	-6	112	140	19*	-10	16	60	65	8
-2	-5	86	42	12	-15	-3	89	64	8	-9	-12	128	137	6
-2	1	66	24	13*	-15	0	72	94	8	-9	-9	47	34	17*
-2	4	74	55	12*	-15	3	105	92	9	-9	-6	130	133	9
-2	7	61	19	11*	-15	6	45	24	9*	-9	-3	132	118	7
-1	-6	70	57	14*	-15	9	111	95	10	-9	0	144	147	9
-1	-3	112	96	10	-14	-16	87	27	12	-9	3	227	239	8
-1	0	139	140	10	-14	-13	75	45	14*	-9	6	99	112	6
-1	3	152	147	8	-14	-10	127	102	9	-9	9	113	102	9
-1	6	45	62	15*	-14	-4	37	71	14*	-9	12	124	118	10
-1	9	57	38	13*	-14	-1	62	68	11*	-9	15	40	14	18*
-1	12	88	51	10	-14	2	48	13	15*	-8	-16	143	122	10
0	-7	64	75	13*	-14	5	59	55	9	-8	-13	121	123	16
0	-4	47	28	13*	-14	8	61	40	11*	-8	-10	111	74	10
0	-1	183	179	7	-14	11	39	43	18*	-8	-7	72	68	6
0	2	195	195	7	-14	14	85	68	11	-8	-4	55	75	14*
0	5	145	196	13	-13	-14	85	74	12	-8	2	117	92	9
0	8	88	133	19*	-13	-11	62	17	14*	-8	5	50	71	15*
					-13	-5	104	126	10	-8	8	85	13	10
^^^^^^^	h =	21	^^^^^^^		-13	-2	60	56	9	-8	14	74	33	15*
					-13	1	89	62	10	-8	17	47	100	21*
-20	-4	41	27	19*	-13	4	112	126	9	-7	-14	72	62	14*
-20	-1	63	42	11*	-13	10	173	164	10	-7	-11	72	49	13*
-19	-8	73	26	12	-13	13	162	116	10	-7	-5	86	50	9
-19	1	125	116	9	-13	16	131	100	11	-7	-2	41	4	20*
-19	4	113	112	13	-12	-15	59	75	16*	-7	1	130	138	5
-18	-12	56	10	15*	-12	-12	75	93	11	-7	4	128	119	9
-18	-9	80	14	12	-12	-9	58	41	13*	-7	7	72	98	12*
-18	-6	72	125	16*	-12	0	104	121	10	-7	10	71	64	7
-18	-3	265	275	9	-12	3	207	205	4	-7	13	42	55	17*
-18	0	224	228	7	-12	6	168	154	10	-6	-15	151	141	10
-18	3	84	96	14*	-12	9	69	7	14*	-6	-9	210	216	9
-18	6	60	13	14*	-12	12	93	84	10	-6	-6	220	222	6

10|F|o vs 10|F|c for Phosphazene Clathrate (Data Set II) page 26

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-6	-3	64	32	10	-15	1	124	119	8	-8	9	53	1	14*
-6	0	171	177	5	-15	7	93	89	8	-7	-10	127	114	10
-6	3	181	186	8	-15	10	147	167	11	-7	-7	237	220	9
-6	6	181	195	9	-14	-9	113	76	10	-7	-4	145	161	12
-6	9	216	195	8	-14	-6	90	86	11	-7	2	112	76	16
-6	12	91	63	10	-14	6	99	57	10	-7	5	157	153	9
-5	-13	117	120	10	-14	9	77	80	14*	-7	8	216	213	9
-5	-7	246	251	7	-14	12	124	68	11	-6	-8	64	25	14*
-5	-4	190	154	22	-13	-10	90	15	12	-6	-5	166	168	20
-5	-1	88	87	21*	-13	-1	92	75	11	-6	-2	181	212	15
-5	2	114	116	9	-13	2	64	59	13*	-6	4	164	195	9
-5	8	181	180	9	-13	5	59	38	9	-6	7	119	123	10
-5	11	161	163	8	-13	8	63	19	15*	-5	-6	96	118	10
-4	-8	93	38	12	-12	-11	89	113	12	-5	-3	56	69	17*
-4	-5	85	74	12	-12	-8	191	181	9	-5	0	194	199	9
-4	-2	171	168	8	-12	-5	213	198	9	-5	3	190	222	9
-4	1	155	163	10	-12	-2	76	93	12	-4	-7	78	88	12
-4	4	65	90	12*	-12	4	100	75	11	-4	-4	109	128	9
-4	10	54	71	14*	-12	7	164	180	7	-4	-1	90	126	10
-3	-9	81	37	12	-12	10	102	101	15					
-3	0	77	80	12	-11	-15	78	111	16*	^^^^^^^ h = 23 ^^^^^^^				
-3	6	83	39	11	-11	-12	55	59	16*					
-2	-7	128	151	9	-11	-9	205	223	23	-17	4	97	20	11
-2	-4	69	4	12*	-11	-6	296	276	9	-16	3	164	234	10
-2	-1	116	129	7	-11	-3	190	194	9	-15	8	172	248	10
-2	2	181	200	20	-11	3	49	62	15*	-14	-5	183	209	9
-2	5	202	277	16	-11	6	130	131	9	-14	-2	138	133	10
-2	8	223	259	9	-11	9	265	272	9	-14	1	136	104	10
-1	-2	210	254	9	-11	12	181	206	9	-14	7	118	104	10
-1	4	93	38	10	-10	-13	114	100	11	-13	-3	82	94	12
					-10	-10	68	37	19*	-13	0	70	51	13*
^^^^^^^ h = 22 ^^^^^^^					-10	-7	102	94	15	-12	-4	132	125	10
					-10	-4	116	127	10	-12	-1	149	123	9
-19	-4	54	64	15*	-10	-1	217	207	9	-12	2	225	205	9
-18	-5	68	97	24*	-10	2	234	244	9	-12	5	215	196	9
-18	-2	76	40	8	-10	5	185	174	9	-11	-5	195	175	9
-18	1	73	46	12*	-10	8	72	62	12	-11	-2	96	118	11
-18	4	126	103	9	-10	11	63	40	14*	-11	4	229	225	9
-17	-3	51	13	18*	-9	-11	204	195	7	-10	-3	179	181	9
-17	0	48	9	16*	-9	-8	242	248	5	-10	3	75	42	12
-17	3	43	24	20*	-9	-5	162	162	7	-9	-1	82	73	12
-16	-7	54	58	15*	-9	-2	64	29	14*	-9	2	125	116	10
-16	-1	51	69	13*	-9	1	112	104	16					
-16	2	59	50	9	-9	4	66	51	13*					
-16	5	89	44	19*	-9	7	140	129	9					
-16	8	88	103	11	-9	10	136	131	9					
-15	-11	139	148	9	-8	-12	51	61	18*					
-15	-8	162	176	14	-8	-3	54	56	16*					
-15	-5	102	145	10	-8	3	64	30	13*					
-15	-2	159	148	9	-8	6	44	38	17*					

Intramolecular Distances Involving the Hydrogen Atoms for $C_6H_4S_2P^+$ $AlCl_4^-$

atom	atom	distance	atom	atom	distance
C3	H3	1.074	C5	H5	1.092
C4	H4	1.072	C6	H6	1.072

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Intramolecular Distances Involving the Hydrogen Atoms for $C_{13}H_{11}PS_2$

atom	atom	distance	atom	atom	distance
C3	H3	0.93(3)	C11	H11	0.91(4)
C5	H5	0.93(4)	C12	H12	0.95(4)
C6	H6	1.01(4)	C13	H131	1.01(6)
C8	H8	0.90(4)	C13	H132	0.94(6)
C9	H9	1.05(4)	C13	H133	0.96(5)
C10	H10	0.99(4)			

Distances are in angstroms. Estimated standard deviations in the least significant figure are given in parentheses.

Table . Torsional Angles (degrees) for $C_6H_4S_2P^+ AlCl_4^-$

P(1)	-S(1)	-C(1)	-C(2)	-0.7 (4)
P(1)	-S(1)	-C(1)	-C(6)	178.4 (3)
C(1)	-S(1)	-P(1)	-S(2)	0.7 (2)
P(1)	-S(2)	-C(2)	-C(1)	0.2 (4)
P(1)	-S(2)	-C(2)	-C(3)	-178.5 (4)
C(2)	-S(2)	-P(1)	-S(1)	-0.5 (2)
S(1)	-C(1)	-C(2)	-S(2)	0.4 (4)
S(1)	-C(1)	-C(2)	-C(3)	179.1 (3)
S(1)	-C(1)	-C(6)	-C(5)	-178.4 (3)
C(2)	-C(1)	-C(6)	-C(5)	0.7 (6)
C(6)	-C(1)	-C(2)	-S(2)	-178.8 (3)
C(6)	-C(1)	-C(2)	-C(3)	-0.1 (6)
S(2)	-C(2)	-C(3)	-C(4)	178.3 (4)
C(1)	-C(2)	-C(3)	-C(4)	-0.4 (6)
C(2)	-C(3)	-C(4)	-C(5)	0.2 (7)
C(3)	-C(4)	-C(5)	-C(6)	0.5 (7)
C(4)	-C(5)	-C(6)	-C(1)	-1.0 (6)

Observed and Calculated Structure Factors for $C_6H_4S_2P^+ AlCl_4^-$

10|F|o vs 10|F|c for br135

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
^^^^^^^ h = -7 ^^^^^^^					1	1	349	357	8	-7	-4	161	140	11
					1	7	191	171	9	-5	-5	110	126	16
-1	2	345	358	8	2	5	136	130	12	-5	-4	321	315	9
0	0	160	153	10	3	1	351	349	8	-3	-5	178	158	11
0	4	232	223	8	3	4	303	304	8	-2	-2	394	380	8
6	2	116	91	12	4	5	472	466	9	-1	-6	164	148	12
					5	-1	159	160	11	-1	-4	330	310	8
^^^^^^^ h = -6 ^^^^^^^					5	1	171	156	10	-1	3	234	239	7
					5	5	147	121	11	0	-6	189	186	11
-9	-2	100	98	16	6	-4	120	126	15	0	-4	188	181	11
-6	-3	108	109	16	6	-2	104	79	16	0	2	375	376	7
-4	-2	102	108	16	6	4	157	159	11	1	-5	201	194	11
-3	-3	125	122	14	7	-3	308	295	8	1	-5	265	261	8
-3	-1	136	154	12	7	0	294	288	8	1	-2	276	277	8
-1	-1	114	94	13	8	0	221	222	9	2	-5	293	301	9
0	-2	170	172	11	9	-1	177	200	10	2	3	310	315	7
0	0	246	259	8	9	0	307	306	8	2	6	261	270	8
2	-2	214	203	9	9	4	279	280	8	2	7	173	153	10
2	6	150	158	11	9	6	314	312	8	3	-1	214	212	7
3	5	177	176	10	10	-1	247	253	8	3	0	336	344	7
4	0	334	341	8	10	0	120	124	13	4	-6	251	240	10
7	-3	190	189	10	10	2	107	106	14	4	-2	141	159	11
8	-2	181	180	10	10	3	332	320	8	4	-1	426	426	8
8	-1	169	150	10	11	-1	242	256	8	4	5	118	111	13
8	2	315	320	8	11	0	235	237	8	4	6	390	390	8
9	-1	152	154	12	11	4	107	119	15	4	8	211	217	10
9	1	155	137	10	11	6	135	117	11	5	-3	394	379	8
10	0	122	132	13	12	-1	127	92	11	5	1	467	467	8
10	5	176	169	10	12	0	172	159	10	5	3	484	482	9
11	4	133	131	12	12	2	139	157	11	5	6	170	156	10
12	2	287	294	8	13	-1	104	104	14	6	-3	149	140	12
13	1	210	201	9	13	0	182	180	9	6	-1	486	489	9
13	3	176	167	10	13	4	287	281	8	6	2	284	288	7
14	2	157	169	10	13	6	112	100	12	6	7	128	111	12
					14	3	109	110	14	7	-1	503	513	9
^^^^^^^ h = -5 ^^^^^^^					15	0	109	120	14	7	0	528	537	10
					15	1	266	259	8	7	2	377	383	7
-16	-1	120	128	13	15	4	230	234	9	8	-1	395	401	8
-11	-2	102	140	16	17	0	151	180	11	8	2	293	307	7
-9	-2	155	122	11	18	1	109	97	13	8	4	285	288	8
-5	-4	134	135	14						9	-4	239	228	9
-4	-1	183	180	10	^^^^^^^ h = -4 ^^^^^^^					9	-1	347	346	8
-3	-3	255	249	9						9	0	267	274	8
-2	-5	271	264	9	-20	-1	100	93	15	9	6	139	144	11
-1	0	229	242	8	-15	-3	218	213	9	10	-1	418	421	8
-1	2	240	239	8	-13	-2	309	304	8	10	0	179	176	9
0	-2	299	271	8	-11	-5	283	275	9	10	2	312	311	7
0	0	205	214	9	-10	-5	190	202	12	10	4	140	129	12
0	4	590	593	11	-9	-5	196	181	11	11	-2	162	165	11
1	-5	169	173	12	-7	-5	176	189	12	11	0	232	226	8

Observed and Calculated Structure Factors for $C_6H_4S_2P^+ AlCl_4^-$

10|F|o vs 10|F|c for br135

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
11	3	178	159	10	-1	-4	105	93	15	10	-3	470	499	9
11	5	443	424	9	-1	-1	671	660	11	10	-2	343	338	7
12	-4	106	245	10	-1	6	363	368	8	10	-1	192	207	8
12	-2	119	119	14	0	-6	322	321	9	10	0	206	199	7
12	-1	153	143	11	0	-4	137	139	12	10	1	655	659	11
12	2	180	184	9	0	-2	724	717	12	10	5	195	187	9
12	4	200	211	9	0	0	894	917	14	10	6	121	117	13
13	-3	165	155	10	0	2	1053	1043	16	11	-4	271	276	9
13	-1	237	240	8	0	6	332	335	8	11	-3	236	235	9
13	0	240	241	8	1	3	99	75	9	11	-1	284	274	7
13	1	228	240	9	1	8	144	144	12	11	0	448	454	8
13	2	267	255	8	2	0	422	414	8	11	2	117	110	10
13	4	145	141	11	2	3	456	452	8	12	-5	114	113	18
14	-3	148	142	12	2	5	480	477	8	12	0	369	369	8
14	-2	195	183	9	3	-2	175	186	7	12	2	276	264	7
14	0	232	241	9	3	0	698	719	11	13	-4	157	189	11
14	2	214	237	9	3	1	338	316	6	13	-1	137	142	12
15	-2	136	118	12	3	2	96	95	8	13	1	133	130	11
16	0	141	154	12	3	3	439	454	8	13	2	120	102	12
16	2	101	94	14	3	4	536	549	10	14	-2	115	104	15
17	2	114	132	14	3	8	315	317	8	14	0	262	264	8
17	3	124	126	13	4	-6	368	384	10	14	2	129	130	12
17	5	152	147	11	4	-2	332	328	7	15	-4	155	152	13
18	-2	148	119	12	4	-1	599	587	10	15	-3	155	156	12
20	3	165	154	10	4	0	394	377	7	15	2	304	299	8
					4	1	405	397	7	15	5	178	189	10
^^^^^^^ h = -3 ^^^^^^^					4	5	173	169	9	15	6	112	123	14
					5	-5	187	196	12	15	7	99	95	14
-22	-2	142	147	12	5	1	209	223	6	17	0	230	250	9
-19	-2	102	79	15	5	8	305	297	8	17	1	363	359	8
-17	-1	225	249	9	6	-3	428	414	8	17	2	131	128	13
-15	-2	192	182	10	6	-1	324	320	6	18	-3	169	188	11
-14	-5	233	243	10	6	1	122	125	8	18	-2	147	129	12
-14	-1	354	343	8	6	5	243	235	8	18	-1	359	372	9
-12	-4	175	155	12	6	6	109	116	14	18	0	104	125	16
-12	-3	371	374	9	7	-4	182	171	11	18	2	179	174	10
-12	-1	413	394	8	7	0	178	166	6	19	-1	238	271	9
-11	-5	196	195	11	7	1	429	427	8	19	1	193	165	9
-8	-5	157	157	14	7	2	187	195	6	20	-1	250	251	9
-7	-6	225	224	10	7	6	199	206	9	20	0	149	149	11
-7	-1	276	288	6	8	-4	428	427	9	21	-2	153	156	12
-6	-5	167	154	13	8	-2	170	180	8					
-5	-2	188	203	7	8	0	318	333	6	^^^^^^^ h = -2 ^^^^^^^				
-5	-1	616	623	11	8	1	256	262	6					
-4	-5	445	434	9	8	3	732	734	12	-21	-2	154	140	11
-3	-6	368	372	9	8	6	237	230	8	-20	-2	202	191	9
-3	-4	270	247	8	9	-4	158	139	13	-19	-1	164	164	11
-3	-1	258	253	6	9	2	142	143	8	-18	-3	145	145	13
-2	-2	651	645	11	9	6	224	227	9	-14	-2	495	504	9
-1	-5	189	195	11	10	-5	201	187	11	-11	-7	182	170	12

Observed and Calculated Structure Factors for $C_6H_4S_2P^+\ AlCl_4^-$

10|F|o vs 10|F|c for br135

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
-9	-7	211	212	11	7	-5	152	130	14	16	-2	268	256	9
-9	-6	190	178	11	7	-4	241	231	9	17	-4	465	445	9
-9	-2	654	641	11	7	-1	454	445	8	17	1	114	161	15
-7	-7	112	101	17	7	1	505	512	9	17	2	101	68	16
-6	-7	130	131	15	7	2	104	99	8	18	-4	118	123	17
-5	-4	190	196	9	7	9	259	265	8	18	1	207	202	10
-5	-2	173	171	7	8	-8	185	189	12	18	2	259	244	9
-4	-5	152	146	12	8	-6	139	122	16	21	3	236	239	9
-3	-2	325	325	6	8	-4	482	479	9	22	-3	237	215	9
-2	-7	270	272	9	8	-3	161	153	9	22	0	138	140	13
-2	-6	362	363	8	8	-2	909	948	15	23	-1	102	87	17
-2	-4	619	616	11	8	0	210	215	6	23	0	215	212	10
-2	-2	138	144	7	8	1	246	240	6					
-1	-7	187	175	11	8	3	470	460	9	^^^^^^^ h = -1 ^^^^^^^				
-1	-6	233	229	10	8	5	441	451	8					
-1	-4	491	466	9	8	8	189	184	9	-22	-3	155	141	12
-1	-3	646	614	11	9	1	364	375	7	-21	-2	308	322	9
0	-8	273	278	10	9	2	350	357	7	-20	-4	156	144	12
0	-6	113	93	17	9	5	134	111	10	-15	-6	216	223	10
0	-4	212	210	7	10	-7	137	146	16	-14	-5	194	189	11
0	0	282	274	5	10	-3	364	366	8	-13	-1	608	606	11
0	2	98	112	7	10	0	197	182	6	-12	-7	121	132	16
0	8	222	231	9	10	2	500	506	9	-12	-4	336	352	8
1	0	625	609	10	11	-3	156	149	12	-10	-2	447	442	8
1	2	920	960	14	11	-2	279	273	7	-10	-1	363	359	7
1	4	354	343	6	11	-1	426	416	8	-9	-2	388	389	7
2	-5	216	214	9	11	1	517	524	9	-7	-5	103	106	15
2	-1	522	506	9	11	2	240	239	6	-7	-1	205	226	6
3	-5	251	246	9	11	3	471	483	9	-6	-6	109	60	16
3	-4	798	799	14	11	5	232	233	8	-5	-5	238	238	7
3	3	857	842	14	12	-6	275	313	10	-5	-1	264	262	6
3	6	228	229	8	12	-3	169	182	12	-4	-8	117	101	15
3	7	269	273	9	12	-1	251	257	7	-4	-6	153	121	11
3	9	134	133	13	12	1	381	386	7	-4	-4	853	852	14
4	-3	623	619	11	13	-6	110	173	16	-3	-8	209	218	10
4	-2	100	101	9	13	-2	357	379	8	-3	-2	264	257	6
4	0	713	688	11	13	-1	155	146	9	-2	-6	106	118	15
4	1	165	148	5	13	0	233	227	7	-2	-4	571	581	10
4	2	878	880	14	13	1	317	307	7	-2	-2	985	996	15
4	3	441	451	8	13	3	473	483	9	-1	-5	320	323	7
5	-7	187	190	11	14	-3	240	246	10	-1	-2	2469	2462	37
5	-6	277	265	10	14	-1	311	314	8	-1	-1	98	74	6
5	1	398	393	7	14	0	511	518	9	-1	2	164	154	5
5	4	313	298	6	14	4	230	230	8	-1	7	230	244	9
5	6	186	178	9	15	-5	227	228	11	-1	8	124	141	14
6	-3	157	154	9	15	-1	218	202	9	0	-8	224	211	10
6	-2	83	93	12	15	2	339	338	8	0	-4	502	518	9
6	-1	371	354	7	15	5	104	100	15	0	-2	1431	1426	22
6	0	605	630	10	16	-6	148	129	13	0	0	307	317	5
6	6	267	279	8	16	-5	144	150	14	0	4	951	963	15

Observed and Calculated Structure Factors for $C_6H_4S_2P^+$ $AlCl_4^-$

10|F|o vs 10|F|c for br135

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
0	8	189	175	9	11	-4	139	149	13	-16	-4	222	213	10
1	-6	315	313	8	11	-3	410	398	8	-14	-7	360	359	9
1	3	435	439	8	11	-2	122	105	11	-14	-6	150	159	13
2	-7	364	366	9	11	-1	104	97	11	-14	-4	393	405	8
2	-3	461	462	8	11	0	568	563	10	-13	-1	184	200	8
2	0	129	128	4	11	2	128	127	8	-12	-7	179	194	11
2	5	472	480	9	12	-6	363	413	9	-12	-3	275	269	7
3	-5	208	202	8	12	-5	134	93	15	-11	-8	120	109	15
3	-4	344	347	7	12	-3	129	129	12	-11	-2	389	380	7
3	-1	139	109	6	12	-1	176	180	8	-9	-1	472	481	8
3	0	68	84	7	12	0	222	212	7	-8	-1	355	367	6
3	1	671	664	11	12	2	384	383	7	-7	-8	119	125	15
3	4	336	328	6	12	8	97	116	15	-7	-5	111	120	12
3	9	127	98	14	13	-6	276	334	9	-6	-9	141	138	12
4	-2	385	385	7	13	-2	210	209	8	-6	-7	140	103	12
4	0	357	357	6	13	0	1008	996	16	-5	-7	140	126	12
4	3	125	138	6	13	8	96	71	15	-5	-1	199	186	5
4	5	421	413	8	14	-3	158	172	13	-4	-5	227	224	7
4	6	226	216	8	14	0	600	595	10	-4	-1	412	397	7
5	-4	302	296	7	14	5	417	410	8	-3	-8	166	165	11
5	-3	88	68	12	15	-4	222	210	11	-3	-3	373	367	7
5	-2	405	4[illegible]2	7	15	-2	155	197	14	-2	-4	89	80	10
5	0	143	134	6	15	0	206	202	8	-2	-3	169	165	6
5	6	182	187	9	15	1	129	141	11	-1	-9	176	183	12
6	-5	260	268	8	15	3	128	130	13	-1	-2	597	590	10
6	-3	397	387	7	15	6	166	160	10	-1	1	307	309	5
6	-2	236	241	6	15	7	194	180	9	-1	4	79	65	11
6	-1	702	678	11	16	-6	168	150	12	-1	6	477	464	9
6	0	815	800	13	16	-2	415	402	9	0	-8	256	271	9
6	2	300	288	6	16	-1	190	197	10	0	-6	544	550	10
6	5	601	599	11	16	1	433	439	8	0	-4	252	248	6
6	7	321	328	8	17	-4	122	144	16	0	2	1281	1240	19
6	9	109	89	14	17	1	210	224	9	1	-8	118	137	15
7	-6	187	192	11	18	-2	342	346	10	1	3	254	261	5
7	-4	256	263	7	18	-1	169	139	12	1	5	594	595	11
7	0	974	961	15	18	3	193	178	10	2	-9	161	153	12
7	1	828	820	13	19	-5	270	283	10	2	-8	190	195	11
8	-4	313	309	7	20	2	169	170	11	2	-5	144	147	9
8	-2	282	272	6	21	-1	216	201	10	2	-2	133	128	6
8	0	204	204	6	22	-2	114	98	16	2	6	146	150	10
8	6	202	195	9	23	2	172	166	11	2	7	175	171	11
8	7	194	198	10	24	-2	133	140	13	3	-9	145	157	14
9	-1	499	489	9						3	-6	234	235	8
9	0	1067	1025	17	^^^^^^^	h =	0	^^^^^^^		3	-5	601	588	11
9	1	191	178	6						3	-1	248	244	4
9	8	105	110	15	-22	-3	131	134	13	4	-6	360	362	8
10	-6	135	119	15	-20	-4	258	266	9	4	-4	564	561	10
10	-4	458	443	9	-20	-1	142	184	14	4	-2	197	242	5
10	1	149	159	7	-18	-6	123	93	15	4	0	1083	1109	16
11	-5	205	192	11	-18	-2	215	191	9	4	3	505	510	9

Observed and Calculated Structure Factors for $C_6H_4S_2P^+ AlCl_4^-$

10|F|o vs 10|F|c for br135 page 5

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
4	7	452	446	9	15	-5	189	192	11	-1	-9	208	229	10
5	-4	177	179	7	15	-3	243	253	9	-1	-6	356	360	8
5	-2	1272	1342	19	15	-2	398	398	8	-1	-4	366	370	7
5	6	96	74	15	15	7	122	107	13	-1	-1	54	61	7
6	-6	140	156	12	16	-7	134	136	14	-1	0	90	96	4
6	-5	386	407	7	16	-6	105	97	17	-1	3	97	90	9
6	-2	871	824	14	16	-5	358	348	9	-1	8	176	191	11
6	-1	234	237	6	16	2	175	168	10	0	-2	118	114	6
6	0	686	699	11	17	-4	169	152	12	1	4	507	507	9
6	3	348	361	6	17	-3	162	186	13	2	-7	388	385	9
6	4	869	895	14	17	1	182	188	10	2	-6	250	237	8
7	-1	1173	1178	18	18	-5	234	212	10	2	-4	192	253	6
7	2	460	441	8	18	0	173	157	11	2	-3	944	1057	15
7	3	455	449	8	18	1	150	148	12	2	-1	1359	1323	21
7	4	498	500	9	18	3	380	382	9	2	1	1577	1532	24
7	9	125	140	13	19	-2	172	158	12	2	5	243	252	7
8	-8	131	67	13	20	-3	260	245	9	3	-7	168	151	11
8	-5	358	363	7	20	0	426	409	9	3	-6	165	158	10
8	-3	626	597	11	21	-5	171	192	12	3	-5	560	541	10
8	-2	625	612	11	21	-2	125	92	14	3	-2	357	354	6
8	4	185	164	7	21	1	147	147	13	4	-7	274	277	9
9	-5	149	143	11	22	0	190	181	11	4	-2	552	553	9
9	-4	542	527	10	24	-2	135	139	14	4	-1	79	15	8
9	-2	486	456	9	25	-2	206	198	10	4	1	535	528	9
9	3	581	591	10						4	3	325	333	6
10	-5	186	174	9	^^^^^^^	h =		1	^^^^^^^	4	7	177	183	11
10	-4	352	340	7						5	-9	148	154	12
10	-3	332	330	7	-24	-3	157	173	12	5	-7	212	212	10
10	-2	153	147	8	-22	-3	418	419	9	5	-5	335	333	7
10	0	277	248	6	-22	-2	145	137	12	5	-4	161	148	7
10	1	239	240	6	-21	-5	101	79	16	5	-2	1490	1538	23
10	7	201	199	9	-20	-5	136	131	13	5	7	308	293	8
11	-7	113	100	15	-18	-2	309	312	8	6	-8	120	134	15
11	-6	166	178	12	-17	-3	266	272	9	6	-4	110	112	9
11	-5	179	168	10	-16	-7	107	104	16	6	4	766	767	13
11	-4	350	342	8	-16	-6	188	199	11	7	-5	400	399	8
11	-3	532	526	10	-16	-3	224	231	9	7	-3	213	211	6
11	1	106	119	10	-13	-2	207	226	7	7	-2	367	369	7
12	-5	252	263	9	-13	-1	231	238	7	7	2	230	226	6
12	-4	235	232	9	-11	-1	357	355	7	7	3	231	228	6
12	1	909	917	15	-9	-7	212	205	9	7	7	160	157	11
12	2	659	686	12	-9	-3	136	124	7	8	-5	398	405	8
13	-5	301	278	9	-9	-2	642	658	11	8	-4	128	142	9
13	-4	567	567	10	-7	-6	145	147	11	8	-3	509	510	9
13	2	154	163	8	-6	-3	353	354	6	8	-2	618	633	10
13	7	147	152	11	-5	-1	186	183	5	8	-1	330	388	6
14	-2	414	400	8	-4	-9	122	148	15	8	1	510	492	9
14	-1	514	605	9	-4	-4	250	247	6	8	3	799	793	13
14	0	676	653	12	-3	-3	429	419	8	8	5	487	472	9
15	-6	130	127	14	-2	-2	324	314	6	8	6	362	352	8

Observed and Calculated Structure Factors for $C_6H_4S_2P^+\ AlCl_4^-$

10|F|o vs 10|F|c for br135

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
9	-6	225	234	9	^^^^^^^ h = 2 ^^^^^^^					5	5	156	138	12
9	-4	219	207	7						6	-7	292	294	9
9	5	166	161	11	-21	-2	335	323	9	6	-4	729	709	12
10	-7	119	107	15	-21	-1	297	316	8	6	-3	118	118	8
10	-6	309	311	8	-20	-1	163	178	11	6	-2	201	211	5
10	-5	255	265	8	-17	-3	144	146	12	7	-6	218	221	9
10	-4	108	130	12	-16	-6	109	102	15	7	-5	688	728	12
10	-3	428	429	8	-16	-1	428	420	8	7	-4	258	256	6
10	-2	413	396	7	-15	-1	110	78	12	7	0	398	408	7
10	0	709	707	12	-14	-2	144	136	10	7	2	447	457	8
10	5	527	499	9	-13	-4	118	118	13	7	3	200	207	8
10	8	156	160	11	-13	-2	199	192	8	8	-4	140	144	8
11	-7	363	363	9	-12	-8	143	151	12	8	-2	240	244	6
11	-4	200	189	8	-12	-3	247	252	7	8	7	188	181	10
11	-3	119	132	10	-11	-4	107	111	13	9	-7	159	147	11
12	-4	188	181	9	-9	-3	385	387	7	9	-6	108	101	12
12	-3	328	334	7	-7	-3	816	825	13	9	-4	495	481	9
12	-1	340	346	7	-6	-1	520	522	9	9	3	359	365	8
13	-7	104	124	15	-5	-8	101	101	15	10	-5	201	210	9
13	-6	199	212	10	-5	-5	641	663	11	10	-4	320	313	7
13	-5	465	451	9	-5	-2	446	423	8	10	-3	344	348	7
13	-4	210	212	9	-4	-4	381	387	7	10	2	174	174	8
13	3	473	476	9	-3	-4	170	174	6	10	4	280	271	9
14	-6	213	231	10	-2	-8	108	124	15	10	5	259	246	10
14	-2	606	594	11	-2	-6	397	402	8	11	-6	224	207	9
14	1	239	246	7	-2	-1	1416	1456	22	11	5	130	128	15
14	4	132	142	15	-1	-9	113	113	15	12	-7	271	270	9
15	-5	118	146	16	-1	-6	165	156	10	12	-4	171	153	10
15	-2	652	630	12	-1	1	635	621	10	12	-2	400	414	7
15	1	322	315	8	0	-6	665	670	12	12	2	651	658	12
15	3	213	202	10	0	-4	248	237	6	13	-5	115	99	15
15	7	229	220	9	0	2	534	537	9	14	-6	219	227	9
16	-5	130	140	14	1	-7	335	330	8	14	-5	191	186	10
16	-4	259	260	9	1	-1	554	540	9	14	4	121	104	16
16	0	332	337	8	2	-7	570	563	10	15	-6	320	326	9
16	3	200	196	11	2	-3	185	197	6	15	-4	407	393	9
17	-7	132	142	14	2	-2	533	538	9	15	-3	424	423	9
17	-5	209	214	10	2	0	99	111	7	15	0	414	401	8
17	-2	221	229	10	2	8	123	110	14	15	2	233	237	9
18	4	115	121	16	3	-5	239	226	7	16	-5	239	237	9
19	-3	237	218	9	3	-1	592	592	10	16	0	519	500	9
19	-1	202	178	10	3	0	651	660	11	16	1	149	146	12
19	0	125	105	15	3	3	781	761	13	17	0	125	142	15
20	-4	415	415	9	3	8	113	132	14	18	-5	197	193	10
20	-1	195	204	11	4	-5	385	390	7	18	-3	233	237	10
20	2	138	216	18	4	4	144	154	10	19	-6	117	78	14
22	-4	253	246	9	4	8	143	159	12	19	-5	198	178	10
24	0	126	124	15	5	-3	105	116	8	19	-2	321	329	8
25	0	117	122	15	5	0	535	531	9	19	0	270	266	9
					5	3	512	509	9	20	-4	207	182	10

Observed and Calculated Structure Factors for $C_6H_4S_2P^+\ AlCl_4^-$

10|F|o vs 10|F|c for br135

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
20	-2	125	126	14	5	0	529	532	9	-16	-3	332	310	8
20	0	153	175	13	5	4	104	152	10	-15	-3	175	157	10
20	4	176	169	12	6	-8	126	122	14	-14	-6	175	176	10
21	0	149	162	13	6	-4	522	515	9	-14	-4	170	244	9
21	4	135	157	15	6	-3	1046	1040	17	-14	-3	211	209	9
22	1	224	212	10	6	-2	558	552	10	-13	-3	147	151	11
23	-1	252	246	9	6	0	579	571	10	-12	-1	213	201	9
					6	2	696	702	12	-11	-2	103	99	14
^^^^^^^ h = 3 ^^^^^^^					7	-7	159	162	11	-10	-1	363	375	8
					7	-5	224	235	8	-9	-5	240	233	8
-23	-1	116	130	13	7	-4	362	355	7	-9	-1	309	318	7
-21	-2	125	112	13	7	2	121	117	10	-8	-8	173	185	10
-16	-3	241	242	9	8	-7	154	135	11	-8	-1	155	144	9
-15	-3	244	245	8	8	-4	213	212	8	-7	-7	107	110	14
-15	-1	201	206	9	8	3	257	258	8	-7	-4	102	108	14
-14	-5	100	99	15	8	7	119	108	16	-7	-3	182	174	8
-14	-1	506	516	9	9	-8	178	169	11	-7	-1	526	523	9
-13	-7	195	219	10	9	-7	132	149	13	-6	-4	101	70	13
-13	-6	157	175	11	9	-5	107	96	15	-6	-3	108	100	12
-13	-3	122	106	12	9	2	96	75	13	-5	-7	299	303	8
-12	-7	327	343	8	9	6	179	187	12	-4	-1	121	125	9
-12	-1	270	278	7	10	-7	252	251	9	-3	-7	161	171	11
-11	-1	524	523	9	10	4	143	121	14	-3	-2	135	130	8
-9	-3	206	207	7	11	-6	242	231	9	-3	-1	137	141	8
-9	-1	492	494	9	11	-5	241	237	9	-2	-5	149	150	11
-8	-2	529	524	10	11	-3	267	266	7	-2	-2	721	739	12
-7	-3	532	553	10	12	-5	121	126	14	-2	-1	153	163	7
-5	-4	331	328	7	12	-3	299	300	7	-1	-5	143	139	11
-4	-9	128	135	13	12	2	117	80	13	-1	-4	339	319	8
-4	-6	209	203	9	13	-5	315	299	8	-1	-2	277	289	6
-4	-2	602	605	10	13	-4	145	152	12	0	-8	158	138	11
-3	-5	381	368	8	13	2	222	198	9	0	-6	296	298	8
-2	-4	253	258	6	14	-4	240	252	9	0	-4	430	436	8
-1	0	209	204	5	15	0	113	101	15	0	0	122	124	9
-1	3	434	426	8	15	1	341	337	8	0	2	320	327	7
0	-8	362	364	8	16	-2	114	103	14	1	-1	291	290	6
1	-5	213	212	8	16	5	110	96	17	1	0	665	670	11
1	-4	869	819	14	17	-4	268	261	9	1	1	191	203	7
1	-2	81	73	10	17	4	171	181	12	2	0	143	151	8
2	-2	285	285	6	18	-5	321	310	9	2	1	409	424	7
2	-1	174	166	6	19	0	157	168	11	2	3	135	114	11
2	1	94	110	10	20	-5	252	248	9	3	-5	153	139	11
2	3	276	264	7	20	-4	215	206	10	4	-2	454	459	8
2	4	308	287	8						4	3	328	342	8
2	5	184	178	10	^^^^^^^ h = 4 ^^^^^^^					5	-4	413	412	8
3	3	226	217	7						5	-2	204	207	7
4	-3	322	319	7	-19	-3	369	366	8	5	0	336	341	7
4	3	221	212	7	-18	-2	297	292	8	5	1	332	350	7
5	-3	154	166	7	-18	-1	154	127	11	5	2	273	277	8
5	-2	752	745	12	-16	-6	249	248	8	6	-5	134	132	13

Observed and Calculated Structure Factors for $C_6H_4S_2P^+ AlCl_4^-$

10|F|o vs 10|F|c for br135

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
6	-1	270	273	7	5	0	128	135	12	11	-3	153	156	10
6	2	143	160	11	6	-6	129	122	13					
6	6	179	174	10	6	-5	126	145	13	^^^^^^^ h = 7 ^^^^^^^				
7	2	418	427	8	6	-1	318	329	8					
9	-4	464	456	9	6	3	351	336	8	-3	-1	123	137	11
9	-3	122	139	12	6	5	145	151	12	-1	-4	103	112	13
9	-2	146	135	9	7	-4	104	106	14	-1	-1	167	170	9
9	6	130	121	14	7	1	143	126	11	5	-2	145	149	10
10	-5	228	242	9	8	-3	114	108	13					
10	2	103	63	15	8	-1	287	274	8					
11	-6	112	125	14	8	2	338	357	8					
12	-6	167	169	11	8	3	229	225	9					
13	-5	198	175	9	10	-1	166	156	9					
13	5	160	157	12	12	-6	132	98	12					
14	-5	100	77	15	12	2	177	189	9					
14	1	184	196	10	14	3	151	155	12					
15	-5	144	115	12	15	-2	324	337	8					
16	-4	110	119	14	16	-1	114	85	13					
16	2	275	266	9	17	-2	153	146	10					
16	3	173	165	11	17	-1	217	215	8					
16	4	138	136	13										
17	0	188	188	10	^^^^^^^ h = 6 ^^^^^^^									
18	-3	147	107	10										
					-7	-5	233	251	9					
^^^^^^^ h = 5 ^^^^^^^					-7	-4	215	199	9					
					-6	-2	173	160	9					
-13	-2	180	184	10	-3	-2	214	207	8					
-12	-5	126	129	12	-2	-5	101	74	14					
-9	-7	187	173	9	-2	-4	218	224	8					
-8	-4	215	208	8	-2	-3	147	151	10					
-8	-2	280	285	8	-2	-1	176	182	9					
-7	-6	135	128	12	-1	-6	265	250	8					
-7	-2	193	163	9	-1	-4	111	100	13					
-4	-6	125	123	12	-1	-2	435	435	8					
-3	-7	198	190	10	-1	0	149	151	10					
-2	-7	97	89	16	0	-6	188	185	10					
-2	-2	162	160	9	0	-4	286	272	8					
-1	2	227	219	8	2	0	127	135	12					
1	4	197	189	9	2	1	147	159	10					
2	-6	109	115	16	3	-4	171	174	10					
3	-6	229	222	9	3	-3	311	290	8					
3	-5	191	178	10	3	0	125	110	11					
3	-3	139	125	11	4	-3	112	107	13					
3	0	528	524	10	5	-6	234	253	9					
3	5	238	241	9	5	-3	245	266	8					
4	-7	111	130	15	5	-2	241	237	8					
4	-4	367	362	8	6	0	382	392	8					
4	-1	193	191	9	7	1	191	183	9					
5	-6	169	187	11	8	-4	167	168	9					
5	-2	293	297	8	8	-1	202	191	8					

Table . Torsional Angles (degrees) for $C_{13}H_{11}PS_2$

S(1)	-P(1)	-S(2)	-C(2)	24.4 (1)
S(2)	-P(1)	-S(1)	-C(1)	-25.6 (1)
S(1)	-P(1)	-C(7)	-C(8)	-97.5 (3)
S(1)	-P(1)	-C(7)	-C(12)	83.8 (3)
C(7)	-P(1)	-S(1)	-C(1)	80.4 (2)
S(2)	-P(1)	-C(7)	-C(8)	0.5 (3)
S(2)	-P(1)	-C(7)	-C(12)	-178.2 (2)
C(7)	-P(1)	-S(2)	-C(2)	-78.1 (2)
P(1)	-S(1)	-C(1)	-C(2)	21.0 (3)
P(1)	-S(1)	-C(1)	-C(6)	-164.6 (3)
P(1)	-S(2)	-C(2)	-C(1)	-17.2 (3)
P(1)	-S(2)	-C(2)	-C(3)	168.6 (3)
S(1)	-C(1)	-C(2)	-S(2)	-2.7 (3)
S(1)	-C(1)	-C(2)	-C(3)	171.5 (2)
S(1)	-C(1)	-C(6)	-C(5)	-171.6 (3)
C(2)	-C(1)	-C(6)	-C(5)	2.8 (5)
C(6)	-C(1)	-C(2)	-S(2)	-177.3 (2)
C(6)	-C(1)	-C(2)	-C(3)	-3.1 (4)
S(2)	-C(2)	-C(3)	-C(4)	175.7 (2)
C(1)	-C(2)	-C(3)	-C(4)	1.5 (4)
C(2)	-C(3)	-C(4)	-C(13)	-179.6 (3)
C(2)	-C(3)	-C(4)	-C(5)	0.3 (4)
C(3)	-C(4)	-C(5)	-C(6)	-0.6 (5)
C(13)	-C(4)	-C(5)	-C(6)	179.3 (3)
C(4)	-C(5)	-C(6)	-C(1)	-1.0 (5)
P(1)	-C(7)	-C(8)	-C(9)	179.5 (2)
P(1)	-C(7)	-C(12)	-C(11)	-178.8 (3)
C(8)	-C(7)	-C(12)	-C(11)	2.4 (5)
C(12)	-C(7)	-C(8)	-C(9)	-1.9 (4)
C(7)	-C(8)	-C(9)	-C(10)	0.1 (5)
C(8)	-C(9)	-C(10)	-C(11)	1.1 (5)
C(9)	-C(10)	-C(11)	-C(12)	-0.5 (5)
C(10)	-C(11)	-C(12)	-C(7)	-1.3 (5)

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

^^^^^^^ h = -27 ^^^^^^^

k	l	Fo	Fc	sigF
1	6	33	12	8*
3	14	28	31	8*

^^^^^^^ h = -26 ^^^^^^^

k	l	Fo	Fc	sigF
0	18	47	60	10*
1	4	30	7	13*
1	14	60	43	8
1	17	40	25	14*
2	8	48	36	11*
3	14	37	27	14*
3	17	29	2	11*
5	7	7	1	3*

^^^^^^^ h = -25 ^^^^^^^

k	l	Fo	Fc	sigF
0	11	40	26	14*
0	13	43	32	12*
1	11	43	12	13*
1	15	36	53	16*
1	16	41	13	14*
2	6	45	38	10*
2	17	45	15	15*
3	5	49	22	9*
4	1	10	2	3*
4	14	46	30	12*
6	6	2	20	0*

^^^^^^^ h = -24 ^^^^^^^

k	l	Fo	Fc	sigF
0	8	64	72	9
0	16	70	72	8
0	20	36	39	12*
0	22	52	33	8
0	24	14	33	7*
1	7	51	43	11*
2	8	41	52	13*
2	22	34	11	10*
3	10	51	63	12*
3	21	32	6	11*
5	3	29	6	6*

^^^^^^^ h = -23 ^^^^^^^

k	l	Fo	Fc	sigF
0	11	68	50	8
0	15	50	78	12*
1	12	71	68	9
1	14	76	79	9
1	17	48	35	13*
2	14	64	46	9
2	17	49	62	14*
4	10	55	55	11*
4	14	38	52	16*
4	16	54	65	11*
4	18	53	28	13*
5	6	48	43	9*
5	10	43	43	12*

^^^^^^^ h = -22 ^^^^^^^

k	l	Fo	Fc	sigF
0	4	70	83	8
0	8	83	97	7
1	3	44	43	11*
1	11	41	49	14*
1	20	85	80	8
2	18	52	38	13*
3	4	75	74	6
3	12	57	43	10*
3	14	58	67	11*
3	16	63	56	11*
4	7	59	62	9
4	11	36	33	16*
4	17	38	47	16*
5	9	47	53	12*
5	13	44	27	13*
6	19	21	34	7*

^^^^^^^ h = -21 ^^^^^^^

k	l	Fo	Fc	sigF
0	3	63	57	8
0	11	44	48	13*
0	19	80	73	7
1	4	88	97	6
1	8	57	67	10*
1	10	98	106	6
1	11	84	103	7
1	12	78	86	8
2	4	55	42	8
2	12	61	77	10
2	19	69	68	10
3	1	33	50	12*
3	20	49	60	13*
4	6	64	86	9
4	8	86	92	7
4	9	45	24	12*
4	10	39	60	15*
4	11	72	72	8
5	6	41	37	13*
5	14	40	3	14*
5	23	13	5	3*
6	16	35	28	18*
7	1	18	19	7*
7	5	39	35	11*
7	14	40	3	11*
7	17	25	29	7*

^^^^^^^ h = -20 ^^^^^^^

k	l	Fo	Fc	sigF
0	8	152	170	5
0	10	120	117	5
0	12	91	105	7
0	20	70	65	8
1	10	50	52	11*
1	11	77	73	7
1	12	77	83	7
1	14	66	64	9
2	1	49	83	9*
2	2	72	88	6
2	10	42	34	12*
2	14	78	96	8
3	3	45	31	10*
3	4	81	81	6
3	6	77	77	7
3	8	36	7	14*
3	10	82	69	7
3	11	56	55	10*
3	12	87	99	7
4	1	41	46	9*
4	3	37	42	12*
4	5	50	40	9*
4	6	58	67	9
4	14	55	48	11*
5	9	51	62	11*
5	11	37	37	15*
6	20	31	6	12*
7	13	46	34	14*
8	6	32	12	10*

^^^^^^^ h = -19 ^^^^^^^

k	l	Fo	Fc	sigF
0	1	64	86	7
0	3	52	72	9*
0	7	80	92	7
0	25	52	40	8
1	2	105	120	5
1	4	57	67	8
1	10	136	140	5
1	11	65	62	8

k	l	Fo	Fc	sigF
1	12	117	114	5
2	1	57	65	7
2	3	42	59	10*
2	4	56	75	8
2	5	61	64	7
2	11	136	150	5
2	13	120	131	6
3	5	35	39	12*
3	8	54	32	8
3	10	94	100	6
3	12	79	77	7
3	14	127	126	6
4	3	121	137	5
4	4	59	65	9
4	5	118	118	5
4	8	77	71	7
4	23	41	57	11*
5	6	47	38	10*
5	10	51	51	10*
5	12	60	60	9
6	9	45	55	12*
7	9	49	40	11*
7	13	52	60	10*
7	18	45	24	8*
8	9	37	5	15*

^^^^^^^ h = -18 ^^^^^^^

k	l	Fo	Fc	sigF
1	1	55	70	8
1	3	78	96	6
1	4	91	104	5
1	8	162	176	4
1	10	121	120	5
1	12	70	86	8
1	13	98	95	6
2	3	89	106	5
2	4	45	61	10*
2	8	89	102	6
2	14	46	47	12*
3	2	127	144	4
3	4	77	85	6
3	5	94	99	5
3	8	77	86	6
3	9	62	58	7
4	3	83	106	6
4	4	62	79	8
4	5	66	63	7
4	6	41	60	11*
4	23	69	55	10
4	25	39	49	5
5	6	45	36	11*
5	10	66	58	8
5	11	41	31	13*
5	13	51	51	10*
5	14	44	49	12*
6	11	74	78	7
6	13	71	73	8
6	15	55	67	11*
7	12	56	67	10*
7	18	36	14	14*
8	1	31	28	13*
8	9	42	11	11*
8	11	61	41	10
8	12	35	17	17*
8	14	38	9	13*
8	15	45	43	9*
8	17	35	35	6*
9	5	24	33	10*

^^^^^^^ h = -17 ^^^^^^^

k	l	Fo	Fc	sigF
0	3	100	109	5
0	5	193	214	4
0	9	76	66	6
0	11	99	89	6
0	13	89	92	7
0	23	88	111	7
0	25	68	84	8
1	2	186	204	4
1	4	182	181	4
1	7	196	208	4
1	8	110	123	5
1	9	103	111	5
1	10	116	129	5
1	11	127	135	5
1	12	133	137	5
1	13	71	68	7
1	14	73	80	7
1	24	68	60	9
2	1	68	85	6
2	3	106	115	4
2	4	86	97	5
2	5	63	72	7
2	8	183	192	4
2	10	64	53	7
2	11	84	88	6
2	13	133	133	5
2	14	101	109	6
3	1	73	85	5
3	3	87	97	5
3	4	43	34	9*
3	5	126	125	4
3	6	56	54	8
3	8	32	52	14*
3	9	72	76	7
3	10	62	61	7
3	12	84	79	6
3	14	159	158	5
4	1	72	78	6
4	2	43	47	9*
4	6	31	11	13*
4	9	57	69	8
4	11	101	107	5
4	12	105	109	5
4	14	70	75	8
4	20	58	64	10*
5	5	84	77	6
5	6	105	95	5
5	8	70	78	7
5	9	67	66	7
6	1	79	90	6
6	6	74	74	7
6	8	78	84	7
6	10	94	99	6
6	11	44	43	12*
6	12	69	67	8
7	5	71	72	8
7	7	65	60	8
8	6	48	33	11*
8	12	52	52	9*
8	16	55	38	8
9	2	26	7	11*

^^^^^^^ h = -16 ^^^^^^^

k	l	Fo	Fc	sigF
0	2	146	147	4
0	4	96	96	5
0	6	105	112	5
0	12	261	254	5
0	14	148	169	5
1	1	79	73	5
1	2	248	250	4
1	3	70	65	6
1	5	199	202	4
1	8	73	74	6
1	9	113	120	4
1	11	84	91	6
2	3	122	122	4
2	4	104	84	4
2	6	220	213	4

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF
2	7	189	185	4
2	8	150	145	4
2	9	52	62	8
2	10	124	120	4
2	12	50	43	9*
2	13	134	134	4
2	14	52	52	10*
3	5	163	172	4
3	6	53	70	7
3	7	167	157	4
3	8	155	147	4
3	9	96	102	5
3	10	153	154	4
4	2	72	74	6
4	3	29	19	13*
4	5	53	51	8
4	8	32	21	13*
4	11	67	70	7
5	2	53	54	8
5	3	71	63	6
5	5	53	37	8
5	8	55	45	8
5	9	163	151	4
5	11	99	91	5
5	12	67	66	7
5	13	86	93	6
5	15	65	86	9
5	19	39	53	14*
6	1	91	92	5
6	2	67	76	7
6	8	82	80	6
6	12	47	57	10*
7	4	67	45	7
7	6	67	73	8
7	14	68	64	8
8	9	86	89	7
8	11	51	34	10*
8	16	37	38	14*
9	5	53	47	12*
10	1	2	16	1*
10	12	5	25	1*

^^^^^^^ h = -15 ^^^^^^^

k	l	Fo	Fc	sigF
0	3	161	160	4
0	5	182	186	4
0	9	157	158	4
0	11	158	144	4
0	13	360	350	6
0	25	50	30	11*
1	2	217	221	4
1	3	85	83	5
1	4	65	59	6
1	8	197	200	4
1	9	110	111	4
1	10	123	119	4
1	11	122	129	4
1	12	155	158	4
1	13	165	170	4
1	14	125	117	5
2	1	181	181	4
2	2	74	69	5
2	3	176	178	4
2	4	173	153	4
2	5	218	213	4
2	6	101	95	4
2	7	208	199	4
2	9	143	139	4
2	10	85	70	5
2	12	54	66	8
2	23	75	58	9
3	2	117	112	4
3	3	90	93	4
3	4	166	164	4
3	6	168	158	4
3	8	147	137	4
3	10	62	55	7
3	11	136	122	4
3	23	38	11	17*
4	2	88	89	5
4	6	74	70	5
4	9	70	68	6
4	11	83	104	6
4	14	85	86	6
4	24	41	1	12*
5	1	37	46	11*
5	5	52	38	8
5	6	72	61	6
5	9	49	58	9*
5	10	51	51	9*
5	11	72	80	7
5	12	151	151	4
5	13	40	20	12*
5	14	118	117	5
5	15	68	56	8
6	2	102	112	5
6	6	84	85	6
6	8	131	132	4
6	9	53	69	9*
6	10	106	106	5
6	11	57	55	8
6	12	76	77	7
6	15	54	49	9
7	5	85	78	6
7	6	88	75	6
7	7	59	60	9
7	8	53	53	10*
7	9	71	64	7
7	10	51	38	9*
8	8	58	53	9
8	10	48	52	11*
8	17	38	0	13*
8	20	16	42	7*
9	6	40	41	13*
9	14	34	1	11*

^^^^^^^ h = -14 ^^^^^^^

k	l	Fo	Fc	sigF
0	2	112	108	4
0	4	586	575	9
0	6	72	76	6
0	8	68	66	6
0	14	120	124	5
1	1	214	218	4
1	2	121	130	4
1	3	39	32	9*
1	4	195	196	4
1	5	98	96	4
1	6	34	36	10*
1	7	101	103	4
1	8	82	84	5
1	9	120	119	4
1	10	42	72	9*
1	11	172	182	4
1	12	171	176	4
1	14	151	150	4
1	15	73	71	7
2	2	89	90	4
2	3	221	208	4
2	4	68	51	5
2	5	318	298	5
2	6	90	80	4
2	7	235	225	4
2	8	86	84	4
2	9	102	98	4
2	12	101	109	5
2	23	77	79	9
3	1	71	68	5
3	3	51	61	7
3	6	75	64	5

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
3	7	110	104	4	0	5	465	459	8	4	12	100	94	5
3	8	166	158	4	0	7	496	483	8	4	14	58	45	8
3	10	269	254	5	0	9	283	268	5	5	1	77	73	5
3	11	61	49	7	0	11	351	334	6	5	2	96	98	5
3	12	100	105	5	0	13	314	300	5	5	3	65	88	6
3	13	101	104	5	0	15	377	378	6	5	4	153	161	4
3	23	51	38	12*	1	1	248	249	4	5	6	71	71	6
4	2	58	60	6	1	3	274	277	5	5	7	103	96	4
4	5	97	94	4	1	4	135	133	3	5	9	78	80	5
4	8	125	114	4	1	5	119	126	3	5	10	54	59	7
4	9	165	146	4	1	6	139	133	3	5	12	125	130	4
4	10	172	167	4	1	7	57	42	6	5	13	67	69	7
4	11	199	198	4	1	10	170	180	4	5	14	143	154	4
4	12	77	82	6	1	11	123	130	4	5	15	38	59	13*
5	1	176	174	4	1	12	113	110	4	6	2	188	184	4
5	2	92	97	5	1	13	61	62	7	6	3	73	82	6
5	3	133	131	4	1	14	104	106	5	6	5	123	121	4
5	4	56	64	8	1	15	109	115	5	6	8	72	79	6
5	11	97	86	5	1	16	93	90	6	6	10	35	42	11*
5	12	47	40	10*	2	1	162	153	3	6	20	52	58	11*
5	14	49	41	10*	2	2	82	76	4	7	8	83	89	6
5	15	39	9	12*	2	3	261	250	4	7	10	58	52	8
6	1	109	116	5	2	5	173	161	3	7	12	40	12	11*
6	3	75	68	6	2	7	154	150	3	8	5	58	42	9
6	6	77	68	6	2	8	66	59	5	8	7	56	49	8
6	8	80	84	6	2	9	105	104	4	8	10	86	87	6
6	11	60	61	7	2	10	117	113	4	8	12	69	67	6
7	4	63	66	8	2	12	179	186	4	9	14	34	26	13*
7	6	85	78	6	2	13	153	152	4	11	6	6	20	2*
7	8	94	99	5	2	14	69	73	7					
7	9	69	56	7	2	25	49	71	13*	^^^^^^^ h = -12 ^^^^^^^				
7	14	87	93	6	3	1	109	103	4					
7	18	33	29	14*	3	2	211	210	4	0	2	253	252	4
7	19	43	38	11*	3	3	83	79	4	0	4	341	341	6
8	6	33	12	15*	3	4	107	104	4	0	6	328	340	6
8	8	63	55	8	3	5	89	78	4	0	8	185	176	4
8	10	36	34	12*	3	6	172	161	3	0	10	118	110	4
8	16	42	21	10*	3	7	195	181	4	0	12	122	122	4
8	18	34	44	14*	3	9	376	346	6	0	14	166	166	4
9	10	32	20	13*	3	10	131	136	4	0	24	67	87	9
9	12	30	59	12*	3	11	251	242	4	1	2	123	121	3
9	14	31	54	14*	3	12	107	111	4	1	3	96	90	4
10	2	35	38	11*	4	1	104	96	4	1	4	242	245	4
10	3	31	16	14*	4	2	166	170	4	1	5	259	263	4
10	8	35	34	10*	4	4	177	170	4	1	6	207	211	4
					4	6	136	127	4	1	7	275	289	5
^^^^^^^ h = -13 ^^^^^^^					4	7	60	66	6	1	9	307	322	5
					4	8	150	129	4	1	10	114	125	4
0	1	125	128	4	4	9	102	92	4	1	11	202	209	4
0	3	243	251	4	4	10	121	124	4	1	15	83	86	6

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
1	16	61	56	8	6	11	69	73	6	2	15	188	183	4
2	2	112	115	3	6	21	56	62	10*	3	1	350	323	6
2	3	111	105	3	7	2	99	91	5	3	2	95	91	4
2	4	65	61	5	7	4	120	117	5	3	3	72	68	4
2	5	145	141	3	7	6	105	108	5	3	4	117	122	3
2	6	112	107	3	7	9	76	78	5	3	5	310	299	5
2	7	117	125	3	7	10	68	75	6	3	7	351	329	6
2	9	151	146	3	7	11	103	108	5	3	8	58	57	5
2	10	126	117	4	7	13	87	84	6	3	9	191	178	4
2	11	71	71	5	7	20	38	58	13*	3	10	199	196	4
2	12	42	45	10*	7	22	28	46	13*	3	11	173	167	4
2	13	250	262	4	8	10	77	76	6	3	12	123	126	4
2	14	232	243	4	8	12	67	56	7	3	13	153	152	4
2	15	109	123	5	9	6	65	71	8	3	14	235	235	4
3	1	174	169	4	9	10	35	33	11*	3	25	65	63	9
3	3	101	94	4	9	18	32	15	5	4	2	56	50	6
3	5	134	127	3	11	6	14	25	5*	4	4	68	76	5
3	7	32	14	9*						4	5	91	86	4
3	9	103	94	4	^^^^^^^		h = -11		^^^^^^^	4	6	112	102	3
3	10	113	117	4						4	7	204	188	4
3	11	53	54	7	0	1	648	655	10	4	8	86	72	4
3	13	148	145	4	0	3	575	583	9	4	10	92	82	4
3	14	74	102	7	0	5	479	487	8	4	11	77	72	5
4	1	161	153	4	0	7	455	442	8	4	12	107	119	4
4	2	124	123	4	0	9	352	336	6	4	14	188	182	4
4	3	229	232	4	0	11	185	182	4	5	2	78	93	5
4	4	74	72	5	0	13	165	157	4	5	4	382	390	6
4	5	252	241	4	0	15	89	87	5	5	5	60	77	6
4	6	120	103	3	0	17	64	90	8	5	6	388	355	7
4	7	99	83	4	1	1	129	127	3	5	7	98	91	4
4	8	257	233	4	1	2	157	159	3	5	8	143	131	3
4	9	36	41	10*	1	3	114	117	3	5	9	145	141	3
4	10	125	118	4	1	4	113	115	3	5	11	65	68	6
4	11	132	125	4	1	5	79	75	4	5	12	77	69	6
4	12	111	112	4	1	7	144	149	3	6	1	111	111	5
4	13	228	235	4	1	8	239	250	4	6	2	100	84	5
4	24	45	40	13*	1	9	200	208	4	6	3	96	86	5
4	26	31	55	10*	1	10	99	97	4	6	5	67	75	6
5	1	201	190	4	1	11	132	137	4	6	8	79	85	5
5	2	106	121	4	1	13	199	203	4	6	9	31	22	11*
5	3	197	199	4	1	15	121	111	5	6	10	113	111	4
5	4	75	92	5	1	16	101	126	6	6	11	72	64	6
5	5	151	140	4	2	2	58	49	5	6	13	51	47	9*
5	10	99	96	4	2	3	201	191	3	6	14	92	84	5
5	12	135	130	4	2	8	78	76	4	6	21	51	59	11*
5	14	80	84	6	2	9	181	181	3	6	25	16	18	5*
5	15	95	98	5	2	10	132	141	3	7	2	96	85	6
6	8	59	62	6	2	11	117	116	4	7	5	29	14	13*
6	9	45	53	9*	2	12	140	149	4	7	15	76	67	7
6	10	80	82	5	2	13	301	300	5	8	2	61	51	9

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
8	5	60	53	7	3	8	158	157	3	8	9	53	66	7
8	6	72	69	6	3	9	180	173	3	9	2	70	61	9
8	8	103	103	4	3	10	40	46	8*	9	4	74	83	7
8	10	98	107	5	3	11	64	70	6	10	8	54	57	6
8	13	37	1	10*	3	12	173	178	4	11	2	34	7	11*
8	16	47	36	10*	3	14	118	126	5	11	10	13	10	4*
9	8	32	37	12*	3	15	131	137	5					
10	1	59	26	14*	4	1	267	249	4	^^^^^^^ h = -9 ^^^^^^^				
11	7	17	15	7*	4	3	368	362	6					
11	9	13	4	4*	4	4	158	161	3	0	1	272	283	5
					4	5	485	428	8	0	3	484	505	8
^^^^^^^ h = -10 ^^^^^^^					4	6	91	78	4	0	5	825	789	13
					4	7	336	314	6	0	7	296	281	5
0	4	136	138	3	4	8	45	52	7	0	11	87	83	4
0	6	179	160	3	4	10	121	120	4	0	13	168	165	4
0	8	56	48	6	4	11	54	49	7	0	15	48	53	9*
0	10	87	86	4	4	13	59	36	7	0	17	59	61	8
0	12	172	177	4	4	14	128	123	4	1	2	65	55	4
0	24	88	97	7	5	1	89	82	4	1	3	166	180	3
0	26	57	95	9	5	2	150	164	4	1	4	199	203	3
1	1	254	254	4	5	3	64	60	5	1	5	305	327	5
1	2	298	298	5	5	4	145	153	3	1	6	205	221	3
1	3	153	151	3	5	6	110	101	3	1	7	291	313	5
1	4	187	198	3	5	7	247	224	4	1	8	184	196	3
1	5	280	284	5	5	8	70	67	5	1	9	368	391	6
1	6	399	425	7	5	9	134	129	4	1	10	154	158	3
1	7	480	503	8	5	12	145	142	4	1	11	406	407	7
1	8	286	299	5	5	13	40	54	12*	1	12	66	70	6
1	9	352	383	6	5	14	155	149	4	1	14	98	98	5
1	11	107	129	4	5	15	84	66	6	1	15	70	76	7
1	12	44	42	9*	6	2	50	49	7	2	1	139	130	3
1	14	155	145	4	6	5	86	76	4	2	2	87	91	3
1	15	180	179	4	6	6	106	108	4	2	3	211	214	4
1	16	147	152	4	6	7	106	105	4	2	4	185	171	3
1	17	144	155	5	6	8	98	102	4	2	5	234	220	4
1	25	50	84	13*	6	10	67	75	6	2	6	79	79	3
2	1	179	163	3	6	11	86	85	5	2	7	51	58	5
2	3	131	128	3	6	13	145	151	4	2	10	376	377	6
2	5	114	118	3	6	15	139	126	4	2	11	232	228	4
2	6	179	185	3	6	23	32	23	14*	2	12	178	169	4
2	7	91	96	3	7	1	94	71	6	2	13	280	273	5
2	8	314	318	5	7	2	102	101	5	2	15	252	242	5
2	9	229	223	4	7	3	54	51	8	3	1	276	245	5
2	11	282	272	5	7	4	87	94	5	3	2	95	115	3
2	13	165	154	4	7	6	44	47	8*	3	3	154	153	3
2	15	197	193	4	7	10	95	91	5	3	4	223	217	4
2	16	93	98	6	7	12	150	144	4	3	7	160	156	3
3	1	120	123	3	7	13	31	35	15*	3	8	82	78	4
3	5	124	119	3	7	14	97	98	5	3	9	226	215	4
3	6	282	261	5	8	4	30	6	14*	3	10	229	233	4

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
3	11	135	130	4	8	2	92	88	6	2	10	620	624	10
3	12	186	175	4	8	3	38	19	11*	2	11	152	152	4
3	13	176	179	4	8	6	91	96	4	2	12	133	144	4
3	14	238	243	4	8	8	57	58	7	2	13	151	149	4
3	15	193	196	4	8	9	51	37	7	2	14	80	85	6
3	16	145	150	5	8	15	43	12	11*	2	15	122	132	5
4	2	174	192	3	8	16	42	59	12*	3	1	100	85	3
4	3	49	55	5	8	18	50	63	10*	3	3	87	86	3
4	4	58	52	4	9	1	64	47	10	3	4	53	54	4
4	5	72	76	4	9	2	105	87	6	3	5	300	267	5
4	6	304	262	5	9	5	36	29	10*	3	7	343	329	6
4	7	160	152	3	9	10	59	48	6	3	8	175	170	3
4	8	124	107	3	9	12	35	59	13*	3	9	329	328	5
4	9	203	203	4	9	13	31	30	13*	3	10	136	139	4
4	11	39	40	10*	9	14	45	24	9*	3	11	199	195	4
4	12	37	51	11*	11	9	22	29	6*	3	13	82	88	6
4	13	58	71	8						3	14	66	48	8
5	1	134	131	4	^^^^^^^	h =	-8	^^^^^^^		3	16	124	133	5
5	2	242	270	4						4	1	59	61	5
5	3	68	73	5	0	2	280	308	5	4	2	147	166	3
5	4	229	232	4	0	4	440	452	7	4	3	276	286	5
5	5	82	77	4	0	6	381	369	6	4	5	141	123	3
5	6	220	203	4	0	8	225	224	4	4	6	533	488	8
5	7	74	66	4	0	10	114	106	3	4	7	163	150	3
5	8	88	98	4	0	12	98	104	4	4	8	101	101	4
5	9	120	113	4	0	14	72	78	5	4	9	57	60	6
5	11	115	119	4	0	16	194	204	4	4	10	87	93	5
5	13	39	43	12*	1	1	326	309	5	4	11	139	143	4
5	24	68	51	10	1	3	338	317	5	4	12	121	126	4
5	25	35	14	12*	1	4	28	40	6*	4	13	105	106	5
6	3	109	111	4	1	5	121	131	2	4	14	124	128	5
6	4	131	132	3	1	6	104	110	3	4	25	40	53	13*
6	5	55	49	5	1	7	218	232	4	5	1	144	141	3
6	6	242	230	4	1	8	167	174	3	5	3	250	261	4
6	8	242	260	4	1	9	375	386	6	5	4	229	224	4
6	9	91	92	4	1	10	164	163	3	5	5	190	166	3
6	10	125	119	4	1	11	67	76	5	5	6	182	157	3
6	11	124	118	4	1	15	226	215	4	5	7	140	119	3
6	12	59	52	7	1	16	201	201	4	5	8	78	77	5
6	13	53	64	9*	1	17	217	218	5	5	9	215	229	4
7	2	56	25	8	1	25	45	35	14*	5	11	112	112	4
7	3	66	59	6	2	1	602	532	9	5	14	123	123	5
7	4	63	60	6	2	2	435	416	7	5	15	74	69	7
7	6	47	52	7	2	3	399	398	6	5	24	41	39	17*
7	7	61	62	5	2	4	221	212	4	6	2	47	36	7
7	8	51	53	7	2	5	197	196	3	6	3	79	89	4
7	10	48	46	8*	2	6	177	187	3	6	4	91	90	4
7	13	58	52	8	2	7	185	181	3	6	5	108	108	3
7	18	38	46	15*	2	8	348	353	6	6	6	115	116	3
7	19	42	40	13*	2	9	266	273	4	6	7	109	110	4

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF
6	8	87	93	4
6	12	72	60	6
6	13	80	72	6
6	14	116	107	5
6	15	93	98	6
7	2	220	209	4
7	4	106	105	4
7	5	40	42	8*
7	6	50	60	6
7	7	49	43	7
7	8	46	46	8*
7	9	88	82	5
7	10	109	109	4
7	11	76	65	6
7	12	183	174	4
7	13	67	61	8
7	14	41	57	12*
8	3	54	68	8
8	6	39	30	8*
8	7	50	63	7
9	4	52	58	7
9	5	44	34	8*
9	10	61	53	6
9	12	45	48	10*
9	13	38	51	12*
9	18	26	37	12*
10	8	63	81	5

^^^^^^^ h = -7 ^^^^^^^

k	l	Fo	Fc	sigF
0	1	218	227	4
0	3	339	354	6
0	5	111	104	3
0	7	126	121	3
0	9	377	368	6
0	11	556	559	9
0	13	281	283	5
0	15	88	86	5
1	1	56	41	3
1	2	57	63	3
1	3	186	187	3
1	4	143	150	3
1	5	43	53	3
1	6	346	357	6
1	7	533	565	8
1	8	129	140	3
1	9	277	281	5
1	11	127	139	4
1	12	59	52	7
1	13	123	115	4
1	14	171	162	4
1	15	136	137	5
1	16	99	87	6
1	17	98	95	6
2	1	351	339	6
2	2	181	177	3
2	3	485	467	7
2	4	248	244	4
2	5	643	636	10
2	6	87	78	3
2	8	182	180	3
2	9	117	130	3
2	11	49	51	8
2	12	408	412	7
2	14	237	243	4
2	15	115	113	5
2	16	152	150	5
3	1	210	206	4
3	2	365	390	6
3	3	30	15	6*
3	4	280	275	5
3	5	348	329	6
3	6	250	250	4
3	7	238	231	4
3	8	111	101	3
3	9	116	113	4
3	10	142	149	4
3	11	65	65	6
3	14	50	61	10*
3	15	174	162	4
3	23	69	49	10
4	1	220	213	4
4	2	217	240	4
4	3	231	230	4
4	4	185	176	3
4	5	48	37	5
4	7	192	187	3
4	8	121	122	3
4	9	223	232	4
4	10	37	63	11*
4	13	58	53	8
5	3	118	118	3
5	4	111	113	3
5	5	123	111	3
5	7	96	99	4
5	8	113	111	4
5	9	190	190	4
5	10	229	219	4
5	11	49	53	9*
5	12	163	167	4
5	14	51	52	10*
6	1	184	184	4
6	3	122	123	3
6	4	131	128	3
6	6	163	169	3
6	7	73	74	5
6	8	254	272	4
6	9	90	97	5
6	10	227	219	4
6	11	88	75	5
6	12	94	81	5
7	1	83	78	6
7	2	120	115	4
7	3	65	75	5
7	4	78	90	4
7	5	82	89	4
7	9	109	109	4
7	11	170	176	4
7	12	58	52	8
7	13	84	85	6
8	1	82	70	6
8	4	52	58	6
8	6	43	45	7*
8	14	82	85	7
9	2	96	93	6
9	4	73	77	5
9	5	57	68	6
9	7	64	62	5
10	11	33	17	10*
10	15	29	25	9*
11	2	47	36	11*
11	10	29	41	6*
12	3	3	10	1*

^^^^^^^ h = -6 ^^^^^^^

k	l	Fo	Fc	sigF
0	2	389	405	6
0	4	287	282	5
0	6	55	40	4
0	8	140	135	3
0	10	297	293	5
0	12	146	146	3
0	14	100	111	4
0	16	101	101	5
0	24	78	99	8
1	1	556	500	9
1	2	509	504	8
1	3	183	192	3
1	4	302	322	5
1	5	488	504	8

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
1	6	506	541	8	4	9	179	172	4	10	17	6	8	2*
1	7	543	554	8	4	10	95	97	5	11	5	27	39	10*
1	8	481	499	8	4	11	377	384	6					
1	9	144	148	3	4	12	95	101	6	^^^^^^^ h = -5 ^^^^^^^				
1	10	180	195	4	4	13	217	219	4					
1	11	115	109	4	4	14	99	90	6	0	1	144	154	3
1	12	196	187	4	5	2	39	48	6	0	3	135	133	3
1	13	103	101	5	5	3	35	33	6	0	5	196	198	3
1	14	65	77	8	5	4	199	188	3	0	7	82	60	3
1	15	129	123	5	5	5	188	174	3	0	9	282	295	5
1	16	97	110	6	5	6	129	130	3	0	11	499	495	8
1	17	152	151	5	5	7	36	27	9*	0	13	438	444	7
1	24	55	69	12*	5	8	100	94	4	0	15	290	290	5
2	1	617	576	9	5	11	62	76	7	0	17	55	40	8
2	2	612	605	9	5	13	52	58	10*	1	1	386	373	6
2	3	634	615	10	5	14	51	32	10*	1	2	98	102	2
2	4	38	23	4	6	1	153	157	4	1	3	107	106	2
2	5	85	95	2	6	2	104	120	3	1	4	144	143	2
2	6	313	298	5	6	3	189	186	3	1	5	88	96	2
2	7	335	328	6	6	4	177	172	3	1	6	700	733	11
2	8	163	167	3	6	5	221	224	4	1	7	574	574	9
2	9	181	181	3	6	6	112	101	3	1	8	345	337	6
2	10	377	388	6	6	7	188	199	4	1	10	87	85	4
2	11	199	202	4	6	9	167	178	4	1	11	56	72	7
2	12	235	236	4	6	11	172	149	4	1	12	261	258	4
2	13	100	100	5	6	12	83	78	7	1	13	79	87	6
2	15	183	190	4	6	14	77	65	7	1	14	295	283	5
2	16	86	101	7	6	15	40	44	14*	1	15	218	213	4
3	1	232	230	4	7	2	247	260	4	1	16	275	266	5
3	2	267	283	4	7	4	165	174	3	2	1	388	374	6
3	3	66	65	3	7	5	69	82	5	2	2	585	585	9
3	4	39	33	4	7	8	62	68	6	2	3	184	199	3
3	5	62	59	3	7	10	58	42	7	2	4	454	437	7
3	6	158	159	3	7	14	58	67	9	2	5	293	298	5
3	7	270	259	5	8	1	114	109	5	2	6	458	464	7
3	8	296	290	5	8	4	44	62	7	2	7	335	347	6
3	9	297	310	5	8	7	40	38	9*	2	10	185	184	4
3	10	118	117	4	8	13	97	97	6	2	11	73	81	6
3	11	296	294	5	8	15	114	116	6	2	12	206	207	4
3	12	326	332	5	8	17	79	65	7	2	13	140	137	4
3	13	92	83	6	9	1	45	32	12*	2	14	121	121	5
3	14	162	164	4	9	3	63	66	5	2	16	51	58	11*
3	16	148	144	5	9	5	77	83	5	2	23	55	51	13*
4	2	252	289	4	9	8	66	63	6	2	25	64	67	10
4	3	52	47	4	9	9	29	19	14*	3	1	281	269	5
4	4	253	236	4	9	10	66	72	7	3	2	221	243	4
4	5	47	43	5	9	12	45	60	11*	3	3	257	248	4
4	6	198	194	3	9	14	56	64	9	3	4	301	283	5
4	7	126	116	3	9	19	20	13	6*	3	5	367	371	6
4	8	327	322	5	10	12	38	12	9*	3	6	196	186	3

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
3	7	400	399	7	8	2	71	79	4	2	11	94	99	5
3	9	131	137	4	8	4	114	127	3	2	13	57	63	9
3	10	121	125	4	8	6	138	131	4	2	14	128	134	5
3	11	100	101	5	8	8	76	86	6	2	15	77	89	7
3	12	103	113	5	8	12	48	29	10*	2	16	122	114	5
3	13	75	79	7	8	13	63	48	9	2	25	53	33	11*
3	14	151	146	4	8	14	39	5	14*	3	1	500	534	8
3	25	37	8	14*	8	15	50	57	12*	3	2	132	130	2
4	1	367	386	6	8	21	19	17	7*	3	3	545	538	8
4	2	53	58	4	9	2	81	90	4	3	4	448	442	7
4	3	170	163	3	9	4	63	71	5	3	5	301	282	5
4	4	82	74	3	9	8	50	55	8	3	6	243	241	4
4	5	49	51	5	9	10	40	35	11*	3	7	90	77	4
4	6	197	201	4	9	19	15	25	6*	3	8	250	252	4
4	7	58	47	6	10	9	51	57	8	3	9	130	129	4
4	8	217	212	4	10	17	4	22	2*	3	10	217	221	4
4	9	139	137	4						3	11	211	217	4
4	10	226	226	4	^^^^^^^	h =	-4	^^^^^^^		3	12	140	141	4
4	12	246	240	4						3	14	332	342	6
4	13	88	99	6	0	2	567	586	9	3	23	48	29	15*
4	14	98	104	6	0	4	772	754	12	4	1	237	272	4
5	1	246	258	4	0	6	524	528	8	4	2	85	88	2
5	2	75	90	3	0	8	739	731	11	4	3	111	108	3
5	4	39	36	6	0	10	463	474	7	4	4	314	325	5
5	6	283	281	5	0	12	585	589	9	4	5	87	86	4
5	7	53	50	7	0	14	299	297	5	4	6	315	307	5
5	8	297	297	5	1	1	135	133	2	4	8	218	214	4
5	9	105	109	4	1	2	247	257	4	4	9	85	87	5
5	10	186	182	4	1	3	448	465	7	4	10	90	104	5
5	11	198	196	4	1	4	647	671	10	4	11	87	87	6
5	12	195	185	4	1	5	549	570	8	4	12	75	91	7
6	1	191	199	3	1	6	108	118	3	4	13	213	230	5
6	2	118	134	3	1	7	477	465	7	4	14	65	50	9
6	4	64	55	4	1	8	234	244	4	5	1	80	81	3
6	7	56	70	7	1	9	185	185	3	5	2	139	142	3
6	8	68	64	6	1	10	142	144	3	5	3	71	65	3
6	14	82	73	7	1	11	154	156	4	5	4	73	78	4
6	24	22	8	6*	1	12	212	215	4	5	5	104	103	4
7	1	130	133	4	1	16	84	76	7	5	6	165	168	4
7	2	63	79	4	1	17	44	43	13*	5	7	237	243	4
7	3	253	259	4	1	24	70	63	9	5	9	296	302	5
7	4	61	63	5	2	1	292	287	5	5	11	266	268	5
7	5	100	124	4	2	2	747	712	11	5	13	225	207	5
7	6	31	35	11*	2	3	511	470	8	5	14	110	104	6
7	7	34	37	11*	2	4	512	519	8	6	2	125	130	3
7	9	149	140	4	2	5	89	96	3	6	3	130	128	3
7	10	47	48	9*	2	6	239	241	4	6	4	187	205	3
7	12	72	68	7	2	7	430	413	7	6	5	196	199	4
7	13	110	108	5	2	8	197	186	4	6	6	84	66	5
7	14	114	98	6	2	10	208	209	4	6	7	144	149	4

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF
6	8	67	72	6
6	9	70	59	6
6	10	59	59	8
6	11	36	5	12*
6	12	79	67	7
6	14	81	71	7
6	23	40	57	12*
7	1	86	89	4
7	2	107	118	3
7	3	80	89	4
7	4	65	81	5
7	5	124	131	4
7	7	78	71	5
7	9	42	40	10*
7	10	99	88	5
7	11	47	32	10*
7	13	72	70	8
7	17	67	45	9
7	22	32	34	9*
8	4	59	59	6
8	5	146	148	4
8	6	65	56	6
8	7	197	185	4
8	8	42	28	10*
8	9	101	89	5
8	11	99	93	5
8	13	59	69	10
8	15	62	64	10
9	1	76	89	5
9	3	89	103	4
9	5	85	85	5
9	10	66	64	7
9	12	54	50	9*
9	16	47	23	14*
11	9	34	15	8*
11	13	7	16	2*

^^^^^^^ h = -3 ^^^^^^^

k	l	Fo	Fc	sigF
0	1	76	76	2
0	3	1339	1359	21
0	5	61	50	3
0	7	119	126	2
0	9	119	116	3
0	11	84	78	4
0	13	67	71	6
0	17	48	24	9*
1	1	167	160	3
1	2	311	317	5
1	3	651	688	10
1	4	929	942	14
1	5	60	62	3
1	6	387	403	6
1	7	88	96	3
1	8	424	437	7
1	9	238	237	4
1	10	80	71	5
1	11	313	315	5
1	12	148	149	4
1	13	281	274	5
1	14	224	217	4
1	15	141	128	4
1	16	211	201	5
2	1	79	81	2
2	2	433	421	7
2	3	155	156	3
2	4	675	685	10
2	5	232	218	4
2	6	43	47	5
2	8	145	151	3
2	9	242	247	4
2	10	272	280	5
2	11	93	97	5
2	12	110	110	5
2	13	98	107	6
2	15	52	11	11*
2	16	78	80	8
3	1	213	211	4
3	2	30	29	4
3	3	595	608	9
3	4	204	181	3
3	5	121	122	3
3	6	79	64	4
3	7	216	216	4
3	8	207	207	4
3	9	291	301	5
3	10	79	75	5
3	12	127	128	4
3	15	138	148	5
4	1	24	35	7*
4	2	167	163	3
4	5	323	310	5
4	6	181	183	3
4	7	281	286	5
4	8	465	461	8
4	9	106	112	4
4	10	341	336	6
4	12	206	220	4
4	13	136	139	5
4	14	172	179	5
5	1	270	285	5
5	2	76	69	3
5	3	178	177	3
5	7	115	118	4
5	9	87	92	5
5	11	92	92	6
5	13	137	129	5
6	1	121	122	3
6	2	137	135	3
6	3	56	57	5
6	4	79	89	5
6	5	44	73	8*
6	6	41	64	10*
6	7	197	212	4
6	8	89	90	5
6	13	64	58	8
6	15	57	62	10*
7	1	203	209	3
7	2	100	107	3
7	3	146	173	3
7	4	127	139	4
7	5	100	115	4
7	6	113	120	4
7	8	83	70	5
7	9	122	106	4
7	10	42	53	11*
7	11	149	145	4
7	17	91	81	8
7	19	51	54	13*
8	1	55	66	5
8	2	117	136	3
8	3	42	46	8*
8	4	128	130	4
8	5	81	81	5
8	6	117	113	4
8	7	102	94	5
8	15	52	54	12*
9	4	31	39	11*
9	11	68	70	8
10	9	34	21	11*

^^^^^^^ h = -2 ^^^^^^^

k	l	Fo	Fc	sigF
0	2	457	458	7
0	4	951	979	14
0	6	393	396	6
0	8	1079	1081	16
0	10	681	677	11
0	12	286	284	5
0	14	217	213	4

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
1	1	602	545	9	4	8	115	106	4					
1	2	220	223	4	4	9	167	175	4	0	3	588	586	9
1	3	386	397	6	4	11	71	77	7	0	5	461	483	7
1	4	371	378	6	4	14	50	61	12*	0	7	50	58	4
1	5	295	313	5	5	1	430	407	7	0	9	510	492	8
1	6	114	114	3	5	2	161	163	3	0	11	231	227	4
1	7	256	270	4	5	3	206	196	4	0	13	165	157	4
1	8	131	137	3	5	4	133	127	3	0	15	105	105	5
1	9	335	335	6	5	5	138	141	4	0	23	70	77	8
1	10	231	229	4	5	6	134	135	4	1	1	814	762	12
1	11	85	93	5	5	7	156	151	4	1	2	138	131	2
1	12	243	233	4	5	8	85	72	5	1	3	713	708	11
1	13	140	133	4	5	9	243	246	4	1	4	748	787	11
1	14	127	115	5	5	10	115	123	5	1	5	67	82	4
1	16	216	212	5	5	11	179	178	4	1	6	434	467	7
2	2	675	654	10	5	12	99	95	6	1	7	65	60	4
2	3	549	513	8	5	13	134	125	5	1	8	385	404	6
2	4	81	91	3	5	14	135	124	5	1	11	252	249	4
2	5	165	172	3	6	2	68	60	4	1	12	146	147	4
2	7	233	245	4	6	3	71	74	5	1	14	160	164	4
2	8	215	217	4	6	4	238	249	4	1	15	60	68	9
2	9	136	136	4	6	5	116	117	4	1	16	114	117	6
2	10	197	208	4	6	6	106	113	4	2	2	495	460	8
2	11	84	79	6	6	8	106	113	4	2	4	144	137	3
2	12	339	348	6	6	9	87	92	5	2	5	252	248	4
2	14	119	119	5	6	11	173	161	4	2	6	207	221	4
2	15	45	21	13*	6	13	139	128	5	2	7	79	78	4
2	16	153	167	5	6	15	161	153	5	2	8	197	219	4
2	24	39	42	16*	7	6	102	89	4	2	9	259	266	4
3	1	503	478	8	7	8	123	114	4	2	10	386	393	6
3	2	307	311	5	7	9	57	44	8	2	11	198	201	4
3	3	250	245	4	7	15	65	67	10	2	12	325	331	5
3	4	655	619	10	7	17	59	43	11*	2	13	200	206	4
3	5	182	168	3	8	1	33	43	8*	2	14	52	63	11*
3	6	775	754	12	8	3	153	160	4	2	15	142	140	5
3	7	64	65	5	8	4	46	44	7	3	1	309	291	5
3	8	413	411	7	8	5	199	208	4	3	2	94	77	3
3	9	170	176	4	8	6	42	44	9*	3	3	131	115	3
3	10	187	195	4	8	7	132	138	4	3	4	60	44	4
3	11	199	201	4	8	8	44	35	10*	3	5	171	157	3
3	12	70	86	7	8	9	121	113	4	3	6	225	214	4
3	13	57	63	9	8	13	56	55	10*	3	7	222	220	4
3	14	174	177	5	8	15	43	52	16*	3	8	175	178	4
3	15	85	76	8	9	1	81	88	4	3	9	227	239	4
4	1	275	270	5	9	2	54	43	6	3	10	295	304	5
4	2	89	97	3	9	11	53	47	10*	3	11	53	62	9*
4	3	338	323	6	10	8	38	29	10*	3	12	102	100	5
4	4	115	108	3	12	6	7	8	1*	3	13	52	66	11*
4	5	273	261	5						3	14	215	219	5
4	7	262	256	4	^^^^^^^ h = -1 ^^^^^^^					4	1	125	122	3

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
4	2	558	523	9	9	18	18	16	5*	4	1	95	94	4
4	3	432	394	7						4	2	67	53	5
4	4	97	107	4	^^^^^^^	h =	0	^^^^^^^		4	3	50	48	7
4	5	412	376	7						4	4	133	125	4
4	7	245	237	4	0	2	973	950	15	4	5	181	178	4
4	10	174	190	4	0	4	148	154	3	4	6	239	236	4
4	12	138	149	5	0	6	129	124	3	4	7	231	238	4
4	13	160	178	5	0	10	434	420	7	4	8	155	157	4
4	14	39	43	15*	0	12	113	113	4	4	9	106	126	5
4	23	56	66	11*	0	14	69	78	6	4	11	117	110	5
5	1	60	63	5	0	16	53	56	9	4	13	83	77	7
5	3	92	86	4	1	1	1061	1034	16	4	23	41	39	13*
5	8	99	97	5	1	2	437	447	7	5	1	463	459	8
5	9	134	136	4	1	3	40	13	5	5	2	223	211	4
5	10	141	140	4	1	4	70	78	4	5	3	442	417	7
5	11	143	148	4	1	6	110	124	3	5	4	178	176	4
5	12	102	102	6	1	7	117	126	3	5	5	164	157	4
5	14	118	101	6	1	8	105	94	4	5	6	204	206	4
6	1	63	69	5	1	9	74	65	5	5	7	103	115	4
6	2	100	104	4	1	10	276	278	5	5	8	125	129	4
6	5	147	152	4	1	11	145	133	4	5	9	90	103	5
6	7	55	54	7	1	12	191	190	4	5	12	118	109	5
6	8	71	80	6	1	13	136	137	5	5	13	50	66	12*
6	9	48	47	9*	1	14	82	60	7	5	14	64	65	10
6	10	94	87	6	1	15	88	91	7	6	1	132	153	3
6	11	75	67	7	2	1	161	135	3	6	2	62	64	5
7	1	189	212	3	2	2	221	208	4	6	3	271	270	4
7	2	117	136	3	2	3	258	258	4	6	4	214	219	4
7	3	119	141	4	2	4	93	87	3	6	5	185	191	4
7	4	116	123	3	2	5	236	239	4	6	7	101	97	5
7	6	165	186	4	2	6	388	418	6	6	11	140	129	5
7	7	207	182	4	2	7	91	107	4	6	13	180	169	5
7	8	156	138	4	2	8	501	538	8	6	15	136	127	6
7	9	195	177	4	2	9	147	158	4	7	1	51	68	6
7	10	93	85	6	2	10	392	399	7	7	5	54	62	7
7	11	80	78	7	2	12	291	297	5	7	6	47	27	8*
7	17	44	60	16*	2	13	117	118	5	7	7	161	149	4
7	18	50	5	13*	2	14	218	219	5	7	9	106	101	5
8	1	68	70	4	3	1	89	92	3	7	10	53	33	10*
8	3	99	100	3	3	2	237	221	4	7	11	102	96	6
8	5	126	125	4	3	3	238	193	4	7	13	62	53	10
8	7	122	117	4	3	4	556	510	9	7	14	39	48	16*
8	9	89	83	6	3	5	218	225	4	8	3	115	130	3
8	10	65	55	8	3	6	512	536	8	8	4	66	62	5
8	12	59	51	10*	3	7	162	169	4	8	5	120	130	4
9	1	96	126	3	3	8	117	123	4	8	7	124	113	4
9	3	43	63	6	3	9	439	466	7	8	9	54	39	9*
9	7	75	79	5	3	11	189	196	4	8	10	58	69	9
9	9	59	60	8	3	13	251	255	5	8	11	46	35	12*
9	13	40	2	14*	3	14	76	92	8	8	13	84	80	8

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF
8	15	70	43	9
9	2	24	14	9*
9	3	37	39	7*
9	7	92	96	5
9	9	58	65	8
9	11	72	65	8
9	16	32	15	15*
10	0	59	93	3
10	2	42	69	4

^^^^^^^ h = 1 ^^^^^^^

k	l	Fo	Fc	sigF
0	3	1121	1124	17
0	5	153	142	3
0	7	128	122	3
0	11	125	121	3
0	13	146	145	4
0	23	59	73	9
0	25	23	53	9*
1	1	375	370	6
1	2	383	404	6
1	3	200	198	3
1	4	456	484	7
1	5	192	205	3
1	6	482	507	8
1	7	260	283	4
1	9	40	63	10*
1	10	143	136	4
1	11	253	247	4
1	12	249	240	5
1	13	324	305	5
1	14	239	238	5
1	15	141	133	5
2	1	285	282	5
2	2	345	308	6
2	3	328	322	5
2	4	125	114	3
2	5	360	366	6
2	6	411	434	7
2	7	85	99	5
2	8	489	514	8
2	9	124	125	4
2	10	335	346	6
2	11	135	138	5
2	12	210	211	4
2	14	49	66	12*
2	15	85	83	8
3	2	170	149	3
3	3	354	323	6
3	4	347	338	6
3	5	359	371	6
3	6	51	59	7
3	7	160	171	4
3	8	166	172	4
3	11	85	101	6
3	13	81	65	8
3	14	94	83	7
4	1	187	180	4
4	2	572	509	9
4	3	204	188	4
4	4	214	196	4
4	5	247	241	4
4	8	141	141	4
4	11	167	170	4
4	12	71	83	8
4	13	98	110	6
4	14	79	81	8
4	20	50	76	16*
5	1	148	141	4
5	2	224	198	4
5	3	94	81	5
5	4	354	347	6
5	5	51	50	8
5	6	179	177	4
5	7	122	121	4
5	11	83	96	7
5	12	81	69	7
5	13	97	91	7
6	1	183	193	4
6	2	114	115	4
6	3	111	107	4
6	4	111	104	4
6	8	70	68	7
6	9	58	51	9
6	10	141	124	5
6	11	88	81	7
6	12	202	185	5
6	13	50	51	12*
6	17	46	1	15*
6	19	80	68	9
7	0	77	77	9
7	1	106	124	5
7	2	56	70	8
7	4	75	83	5
7	5	63	68	7
7	6	35	43	12*
7	7	142	119	4
7	8	59	40	8
7	9	190	178	5
7	11	164	152	5
8	2	47	51	8*
8	4	54	57	7
8	6	99	92	5
8	7	88	84	5
8	8	63	76	8
9	1	127	127	4
9	3	61	87	6
9	10	58	44	9
10	1	77	82	5

^^^^^^^ h = 2 ^^^^^^^

k	l	Fo	Fc	sigF
0	2	1743	1760	27
0	4	433	432	7
0	6	134	142	3
0	8	414	413	7
0	10	152	152	3
1	1	789	788	12
1	2	1369	1373	21
1	3	544	566	9
1	4	605	630	9
1	5	481	495	8
1	6	213	216	4
1	7	63	76	6
1	8	196	194	4
1	10	113	112	5
1	11	163	165	4
1	12	102	89	5
1	13	172	179	5
1	14	59	29	9
1	23	46	59	11*
2	1	147	153	3
2	3	67	89	5
2	4	210	203	4
2	5	126	103	3
2	6	174	189	4
2	7	139	156	4
2	8	205	216	4
2	9	324	338	5
2	10	434	446	8
2	11	121	119	5
2	12	214	208	5
2	14	153	166	5
3	1	187	192	4
3	2	155	151	4
3	3	66	63	6
3	4	45	98	9*
3	5	85	90	5
3	7	208	225	4
3	8	73	84	7

10|F|o vs 10|F|c for bzn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
3	9	239	241	4	9	6	32	16	14*	4	3	71	82	7
3	10	112	140	5	9	7	43	48	11*	4	4	122	109	4
3	11	269	273	5	11	4	32	47	11*	4	5	240	237	4
3	12	292	308	5	11	7	30	27	11*	4	6	260	278	5
3	13	120	114	6						4	8	160	175	4
3	14	209	194	5	^^^^^^^	h =	3	^^^^^^		4	9	144	153	5
4	1	304	334	5						4	10	106	113	6
4	2	78	88	6	0	1	164	174	3	4	11	175	195	5
4	3	262	248	5	0	3	405	416	6	4	20	52	44	14*
4	4	156	144	4	0	5	460	432	7	5	2	480	462	8
4	5	214	211	4	0	7	126	125	3	5	3	181	182	4
4	7	86	81	5	0	9	90	91	4	5	4	237	239	4
4	8	161	165	4	0	11	95	93	4	5	6	66	69	8
4	9	146	169	4	0	13	155	146	4	5	7	85	87	6
4	19	62	48	12*	1	1	352	346	6	5	8	64	56	8
5	1	428	430	7	1	2	969	950	15	5	9	154	163	4
5	2	122	110	5	1	3	233	240	4	5	11	35	8	16*
5	4	236	224	4	1	4	118	122	3	5	12	81	81	8
5	5	102	102	5	1	5	757	751	12	5	13	49	42	13*
5	6	133	141	4	1	6	154	149	3	5	14	103	94	7
5	7	118	132	5	1	7	85	86	5	5	18	54	47	14*
5	8	182	192	4	1	10	212	208	4	6	2	156	141	5
5	13	77	71	8	1	12	233	219	5	6	3	217	211	5
5	14	44	55	15*	1	13	170	170	5	6	4	144	140	5
6	1	170	171	5	1	14	232	224	5	6	6	102	105	6
6	3	414	399	7	2	1	496	476	8	6	7	69	83	8
6	4	50	53	10*	2	2	174	186	3	6	8	42	35	12*
6	5	361	369	6	2	3	439	419	7	6	9	128	116	5
6	6	177	186	4	2	4	48	35	7	6	10	66	62	9
6	7	224	226	4	2	5	333	346	6	6	11	151	131	5
6	8	79	80	6	2	6	91	106	5	6	12	91	87	7
6	10	52	45	11*	2	7	259	268	4	6	13	92	86	8
7	2	71	55	8	2	8	236	241	4	6	19	51	8	15*
7	4	66	63	7	2	9	292	308	5	7	0	44	33	16*
7	6	153	135	4	2	12	106	106	6	7	1	186	204	5
7	8	43	27	12*	2	14	41	48	15*	7	2	102	93	6
7	9	65	55	8	3	1	184	194	4	7	4	132	114	5
7	12	83	62	8	3	2	264	254	4	7	5	122	100	5
7	13	38	40	17*	3	3	161	157	4	7	7	107	81	5
7	16	61	56	11*	3	4	251	259	4	7	9	130	110	5
8	1	96	69	7	3	5	51	39	9*	7	11	96	90	7
8	3	88	75	6	3	6	380	390	6	8	1	64	51	11*
8	5	106	104	5	3	7	118	126	5	8	6	73	63	7
8	8	33	20	15*	3	8	130	128	4	8	10	38	43	16*
8	9	99	87	6	3	9	74	52	7	9	0	106	74	9
8	11	77	73	8	3	10	194	202	5	9	1	39	17	18*
8	13	65	61	10	3	11	130	132	5	9	2	56	38	11*
8	15	47	55	14*	3	13	151	151	5	9	8	58	69	10*
9	1	84	61	8	3	14	67	59	10	9	9	57	40	10*
9	2	75	75	7	4	2	89	92	6					

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
^^^^^^^ h = 4 ^^^^^^^					4	9	80	82	7	1	1	313	308	5
					4	10	130	139	5	1	2	458	450	7
0	2	319	303	5	4	12	138	138	5	1	3	171	171	3
0	4	492	502	8	5	1	39	28	14*	1	4	546	509	9
0	6	408	417	7	5	3	202	198	5	1	5	457	425	8
0	8	325	330	5	5	4	130	140	5	1	6	232	227	4
0	10	349	352	6	5	5	222	229	5	1	7	584	543	9
0	12	89	90	5	5	6	60	78	10	1	10	118	109	5
0	20	62	71	9	5	7	250	263	5	1	11	61	55	9
1	1	403	391	7	5	8	92	105	6	1	12	196	190	5
1	2	615	601	10	5	9	150	157	5	1	14	102	103	7
1	3	594	580	9	5	18	55	34	13*	2	1	402	380	7
1	4	629	600	10	6	1	160	163	5	2	3	378	352	6
1	5	257	253	4	6	3	185	184	5	2	4	176	172	4
1	6	243	239	4	6	4	135	140	5	2	5	233	234	4
1	7	38	24	11*	6	5	158	157	5	2	6	205	205	4
1	9	94	87	5	6	6	97	114	6	2	7	142	138	5
1	11	266	253	5	6	7	107	129	6	2	12	117	122	6
1	13	156	135	5	6	8	47	41	12*	2	13	110	100	6
1	23	29	30	14*	6	9	95	88	7	2	14	112	101	7
2	1	384	375	6	6	14	70	74	10	3	3	170	179	4
2	2	672	666	10	7	0	154	124	5	3	4	71	79	7
2	3	251	246	4	7	2	66	50	10	3	5	160	175	4
2	4	406	402	7	7	3	42	41	15*	3	6	134	132	5
2	5	303	311	5	7	5	71	71	8	3	8	46	31	12*
2	6	108	102	5	7	6	122	113	5	3	9	253	254	5
2	7	243	256	4	7	7	107	94	6	3	11	205	205	5
2	9	105	105	6	7	8	199	181	5	4	1	369	397	6
2	11	199	196	5	7	9	86	72	7	4	2	107	107	5
2	12	79	76	8	7	10	94	70	7	4	3	169	174	4
2	24	10	10	4*	8	0	74	32	9	4	4	126	131	5
3	1	515	545	8	8	1	130	98	6	4	6	259	272	5
3	2	252	243	4	8	3	128	96	5	4	8	255	261	5
3	3	174	178	4	8	11	71	51	9	4	9	48	89	13*
3	4	306	307	5	8	13	76	77	9	4	10	216	226	5
3	5	253	261	4	8	15	42	38	17*	4	11	99	74	7
3	6	94	98	6	9	12	44	36	12*	4	12	95	88	7
3	7	77	60	7	10	8	42	38	11*	5	1	233	257	4
3	8	175	178	4	11	4	34	41	14*	5	3	83	77	7
3	10	152	151	5	11	9	11	16	5*	5	4	86	75	7
3	11	112	124	6						5	8	124	136	5
3	12	85	76	7	^^^^^^^ h = 5 ^^^^^^^					5	9	124	103	5
3	14	135	129	6						5	10	111	92	6
4	1	162	183	4	0	1	245	247	4	5	11	125	121	6
4	2	97	101	6	0	3	191	186	3	5	14	75	79	9
4	3	174	181	4	0	5	375	357	6	6	0	233	246	5
4	4	75	86	7	0	7	516	521	8	6	1	193	208	5
4	5	140	139	5	0	9	232	232	4	6	2	232	230	5
4	6	123	137	5	0	11	41	51	10*	6	3	117	115	6
4	8	64	73	9	0	13	119	133	5	6	4	255	253	5

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
6	6	142	118	5	2	7	185	177	4	8	8	74	66	8
6	7	92	88	7	2	9	191	192	5	8	10	66	69	10
6	8	79	74	8	2	18	71	76	10	8	13	45	15	12*
6	9	85	77	7	3	1	218	236	4	9	0	44	26	16*
6	11	76	70	8	3	2	282	293	5	9	4	59	52	11*
6	13	68	65	10	3	3	242	265	4	9	6	66	62	9
6	15	41	30	17*	3	4	154	139	4	9	8	65	68	10
6	18	46	57	16*	3	5	149	149	4	10	9	31	2	14*
7	1	95	77	7	3	6	183	179	4	11	3	37	19	13*
7	3	86	63	8	3	7	77	91	8	11	8	9	18	2*
7	5	130	107	6	3	8	94	91	6					
7	7	75	64	8	3	14	52	22	13*	^^^^^^^ h = 7 ^^^^^^^				
8	2	116	92	7	4	1	125	127	5					
8	6	44	40	13*	4	2	489	508	8	0	1	133	125	3
8	14	63	57	12*	4	3	105	108	6	0	3	444	465	7
9	0	96	73	9	4	4	158	165	5	0	5	452	458	7
9	3	73	56	9	4	5	208	209	5	0	7	561	556	9
9	5	75	81	9	4	7	275	292	5	0	9	417	409	7
11	0	52	31	17*	4	9	166	176	5	0	11	171	161	4
11	8	18	38	4*	4	10	92	87	7	0	13	34	52	14*
11	9	5	7	2*	4	11	132	120	6	1	1	72	72	4
					4	12	149	140	5	1	2	271	255	5
^^^^^^^ h = 6 ^^^^^^^					4	14	44	48	15*	1	3	190	177	4
					5	2	98	106	6	1	4	357	319	6
0	4	265	271	4	5	5	267	277	5	1	8	160	147	4
0	6	345	338	6	5	6	91	88	7	2	1	191	200	4
0	8	228	227	4	5	7	150	152	5	2	2	140	144	4
0	10	63	60	6	5	9	82	73	8	2	4	243	235	5
0	12	187	186	4	5	10	65	56	9	2	5	149	140	5
0	14	74	62	7	5	14	59	57	11*	2	6	294	304	5
1	1	113	118	3	6	1	53	17	11*	2	8	147	144	5
1	2	289	263	5	6	2	91	108	7	2	11	104	107	6
1	3	364	336	6	6	4	69	79	9	2	13	189	185	5
1	4	126	112	4	6	6	65	63	9	3	1	445	458	7
1	5	307	288	5	6	7	92	70	7	3	2	65	73	8
1	6	225	222	4	6	8	40	36	15*	3	3	339	345	6
1	8	142	126	5	6	9	80	60	8	3	4	117	112	5
1	9	165	141	4	6	10	56	33	11*	3	6	57	59	10*
1	10	114	100	5	6	11	79	67	9	3	10	102	118	7
1	11	231	214	5	6	14	42	1	16*	3	11	161	146	5
1	12	89	74	7	7	0	200	162	5	3	12	125	119	6
1	13	170	167	5	7	2	118	91	6	3	14	111	121	7
1	14	76	77	8	7	4	48	53	13*	4	1	296	310	5
1	22	37	2	9*	7	6	125	114	6	4	2	201	216	4
2	1	496	514	8	7	8	115	112	6	4	3	191	190	4
2	2	32	34	12*	7	9	80	80	8	4	5	75	88	8
2	3	157	157	4	7	11	72	69	9	4	6	74	55	8
2	4	223	217	4	8	1	132	113	6	4	8	77	85	8
2	5	214	210	4	8	3	86	75	8	4	9	48	52	14*
2	6	360	349	6	8	5	72	57	9	4	10	48	25	13*

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF	k	l	Fo	Fc	sigF
4	12	88	70	8	1	3	567	532	9	8	0	109	93	6
4	14	53	36	13*	1	4	171	156	4	8	1	67	54	9
5	1	172	186	4	1	5	93	83	6	8	2	82	78	9
5	3	91	92	7	1	8	230	210	5	8	4	42	52	15*
5	4	219	227	5	1	9	190	172	4	9	3	69	53	9
5	5	92	103	7	1	10	122	109	5	9	6	43	44	13*
5	6	218	224	5	1	11	71	70	9	10	5	53	9	11*
5	8	212	190	5	1	12	90	75	7					
5	9	89	84	8	1	13	85	84	7	^^^^^^^ h = 9 ^^^^^^^				
5	10	110	99	6	1	21	29	14	8*					
5	11	77	79	9	2	1	146	149	4	0	1	75	72	4
5	13	61	74	12*	2	3	181	178	4	0	3	72	78	5
5	15	47	17	14*	2	4	162	160	4	0	5	363	360	6
6	0	77	68	7	2	5	186	186	4	0	7	285	275	5
6	2	93	99	7	2	7	212	217	5	0	9	262	258	5
6	3	45	45	13*	2	9	68	70	9	0	13	42	63	12*
6	4	136	131	5	2	10	69	79	9	1	2	44	54	10*
6	6	88	84	7	2	11	74	80	9	1	3	230	218	4
6	10	104	94	7	2	12	113	100	6	1	6	84	70	7
6	12	82	83	9	2	17	75	62	9	1	7	149	142	5
7	0	119	103	5	3	1	87	109	6	1	8	99	97	6
7	1	44	43	14*	3	2	174	175	4	1	9	192	177	5
7	2	87	63	7	3	3	94	106	6	1	10	62	63	9
7	3	86	69	8	3	4	97	90	6	1	11	212	207	5
7	4	38	22	16*	3	7	57	63	11*	2	2	235	233	4
8	0	124	99	6	3	8	129	154	6	2	3	168	165	4
8	2	104	82	7	3	11	68	54	10	2	4	83	93	7
8	4	138	108	6	3	14	76	76	9	2	5	331	330	6
8	8	47	51	13*	4	2	143	152	5	2	6	62	63	10
8	10	97	87	7	4	3	183	201	5	2	7	139	154	5
8	11	52	33	12*	4	4	303	326	5	2	8	87	89	7
8	14	42	2	11*	4	5	155	164	5	2	10	40	35	16*
9	0	111	98	7	4	6	133	129	5	2	13	99	104	7
9	2	83	59	8	4	7	271	295	5	3	1	358	377	6
9	6	39	28	15*	4	9	168	164	5	3	2	137	144	5
9	8	53	25	11*	4	12	63	59	11*	3	3	458	473	8
10	7	38	17	14*	5	1	106	95	5	3	4	238	246	5
11	0	60	52	12*	5	3	60	46	10	3	5	198	197	5
11	4	28	11	9*	5	4	129	126	5	3	6	187	198	5
11	6	16	33	5*	5	6	128	110	6	3	8	108	118	6
11	7	7	4	3*	5	9	70	58	9	3	9	74	61	9
					5	11	69	69	10	3	11	74	69	9
^^^^^^^ h = 8 ^^^^^^^					6	0	91	95	6	3	14	110	108	7
					6	3	48	43	12*	3	16	40	51	17*
0	2	364	354	6	7	0	204	160	5	3	18	46	55	15*
0	4	235	233	4	7	1	169	144	5	4	1	137	151	5
0	10	78	74	6	7	3	133	112	5	4	2	200	221	5
0	12	65	78	7	7	5	86	67	7	4	3	91	92	7
1	1	635	606	10	7	6	86	86	7	4	4	147	156	5
1	2	259	240	4	7	8	53	48	12*	4	6	76	88	9

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF
4	8	61	53	11*
4	11	52	49	12*
5	2	113	132	5
5	4	120	127	5
5	6	115	113	6
5	8	115	98	6
5	9	84	71	8
6	1	96	82	6
6	2	41	30	13*
6	7	103	85	6
6	8	103	76	6
6	10	91	84	8
6	12	64	86	10
7	2	62	20	9
7	3	59	55	10*
7	5	39	43	16*
7	7	44	47	14*
8	0	172	163	5
8	2	175	159	5
8	4	49	68	13*
8	8	49	41	12*
8	9	44	0	12*
9	0	58	47	10*
11	3	17	1	6*

^^^^^^^ h = 10 ^^^^^^^

k	l	Fo	Fc	sigF
0	2	80	70	4
0	4	297	297	5
0	6	132	131	4
0	8	133	122	4
0	12	44	53	12*
1	1	404	388	7
1	2	171	164	4
1	3	270	249	5
1	5	193	180	4
1	8	51	23	11*
1	10	71	50	9
1	11	94	95	7
2	1	48	35	9*
2	2	81	82	7
2	3	295	293	5
2	5	124	111	5
2	7	122	114	6
2	10	121	111	6
2	13	43	56	16*
2	14	46	75	15*
3	1	53	70	9*
3	3	40	49	15*
3	4	78	76	8
3	5	103	118	7
3	6	198	212	5
3	8	56	33	11*
3	10	105	109	7
4	2	189	208	4
4	4	80	92	8
4	9	91	93	7
4	15	42	56	16*
5	4	79	89	8
5	5	72	73	9
5	6	112	107	6
5	8	98	93	7
5	9	95	96	7
5	11	71	75	9
6	0	157	123	4
6	2	83	74	7
6	3	63	41	9
6	5	104	99	6
6	7	121	110	6
6	9	46	29	13*
6	14	54	25	12*
7	0	58	63	9
7	1	76	72	7
7	3	65	54	9
7	5	40	42	15*
7	6	144	140	5
7	14	35	17	10*
8	2	75	79	8
8	3	53	60	11*
9	8	38	3	13*

^^^^^^^ h = 11 ^^^^^^^

k	l	Fo	Fc	sigF
0	1	61	60	6
0	3	232	228	4
0	13	79	87	8
0	15	70	87	8
0	17	43	68	12*
1	1	233	218	4
1	2	143	126	4
1	3	120	99	5
1	10	60	58	10
1	11	60	70	10*
1	13	59	84	11*
1	18	40	49	11*
2	1	134	132	4
2	3	197	190	5
2	5	371	368	6
2	6	92	89	8
2	7	213	229	5
2	14	39	66	17*
2	16	44	39	13*
3	1	142	154	4
3	2	74	95	8
3	3	163	187	5
3	4	250	255	5
3	5	112	124	6
3	6	256	241	5
3	8	202	199	5
3	9	143	145	6
4	1	97	103	5
4	3	40	48	14*
4	4	105	127	6
4	6	58	44	10*
4	9	94	100	7
5	1	73	98	7
5	3	55	63	10*
5	6	68	50	8
5	10	43	14	14*
6	0	165	146	4
6	2	110	91	5
6	3	109	95	6
6	11	41	7	14*
6	12	66	60	8
7	0	82	68	7
7	2	70	67	8
7	6	83	89	7
8	0	83	89	6
8	2	90	93	6
8	8	42	44	11*
9	6	50	44	10*
9	9	19	7	9*
11	1	10	9	3*

^^^^^^^ h = 12 ^^^^^^^

k	l	Fo	Fc	sigF
0	2	70	64	6
0	4	115	104	4
0	6	70	82	6
0	12	62	60	9
1	1	242	244	4
1	3	140	122	5
1	4	133	121	5
1	6	122	125	5
1	8	74	69	8
1	11	65	93	10
2	1	54	48	9
2	2	131	119	5
2	3	183	172	5
2	4	72	83	9

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF
2	5	238	238	5
2	8	95	90	8
3	1	54	35	9
3	2	180	189	4
3	4	83	86	7
3	5	42	44	15*
3	8	42	6	15*
4	1	69	50	7
4	5	48	38	12*
4	6	96	94	7
4	8	91	102	7
4	15	36	28	17*
4	16	35	24	10*
5	0	84	71	6
5	1	89	93	6
5	3	99	89	6
5	6	83	70	7
6	0	55	60	9
6	3	37	26	14*
6	7	71	75	8
6	9	60	61	9
7	2	74	68	7
7	6	37	50	15*
7	8	44	52	12*
8	10	30	21	9*
8	12	3	10	1*
10	0	49	57	9*

^^^^^^^ h = 13 ^^^^^^^

k	l	Fo	Fc	sigF
0	1	85	94	5
0	3	237	242	4
0	5	130	134	4
0	7	118	129	5
1	1	198	197	4
1	2	83	73	6
1	3	88	80	6
1	5	63	45	9
1	7	106	105	6
1	8	101	103	6
1	10	35	52	17*
1	16	35	47	13*
1	18	7	34	3*
2	2	47	46	11*
2	3	80	74	7
2	5	123	121	6
2	8	152	146	5
3	1	136	144	5
3	4	65	66	9
3	6	159	160	5
3	8	60	61	10*
3	9	86	93	8
3	10	76	90	9
3	11	81	88	8
4	1	97	107	6
4	10	72	98	9
4	12	52	64	12*
5	1	43	69	12*
5	2	105	104	6
5	3	81	79	7
5	4	112	100	6
6	0	134	130	4
6	2	121	130	5
7	2	62	56	8
7	3	54	58	9*
8	0	33	49	14*
9	3	30	24	14*
9	4	35	34	11*

^^^^^^^ h = 14 ^^^^^^^

k	l	Fo	Fc	sigF
0	2	37	46	11*
0	10	70	64	8
0	12	43	37	12*
0	14	47	58	11*
1	1	59	59	9
1	2	148	144	5
1	4	93	85	7
1	5	68	54	9
1	7	53	55	11*
1	8	54	52	11*
1	17	8	19	4*
2	2	160	158	5
2	3	67	63	9
2	5	109	91	6
2	14	37	1	17*
2	17	4	3	1*
3	1	131	136	5
3	3	35	39	15*
3	5	94	76	7
4	0	71	68	7
4	1	105	103	5
4	3	54	52	10*
4	5	68	73	8
4	6	47	38	12*
4	8	88	102	7
5	1	111	112	5
5	8	47	35	11*
5	13	34	8	9*
6	0	75	76	7
6	1	89	98	6
6	3	64	64	8
6	6	59	59	9
8	9	15	25	4*
9	0	34	27	9*
9	2	33	46	11*

^^^^^^^ h = 15 ^^^^^^^

k	l	Fo	Fc	sigF
0	1	145	154	4
0	3	201	216	4
0	5	137	160	4
1	2	77	78	7
1	4	92	94	7
1	7	42	4	13*
1	8	114	119	6
1	10	72	88	8
2	1	167	160	4
2	2	95	94	6
2	4	89	80	7
3	1	66	79	8
3	3	54	42	10*
3	12	35	3	13*
4	2	100	100	6
4	4	105	101	6
4	11	40	61	12*
5	0	159	152	4
5	1	78	84	6
5	2	93	90	6
5	4	53	66	10*
5	6	50	45	10*
5	13	15	33	6*
6	0	96	108	6
8	4	38	15	10*

^^^^^^^ h = 16 ^^^^^^^

k	l	Fo	Fc	sigF
0	0	39	64	10*
0	2	110	114	5
0	4	145	151	4
1	2	77	94	7
1	3	72	56	8
1	4	79	76	7
1	5	46	24	12*
1	7	36	44	16*
3	6	43	65	14*
3	8	79	86	8
3	10	39	47	13*
4	0	80	98	6
4	1	89	98	6

10|F|o vs 10|F|c for brn $C_{13}H_{11}PS_2$

k	l	Fo	Fc	sigF
4	3	57	73	10*
5	0	59	63	8
5	2	43	47	11*
6	1	60	80	7
6	8	31	15	14*
8	0	28	20	11*
8	6	16	14	5*
9	0	22	9	8*
9	2	17	25	5*

^^^^^^^ h = 17 ^^^^^^^

k	l	Fo	Fc	sigF
0	1	50	59	9*
0	5	70	69	7
0	11	47	84	10*
1	1	111	108	5
1	2	63	69	9
1	3	47	56	12*
1	5	58	71	10*
1	8	60	73	9
2	3	55	37	10*
2	4	39	41	15*
3	8	41	41	13*
4	0	45	29	10*
4	1	61	62	8
4	2	99	120	6
4	4	75	95	7
4	6	70	81	8
4	10	34	14	13*
6	7	34	23	11*
7	0	30	38	12*
8	0	29	36	11*

^^^^^^^ h = 18 ^^^^^^^

k	l	Fo	Fc	sigF
0	0	147	176	4
0	2	107	128	5
0	4	72	93	7
0	10	47	57	12*
1	12	22	5	7*
3	0	89	96	6
3	4	42	35	13*
3	9	30	27	13*
4	3	56	47	8
4	8	44	6	11*
7	5	18	31	7*
9	0	3	8	1*

^^^^^^^ h = 19 ^^^^^^^

k	l	Fo	Fc	sigF
0	3	68	81	7
1	3	59	59	9
1	6	42	37	12*
2	3	52	20	10*
3	5	33	31	15*
3	8	42	35	11*
4	8	25	11	12*
5	5	32	22	13*
5	6	38	33	9*
5	7	23	24	9*
7	1	26	53	11*
8	1	9	0	4*

^^^^^^^ h = 20 ^^^^^^^

k	l	Fo	Fc	sigF
0	2	67	78	7
0	10	15	45	7*
1	10	13	19	5*
2	2	35	26	15*
2	7	42	17	12*

^^^^^^^ h = 21 ^^^^^^^

k	l	Fo	Fc	sigF
1	8	24	8	7*
2	6	41	11	10*
4	3	33	6	13*
5	3	28	8	9*
7	1	7	18	2*

^^^^^^^ h = 22 ^^^^^^^

k	l	Fo	Fc	sigF
0	8	7	24	1*
2	5	29	3	11*

^^^^^^^ h = 23 ^^^^^^^

k	l	Fo	Fc	sigF
5	0	19	10	8*

^^^^^^^ h = 24 ^^^^^^^

k	l	Fo	Fc	sigF
3	1	25	49	8*
3	2	15	42	6*

^^^^^^^ h = 26 ^^^^^^^

k	l	Fo	Fc	sigF
0	0	11	37	4*

Table . Hydrogen atom positional parameters for $(C_6H_6)_4Sn$

ATOM	x/a	y/b	z/c	U(iso)
H2	0.089 (6)	-0.152 (5)	-0.339 (9)	0.099 (21)
H3	0.253 (5)	-0.168 (5)	-0.554 (10)	0.095 (20)
H4	0.399 (4)	-0.048 (4)	-0.501 (7)	0.071 (14)
H5	0.389 (3)	0.091 (3)	-0.279 (9)	0.086 (18)
H6	0.229 (3)	0.120 (3)	-0.098 (7)	0.033 (10)

Table . Hydrogen atom positional parameters for $(C_6H_5)_4Pb$

ATOM	x/a	y/b	z/c	U(iso)
H2	0.083 (3)	-0.133 (5)	-0.346 (7)	0.064 (7)
H3	0.247 (5)	-0.170 (3)	-0.559 (5)	0.047 (7)
H4	0.400 (5)	-0.051 (6)	-0.515 (6)	0.067 (7)
H5	0.391 (5)	0.084 (5)	-0.288 (7)	0.072 (7)
H6	0.223 (6)	0.113 (5)	-0.084 (7)	0.069 (7)

Table . Hydrogen atom positional parameters for $(C_6H_5)_4Si$

ATOM	x/a	y/b	z/c	U(iso)
H2	0.068 (3)	-0.146 (3)	-0.326 (5)	0.048 (7)
H3	0.228 (3)	-0.172 (3)	-0.514 (6)	0.055 (8)
H4	0.396 (3)	-0.054 (3)	-0.461 (5)	0.067 (10)
H5	0 394 (2)	0.087 (2)	-0.243 (7)	0.076 (10)
H6	0.241 (3)	0.112 (3)	-0.046 (5)	0.051 (8)

Table . Hydrogen atom positional parameters for $GePh_4$

ATOM	x/a	y/b	z/c	U(iso)
H2	0.071 (3)	-0.151 (3)	-0.328 (3)	0.084 (3)
H3	0.239 (3)	-0.168 (2)	-0.511 (3)	0.079 (3)
H4	0.399 (2)	-0.056 (2)	-0.476 (3)	0.072 (3)
H5	0.391 (2)	0.086 (2)	-0.248 (3)	0.070 (3)
H6	0.236 (3)	0.116 (2)	-0.052 (3)	0.064 (3)

Table . Hydrogen atom positional parameters for $GePh_4$ (lt)

ATOM	x/a	y/b	z/c	U(iso)
H2	0.068 (2)	-0.157 (2)	-0.326 (3)	0.062 (3)
H3	0.246 (3)	-0.170 (2)	-0.522 (3)	0.072 (3)
H4	0.391 (2)	-0.056 (2)	-0.482 (3)	0.084 (3)
H5	0.390 (2)	0.088 (2)	-0.251 (3)	0.073 (3)
H6	0.236 (2)	0.119 (2)	-0.054 (3)	0.042 (3)

Intermolecular Distances (Å) Involving the Hydrogen Atoms for $SiPh_4$

C(2)	-H(2)	0.93 (3)
C(3)	-H(3)	0.97 (3)
C(4)	-H(4)	0.94 (4)
C(5)	-H(5)	0.95 (3)
C(6)	-H(6)	0.94 (3)

Intramolecular Distances (Å) Involving the Hydrogen Atoms for $GePh_4$ (RT)

C(2)	-H(2)	0.99 (3)
C(3)	-H(3)	0.86 (3)
C(4)	-H(4)	0.98 (3)
C(5)	-H(5)	0.92 (3)
C(6)	-H(6)	0.97 (3)

Intramolecular Distances (Å) Involving the Hydrogen Atoms for $GePh_4$ (LT)

C(2)	-H(2)	1.06 (3)
C(3)	-H(3)	0.91 (3)
C(4)	-H(4)	0.91 (3)
C(5)	-H(5)	0 93 (2)
C(6)	-H(6)	0 98 (2)

Intramolecular Distances (Å) Involving the Hydrogen Atoms for $SnPh_4$

C(2)	-H(2)	0 96 (7)
C(3)	-H(3)	0.94 (6)
C(4)	-H(4)	0.92 (5)
C(5)	-H(5)	0.95 (4)
C(6)	-H(6)	0.92 (4)

Intermolecular Distances (Å) Involving the Hydrogen Atoms for $PbPh_4$

C(2)	-H(2)	0.96 (5)
C(3)	-H(3)	0.95 (5)
C(4)	-H(4)	0.94 (6)
C(5)	-H(5)	0.90 (6)
C(6)	-H(6)	0.96 (6)

Table Torsional Angles (degrees) for $(C_6H_5)_4Si$

C(1)	-SI(1)	-C'(1)	-C'(2)	-52.1 (3)
C(1)	-SI(1)	-C'(1)	-C'(6)	127.6 (3)
C(1)	-SI(1)	-C''(1)	-C''(2)	172.5 (2)
C(1)	-SI(1)	-C''(1)	-C''(6)	-7.2 (3)
C''(1)	-SI(1)	-C(1)	-C(2)	68.3 (3)
C''(1)	-SI(1)	-C(1)	-C(6)	-112.0 (3)
SI(1)	-C(1)	-C(2)	-C(3)	-178.9 (3)
C(2)	-C(1)	-SI(1)	-C'''(1)	-172.5 (2)
SI(1)	-C(1)	-C(6)	-C(5)	179.6 (2)
C(6)	-C(1)	-SI(1)	-C'''(1)	7.2 (2)
C(2)	-C(1)	-C(6)	-C(5)	-0.7 (4)
C(6)	-C(1)	-C(2)	-C(3)	1.4 (4)
C(1)	-C(2)	-C(3)	-C(4)	-1.0 (5)
C(2)	-C(3)	-C(4)	-C(5)	-0.1 (5)
C(3)	-C(4)	-C(5)	-C(6)	0.8 (5)
C(4)	-C(5)	-C(6)	-C(1)	-0.3 (4)

Primed atoms have symmetry operation:

' - -x,-y,z

'' - y,-x,-z

''' - -y,x,-z

Table Torsional Angles (degrees) for GEPH4 (RT)

C(1)	-GE(1)	-C'(1)	-C'(2)	-54.1 (3)
C(1)	-GE(1)	-C'(1)	-C'(6)	125.4 (3)
C(1)	-GE(1)	-C''(1)	-C''(2)	174.3 (3)
C(1)	-GE(1)	-C''(1)	-C''(6)	-5.2 (3)
C''(1)	-GE(1)	-C(1)	-C(2)	66.1 (3)
C''(1)	-GE(1)	-C(1)	-C(6)	-114.4 (3)
GE(1)	-C(1)	-C(2)	-C(3)	-179.4 (3)
C(2)	-C(1)	-GE(1)	-C'''(1)	-174.3 (2)
GE(1)	-C(1)	-C(6)	-C(5)	179.9 (3)
C(6)	-C(1)	-GE(1)	-C'''(1)	5.2 (3)
C(2)	-C(1)	-C(6)	-C(5)	-0.6 (5)
C(6)	-C(1)	-C(2)	-C(3)	1.1 (5)
C(1)	-C(2)	-C(3)	-C(4)	-0.6 (6)
C(2)	-C(3)	-C(4)	-C(5)	-0 5 (6)
C(3)	-C(4)	-C(5)	-C(6)	1.0 (6)
C(4)	-C(5)	-C(6)	-C(1)	-0 4 (5)

Primed atoms have symmetry operations:

'	-	-X + 0.000	-Y + 0.000	Z + 0.000
''	-	Y + 0.000	-X + 0.000	-Z + 0.000
'''	-	-Y + 0.000	X + 0.000	-Z + 0.000

Table Torsional Angles (degrees) for $GePh_4$ (LT)

C(1)	-GE(1)	-C'(1)	-C'(2)	-55.3 (3)
C(1)	-GE(1)	-C'(1)	-C'(6)	125.0 (3)
C(1)	-GE(1)	-C''(1)	-C''(2)	175.4 (3)
C(1)	-GE(1)	-C''(1)	-C''(6)	-4.8 (3)
C''(1)	-GE(1)	-C(1)	-C(2)	64.9 (3)
C''(1)	-GE(1)	-C(1)	-C(6)	-114.9 (3)
GE(1)	-C(1)	-C(2)	-C(3)	-179.1 (3)
C(2)	-C(1)	-GE(1)	-C'''(1)	-175.4 (2)
GE(1)	-C(1)	-C(6)	-C(5)	179.3 (3)
C(6)	-C(1)	-GE(1)	-C'''(1)	4.8 (2)
C(2)	-C(1)	-C(6)	-C(5)	-0.5 (4)
C(6)	-C(1)	-C(2)	-C(3)	0.7 (5)
C(1)	-C(2)	-C(3)	-C(4)	-0.2 (5)
C(2)	-C(3)	-C(4)	-C(5)	-0.6 (5)
C(3)	-C(4)	-C(5)	-C(6)	0.9 (5)
C(4)	-C(5)	-C(6)	-C(1)	-0.3 (5)

Primed atoms have symmetry operations:

'	-	-X + 0.000	-Y + 0.000	Z + 0.000
''	-	Y + 0.000	-X + 0.000	-Z + 0.000
'''	-	-Y + 0.000	X + 0.000	-Z + 0.000

Table Torsional Angles (degrees) for $(C_6H_5)_4Sn$

C(1)	-SN(1)	-C(1)'	-C(2)'	-57.9 (4)
C(1)	-SN(1)	-C(1)'	-C(6)'	122.3 (3)
C(1)	-SN(1)	-C(1)''	-C(2)''	177.5 (3)
C(1)	-SN(1)	-C(1)''	-C(6)''	-2.6 (4)
C(1)''	-SN(1)	-C(1)	-C(2)	61.7 (4)
C(1)''	-SN(1)	-C(1)	-C(6)	-118.1 (3)
SN(1)	-C(1)	-C(2)	-C(3)	-179.3 (4)
C(2)	-C(1)	-SN(1)	-C(1)'''	-177.5 (3)
SN(1)	-C(1)	-C(6)	-C(5)	-179.0 (3)
C(6)	-C(1)	-SN(1)	-C(1)'''	2.6 (3)
C(2)	-C(1)	-C(6)	-C(5)	1.1 (6)
C(6)	-C(1)	-C(2)	-C(3)	0.6 (6)
C(1)	-C(2)	-C(3)	-C(4)	-1.9 (7)
C(2)	-C(3)	-C(4)	-C(5)	1.6 (7)
C(3)	-C(4)	-C(5)	-C(6)	0.1 (6)
C(4)	-C(5)	-C(6)	-C(1)	-1.5 (6)

Primed atoms have symmetry operation:

' - -x,-y,z

'' - y,-x,-z

'''- -y,x,-z

Table Torsional Angles (degrees) for C24H20PB P4-2121

C(1)	-PB(1)	-C'(1)	-C'(2)	-57.9 (8)
C(1)	-PB(1)	-C'(1)	-C'(6)	121.0 (7)
C(1)	-PB(1)	-C''(1)	-C''(2)	177.5 (7)
C(1)	-PB(1)	-C''(1)	-C''(6)	-1.4 (8)
C''(1)	-PB(1)	-C(1)	-C(2)	61.7 (8)
C''(1)	-PB(1)	-C(1)	-C(6)	-119.4 (7)
PB(1)	-C(1)	-C(2)	-C(3)	-179.8 (8)
C(2)	-C(1)	-PB(1)	-C'''(1)	-177.5 (6)
PB(1)	-C(1)	-C(6)	-C(5)	-179.4 (8)
C(6)	-C(1)	-PB(1)	-C'''(1)	1.4 (6)
C(2)	-C(1)	-C(6)	-C(5)	-0.4 (13)
C(6)	-C(1)	-C(2)	-C(3)	1.2 (13)
C(1)	-C(2)	-C(3)	-C(4)	-1.5 (14)
C(2)	-C(3)	-C(4)	-C(5)	0.9 (15)
C(3)	-C(4)	-C(5)	-C(6)	-0.1 (14)
C(4)	-C(5)	-C(6)	-C(1)	-0.2 (13)

Primed atoms have symmetry operation:

' - -x,-y,z

'' - y,-x,-z

'''- -y,x,-z

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Si$

An * indicates weak or extinct reflections not used in the final refinements.

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	1	0	434	442	0	2	0	369	375	1	2	0	79	79
2	2	0	455	448	1	3	0	130	135	2	3	0	109	107
3	3	0	429	419	0	4	0	41	41	1	4	0	5	3*
2	4	0	49	48	3	4	0	156	153	4	4	0	91	85
1	5	0	18	18	2	5	0	67	59	3	5	0	91	100
4	5	0	173	164	5	5	0	7	18*	0	6	0	134	129
1	6	0	99	100	2	6	0	298	296	3	6	0	218	211
4	6	0	165	175	5	6	0	7	14*	6	6	0	157	158
1	7	0	162	163	2	7	0	7	7*	3	7	0	92	92
4	7	0	25	24	5	7	0	107	105	6	7	0	49	47
7	7	0	108	115	0	8	0	188	192	1	8	0	50	46
2	8	0	155	157	3	8	0	7	12*	4	8	0	26	30
5	8	0	66	70	6	8	0	60	64	7	8	0	13	21*
8	8	0	127	137	1	9	0	295	302	2	9	0	10	10*
3	9	0	64	66	4	9	0	33	34	5	9	0	70	71
6	9	0	7	11*	7	9	0	85	88	8	9	0	14	11*
9	9	0	10	18*	0	10	0	19	20	1	10	0	22	20
2	10	0	62	63	3	10	0	16	18*	4	10	0	9	16*
5	10	0	10	13*	6	10	0	44	44	7	10	0	9	4*
8	10	0	72	72	9	10	0	3	16*	10	10	0	8	12*
1	11	0	29	32	2	11	0	48	49	3	11	0	36	36
4	11	0	39	41	5	11	0	49	47	6	11	0	27	25
7	11	0	88	84	8	11	0	12	12*	9	11	0	13	13*
10	11	0	22	17*	11	11	0	31	34	0	12	0	28	28
1	12	0	60	62	2	12	0	94	95	3	12	0	9	5*
4	12	0	35	31	5	12	0	27	29	6	12	0	33	33
7	12	0	42	46	8	12	0	20	23*	9	12	0	29	29
10	12	0	11	4*	11	12	0	14	15*	12	12	0	12	6*
1	13	0	64	64	2	13	0	57	60	3	13	0	24	26
4	13	0	9	1*	5	13	0	12	20*	6	13	0	10	15*
7	13	0	24	28	8	13	0	23	10	9	13	0	16	2*
10	13	0	36	31	11	13	0	23	17*	12	13	0	12	3*
13	13	0	14	6*	0	14	0	10	1*	1	14	0	28	28
2	14	0	39	37	3	14	0	30	25	4	14	0	31	24
5	14	0	20	6*	6	14	0	18	27*	7	14	0	14	4*
8	14	0	26	28	9	14	0	20	20*	10	14	0	37	31
11	14	0	12	5*	12	14	0	9	13*	1	15	0	51	48
2	15	0	9	17*	3	15	0	47	42	4	15	0	11	1*
5	15	0	46	42	6	15	0	11	8*	7	15	0	15	21*
8	15	0	12	1*	9	15	0	12	16*	10	15	0	12	5*
0	16	0	35	28	1	16	0	29	3*	2	16	0	12	23*
3	16	0	7	3*	4	16	0	40	33	5	16	0	12	11*
6	16	0	5	11*	7	16	0	16	7*	8	16	0	12	11*
9	16	0	12	3*	1	17	0	12	9*	2	17	0	8	2*
3	17	0	15	8*	4	17	0	12	9*	5	17	0	16	16*
6	17	0	12	7*	7	17	0	8	6*	0	18	0	28	20
1	18	0	13	4*	2	18	0	12	8*	3	18	0	12	2*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Si$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	18	0	13	17*	0	1	1	253	232	0	2	1	966	1023
1	2	1	519	505	0	3	1	218	212	1	3	1	449	439
2	3	1	320	305	0	4	1	224	211	1	4	1	306	300
2	4	1	120	115	3	4	1	109	108	0	5	1	307	293
1	5	1	93	87	2	5	1	141	146	3	5	1	172	154
4	5	1	145	146	0	6	1	127	125	1	6	1	195	194
2	6	1	158	150	3	6	1	36	40	4	6	1	97	97
5	6	1	108	110	0	7	1	156	164	1	7	1	19	23
2	7	1	150	155	3	7	1	42	40	4	7	1	47	52
5	7	1	24	25	6	7	1	146	153	0	8	1	46	47
1	8	1	148	153	2	8	1	7	2*	3	8	1	187	187
4	8	1	58	59	5	8	1	86	88	6	8	1	38	40
7	8	1	105	108	0	9	1	50	52	1	9	1	65	69
2	9	1	133	136	3	9	1	125	127	4	9	1	48	51
5	9	1	17	27*	6	9	1	100	102	7	9	1	57	57
8	9	1	11	23*	0	10	1	43	47	1	10	1	68	68
2	10	1	80	82	3	10	1	80	79	4	10	1	46	48
5	10	1	36	37	6	10	1	22	18	7	10	1	73	75
8	10	1	34	43	9	10	1	42	40	0	11	1	66	69
1	11	1	127	126	2	11	1	74	78	3	11	1	9	5*
4	11	1	9	14*	5	11	1	21	27*	6	11	1	45	49
7	11	1	21	26*	8	11	1	31	28	9	11	1	10	15*
10	11	1	45	39	0	12	1	18	26*	1	12	1	49	47
2	12	1	26	25	3	12	1	34	31	4	12	1	36	32
5	12	1	32	25	6	12	1	9	10*	7	12	1	17	29*
8	12	1	22	25*	9	12	1	35	36	10	12	1	19	19*
11	12	1	10	15*	0	13	1	60	56	1	13	1	22	18
2	13	1	40	37	3	13	1	10	9*	4	13	1	52	49
5	13	1	23	16	6	13	1	42	42	7	13	1	20	19*
8	13	1	8	19*	9	13	1	11	10*	10	13	1	10	12*
11	13	1	12	12*	12	13	1	24	21*	0	14	1	32	15*
1	14	1	51	48	2	14	1	8	22*	3	14	1	43	39
4	14	1	15	12*	5	14	1	41	38	6	14	1	11	9*
7	14	1	27	25	8	14	1	11	14*	9	14	1	21	20*
10	14	1	12	14*	11	14	1	12	8*	0	15	1	31	29
1	15	1	31	33	2	15	1	23	22*	3	15	1	20	17*
4	15	1	9	22*	5	15	1	8	2*	6	15	1	21	26*
7	15	1	12	13*	8	15	1	22	26*	9	15	1	12	12*
10	15	1	19	16*	0	16	1	30	13*	1	16	1	10	23*
2	16	1	11	11*	3	16	1	20	21*	4	16	1	12	8*
5	16	1	13	20*	6	16	1	10	6*	7	16	1	12	20*
8	16	1	12	5*	9	16	1	12	14*	0	17	1	14	21*
1	17	1	12	9*	2	17	1	28	22	3	17	1	12	3*
4	17	1	10	17*	5	17	1	12	9*	6	17	1	12	11*
7	17	1	13	8*	0	18	1	12	0*	1	18	1	12	10*
2	18	1	12	8*	3	18	1	12	8*	0	0	2	296	276
0	1	2	160	153	1	1	2	468	446	0	2	2	30	28
1	2	2	248	230	2	2	2	354	334	0	3	2	397	358

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Si$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	3	2	302	293	2	3	2	154	149	3	3	2	307	287
0	4	2	317	304	1	4	2	148	128	2	4	2	336	321
3	4	2	190	181	4	4	2	32	35	0	5	2	118	110
1	5	2	309	295	2	5	2	170	167	3	5	2	106	105
4	5	2	83	86	5	5	2	93	96	0	6	2	26	31
1	6	2	135	127	2	6	2	93	97	3	6	2	50	46
4	6	2	108	112	5	6	2	52	53	6	6	2	107	108
0	7	2	8	11*	1	7	2	70	75	2	7	2	46	49
3	7	2	119	125	4	7	2	109	110	5	7	2	130	129
6	7	2	65	64	7	7	2	83	89	0	8	2	84	86
1	8	2	97	100	2	8	2	136	138	3	8	2	70	71
4	8	2	124	128	5	8	2	112	112	6	8	2	68	69
7	8	2	43	46	8	8	2	57	56	0	9	2	20	23
1	9	2	22	24	2	9	2	40	43	3	9	2	63	66
4	9	2	86	92	5	9	2	66	67	6	9	2	37	37
7	9	2	29	33	8	9	2	9	13*	9	9	2	66	65
0	10	2	80	84	1	10	2	8	2*	2	10	2	71	69
3	10	2	46	50	4	10	2	104	106	5	10	2	16	19*
6	10	2	56	59	7	10	2	17	22*	8	10	2	39	36
9	10	2	19	22*	10	10	2	37	38	0	11	2	10	3*
1	11	2	75	78	2	11	2	31	33	3	11	2	102	102
4	11	2	21	25*	5	11	2	51	49	6	11	2	50	52
7	11	2	29	25	8	11	2	10	16*	9	11	2	40	36
10	11	2	11	1*	11	11	2	29	25	0	12	2	46	47
1	12	2	26	27	2	12	2	56	55	3	12	2	33	32
4	12	2	39	39	5	12	2	30	32	6	12	2	35	35
7	12	2	13	16*	8	12	2	23	26*	9	12	2	5	9*
10	12	2	31	31	11	12	2	12	8*	12	12	2	32	26
0	13	2	13	14*	1	13	2	50	47	2	13	2	40	40
3	13	2	41	43	4	13	2	16	23*	5	13	2	28	30
6	13	2	15	9*	7	13	2	40	38	8	13	2	20	15*
9	13	2	26	26	10	13	2	10	15*	11	13	2	19	14*
12	13	2	12	1*	0	14	2	44	39	1	14	2	23	23
2	14	2	30	33	3	14	2	11	22*	4	14	2	28	24
5	14	2	20	13*	6	14	2	33	33	7	14	2	11	8*
8	14	2	15	19*	9	14	2	12	7*	10	14	2	9	11*
11	14	2	12	6*	0	15	2	17	16*	1	15	2	24	26
2	15	2	11	2*	3	15	2	11	14*	4	15	2	6	10*
5	15	2	14	13*	6	15	2	5	12*	7	15	2	15	19*
8	15	2	12	8*	9	15	2	11	13*	10	15	2	18	12*
0	16	2	12	21*	1	16	2	4	5*	2	16	2	19	18*
3	16	2	14	7*	4	16	2	20	12*	5	16	2	20	10*
6	16	2	12	17*	7	16	2	5	9*	8	16	2	19	11*
0	17	2	14	8*	1	17	2	25	24*	2	17	2	12	10*
3	17	2	17	16*	4	17	2	12	4*	5	17	2	10	11*
6	17	2	10	2*	0	18	2	12	11*	1	18	2	13	3*
2	18	2	24	10*	0	1	3	54	59	0	2	3	229	208
1	2	3	133	130	0	3	3	111	107	1	3	3	124	110

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Si$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	3	3	348	329	0	4	3	177	170	1	4	3	107	99
2	4	3	27	29	3	4	3	290	282	0	5	3	52	44
1	5	3	67	67	2	5	3	138	142	3	5	3	73	75
4	5	3	209	216	0	6	3	72	65	1	6	3	116	116
2	6	3	90	89	3	6	3	197	200	4	6	3	74	76
5	6	3	181	187	0	7	3	83	85	1	7	3	64	59
2	7	3	54	55	3	7	3	64	66	4	7	3	157	157
5	7	3	61	64	6	7	3	14	16*	0	8	3	8	13*
1	8	3	28	25	2	8	3	51	54	3	8	3	21	22
4	8	3	46	46	5	8	3	75	79	6	8	3	86	85
7	8	3	34	33	0	9	3	80	78	1	9	3	38	41
2	9	3	42	45	3	9	3	45	47	4	9	3	79	79
5	9	3	35	39	6	9	3	36	36	7	9	3	31	33
8	9	3	59	58	0	10	3	10	8*	1	10	3	81	83
2	10	3	52	53	3	10	3	55	58	4	10	3	16	22*
5	10	3	76	78	6	10	3	5	20*	7	10	3	44	43
8	10	3	10	10*	9	10	3	38	38	0	11	3	77	78
1	11	3	9	17*	2	11	3	64	65	3	11	3	14	14*
4	11	3	84	83	5	11	3	5	19*	6	11	3	45	43
7	11	3	24	21	8	11	3	46	42	9	11	3	11	8*
10	11	3	12	17*	0	12	3	13	14*	1	12	3	61	60
2	12	3	19	18*	3	12	3	59	60	4	12	3	15	15*
5	12	3	62	60	6	12	3	14	21*	7	12	3	38	35
8	12	3	11	2*	9	12	3	22	24*	10	12	3	19	17*
11	12	3	12	16*	0	13	3	10	17*	1	13	3	10	20*
2	13	3	29	31	3	13	3	10	5*	4	13	3	44	41
5	13	3	18	12*	6	13	3	34	30	7	13	3	11	16*
8	13	3	34	26	9	13	3	27	17	10	13	3	3	20*
11	13	3	12	6*	12	13	3	12	12*	0	14	3	11	1*
1	14	3	7	14*	2	14	3	16	11*	3	14	3	13	17*
4	14	3	18	17*	5	14	3	22	18*	6	14	3	9	7*
7	14	3	27	21	8	14	3	14	6*	9	14	3	12	12*
10	14	3	12	13*	11	14	3	9	13*	0	15	3	15	16*
1	15	3	20	21*	2	15	3	14	22*	3	15	3	5	4*
4	15	3	20	19*	5	15	3	12	9*	6	15	3	13	10*
7	15	3	12	3*	8	15	3	12	2*	9	15	3	13	10*
0	16	3	12	10*	1	16	3	7	11*	2	16	3	16	13*
3	16	3	16	16*	4	16	3	12	6*	5	16	3	5	11*
6	16	3	12	12*	7	16	3	12	9*	0	17	3	14	3*
1	17	3	14	11*	2	17	3	12	11*	3	17	3	11	4*
4	17	3	12	9*	5	17	3	13	13*	0	0	4	119	118
0	1	4	115	107	1	1	4	43	47	0	2	4	118	116
1	2	4	124	114	2	2	4	266	257	0	3	4	67	63
1	3	4	136	130	2	3	4	71	73	3	3	4	235	226
0	4	4	11	18*	1	4	4	26	25	2	4	4	90	88
3	4	4	48	46	4	4	4	206	204	0	5	4	8	9*
1	5	4	61	63	2	5	4	50	49	3	5	4	148	150
4	5	4	153	158	5	5	4	144	144	0	6	4	114	114

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Si$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	6	4	53	57	2	6	4	97	94	3	6	4	99	101
4	6	4	119	121	5	6	4	66	66	6	6	4	109	110
0	7	4	35	40	1	7	4	76	78	2	7	4	57	56
3	7	4	94	98	4	7	4	77	78	5	7	4	61	61
6	7	4	100	105	7	7	4	21	17	0	8	4	30	29
1	8	4	38	38	2	8	4	25	23	3	8	4	59	62
4	8	4	51	49	5	8	4	56	58	6	8	4	33	34
7	8	4	34	32	8	8	4	38	38	0	9	4	31	32
1	9	4	30	32	2	9	4	19	24*	3	9	4	40	44
4	9	4	30	35	5	9	4	65	64	6	9	4	15	12*
7	9	4	37	32	8	9	4	10	12*	9	9	4	48	47
0	10	4	78	78	1	10	4	26	28	2	10	4	56	55
3	10	4	20	23*	4	10	4	65	65	5	10	4	31	35
6	10	4	28	31	7	10	4	21	20*	8	10	4	34	32
9	10	4	11	11*	10	10	4	27	35	0	11	4	10	4*
1	11	4	70	69	2	11	4	30	30	3	11	4	57	54
4	11	4	14	22*	5	11	4	53	51	6	11	4	19	10*
7	11	4	16	16*	8	11	4	11	7*	9	11	4	31	28
10	11	4	11	15*	11	11	4	11	11*	0	12	4	50	48
1	12	4	15	20*	2	12	4	27	31	3	12	4	13	12*
4	12	4	57	59	5	12	4	9	13*	6	12	4	29	26
7	12	4	31	19	8	12	4	32	29	9	12	4	3	13*
10	12	4	18	16*	11	12	4	12	3*	12	12	4	9	15*
0	13	4	14	13*	1	13	4	8	18*	2	13	4	9	4*
3	13	4	28	27	4	13	4	25	21	5	13	4	33	35
6	13	4	9	14*	7	13	4	6	19*	8	13	4	9	4*
9	13	4	17	19*	10	13	4	12	6*	11	13	4	24	14*
0	14	4	11	11*	1	14	4	10	11*	2	14	4	11	17*
3	14	4	7	14*	4	14	4	27	21	5	14	4	11	19*
6	14	4	24	14*	7	14	4	12	7*	8	14	4	12	13*
9	14	4	12	16*	10	14	4	13	9*	0	15	4	12	7*
1	15	4	16	18*	2	15	4	16	18*	3	15	4	20	16*
4	15	4	21	16*	5	15	4	12	13*	6	15	4	12	6*
7	15	4	31	7*	8	15	4	12	4*	0	16	4	12	6*
1	16	4	12	2*	2	16	4	16	17*	3	16	4	12	10*
4	16	4	14	6*	5	16	4	20	16*	6	16	4	21	6*
0	17	4	16	3*	1	17	4	12	7*	2	17	4	12	9*
3	17	4	17	9*	0	1	5	70	70	0	2	5	57	55
1	2	5	45	44	0	3	5	160	162	1	3	5	149	146
2	3	5	135	136	0	4	5	74	76	1	4	5	126	125
2	4	5	44	45	3	4	5	88	89	0	5	5	89	88
1	5	5	23	25	2	5	5	102	99	3	5	5	55	54
4	5	5	37	38	0	6	5	49	51	1	6	5	103	108
2	6	5	42	42	3	6	5	66	65	4	6	5	23	21
5	6	5	106	108	0	7	5	45	45	1	7	5	10	24*
2	7	5	57	55	3	7	5	17	24*	4	7	5	98	103
5	7	5	72	72	6	7	5	47	50	0	8	5	47	50
1	8	5	48	50	2	8	5	46	50	3	8	5	37	34

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Si$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	8	5	73	77	5	8	5	85	84	6	8	5	10	25*
7	8	5	38	37	0	9	5	52	59	1	9	5	34	36
2	9	5	38	38	3	9	5	8	18*	4	9	5	73	72
5	9	5	32	32	6	9	5	9	16*	7	9	5	28	28
8	9	5	37	36	0	10	5	10	13*	1	10	5	40	40
2	10	5	25	29	3	10	5	31	33	4	10	5	21	24*
5	10	5	42	43	6	10	5	31	26	7	10	5	16	20*
8	10	5	23	23*	9	10	5	29	26	0	11	5	20	13*
1	11	5	24	21	2	11	5	34	31	3	11	5	17	16*
4	11	5	40	39	5	11	5	9	13*	6	11	5	4	14*
7	11	5	10	15*	8	11	5	22	19*	9	11	5	12	2*
10	11	5	10	21*	0	12	5	27	24	1	12	5	45	42
2	12	5	17	16*	3	12	5	26	28	4	12	5	6	11*
5	12	5	11	17*	6	12	5	18	21*	7	12	5	14	15*
8	12	5	10	5*	9	12	5	17	10*	10	12	5	12	3*
11	12	5	11	15*	0	13	5	11	16*	1	13	5	11	15*
2	13	5	31	31	3	13	5	14	12*	4	13	5	7	10*
5	13	5	10	4*	6	13	5	24	15*	7	13	5	17	6*
8	13	5	16	16*	9	13	5	12	6*	10	13	5	23	14*
0	14	5	11	5*	1	14	5	18	17*	2	14	5	22	18*
3	14	5	13	16*	4	14	5	12	9*	5	14	5	30	24
6	14	5	14	3*	7	14	5	31	27	8	14	5	12	8*
0	15	5	23	19*	1	15	5	12	5*	2	15	5	24	20*
3	15	5	11	9*	4	15	5	27	18	5	15	5	12	4*
6	15	5	18	16*	7	15	5	13	7*	0	16	5	12	0*
1	16	5	16	17*	2	16	5	12	7*	3	16	5	18	13*
4	16	5	12	2*	0	0	6	28	29	0	1	6	5	3*
1	1	6	161	169	0	2	6	112	113	1	2	6	51	50
2	2	6	119	117	0	3	6	75	77	1	3	6	30	30
2	3	6	50	51	3	3	6	95	97	0	4	6	58	59
1	4	6	18	16*	2	4	6	30	27	3	4	6	29	26
4	4	6	72	70	0	5	6	16	18*	1	5	6	90	90
2	5	6	49	47	3	5	6	40	42	4	5	6	29	31
5	5	6	55	52	0	6	6	59	60	1	6	6	42	45
2	6	6	32	33	3	6	6	35	42	4	6	6	32	29
5	6	6	10	1*	6	6	6	38	37	0	7	6	20	26*
1	7	6	89	89	2	7	6	9	3*	3	7	6	62	58
4	7	6	8	12*	5	7	6	18	22*	6	7	6	10	12*
7	7	6	61	63	0	8	6	84	83	1	8	6	25	31
2	8	6	86	91	3	8	6	17	17*	4	8	6	32	37
5	8	6	6	13*	6	8	6	61	61	7	8	6	25	20
8	8	6	19	19*	0	9	6	10	5*	1	9	6	16	22*
2	9	6	10	4*	3	9	6	44	44	4	9	6	23	30
5	9	6	8	13*	6	9	6	25	29	7	9	6	41	40
8	9	6	6	6*	9	9	6	14	16*	0	10	6	33	28
1	10	6	16	15*	2	10	6	31	25	3	10	6	23	16*
4	10	6	13	16*	5	10	6	13	30*	6	10	6	45	42
7	10	6	12	15*	8	10	6	11	15*	9	10	6	12	5*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Si$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
10	10	6	9	14*	0	11	6	30	28	1	11	6	30	30
2	11	6	11	16*	3	11	6	26	20	4	11	6	20	18*
5	11	6	11	5*	6	11	6	7	15*	7	11	6	12	16*
8	11	6	12	6*	9	11	6	12	15*	10	11	6	12	6*
11	11	6	12	6*	0	12	6	8	15*	1	12	6	7	18*
2	12	6	28	19	3	12	6	11	7*	4	12	6	7	2*
5	12	6	4	15*	6	12	6	12	17*	7	12	6	5	3*
8	12	6	12	11*	9	12	6	12	8*	10	12	6	6	9*
0	13	6	17	5*	1	13	6	10	16*	2	13	6	12	14*
3	13	6	2	19*	4	13	6	12	5*	5	13	6	17	17*
6	13	6	9	6*	7	13	6	15	11*	8	13	6	9	4*
0	14	6	39	34	1	14	6	15	19*	2	14	6	3	20*
3	14	6	8	10*	4	14	6	14	21*	5	14	6	12	3*
6	14	6	16	11*	7	14	6	13	0*	0	15	6	12	0*
1	15	6	9	12*	2	15	6	12	9*	3	15	6	16	12*
4	15	6	13	5*	0	1	7	163	159	0	2	7	63	60
1	2	7	30	30	0	3	7	12	17*	1	3	7	70	70
2	3	7	42	43	0	4	7	20	25*	1	4	7	42	43
2	4	7	18	21*	3	4	7	36	34	0	5	7	14	20*
1	5	7	9	13*	2	5	7	47	47	3	5	7	41	44
4	5	7	18	21*	0	6	7	22	18	1	6	7	27	25
2	6	7	14	17*	3	6	7	38	39	4	6	7	36	36
5	6	7	34	30	0	7	7	46	45	1	7	7	30	37
2	7	7	50	48	3	7	7	24	24	4	7	7	27	26
5	7	7	24	16	6	7	7	41	40	0	8	7	10	15*
1	8	7	65	65	2	8	7	15	26*	3	8	7	27	24
4	8	7	18	24*	5	8	7	25	15	6	8	7	15	21*
7	8	7	35	31	0	9	7	63	62	1	9	7	14	21*
2	9	7	37	37	3	9	7	16	13*	4	9	7	8	10*
5	9	7	12	9*	6	9	7	23	21*	7	9	7	9	4*
8	9	7	26	25	0	10	7	13	20*	1	10	7	26	24
2	10	7	17	10*	3	10	7	11	13*	4	10	7	12	13*
5	10	7	22	11*	6	10	7	16	12*	7	10	7	24	22*
8	10	7	8	4*	9	10	7	12	9*	0	11	7	11	6*
1	11	7	11	15*	2	11	7	11	8*	3	11	7	11	5*
4	11	7	12	3*	5	11	7	12	6*	6	11	7	20	21*
7	11	7	12	14*	8	11	7	7	12*	9	11	7	12	14*
0	12	7	37	31	1	12	7	8	7*	2	12	7	25	20
3	12	7	12	10*	4	12	7	13	10*	5	12	7	15	13*
6	12	7	12	11*	7	12	7	14	12*	8	12	7	11	4*
0	13	7	17	16*	1	13	7	12	14*	2	13	7	18	21*
3	13	7	15	7*	4	13	7	12	7*	5	13	7	16	3*
6	13	7	11	11*	0	14	7	12	8*	1	14	7	4	12*
2	14	7	6	16*	3	14	7	12	11*	4	14	7	13	3*
0	0	8	58	63	0	1	8	38	44	1	1	8	38	33
0	2	8	39	39	1	2	8	33	44	2	2	8	10	20*
0	3	8	32	35	1	3	8	56	56	2	3	8	23	22*
3	3	8	42	45	0	4	8	64	64	1	4	8	29	27

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Si$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	4	8	7	17*	3	4	8	12	19*	4	4	8	23	23*
0	5	8	3	7*	1	5	8	31	29	2	5	8	12	25*
3	5	8	16	16*	4	5	8	11	8*	5	5	8	40	36
0	6	8	42	43	1	6	8	10	4*	2	6	8	36	33
3	6	8	11	15*	4	6	8	11	18*	5	6	8	8	15*
6	6	8	30	33	0	7	8	11	1*	1	7	8	11	14*
2	7	8	5	9*	3	7	8	11	15*	4	7	8	13	22*
5	7	8	20	16*	6	7	8	11	7*	7	7	8	30	29
0	8	8	11	5*	1	8	8	5	5*	2	8	8	31	24
3	8	8	15	16*	4	8	8	14	15*	5	8	8	11	7*
6	8	8	28	20	7	8	8	12	3*	8	8	8	10	13*
0	9	8	11	10*	1	9	8	25	31*	2	9	8	17	16*
3	9	8	28	30	4	9	8	12	10*	5	9	8	8	20*
6	9	8	17	3*	7	9	8	12	13*	8	9	8	12	8*
9	9	8	13	8*	0	10	8	16	5*	1	10	8	12	13*
2	10	8	26	30*	3	10	8	12	12*	4	10	8	16	7*
5	10	8	12	5*	6	10	8	6	8*	7	10	8	9	9*
8	10	8	12	8*	0	11	8	14	23*	1	11	8	12	14*
2	11	8	13	19*	3	11	8	12	3*	4	11	8	12	4*
5	11	8	17	7*	6	11	8	18	2*	7	11	8	13	13*
0	12	8	20	14*	1	12	8	7	8*	2	12	8	32	22
3	12	8	12	9*	4	12	8	12	12*	5	12	8	17	1*
0	13	8	13	9*	1	13	8	13	12*	0	1	9	4	9*
0	2	9	19	16*	1	2	9	45	43	0	3	9	11	6*
1	3	9	15	12*	2	3	9	25	21*	0	4	9	26	32*
1	4	9	36	36	2	4	9	11	13*	3	4	9	29	31
0	5	9	11	24*	1	5	9	11	15*	2	5	9	36	29
3	5	9	15	14*	4	5	9	21	28*	0	6	9	8	11*
1	6	9	7	2*	2	6	9	11	4*	3	6	9	11	11*
4	6	9	12	14*	5	6	9	12	10*	0	7	9	11	0*
1	7	9	12	11*	2	7	9	5	19*	3	7	9	12	1*
4	7	9	17	13*	5	7	9	12	15*	6	7	9	12	12*
0	8	9	18	8*	1	8	9	12	9*	2	8	9	3	7*
3	8	9	20	21*	4	8	9	16	19*	5	8	9	17	10*
6	8	9	12	1*	7	8	9	11	3*	0	9	9	12	2*
1	9	9	16	9*	2	9	9	18	4*	3	9	9	10	6*
4	9	9	12	10*	5	9	9	24	12*	6	9	9	8	8*
0	10	9	12	7*	1	10	9	22	11*	2	10	9	12	11*
3	10	9	16	17*	4	10	9	12	7*	5	10	9	8	12*
0	11	9	12	18*	1	11	9	12	6*	2	11	9	13	13*
0	0	10	15	14*	0	1	10	5	0*	1	1	10	9	8*
0	2	10	12	3*	1	2	10	12	15*	2	2	10	12	17*
0	3	10	15	2*	1	3	10	12	10*	2	3	10	9	8*
3	3	10	25	30*	0	4	10	12	4*	1	4	10	24	18*
2	4	10	21	20*	3	4	10	7	8*	4	4	10	20	24*
0	5	10	12	17*	1	5	10	12	6*	2	5	10	12	7*
3	5	10	9	20*	4	5	10	17	7*	5	5	10	29	18
0	6	10	12	1*	1	6	10	12	8*	2	6	10	12	11*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Si$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	6	10	12	6*	4	6	10	12	18*	5	6	10	12	0*
6	6	10	9	7*	0	7	10	12	2*	1	7	10	14	11*
2	7	10	11	11*	3	7	10	12	8*	4	7	10	12	2*
5	7	10	13	7*	0	8	10	12	5*	1	8	10	12	3*
2	8	10	12	3*	3	8	10	13	1*	0	1	11	12	5*
0	2	11	12	4*	1	2	11	29	14	0	3	11	12	10*
1	3	11	12	10*	2	3	11	10	8*	0	4	11	11	5*
1	4	11	16	5*	2	4	11	13	4*					

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

An * indicates weak reflections not used in the final refinements.

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	2	0	694	684	1	2	0	96	92	2	2	0	152	146
1	3	0	468	452	2	3	0	121	115	3	3	0	741	714
0	4	0	352	342	1	4	0	3	5*	2	4	0	365	351
3	4	0	179	171	4	4	0	158	156	1	5	0	322	309
2	5	0	75	71	3	5	0	365	362	4	5	0	180	167
5	5	0	217	221	0	6	0	412	400	1	6	0	103	100
2	6	0	561	555	3	6	0	244	229	4	6	0	380	385
5	6	0	4	3*	6	6	0	332	330	1	7	0	405	394
2	7	0	12	6*	3	7	0	287	278	4	7	0	7	16*
5	7	0	275	270	6	7	0	48	50	7	7	0	260	261
0	8	0	378	385	1	8	0	64	58	2	8	0	332	327
3	8	0	4	2*	4	8	0	183	184	5	8	0	79	80
6	8	0	200	202	7	8	0	5	15*	8	8	0	248	250
1	9	0	457	447	2	9	0	29	23*	3	9	0	204	205
4	9	0	50	48	5	9	0	207	206	6	9	0	20	13*
7	9	0	197	198	8	9	0	5	7*	9	9	0	80	75
0	10	0	120	119	1	10	0	41	41	2	10	0	180	177
3	10	0	15	13*	4	10	0	134	134	5	10	0	12	12*
6	10	0	154	148	7	10	0	27	1*	8	10	0	140	141
9	10	0	30	19*	10	10	0	67	58	1	11	0	69	69
2	11	0	76	74	3	11	0	58	63	4	11	0	35	35*
5	11	0	145	140	6	11	0	45	32	7	11	0	166	162
8	11	0	6	10*	9	11	0	63	61	10	11	0	33	24*
11	11	0	81	83	0	12	0	128	126	1	12	0	75	76
2	12	0	204	197	3	12	0	20	7*	4	12	0	113	110
5	12	0	12	36*	6	12	0	106	100	7	12	0	52	49
8	12	0	70	76	9	12	0	48	41*	10	12	0	66	50
11	12	0	36	16*	12	12	0	15	23*	1	13	0	151	148
2	13	0	60	63	3	13	0	103	99	4	13	0	6	0*
5	13	0	81	81	6	13	0	6	13*	7	13	0	77	77
8	13	0	37	22*	9	13	0	50	42	10	13	0	20	35*
11	13	0	42	52*	12	13	0	7	0*	13	13	0	33	27*
0	14	0	77	61	1	14	0	16	31*	2	14	0	106	101
3	14	0	27	24*	4	14	0	93	83	5	14	0	31	6*
6	14	0	69	72	7	14	0	61	4*	8	14	0	58	67
9	14	0	20	23*	10	14	0	70	69	11	14	0	31	0*
12	14	0	34	34*	13	14	0	49	7*	14	14	0	8	27*
1	15	0	103	98	2	15	0	6	12*	3	15	0	94	92
4	15	0	35	7*	5	15	0	94	87	6	15	0	7	13*
7	15	0	43	51*	8	15	0	7	1*	9	15	0	56	46
10	15	0	7	3*	11	15	0	52	37*	12	15	0	8	9*
13	15	0	25	23*	14	15	0	27	3*	0	16	0	74	63
1	16	0	31	2*	2	16	0	45	56*	3	16	0	7	7*
4	16	0	73	71	5	16	0	18	16*	6	16	0	40	37*
7	16	0	8	7*	8	16	0	32	34*	9	16	0	7	3*
10	16	0	39	33*	11	16	0	8	1*	12	16	0	9	21*
13	16	0	57	7*	1	17	0	49	32*	2	17	0	23	1*
3	17	0	7	34*	4	17	0	29	10*	5	17	0	48	42*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
6	17	0	7	8*	7	17	0	40	25*	8	17	0	31	2*
9	17	0	44	28*	10	17	0	8	1*	11	17	0	23	17*
12	17	0	8	8*	0	18	0	49	42*	1	18	0	54	6*
2	18	0	23	28*	3	18	0	37	0*	4	18	0	42	41*
5	18	0	28	3*	6	18	0	34	21*	7	18	0	8	3*
8	18	0	41	17*	9	18	0	10	1*	10	18	0	19	10*
1	19	0	24	18*	2	19	0	26	10*	3	19	0	39	20*
4	19	0	33	4*	5	19	0	8	21*	6	19	0	8	1*
7	19	0	36	15*	8	19	0	84	3*	0	20	0	8	13*
1	20	0	25	7*	2	20	0	36	11*	3	20	0	50	4*
4	20	0	25	18*	5	20	0	35	3*	6	20	0	26	16*
0	1	1	567	534	0	2	1	1043	1036	1	2	1	831	806
0	3	1	527	494	1	3	1	470	440	2	3	1	361	340
0	4	1	234	208	1	4	1	632	597	2	4	1	122	116
3	4	1	347	334	0	5	1	615	576	1	5	1	88	79
2	5	1	412	395	3	5	1	157	143	4	5	1	374	376
0	6	1	155	147	1	6	1	411	393	2	6	1	162	152
3	6	1	246	247	4	6	1	107	100	5	6	1	278	275
0	7	1	372	360	1	7	1	4	10*	2	7	1	370	362
3	7	1	56	50	4	7	1	246	242	5	7	1	31	27*
6	7	1	319	310	0	8	1	46	50	1	8	1	319	317
2	8	1	4	8*	3	8	1	362	357	4	8	1	69	65
5	8	1	230	227	6	8	1	54	50	7	8	1	211	212
0	9	1	201	193	1	9	1	61	57	2	9	1	274	271
3	9	1	135	134	4	9	1	165	168	5	9	1	54	33*
6	9	1	216	212	7	9	1	70	67	8	9	1	100	102
0	10	1	62	66	1	10	1	194	189	2	10	1	91	91
3	10	1	200	193	4	10	1	52	49	5	10	1	133	134
6	10	1	33	20*	7	10	1	155	150	8	10	1	34	48*
9	10	1	120	110	0	11	1	187	180	1	11	1	135	135
2	11	1	164	160	3	11	1	22	7*	4	11	1	114	110
5	11	1	28	28*	6	11	1	132	130	7	11	1	6	28*
8	11	1	96	89	9	11	1	6	22*	10	11	1	89	81
0	12	1	27	41*	1	12	1	114	113	2	12	1	29	23*
3	12	1	122	115	4	12	1	28	30*	5	12	1	110	103
6	12	1	23	2*	7	12	1	85	87	8	12	1	28	22*
9	12	1	83	79	10	12	1	28	21*	11	12	1	60	53
0	13	1	147	136	1	13	1	25	28*	2	13	1	114	104
3	13	1	11	11*	4	13	1	128	121	5	13	1	30	21*
6	13	1	100	99	7	13	1	36	17*	8	13	1	61	63
9	13	1	32	13*	10	13	1	54	42	11	13	1	7	13*
12	13	1	42	50*	0	14	1	23	25*	1	14	1	109	106
2	14	1	27	23*	3	14	1	97	97	4	14	1	24	14*
5	14	1	96	89	6	14	1	35	11*	7	14	1	78	66
8	14	1	7	19*	9	14	1	68	50	10	14	1	7	16*
11	14	1	38	32*	12	14	1	21	13*	13	14	1	29	30*
0	15	1	76	75	1	15	1	43	38*	2	15	1	75	61
3	15	1	25	19*	4	15	1	62	63	5	15	1	68	3*
6	15	1	57	64	7	15	1	28	18*	8	15	1	75	57
9	15	1	39	12*	10	15	1	40	37*	11	15	1	21	2*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
12	15	1	8	30*	13	15	1	13	4*	14	15	1	18	19*
0	16	1	7	10*	1	16	1	40	58*	2	16	1	38	11*
3	16	1	59	56	4	16	1	27	11*	5	16	1	50	51*
6	16	1	7	10*	7	16	1	38	45*	8	16	1	32	4*
9	16	1	29	33*	10	16	1	9	5*	11	16	1	20	23*
12	16	1	61	6*	13	16	1	8	16*	0	17	1	60	49
1	17	1	35	14*	2	17	1	41	49*	3	17	1	36	6*
4	17	1	42	41*	5	17	1	81	11*	6	17	1	44	32*
7	17	1	35	10*	8	17	1	38	22*	9	17	1	8	3*
10	17	1	13	18*	11	17	1	46	4*	12	17	1	8	15*
0	18	1	24	4*	1	18	1	35	28*	2	18	1	7	8*
3	18	1	48	28*	4	18	1	31	4*	5	18	1	26	26*
6	18	1	33	6*	7	18	1	8	18*	8	18	1	29	6*
9	18	1	42	19*	10	18	1	8	5*	0	19	1	8	21*
1	19	1	27	7*	2	19	1	28	21*	3	19	1	71	8*
4	19	1	29	25*	5	19	1	31	5*	6	19	1	43	21*
7	19	1	29	3*	8	19	1	24	16*	0	20	1	31	8*
1	20	1	8	19*	2	20	1	39	5*	3	20	1	37	20*
4	20	1	41	5*	5	20	1	8	21*	6	20	1	38	3*
0	0	2	69	66	0	1	2	180	176	1	1	2	599	583
0	2	2	292	277	1	2	2	278	253	2	2	2	670	637
0	3	2	394	351	1	3	2	571	529	2	3	2	165	155
3	3	2	478	453	0	4	2	573	535	1	4	2	133	120
2	4	2	586	558	3	4	2	216	203	4	4	2	249	243
0	5	2	96	88	1	5	2	514	490	2	5	2	205	193
3	5	2	333	329	4	5	2	88	87	5	5	2	305	297
0	6	2	228	227	1	6	2	144	134	2	6	2	274	272
3	6	2	51	48	4	6	2	309	304	5	6	2	62	64
6	6	2	270	264	0	7	2	7	13*	1	7	2	239	235
2	7	2	45	43	3	7	2	290	285	4	7	2	128	127
5	7	2	283	279	6	7	2	70	69	7	7	2	181	173
0	8	2	263	258	1	8	2	105	103	2	8	2	232	226
3	8	2	83	79	4	8	2	268	267	5	8	2	107	109
6	8	2	172	169	7	8	2	62	54	8	8	2	139	136
0	9	2	25	26*	1	9	2	175	170	2	9	2	46	51
3	9	2	201	194	4	9	2	77	78	5	9	2	181	173
6	9	2	60	56	7	9	2	124	117	8	9	2	18	18*
9	9	2	144	139	0	10	2	215	206	1	10	2	5	12*
2	10	2	189	182	3	10	2	67	69	4	10	2	217	212
5	10	2	5	16*	6	10	2	136	134	7	10	2	31	20*
8	10	2	108	102	9	10	2	34	23*	10	10	2	93	91
0	11	2	29	3*	1	11	2	185	180	2	11	2	24	36*
3	11	2	194	195	4	11	2	18	29*	5	11	2	133	128
6	11	2	48	56	7	11	2	92	87	8	11	2	25	20*
9	11	2	89	85	10	11	2	64	2*	11	11	2	66	61
0	12	2	133	127	1	12	2	27	33*	2	12	2	131	122
3	12	2	33	32*	4	12	2	106	103	5	12	2	28	35*
6	12	2	108	99	7	12	2	6	13*	8	12	2	83	,8
9	12	2	38	12*	10	12	2	74	67	11	12	2	8	11*
12	12	2	74	55	0	13	2	14	15*	1	13	2	107	97

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	13	2	63	52	3	13	2	106	101	4	13	2	51	29
5	13	2	89	83	6	13	2	6	6*	7	13	2	89	86
8	13	2	39	18*	9	13	2	69	61	10	13	2	27	21*
11	13	2	53	40*	12	13	2	39	2*	13	13	2	7	31*
0	14	2	93	87	1	14	2	37	29*	2	14	2	79	81
3	14	2	27	24*	4	14	2	75	71	5	14	2	20	17*
6	14	2	82	76	7	14	2	27	6*	8	14	2	51	47*
9	14	2	31	7*	10	14	2	17	29*	11	14	2	23	5*
12	14	2	7	29*	13	14	2	30	2*	14	14	2	35	20*
0	15	2	52	20	1	15	2	48	55*	2	15	2	32	4*
3	15	2	54	53	4	15	2	7	12*	5	15	2	61	49
6	15	2	7	13*	7	15	2	55	48	8	15	2	24	11*
9	15	2	43	33*	10	15	2	64	14*	11	15	2	34	23*
12	15	2	30	6*	13	15	2	37	22*	14	15	2	8	1*
0	16	2	61	56	1	16	2	37	8*	2	16	2	41	46*
3	16	2	7	6*	4	16	2	54	40	5	16	2	7	9*
6	16	2	48	43*	7	16	2	44	10*	8	16	2	29	34*
9	16	2	7	5*	10	16	2	39	26*	11	16	2	25	4*
12	16	2	70	20*	13	16	2	33	3*	0	17	2	7	10*
1	17	2	54	51	2	17	2	23	10*	3	17	2	66	40*
4	17	2	34	3*	5	17	2	33	33*	6	17	2	7	6*
7	17	2	57	30*	8	17	2	8	6*	9	17	2	33	28*
10	17	2	40	5*	11	17	2	11	16*	0	18	2	49	35*
1	18	2	28	3*	2	18	2	40	30*	3	18	2	35	10*
4	18	2	32	27*	5	18	2	8	13*	6	18	2	55	27*
7	18	2	21	3*	8	18	2	13	24*	9	18	2	8	2*
10	18	2	9	18*	0	19	2	30	3*	1	19	2	62	26*
2	19	2	67	7*	3	19	2	39	25*	4	19	2	41	13*
5	19	2	40	25*	6	19	2	32	1*	7	19	2	48	20*
8	19	2	9	5*	0	20	2	9	22*	1	20	2	18	3*
2	20	2	22	22*	3	20	2	12	4*	4	20	2	8	18*
5	20	2	8	4*	0	1	3	299	293	0	2	3	185	171
1	2	3	399	375	0	3	3	358	340	1	3	3	81	75
2	3	3	562	536	0	4	3	188	177	1	4	3	223	214
2	4	3	52	46	3	4	3	506	487	0	5	3	155	162
1	5	3	65	59	2	5	3	319	309	3	5	3	85	84
4	5	3	388	382	0	6	3	67	60	1	6	3	303	294
2	6	3	78	72	3	6	3	351	341	4	6	3	84	81
5	6	3	289	282	0	7	3	260	251	1	7	3	62	58
2	7	3	214	206	3	7	3	57	59	4	7	3	240	231
5	7	3	90	88	6	7	3	95	88	0	8	3	5	11*
1	8	3	159	153	2	8	3	62	65	3	8	3	149	145
4	8	3	47	45	5	8	3	181	176	6	8	3	94	96
7	8	3	109	105	0	9	3	201	193	1	9	3	50	53
2	9	3	162	153	3	9	3	47	51	4	9	3	195	189
5	9	3	35	45*	6	9	3	140	132	7	9	3	25	29*
8	9	3	133	132	0	10	3	5	1*	1	10	3	183	177
2	10	3	41	47*	3	10	3	159	153	4	10	3	22	17*
5	10	3	171	168	6	10	3	24	21*	7	10	3	114	108
8	10	3	22	12*	9	10	3	82	80	0	11	3	179	167

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	11	3	31	19*	2	11	3	154	148	3	11	3	26	16*
4	11	3	167	161	5	11	3	25	16*	6	11	3	109	105
7	11	3	28	15*	8	11	3	93	93	9	11	3	6	9*
10	11	3	58	52	0	12	3	6	24*	1	12	3	129	128
2	12	3	36	14*	3	12	3	130	122	4	12	3	35	16*
5	12	3	115	115	6	12	3	31	19*	7	12	3	85	81
8	12	3	25	8*	9	12	3	65	62	10	12	3	7	24*
11	12	3	52	44*	0	13	3	66	70	1	13	3	14	19*
2	13	3	75	75	3	13	3	33	9*	4	13	3	91	84
5	13	3	7	10*	6	13	3	52	58	7	13	3	13	11*
8	13	3	60	61	9	13	3	29	23*	10	13	3	39	49*
11	13	3	43	7*	12	13	3	42	32*	0	14	3	28	1*
1	14	3	56	58	2	14	3	25	19*	3	14	3	60	56
4	14	3	43	18*	5	14	3	63	50	6	14	3	7	6*
7	14	3	51	45*	8	14	3	31	8*	9	14	3	39	40*
10	14	3	7	15*	11	14	3	19	34*	12	14	3	19	6*
13	14	3	8	18*	0	15	3	61	53	1	15	3	7	26*
2	15	3	66	61	3	15	3	7	9*	4	15	3	58	50
5	15	3	37	8*	6	15	3	7	30*	7	15	3	7	8*
8	15	3	31	26*	9	15	3	7	11*	10	15	3	7	26*
11	15	3	12	5*	12	15	3	24	17*	13	15	3	8	5*
0	16	3	32	11*	1	16	3	45	42*	2	16	3	33	16*
3	16	3	27	40*	4	16	3	47	11*	5	16	3	24	31*
6	16	3	7	21*	7	16	3	7	29*	8	16	3	41	5*
9	16	3	12	20*	10	16	3	18	4*	11	16	3	43	21*
12	16	3	22	7*	0	17	3	7	26*	1	17	3	7	13*
2	17	3	38	35*	3	17	3	19	4*	4	17	3	33	31*
5	17	3	36	17*	6	17	3	46	34*	7	17	3	8	11*
8	17	3	34	27*	9	17	3	33	5*	10	17	3	34	21*
11	17	3	30	3*	0	18	3	24	3*	1	18	3	37	34*
2	18	3	18	12*	3	18	3	16	32*	4	18	3	33	6*
5	18	3	56	29*	6	18	3	45	5*	7	18	3	44	32*
8	18	3	35	4*	9	18	3	48	16*	0	19	3	47	30*
1	19	3	37	5*	2	19	3	39	29*	3	19	3	8	5*
4	19	3	46	17*	5	19	3	8	3*	6	19	3	21	22*
7	19	3	43	1*	0	20	3	25	1*	1	20	3	52	21*
2	20	3	8	2*	3	20	3	31	13*	0	0	4	134	130
0	1	4	122	115	1	1	4	241	241	0	2	4	314	308
1	2	4	133	121	2	2	4	416	405	0	3	4	86	77
1	3	4	324	310	2	3	4	77	74	3	3	4	351	347
0	4	4	212	207	1	4	4	20	22*	2	4	4	258	246
3	4	4	49	41	4	4	4	338	328	0	5	4	13	14*
1	5	4	233	226	2	5	4	41	40	3	5	4	273	268
4	5	4	162	157	5	5	4	256	247	0	6	4	256	248
1	6	4	75	72	2	6	4	228	220	3	6	4	107	106
4	6	4	233	229	5	6	4	78	75	6	6	4	176	170
0	7	4	38	49*	1	7	4	215	203	2	7	4	57	57
3	7	4	214	204	4	7	4	87	88	5	7	4	161	152
6	7	4	93	94	7	7	4	118	113	0	8	4	141	134
1	8	4	28	36*	2	8	4	138	125	3	8	4	53	54

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	8	4	158	152	5	8	4	52	50	6	8	4	116	111
7	8	4	44	35*	8	8	4	117	104	0	9	4	41	43
1	9	4	141	134	2	9	4	5	21*	3	9	4	136	131
4	9	4	30	35*	5	9	4	143	137	6	9	4	36	8*
7	9	4	103	94	8	9	4	32	13*	9	9	4	106	100
0	10	4	167	161	1	10	4	38	28*	2	10	4	140	137
3	10	4	28	30*	4	10	4	139	135	5	10	4	30	35*
6	10	4	96	89	7	10	4	10	21*	8	10	4	89	84
9	10	4	6	9*	10	10	4	71	71	0	11	4	6	6*
1	11	4	136	132	2	11	4	37	38*	3	11	4	114	110
4	11	4	20	21*	5	11	4	111	104	6	11	4	29	13*
7	11	4	63	63	8	11	4	6	2*	9	11	4	63	64
10	11	4	23	16*	11	11	4	41	38*	0	12	4	110	101
1	12	4	6	20*	2	12	4	89	84	3	12	4	33	12*
4	12	4	105	101	5	12	4	6	10*	6	12	4	62	65
7	12	4	40	21*	8	12	4	74	63	9	12	4	33	17*
10	12	4	52	40*	11	12	4	28	4*	12	12	4	38	33*
0	13	4	10	12*	1	13	4	77	68	2	13	4	36	5*
3	13	4	75	70	4	13	4	6	25*	5	13	4	72	67
6	13	4	33	13*	7	13	4	60	49	8	13	4	24	3*
9	13	4	42	43*	10	13	4	19	6*	11	13	4	39	33*
12	13	4	26	1*	13	13	4	26	22*	0	14	4	61	49
1	14	4	15	11*	2	14	4	38	51*	3	14	4	26	21*
4	14	4	31	48*	5	14	4	42	23*	6	14	4	54	38
7	14	4	11	7*	8	14	4	29	37*	9	14	4	7	15*
10	14	4	43	27*	11	14	4	26	3*	12	14	4	30	21*
13	14	4	8	3*	14	14	4	16	13*	0	15	4	7	8*
1	15	4	40	49*	2	15	4	14	18*	3	15	4	55	45
4	15	4	11	17*	5	15	4	7	33*	6	15	4	23	6*
7	15	4	14	29*	8	15	4	9	3*	9	15	4	41	23*
10	15	4	8	1*	11	15	4	8	19*	12	15	4	8	5*
13	15	4	8	11*	0	16	4	43	34*	1	16	4	7	1*
2	16	4	37	45*	3	16	4	17	11*	4	16	4	22	29*
5	16	4	27	16*	6	16	4	24	29*	7	16	4	7	17*
8	16	4	41	28*	9	16	4	8	1*	10	16	4	17	20*
11	16	4	8	4*	0	17	4	29	1*	1	17	4	46	27*
2	17	4	7	9*	3	17	4	33	28*	4	17	4	18	10*
5	17	4	8	23*	6	17	4	37	2*	7	17	4	31	26*
8	17	4	25	2*	9	17	4	9	21*	10	17	4	8	3*
0	18	4	55	23*	1	18	4	37	5*	2	18	4	46	30*
3	18	4	8	9*	4	18	4	8	20*	5	18	4	36	9*
6	18	4	8	23*	7	18	4	8	1*	8	18	4	8	17*
0	19	4	31	1*	1	19	4	39	25*	2	19	4	8	3*
3	19	4	43	20*	4	19	4	43	10*	5	19	4	15	16*
0	1	5	238	240	0	2	5	32	36*	1	2	5	194	187
0	3	5	293	284	1	3	5	148	143	2	3	5	245	240
0	4	5	78	76	1	4	5	254	243	2	4	5	74	70
3	4	5	158	150	0	5	5	215	207	1	5	5	23	18*
2	5	5	194	188	3	5	5	46	41	4	5	5	82	80
0	6	5	43	40	1	6	5	203	198	2	6	5	28	35*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	6	5	160	154	4	6	5	45	30	5	6	5	172	168
0	7	5	147	141	1	7	5	27	38*	2	7	5	151	145
3	7	5	5	19*	4	7	5	172	172	5	7	5	89	92
6	7	5	129	125	0	8	5	50	51	1	8	5	144	142
2	8	5	54	48	3	8	5	124	120	4	8	5	79	83
5	8	5	134	134	6	8	5	34	29*	7	8	5	99	98
0	9	5	129	133	1	9	5	48	40	2	9	5	116	113
3	9	5	20	16*	4	9	5	129	124	5	9	5	49	36
6	9	5	56	61	7	9	5	23	33*	8	9	5	82	79
0	10	5	33	19*	1	10	5	88	92	2	10	5	40	32*
3	10	5	93	85	4	10	5	6	27*	5	10	5	74	77
6	10	5	53	37	7	10	5	81	59	8	10	5	39	27*
9	10	5	64	56	0	11	5	74	64	1	11	5	17	22*
2	11	5	85	82	3	11	5	6	17*	4	11	5	75	72
5	11	5	6	13*	6	11	5	55	46	7	11	5	7	13*
8	11	5	50	49*	9	11	5	33	9*	10	11	5	64	47
0	12	5	27	27*	1	12	5	95	82	2	12	5	20	15*
3	12	5	60	63	4	12	5	33	8*	5	12	5	81	46*
6	12	5	7	18*	7	12	5	54	45	8	12	5	7	7*
9	12	5	30	34*	10	12	5	17	5*	11	12	5	35	30*
0	13	5	54	50	1	13	5	17	14*	2	13	5	62	63
3	13	5	30	14*	4	13	5	44	41*	5	13	5	7	7*
6	13	5	57	48	7	13	5	7	2*	8	13	5	42	37*
9	13	5	8	8*	10	13	5	41	30*	11	13	5	8	3*
12	13	5	25	20*	0	14	5	29	12*	1	14	5	50	50*
2	14	5	36	20*	3	14	5	47	43*	4	14	5	7	5*
5	14	5	46	48*	6	14	5	8	4*	7	14	5	33	44*
8	14	5	7	9*	9	14	5	39	25*	10	14	5	8	2*
11	14	5	34	16*	12	14	5	16	3*	13	14	5	37	16*
0	15	5	40	44*	1	15	5	14	1*	2	15	5	41	44*
3	15	5	7	14*	4	15	5	26	38*	5	15	5	35	4*
6	15	5	51	35*	7	15	5	7	10*	8	15	5	41	21*
9	15	5	8	6*	10	15	5	49	18*	11	15	5	37	6*
12	15	5	30	12*	0	16	5	38	0*	1	16	5	42	35*
2	16	5	7	9*	3	16	5	12	29*	4	16	5	20	7*
5	16	5	23	28*	6	16	5	46	14*	7	16	5	8	21*
8	16	5	24	5*	9	16	5	43	23*	10	16	5	21	2*
0	17	5	23	25*	1	17	5	8	7*	2	17	5	8	22*
3	17	5	21	6*	4	17	5	14	21*	5	17	5	32	5*
6	17	5	44	16*	7	17	5	8	3*	8	17	5	8	17*
9	17	5	41	5*	0	18	5	13	4*	1	18	5	8	18*
2	18	5	46	7*	3	18	5	8	18*	4	18	5	39	6*
5	18	5	8	13*	6	18	5	8	3*	0	19	5	47	11*
1	19	5	41	5*	2	19	5	38	14*	3	19	5	45	5*
0	0	6	147	145	0	1	6	5	17*	1	1	6	277	274
0	2	6	202	201	1	2	6	57	49	2	2	6	191	185
0	3	6	35	41*	1	3	6	111	102	2	3	6	40	37*
3	3	6	63	66	0	4	6	143	140	1	4	6	27	20*
2	4	6	109	107	3	4	6	40	31*	4	4	6	158	156
0	5	6	15	28*	1	5	6	157	159	2	5	6	61	57

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	5	6	128	122	4	5	6	36	30*	5	5	6	110	109
0	6	6	129	127	1	6	6	35	33*	2	6	6	93	88
3	6	6	30	39*	4	6	6	71	69	5	6	6	27	10*
6	6	6	99	93	0	7	6	6	19*	1	7	6	151	150
2	7	6	36	8*	3	7	6	125	118	4	7	6	6	8*
5	7	6	73	73	6	7	6	6	10*	7	7	6	109	114
0	8	6	144	142	1	8	6	32	15*	2	8	6	150	149
3	8	6	31	22*	4	8	6	78	78	5	8	6	37	12*
6	8	6	116	113	7	8	6	38	14*	8	8	6	45	47*
0	9	6	6	0*	1	9	6	74	67	2	9	6	15	9*
3	9	6	93	84	4	9	6	6	17*	5	9	6	57	51
6	9	6	6	26*	7	9	6	78	74	8	9	6	21	3*
9	9	6	65	41	0	10	6	82	73	1	10	6	18	15*
2	10	6	66	65	3	10	6	36	22*	4	10	6	39	30*
5	10	6	33	26*	6	10	6	82	76	7	10	6	7	8*
8	10	6	47	35*	9	10	6	24	3*	10	10	6	17	31*
0	11	6	19	24*	1	11	6	54	58	2	11	6	33	19*
3	11	6	54	49	4	11	6	15	15*	5	11	6	23	35*
6	11	6	34	15*	7	11	6	55	42*	8	11	6	7	7*
9	11	6	7	35*	10	11	6	23	6*	11	11	6	37	13*
0	12	6	31	42*	1	12	6	7	14*	2	12	6	7	27*
3	12	6	37	7*	4	12	6	38	31*	5	12	6	7	16*
6	12	6	14	45*	7	12	6	7	3*	8	12	6	47	31*
9	12	6	12	10*	10	12	6	44	23*	11	12	6	42	6*
12	12	6	8	21*	0	13	6	7	14*	1	13	6	64	45
2	13	6	32	21*	3	13	6	58	48	4	13	6	7	2*
5	13	6	40	37*	6	13	6	7	6*	7	13	6	7	24*
8	13	6	39	3*	9	13	6	35	27*	10	13	6	28	14*
11	13	6	8	14*	12	13	6	41	2*	13	13	6	27	13*
0	14	6	59	59	1	14	6	43	21*	2	14	6	64	44
3	14	6	17	9*	4	14	6	29	40*	5	14	6	7	5*
6	14	6	33	25*	7	14	6	7	2*	8	14	6	41	21*
9	14	6	34	12*	10	14	6	8	18*	11	14	6	14	3*
0	15	6	38	1*	1	15	6	50	26*	2	15	6	9	8*
3	15	6	41	29*	4	15	6	32	6*	5	15	6	7	25*
6	15	6	8	3*	7	15	6	42	23*	8	15	6	32	5*
9	15	6	8	24*	10	15	6	47	6*	0	16	6	29	21*
1	16	6	35	6*	2	16	6	34	24*	3	16	6	8	7*
4	16	6	8	25*	5	16	6	23	5*	6	16	6	19	21*
7	16	6	27	7*	8	16	6	8	16*	9	16	6	31	2*
0	17	6	8	1*	1	17	6	24	20*	2	17	6	37	3*
3	17	6	30	21*	4	17	6	32	3*	5	17	6	26	17*
6	17	6	37	5*	7	17	6	8	9*	0	18	6	28	6*
1	18	6	33	3*	2	18	6	8	9*	3	18	6	35	4*
0	1	7	204	203	0	2	7	34	23*	1	2	7	75	67
0	3	7	107	102	1	3	7	81	82	2	3	7	94	91
0	4	7	6	18*	1	4	7	100	99	2	4	7	35	16*
3	4	7	92	87	0	5	7	73	71	1	5	7	30	20*
2	5	7	96	95	3	5	7	32	36*	4	5	7	57	56
0	6	7	6	16*	1	6	7	91	82	2	6	7	6	16*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	6	7	96	89	4	6	7	6	28*	5	6	7	78	75
0	7	7	80	74	1	7	7	30	35*	2	7	7	82	81
3	7	7	15	28*	4	7	7	65	64	5	7	7	34	26*
6	7	7	69	68	0	8	7	13	13*	1	8	7	93	89
2	8	7	32	27*	3	8	7	17	51*	4	8	7	37	31*
5	8	7	54	48	6	8	7	23	21*	7	8	7	56	54*
0	9	7	88	91	1	9	7	19	20*	2	9	7	82	71
3	9	7	6	9*	4	9	7	42	42*	5	9	7	7	9*
6	9	7	11	42*	7	9	7	28	7*	8	9	7	46	43*
0	10	7	30	25*	1	10	7	61	45	2	10	7	36	8*
3	10	7	32	34*	4	10	7	28	15*	5	10	7	41	41*
6	10	7	7	16*	7	10	7	46	41*	8	10	7	19	3*
9	10	7	7	19*	0	11	7	7	11*	1	11	7	38	17*
2	11	7	38	30*	3	11	7	42	6*	4	11	7	31	26*
5	11	7	7	4*	6	11	7	41	38*	7	11	7	35	16*
8	11	7	45	29*	9	11	7	42	14*	10	11	7	34	18*
0	12	7	34	30*	1	12	7	39	37*	2	12	7	36	18*
3	12	7	33	32*	4	12	7	33	10*	5	12	7	36	31*
6	12	7	7	12*	7	12	7	16	28*	8	12	7	42	2*
9	12	7	33	13*	10	12	7	75	9*	11	12	7	49	17*
0	13	7	41	32*	1	13	7	25	12*	2	13	7	54	41
3	13	7	42	4*	4	13	7	60	23	5	13	7	58	3*
6	13	7	29	25*	7	13	7	28	4*	8	13	7	8	15*
9	13	7	42	10*	10	13	7	20	14*	11	13	7	8	4*
0	14	7	30	14*	1	14	7	30	24*	2	14	7	7	14*
3	14	7	75	22*	4	14	7	22	3*	5	14	7	28	23*
6	14	7	32	1*	7	14	7	21	20*	8	14	7	8	4*
9	14	7	8	15*	10	14	7	8	2*	0	15	7	36	20*
1	15	7	27	3*	2	15	7	44	22*	3	15	7	40	6*
4	15	7	33	22*	5	15	7	40	1*	6	15	7	14	19*
7	15	7	43	6*	8	15	7	33	14*	0	16	7	8	3*
1	16	7	25	19*	2	16	7	8	1*	3	16	7	45	16*
4	16	7	72	4*	5	16	7	21	17*	6	16	7	43	4*
0	17	7	44	14*	1	17	7	8	3*	2	17	7	24	8*
3	17	7	32	2*	0	0	8	6	51*	0	1	8	32	55*
1	1	8	6	34*	0	2	8	69	76	1	2	8	31	42*
2	2	8	47	52*	0	3	8	31	28*	1	3	8	92	88
2	3	8	40	23*	3	3	8	84	76	0	4	8	91	91
1	4	8	6	26*	2	4	8	44	51*	3	4	8	37	19*
4	4	8	65	61	0	5	8	20	16*	1	5	8	69	60
2	5	8	34	19*	3	5	8	54	52	4	5	8	6	8*
5	5	8	68	67	0	6	8	61	65	1	6	8	6	4*
2	6	8	63	54	3	6	8	6	21*	4	6	8	34	48*
5	6	8	7	16*	6	6	8	26	49*	0	7	8	6	2*
1	7	8	43	34*	2	7	8	6	2*	3	7	8	7	38*
4	7	8	27	18*	5	7	8	22	38*	6	7	8	7	6*
7	7	8	46	38*	0	8	8	18	13*	1	8	8	15	3*
2	8	8	44	45*	3	8	8	7	12*	4	8	8	52	39*
5	8	8	7	1*	6	8	8	26	35*	7	8	8	37	2*
8	8	8	43	20*	0	9	8	34	20*	1	9	8	45	41*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	9	8	27	14*	3	9	8	57	49	4	9	8	16	12*
5	9	8	31	36*	6	9	8	30	3*	7	9	8	36	24*
8	9	8	7	10*	9	9	8	7	11*	0	10	8	27	20*
1	10	8	7	16*	2	10	8	48	42*	3	10	8	7	11*
4	10	8	37	27*	5	10	8	41	5*	6	10	8	42	22*
7	10	8	7	11*	8	10	8	7	19*	9	10	8	26	1*
10	10	8	8	26*	0	11	8	8	17*	1	11	8	48	30*
2	11	8	36	25*	3	11	8	16	24*	4	11	8	41	2*
5	11	8	44	23*	6	11	8	30	4*	7	11	8	51	23*
8	11	8	8	4*	9	11	8	44	20*	10	11	8	26	3*
11	11	8	76	18*	0	12	8	37	29*	1	12	8	7	10*
2	12	8	56	31*	3	12	8	42	11*	4	12	8	24	27*
5	12	8	30	1*	6	12	8	33	17*	7	12	8	33	7*
8	12	8	8	15*	9	12	8	46	6*	10	12	8	24	12*
0	13	8	7	10*	1	13	8	44	19*	2	13	8	7	7*
3	13	8	38	14*	4	13	8	8	2*	5	13	8	57	20*
6	13	8	8	6*	7	13	8	44	16*	8	13	8	8	3*
9	13	8	37	8*	0	14	8	25	13*	1	14	8	46	2*
2	14	8	8	11*	3	14	8	13	3*	4	14	8	8	17*
5	14	8	9	4*	6	14	8	73	15*	7	14	8	50	3*
0	15	8	41	5*	1	15	8	8	15*	2	15	8	8	5*
3	15	8	13	10*	4	15	8	30	3*	5	15	8	8	12*
0	16	8	33	11*	1	16	8	8	3*	0	1	9	33	18*
0	2	9	29	1*	1	2	9	64	61	0	3	9	7	15*
1	3	9	7	4*	2	3	9	40	47*	0	4	9	40	17*
1	4	9	55	53	2	4	9	19	16*	3	4	9	56	51*
0	5	9	43	33*	1	5	9	7	9*	2	5	9	62	49
3	5	9	13	17*	4	5	9	49	45*	0	6	9	7	9*
1	6	9	7	17*	2	6	9	7	9*	3	6	9	19	27*
4	6	9	43	5*	5	6	9	24	25*	0	7	9	31	21*
1	7	9	12	9*	2	7	9	33	26*	3	7	9	40	4*
4	7	9	39	32*	5	7	9	7	12*	6	7	9	23	21*
0	8	9	7	8*	1	8	9	11	21*	2	8	9	32	7*
3	8	9	7	27*	4	8	9	30	15*	5	8	9	42	21*
6	8	9	29	4*	7	8	9	7	9*	0	9	9	7	18*
1	9	9	39	7*	2	9	9	7	12*	3	9	9	31	1*
4	9	9	33	22*	5	9	9	7	9*	6	9	9	7	17*
7	9	9	31	8*	8	9	9	8	14*	0	10	9	40	10*
1	10	9	67	26	2	10	9	30	9*	3	10	9	36	30*
4	10	9	13	3*	5	10	9	39	24*	6	10	9	8	9*
7	10	9	38	14*	8	10	9	14	6*	9	10	9	23	16*
0	11	9	46	30*	1	11	9	29	4*	2	11	9	41	23*
3	11	9	24	7*	4	11	9	8	25*	5	11	9	23	5*
6	11	9	42	18*	7	11	9	39	2*	8	11	9	8	10*
9	11	9	8	5*	0	12	9	8	1*	1	12	9	8	12*
2	12	9	27	4*	3	12	9	8	18*	4	12	9	27	2*
5	12	9	43	12*	6	12	9	8	3*	7	12	9	16	11*
8	12	9	8	3*	0	13	9	8	14*	1	13	9	13	3*
2	13	9	23	13*	3	13	9	40	4*	4	13	9	8	11*
5	13	9	8	2*	6	13	9	22	11*	0	14	9	8	3*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	14	9	19	9*	2	14	9	36	7*	3	14	9	48	12*
0	0	10	18	26*	0	1	10	32	1*	1	1	10	18	20*
0	2	10	8	22*	1	2	10	38	12*	2	2	10	7	29*
0	3	10	12	10*	1	3	10	7	25*	2	3	10	53	4*
3	3	10	9	41*	0	4	10	7	12*	1	4	10	28	18*
2	4	10	7	25*	3	4	10	45	7*	4	4	10	16	28*
0	5	10	7	20*	1	5	10	23	14*	2	5	10	37	6*
3	5	10	7	26*	4	5	10	44	7*	5	5	10	47	25*
0	6	10	10	21*	1	6	10	31	7*	2	6	10	7	23*
3	6	10	7	7*	4	6	10	34	25*	5	6	10	7	3*
6	6	10	47	10*	0	7	10	8	1*	1	7	10	23	20*
2	7	10	13	10*	3	7	10	41	15*	4	7	10	7	5*
5	7	10	35	12*	6	7	10	39	1*	7	7	10	8	8*
0	8	10	43	14*	1	8	10	24	2*	2	8	10	82	12*
3	8	10	46	3*	4	8	10	28	13*	5	8	10	19	10*
6	8	10	8	6*	7	8	10	8	8*	8	8	10	48	13*
0	9	10	39	2*	1	9	10	45	14*	2	9	10	8	7*
3	9	10	45	12*	4	9	10	20	7*	5	9	10	42	14*
6	9	10	38	6*	7	9	10	8	11*	8	9	10	31	1*
0	10	10	40	14*	1	10	10	40	3*	2	10	10	8	12*
3	10	10	32	7*	4	10	10	31	16*	5	10	10	8	4*
6	10	10	37	10*	7	10	10	36	2*	0	11	10	39	1*
1	11	10	8	13*	2	11	10	8	2*	3	11	10	33	14*
4	11	10	39	6*	5	11	10	29	13*	6	11	10	8	3*
0	12	10	8	11*	1	12	10	60	2*	2	12	10	8	12*
3	12	10	19	4*	0	1	11	32	9*	0	2	11	22	10*
1	2	11	7	21*	0	3	11	38	16*	1	3	11	35	10*
2	3	11	8	11*	0	4	11	8	1*	1	4	11	8	11*
2	4	11	23	6*	3	4	11	8	9*	0	5	11	8	17*
1	5	11	27	3*	2	5	11	32	13*	3	5	11	8	5*
4	5	11	8	10*	0	6	11	8	5*	1	6	11	28	14*
2	6	11	8	4*	3	6	11	49	12*	4	6	11	19	10*
5	6	11	8	10*	0	7	11	30	15*	1	7	11	48	3*
2	7	11	8	12*	3	7	11	29	7*	4	7	11	40	10*
5	7	11	8	8*	6	7	11	36	11*	0	8	11	48	1*
1	8	11	46	8*	2	8	11	39	5*	3	8	11	8	13*
4	8	11	31	4*	5	8	11	8	9*	0	9	11	28	7*
1	9	11	8	1*	2	9	11	39	9*	3	9	11	32	1*
4	9	11	8	8*	0	0	12	39	20*	0	1	12	37	3*
1	1	12	41	11*	0	2	12	37	8*	1	2	12	24	3*
2	2	12	8	5*	0	3	12	8	2*	1	3	12	43	8*
2	3	12	37	3*	3	3	12	8	7*	0	4	12	24	8*
1	4	12	8	2*	2	4	12	41	7*	3	4	12	46	0*
4	4	12	8	6*	0	5	12	8	1*	1	5	12	46	7*
2	5	12	8	1*										

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60°C)

An * indicates weak reflections not used in the final refinements.

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	1	0	791	752	0	2	0	698	671	1	2	0	96	93
2	2	0	144	143	1	3	0	455	463	2	3	0	114	113
3	3	0	733	720	0	4	0	346	344	1	4	0	18	13*
2	4	0	363	363	3	4	0	181	173	4	4	0	143	147
1	5	0	315	324	2	5	0	65	63	3	5	0	367	383
4	5	0	180	175	5	5	0	225	230	0	6	0	426	414
1	6	0	105	107	2	6	0	580	590	3	6	0	250	240
4	6	0	396	415	5	6	0	20	11*	6	6	0	348	345
1	7	0	413	407	2	7	0	26	6*	3	7	0	281	283
4	7	0	23	19*	5	7	0	278	288	6	7	0	52	53
7	7	0	301	300	0	8	0	411	418	1	8	0	69	65
2	8	0	343	347	3	8	0	17	10*	4	8	0	182	191
5	8	0	79	82	6	8	0	204	212	7	8	0	5	16*
8	8	0	305	298	1	9	0	493	491	2	9	0	39	37
3	9	0	206	218	4	9	0	47	53	5	9	0	213	227
6	9	0	31	21*	7	9	0	220	229	8	9	0	20	5*
9	9	0	80	78	0	10	0	117	116	1	10	0	58	56
2	10	0	197	202	3	10	0	18	15*	4	10	0	151	163
5	10	0	18	26*	6	10	0	159	169	7	10	0	16	0*
8	10	0	166	170	9	10	0	20	29*	10	10	0	83	73
1	11	0	83	83	2	11	0	89	91	3	11	0	69	70
4	11	0	33	38*	5	11	0	157	168	6	11	0	37	36
7	11	0	186	196	8	11	0	32	11*	9	11	0	75	71
10	11	0	14	37*	11	11	0	105	114	0	12	0	140	140
1	12	0	93	93	2	12	0	236	236	3	12	0	27	3*
4	12	0	122	126	5	12	0	48	48	6	12	0	106	113
7	12	0	63	65	8	12	0	91	93	9	12	0	52	52
10	12	0	71	66	11	12	0	7	18*	12	12	0	27	25*
1	13	0	178	179	2	13	0	64	70	3	13	0	112	113
4	13	0	15	3*	5	13	0	95	98	6	13	0	27	13*
7	13	0	87	97	8	13	0	40	24*	9	13	0	62	53
10	13	0	32	40*	11	13	0	82	71	12	13	0	9	2*
13	13	0	6	35*	0	14	0	73	68	1	14	0	34	33*
2	14	0	125	126	3	14	0	36	28*	4	14	0	110	107
5	14	0	6	9*	6	14	0	84	83	7	14	0	6	9*
8	14	0	78	86	9	14	0	8	24*	10	14	0	94	93
11	14	0	27	2*	12	14	0	43	46*	13	14	0	28	9*
14	14	0	33	39	1	15	0	89	119*	2	15	0	25	12*
3	15	0	96	113	4	15	0	16	9*	5	15	0	105	112
6	15	0	21	13*	7	15	0	63	63	8	15	0	36	2*
9	15	0	48	62*	10	15	0	33	2*	11	15	0	52	51
12	15	0	52	12*	13	15	0	28	33*	14	15	0	3	4*
0	16	0	74	81	1	16	0	7	1*	2	16	0	60	66
3	16	0	29	10*	4	16	0	75	94*	5	16	0	20	19*
6	16	0	37	45*	7	16	0	7	6*	8	16	0	53	54
9	16	0	7	2*	10	16	0	37	49*	11	16	0	55	2*
12	16	0	24	32*	13	16	0	4	8*	1	17	0	50	48*
2	17	0	22	6*	3	17	0	46	43*	4	17	0	8	12*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60°C)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
5	17	0	43	57	6	17	0	7	6*	7	17	0	53	37
8	17	0	27	4*	9	17	0	42	43*	10	17	0	6	3*
11	17	0	21	24*	12	17	0	11	9*	0	18	0	64	66
1	18	0	9	8*	2	18	0	8	39*	3	18	0	13	2*
4	18	0	35	59*	5	18	0	50	0*	6	18	0	34	29*
7	18	0	7	4*	8	18	0	50	27*	9	18	0	6	1*
10	18	0	13	12*	1	19	0	12	28*	2	19	0	7	14*
3	19	0	7	30*	4	19	0	23	8*	5	19	0	19	32*
6	19	0	22	0*	7	19	0	6	25*	8	19	0	18	3*
9	19	0	19	22*	0	20	0	31	21*	1	20	0	45	10*
2	20	0	6	17*	3	20	0	5	7*	4	20	0	22	24*
5	20	0	17	6*	6	20	0	16	26*	1	21	0	4	33*
0	1	1	539	528	0	2	1	995	1031	1	2	1	788	821
0	3	1	500	485	1	3	1	436	450	2	3	1	340	347
0	4	1	224	208	1	4	1	588	616	2	4	1	123	121
3	4	1	343	353	0	5	1	601	602	1	5	1	84	81
2	5	1	401	411	3	5	1	147	142	4	5	1	378	394
0	6	1	163	155	1	6	1	406	412	2	6	1	164	157
3	6	1	245	253	4	6	1	110	107	5	6	1	288	290
0	7	1	367	376	1	7	1	23	21*	2	7	1	373	389
3	7	1	63	59	4	7	1	252	258	5	7	1	39	41
6	7	1	340	344	0	8	1	53	55	1	8	1	323	329
2	8	1	23	10*	3	8	1	393	393	4	8	1	70	75
5	8	1	247	251	6	8	1	60	59	7	8	1	227	231
0	9	1	203	210	1	9	1	59	61	2	9	1	292	297
3	9	1	153	157	4	9	1	176	182	5	9	1	32	37*
6	9	1	235	245	7	9	1	86	86	8	9	1	112	115
0	10	1	67	72	1	10	1	214	218	2	10	1	106	104
3	10	1	222	224	4	10	1	60	61	5	10	1	146	151
6	10	1	35	20	7	10	1	173	178	8	10	1	55	60
9	10	1	137	139	0	11	1	199	210	1	11	1	153	157
2	11	1	176	178	3	11	1	17	7*	4	11	1	129	128
5	11	1	26	29*	6	11	1	151	154	7	11	1	27	34*
8	11	1	114	112	9	11	1	16	34*	10	11	1	99	100
0	12	1	57	58	1	12	1	121	128	2	12	1	36	33*
3	12	1	145	140	4	12	1	30	32*	5	12	1	126	122
6	12	1	21	4*	7	12	1	103	105	8	12	1	14	28*
9	12	1	100	104	10	12	1	49	28	11	12	1	73	72
0	13	1	161	170	1	13	1	31	36*	2	13	1	125	122
3	13	1	14	12*	4	13	1	156	149	5	13	1	35	29*
6	13	1	123	118	7	13	1	6	18*	8	13	1	79	79
9	13	1	6	16*	10	13	1	36	49*	11	13	1	20	20*
12	13	1	54	69	0	14	1	38	35*	1	14	1	127	131
2	14	1	6	28*	3	14	1	125	119	4	14	1	6	22*
5	14	1	115	107	6	14	1	30	18*	7	14	1	88	83
8	14	1	33	22*	9	14	1	81	67	10	14	1	35	22*
11	14	1	24	42*	12	14	1	21	19*	13	14	1	20	40*
0	15	1	88	95	1	15	1	52	46	2	15	1	81	73
3	15	1	33	24*	4	15	1	77	76	5	15	1	14	2*
6	15	1	92	83	7	15	1	31	23*	8	15	1	82	79

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60°C)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
9	15	1	6	16*	10	15	1	60	52	11	15	1	31	5*
12	15	1	30	43*	13	15	1	3	5*	14	15	1	2	28*
0	16	1	15	8*	1	16	1	75	74	2	16	1	6	12*
3	16	1	74	73	4	16	1	18	17*	5	16	1	71	68
6	16	1	28	16*	7	16	1	61	62	8	16	1	24	5*
9	16	1	51	47	10	16	1	6	6*	11	16	1	34	34*
12	16	1	16	8*	13	16	1	9	25*	0	17	1	65	64
1	17	1	27	18*	2	17	1	64	68	3	17	1	17	6*
4	17	1	61	55	5	17	1	31	16*	6	17	1	47	44
7	17	1	6	13*	8	17	1	17	30*	9	17	1	32	5*
10	17	1	16	27*	11	17	1	4	6*	12	17	1	15	23*
0	18	1	6	7*	1	18	1	39	41*	2	18	1	30	14*
3	18	1	57	40*	4	18	1	18	4*	5	18	1	42	37
6	18	1	22	9*	7	18	1	9	27*	8	18	1	6	13*
9	18	1	17	30*	10	18	1	6	8*	0	19	1	6	32*
1	19	1	6	10*	2	19	1	8	33*	3	19	1	6	11*
4	19	1	23	38*	5	19	1	35	5*	6	19	1	21	31*
7	19	1	5	7*	8	19	1	34	27*	0	20	1	38	14
1	20	1	27	28*	2	20	1	9	7*	3	20	1	27	29*
4	20	1	4	6*	5	20	1	27	32	6	20	1	4	3*
0	0	2	76	80	0	1	2	172	180	1	1	2	552	583
0	2	2	271	283	1	2	2	273	276	2	2	2	624	666
0	3	2	379	362	1	3	2	529	557	2	3	2	165	164
3	3	2	473	480	0	4	2	561	556	1	4	2	126	122
2	4	2	569	582	3	4	2	221	217	4	4	2	229	243
0	5	2	86	81	1	5	2	487	504	2	5	2	211	206
3	5	2	339	353	4	5	2	100	101	5	5	2	317	322
0	6	2	233	239	1	6	2	148	145	2	6	2	278	290
3	6	2	57	52	4	6	2	330	340	5	6	2	79	82
6	6	2	291	296	0	7	2	12	12*	1	7	2	237	250
2	7	2	49	46	3	7	2	299	310	4	7	2	145	146
5	7	2	301	309	6	7	2	87	84	7	7	2	188	189
0	8	2	282	296	1	8	2	116	113	2	8	2	237	244
3	8	2	86	88	4	8	2	290	300	5	8	2	120	123
6	8	2	182	186	7	8	2	64	68	8	8	2	159	165
0	9	2	35	31	1	9	2	193	192	2	9	2	57	57
3	9	2	219	224	4	9	2	87	89	5	9	2	190	200
6	9	2	73	68	7	9	2	133	137	8	9	2	31	26*
9	9	2	166	172	0	10	2	224	231	1	10	2	23	25*
2	10	2	207	204	3	10	2	82	89	4	10	2	243	247
5	10	2	25	18*	6	10	2	148	154	7	10	2	35	22*
8	10	2	122	119	9	10	2	25	29*	10	10	2	106	113
0	11	2	25	8*	1	11	2	202	209	2	11	2	39	39
3	11	2	227	231	4	11	2	41	38	5	11	2	151	152
6	11	2	65	64	7	11	2	100	104	8	11	2	29	27*
9	11	2	104	106	10	11	2	26	2*	11	11	2	75	79
0	12	2	145	154	1	12	2	36	42*	2	12	2	150	148
3	12	2	23	41*	4	12	2	116	117	5	12	2	45	43
6	12	2	129	126	7	12	2	6	14*	8	12	2	102	100
9	12	2	29	16*	10	12	2	90	91	11	12	2	5	16*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60°C)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
12	12	2	50	73	0	13	2	5	24*	1	13	2	117	117
2	13	2	67	67	3	13	2	122	122	4	13	2	40	38*
5	13	2	96	96	6	13	2	35	9*	7	13	2	118	112
8	13	2	18	27*	9	13	2	81	80	10	13	2	36	30*
11	13	2	57	54	12	13	2	8	6*	13	13	2	32	42
0	14	2	92	107	1	14	2	39	39*	2	14	2	104	102
3	14	2	34	27*	4	14	2	93	89	5	14	2	6	23*
6	14	2	106	103	7	14	2	16	10*	8	14	2	65	60
9	14	2	26	14*	10	14	2	49	40	11	14	2	9	5*
12	14	2	27	40*	13	14	2	13	3*	14	14	2	8	32*
0	15	2	35	34*	1	15	2	65	72	2	15	2	29	9*
3	15	2	77	73	4	15	2	7	14*	5	15	2	85	66
6	15	2	35	15*	7	15	2	70	65	8	15	2	6	16*
9	15	2	36	45*	10	15	2	25	21*	11	15	2	38	33*
12	15	2	4	11*	13	15	2	15	35*	14	15	2	7	2*
0	16	2	66	78	1	16	2	6	10*	2	16	2	64	61
3	16	2	59	10*	4	16	2	60	54	5	16	2	15	14*
6	16	2	64	58	7	16	2	30	15*	8	16	2	35	46*
9	16	2	21	6*	10	16	2	31	36*	11	16	2	26	8*
12	16	2	18	32*	13	16	2	2	1*	0	17	2	6	14*
1	17	2	68	70	2	17	2	34	16*	3	17	2	66	56
4	17	2	35	2*	5	17	2	51	47	6	17	2	21	10*
7	17	2	43	43	8	17	2	10	11*	9	17	2	35	41*
10	17	2	5	7*	11	17	2	14	24*	0	18	2	47	47
1	18	2	6	2*	2	18	2	39	41*	3	18	2	6	12*
4	18	2	40	41*	5	18	2	27	19*	6	18	2	38	40*
7	18	2	5	3*	8	18	2	35	36	9	18	2	21	4*
10	18	2	15	28*	0	19	2	5	3*	1	19	2	38	36
2	19	2	5	9*	3	19	2	25	38*	4	19	2	21	20*
5	19	2	33	39	6	19	2	4	4*	7	19	2	20	29*
8	19	2	15	7*	0	20	2	14	31*	1	20	2	24	3*
2	20	2	27	35*	3	20	2	4	6*	4	20	2	17	28*
5	20	2	15	8*	0	1	3	287	305	0	2	3	176	171
1	2	3	399	406	0	3	3	355	361	1	3	3	63	65
2	3	3	563	574	0	4	3	192	189	1	4	3	217	226
2	4	3	70	67	3	4	3	534	537	0	5	3	163	179
1	5	3	60	63	2	5	3	328	332	3	5	3	98	96
4	5	3	422	434	0	6	3	71	68	1	6	3	319	330
2	6	3	74	74	3	6	3	370	371	4	6	3	95	95
5	6	3	306	314	0	7	3	289	289	1	7	3	69	66
2	7	3	229	237	3	7	3	57	60	4	7	3	257	264
5	7	3	111	114	6	7	3	101	100	0	8	3	26	16*
1	8	3	173	177	2	8	3	73	78	3	8	3	165	166
4	8	3	55	57	5	8	3	210	212	6	8	3	112	116
7	8	3	127	130	0	9	3	216	216	1	9	3	60	65
2	9	3	176	175	3	9	3	52	55	4	9	3	215	219
5	9	3	41	47	6	9	3	164	161	7	9	3	29	36*
8	9	3	156	163	0	10	3	31	7*	1	10	3	206	210
2	10	3	49	53	3	10	3	173	174	4	10	3	45	17*
5	10	3	198	204	6	10	3	45	19*	7	10	3	134	133

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60°C)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
8	10	3	17	17*	9	10	3	100	101	0	11	3	192	200
1	11	3	26	25*	2	11	3	180	181	3	11	3	26	21*
4	11	3	196	196	5	11	3	17	16*	6	11	3	125	128
7	11	3	23	19*	8	11	3	117	117	9	11	3	34	13*
10	11	3	65	67	0	12	3	15	35*	1	12	3	153	157
2	12	3	18	20*	3	12	3	152	150	4	12	3	26	24*
5	12	3	146	148	6	12	3	34	27*	7	12	3	107	100
8	12	3	17	15*	9	12	3	80	78	10	12	3	10	31*
11	12	3	55	60	0	13	3	80	82	1	13	3	9	18*
2	13	3	93	95	3	13	3	20	21*	4	13	3	115	111
5	13	3	6	14*	6	13	3	83	76	7	13	3	28	14*
8	13	3	81	82	9	13	3	36	27*	10	13	3	69	72
11	13	3	6	8*	12	13	3	37	48	0	14	3	25	4*
1	14	3	73	76	2	14	3	9	25*	3	14	3	81	75
4	14	3	37	27*	5	14	3	70	70	6	14	3	10	12*
7	14	3	72	63	8	14	3	12	9*	9	14	3	57	58
10	14	3	6	18*	11	14	3	51	54	12	14	3	16	11*
13	14	3	21	30*	0	15	3	62	70	1	15	3	23	34*
2	15	3	87	86	3	15	3	6	16*	4	15	3	68	70
5	15	3	23	10*	6	15	3	32	40*	7	15	3	35	11*
8	15	3	33	35*	9	15	3	23	14*	10	15	3	41	40*
11	15	3	13	9*	12	15	3	27	26*	13	15	3	3	7*
0	16	3	34	17*	1	16	3	68	60	2	16	3	23	24*
3	16	3	68	59	4	16	3	17	18*	5	16	3	35	45*
6	16	3	31	31*	7	16	3	6	43*	8	16	3	23	8*
9	16	3	16	27*	10	16	3	51	8*	11	16	3	21	32*
12	16	3	18	7*	0	17	3	26	33*	1	17	3	6	20*
2	17	3	46	50	3	17	3	6	6*	4	17	3	38	45*
5	17	3	28	24*	6	17	3	63	53	7	17	3	23	15*
8	17	3	38	39*	9	17	3	19	8*	10	17	3	29	32*
11	17	3	3	3*	0	18	3	6	4*	1	18	3	43	47
2	18	3	27	18*	3	18	3	44	45	4	18	3	6	9*
5	18	3	28	42*	6	18	3	9	6*	7	18	3	45	49
8	18	3	21	7*	9	18	3	11	23*	0	19	3	42	44
1	19	3	18	6*	2	19	3	35	43*	3	19	3	5	8*
4	19	3	4	25*	5	19	3	4	3*	6	19	3	23	35*
7	19	3	5	3*	0	20	3	4	3*	1	20	3	18	33*
2	20	3	7	2*	3	20	3	13	21*	4	20	3	3	2*
0	0	4	156	162	0	1	4	132	129	1	1	4	256	271
0	2	4	332	339	1	2	4	141	136	2	2	4	433	450
0	3	4	94	95	1	3	4	350	353	2	3	4	89	89
3	3	4	371	391	0	4	4	245	242	1	4	4	21	23*
2	4	4	284	283	3	4	4	46	41	4	4	4	360	374
0	5	4	28	18*	1	5	4	259	259	2	5	4	42	44
3	5	4	300	303	4	5	4	181	185	5	5	4	299	297
0	6	4	291	291	1	6	4	85	85	2	6	4	255	258
3	6	4	123	125	4	6	4	265	267	5	6	4	94	97
6	6	4	204	208	0	7	4	54	66	1	7	4	240	243
2	7	4	74	72	3	7	4	243	244	4	7	4	101	106
5	7	4	191	192	6	7	4	103	110	7	7	4	145	152

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60°C)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	8	4	166	163	1	8	4	40	46*	2	8	4	149	146
3	8	4	50	53	4	8	4	182	188	5	8	4	53	56
6	8	4	141	136	7	8	4	39	45*	8	8	4	142	135
0	9	4	58	57	1	9	4	166	167	2	9	4	5	26*
3	9	4	152	156	4	9	4	48	47	5	9	4	172	172
6	9	4	5	13*	7	9	4	123	118	8	9	4	19	16*
9	9	4	134	133	0	10	4	191	197	1	10	4	46	35
2	10	4	166	165	3	10	4	41	39	4	10	4	170	171
5	10	4	28	37*	6	10	4	104	112	7	10	4	33	25*
8	10	4	111	110	9	10	4	14	12*	10	10	4	91	94
0	11	4	11	6*	1	11	4	162	164	2	11	4	55	49
3	11	4	138	138	4	11	4	16	25*	5	11	4	132	134
6	11	4	21	19*	7	11	4	78	80	8	11	4	32	2*
9	11	4	85	83	10	11	4	29	23*	11	11	4	12	54*
0	12	4	122	128	1	12	4	6	23*	2	12	4	111	110
3	12	4	21	17*	4	12	4	127	133	5	12	4	6	13*
6	12	4	82	86	7	12	4	27	27*	8	12	4	85	84
9	12	4	31	22*	10	12	4	57	56	11	12	4	30	6*
12	12	4	31	50*	0	13	4	6	16*	1	13	4	85	90
2	13	4	6	8*	3	13	4	94	95	4	13	4	33	36*
5	13	4	95	95	6	13	4	18	20*	7	13	4	77	70
8	13	4	31	7*	9	13	4	71	63	10	13	4	6	8*
11	13	4	43	51	12	13	4	22	2*	13	13	4	3	34*
0	14	4	60	64	1	14	4	31	16*	2	14	4	72	72
3	14	4	20	33*	4	14	4	63	65	5	14	4	47	36*
6	14	4	61	58	7	14	4	18	8*	8	14	4	53	55
9	14	4	19	19*	10	14	4	50	43	11	14	4	22	4*
12	14	4	16	34*	13	14	4	6	7*	14	14	4	1	23*
0	15	4	6	20*	1	15	4	77	71	2	15	4	23	26*
3	15	4	73	64	4	15	4	38	26*	5	15	4	42	49*
6	15	4	27	11*	7	15	4	58	43	8	15	4	33	4*
9	15	4	22	34*	10	15	4	26	3*	11	15	4	17	31*
12	15	4	18	8*	13	15	4	10	18*	0	16	4	51	49
1	16	4	16	3*	2	16	4	74	68	3	16	4	25	16*
4	16	4	7	43*	5	16	4	6	20*	6	16	4	33	46*
7	16	4	29	26*	8	16	4	35	42*	9	16	4	40	1*
10	16	4	28	29*	11	16	4	20	9*	0	17	4	30	1*
1	17	4	24	38*	2	17	4	31	16*	3	17	4	32	41*
4	17	4	28	19*	5	17	4	34	35*	6	17	4	6	2*
7	17	4	55	40*	8	17	4	12	3*	9	17	4	4	32*
10	17	4	3	3*	0	18	4	44	34*	1	18	4	12	7*
2	18	4	40	46*	3	18	4	9	13*	4	18	4	18	30*
5	18	4	29	14*	6	18	4	37	36*	7	18	4	24	3*
8	18	4	21	27*	0	19	4	5	2*	1	19	4	38	39
2	19	4	16	5*	3	19	4	29	33*	4	19	4	4	15*
5	19	4	12	25*	0	1	5	280	286	0	2	5	45	38
1	2	5	237	232	0	3	5	341	340	1	3	5	175	172
2	3	5	284	282	0	4	5	95	94	1	4	5	293	292
2	4	5	95	93	3	4	5	177	175	0	5	5	265	267
1	5	5	35	26*	2	5	5	235	228	3	5	5	56	48

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60°C)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	5	5	98	99	0	6	5	46	43	1	6	5	238	239
2	6	5	45	45	3	6	5	195	195	4	6	5	6	39*
5	6	5	208	210	0	7	5	185	180	1	7	5	56	56
2	7	5	183	181	3	7	5	32	19*	4	7	5	215	218
5	7	5	121	126	6	7	5	165	167	0	8	5	61	67
1	8	5	182	182	2	8	5	59	58	3	8	5	165	163
4	8	5	109	116	5	8	5	166	170	6	8	5	42	45*
7	8	5	125	131	0	9	5	165	168	1	9	5	51	55
2	9	5	147	146	3	9	5	27	17*	4	9	5	156	161
5	9	5	49	52	6	9	5	81	84	7	9	5	41	48*
8	9	5	97	105	0	10	5	54	21*	1	10	5	114	115
2	10	5	34	40*	3	10	5	108	113	4	10	5	33	39*
5	10	5	98	100	6	10	5	41	54*	7	10	5	73	79
8	10	5	28	40*	9	10	5	66	77	0	11	5	86	88
1	11	5	31	31*	2	11	5	114	112	3	11	5	41	25*
4	11	5	92	94	5	11	5	19	22*	6	11	5	62	64
7	11	5	36	14*	8	11	5	64	68	9	11	5	40	16*
10	11	5	66	71	0	12	5	57	49	1	12	5	116	114
2	12	5	26	18*	3	12	5	78	85	4	12	5	7	8*
5	12	5	56	65	6	12	5	26	24*	7	12	5	64	69
8	12	5	36	12*	9	12	5	43	53*	10	12	5	7	5*
11	12	5	17	45*	0	13	5	77	73	1	13	5	25	24*
2	13	5	83	86	3	13	5	7	22*	4	13	5	57	57
5	13	5	36	10*	6	13	5	67	72	7	13	5	58	6*
8	13	5	45	56*	9	13	5	7	18*	10	13	5	32	47*
11	13	5	6	4*	12	13	5	21	31*	0	14	5	17	17*
1	14	5	76	77	2	14	5	26	32*	3	14	5	62	64
4	14	5	7	3*	5	14	5	70	71	6	14	5	36	8*
7	14	5	67	65	8	14	5	7	15*	9	14	5	44	37*
10	14	5	18	3*	11	14	5	24	24*	12	14	5	9	5*
13	14	5	11	29*	0	15	5	73	67	1	15	5	7	1*
2	15	5	46	63*	3	15	5	34	24*	4	15	5	56	60
5	15	5	29	7*	6	15	5	47	53*	7	15	5	58	18*
8	15	5	32	35*	9	15	5	6	11*	10	15	5	26	29*
11	15	5	4	10*	12	15	5	14	21*	0	16	5	37	2*
1	16	5	33	54*	2	16	5	7	18*	3	16	5	45	43*
4	16	5	7	14*	5	16	5	36	44*	6	16	5	27	24*
7	16	5	18	35*	8	16	5	46	7*	9	16	5	17	38*
10	16	5	4	3*	0	17	5	29	41*	1	17	5	37	11*
2	17	5	18	35*	3	17	5	6	11*	4	17	5	25	34*
5	17	5	29	7*	6	17	5	15	25*	7	17	5	27	5*
8	17	5	24	30*	0	18	5	14	6*	1	18	5	30	28*
2	18	5	26	11*	3	18	5	5	31*	4	18	5	5	8*
5	18	5	23	22*	6	18	5	17	4*	0	19	5	15	16*
1	19	5	18	8*	2	19	5	4	23*	0	0	6	215	211
0	1	6	6	34*	1	1	6	368	362	0	2	6	249	258
1	2	6	70	67	2	2	6	233	231	0	3	6	33	36*
1	3	6	128	125	2	3	6	25	42*	3	3	6	69	73
0	4	6	175	176	1	4	6	35	33*	2	4	6	146	144
3	4	6	45	44*	4	4	6	213	211	0	5	6	41	43*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60^oC)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	5	6	204	209	2	5	6	80	81	3	5	6	172	166
4	5	6	35	42*	5	5	6	147	145	0	6	6	163	162
1	6	6	36	38*	2	6	6	123	122	3	6	6	56	52
4	6	6	92	88	5	6	6	6	23*	6	6	6	128	132
0	7	6	14	22*	1	7	6	202	205	2	7	6	36	18*
3	7	6	161	160	4	7	6	30	8*	5	7	6	91	100
6	7	6	25	11*	7	7	6	151	162	0	8	6	195	191
1	8	6	6	19*	2	8	6	197	207	3	8	6	32	36*
4	8	6	99	102	5	8	6	6	20*	6	8	6	150	162
7	8	6	30	18*	8	8	6	61	64	0	9	6	7	8*
1	9	6	91	97	2	9	6	36	15*	3	9	6	109	118
4	9	6	6	21*	5	9	6	75	69	6	9	6	6	32*
7	9	6	95	109	8	9	6	13	10*	9	9	6	39	62*
0	10	6	119	112	1	10	6	7	24*	2	10	6	94	94
3	10	6	15	35*	4	10	6	53	39	5	10	6	13	36*
6	10	6	112	115	7	10	6	20	10*	8	10	6	50	56*
9	10	6	37	3*	10	10	6	40	45*	0	11	6	25	33*
1	11	6	87	81	2	11	6	30	30*	3	11	6	78	72
4	11	6	23	26*	5	11	6	42	55*	6	11	6	7	20*
7	11	6	65	68	8	11	6	18	9*	9	11	6	63	57
10	11	6	30	9*	11	11	6	6	19*	0	12	6	67	63
1	12	6	45	23*	2	12	6	12	35*	3	12	6	19	7*
4	12	6	24	49*	5	12	6	23	23*	6	12	6	67	70
7	12	6	7	6*	8	12	6	33	50*	9	12	6	7	16*
10	12	6	19	36*	11	12	6	28	12*	12	12	6	24	40*
0	13	6	38	27*	1	13	6	81	70	2	13	6	36	35*
3	13	6	82	78	4	13	6	18	2*	5	13	6	59	54
6	13	6	7	12*	7	13	6	7	34*	8	13	6	12	2*
9	13	6	35	43*	10	13	6	29	25*	11	13	6	5	23*
12	13	6	20	4*	0	14	6	95	96	1	14	6	34	36*
2	14	6	75	67	3	14	6	35	15*	4	14	6	54	62
5	14	6	7	9*	6	14	6	47	39*	7	14	6	7	6*
8	14	6	33	36*	9	14	6	6	19*	10	14	6	32	30*
11	14	6	4	3*	0	15	6	27	2*	1	15	6	13	39*
2	15	6	19	11*	3	15	6	31	46*	4	15	6	7	9*
5	15	6	47	40*	6	15	6	15	2*	7	15	6	48	39*
8	15	6	6	7*	9	15	6	38	45	10	15	6	4	9*
0	16	6	41	34*	1	16	6	7	8*	2	16	6	30	38*
3	16	6	62	13*	4	16	6	35	42*	5	16	6	6	7*
6	16	6	28	36*	7	16	6	8	10*	8	16	6	20	27*
9	16	6	3	4*	0	17	6	38	5*	1	17	6	32	34*
2	17	6	48	5*	3	17	6	26	37*	4	17	6	16	5*
5	17	6	23	31*	6	17	6	35	9*	0	18	6	6	14*
1	18	6	22	4*	2	18	6	20	16*	3	18	6	15	10*
0	1	7	275	284	0	2	7	13	9*	1	2	7	85	87
0	3	7	154	155	1	3	7	113	120	2	3	7	137	136
0	4	7	34	19*	1	4	7	137	141	2	4	7	33	24*
3	4	7	116	126	0	5	7	94	100	1	5	7	6	37*
2	5	7	138	140	3	5	7	47	52*	4	5	7	75	82
0	6	7	7	16*	1	6	7	123	123	2	6	7	39	24*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60^oC)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
3	6	7	126	132	4	6	7	8	39*	5	6	7	110	114
0	7	7	102	98	1	7	7	46	51*	2	7	7	111	116
3	7	7	33	44*	4	7	7	89	93	5	7	7	36	42*
6	7	7	96	99	0	8	7	12	19*	1	8	7	129	133
2	8	7	45	41*	3	8	7	60	70	4	8	7	28	46*
5	8	7	66	70	6	8	7	19	31*	7	8	7	96	90
0	9	7	136	139	1	9	7	7	28*	2	9	7	107	118
3	9	7	7	15*	4	9	7	65	69	5	9	7	8	15*
6	9	7	56	61*	7	9	7	26	15*	8	9	7	54	68*
0	10	7	40	47*	1	10	7	37	70*	2	10	7	33	13*
3	10	7	60	54	4	10	7	7	26*	5	10	7	48	70*
6	10	7	14	28*	7	10	7	54	71*	8	10	7	7	9*
9	10	7	38	28*	0	11	7	32	12*	1	11	7	63	33
2	11	7	30	53*	3	11	7	46	10*	4	11	7	42	46*
5	11	7	29	12*	6	11	7	59	63	7	11	7	28	29*
8	11	7	36	51*	9	11	7	41	25*	10	11	7	34	38*
0	12	7	69	48	1	12	7	35	65*	2	12	7	28	27*
3	12	7	57	51	4	12	7	25	18*	5	12	7	40	49*
6	12	7	16	22*	7	12	7	44	48*	8	12	7	7	6*
9	12	7	7	20*	10	12	7	31	18*	11	12	7	26	33*
0	13	7	32	49*	1	13	7	33	22*	2	13	7	64	70
3	13	7	32	6*	4	13	7	7	38*	5	13	7	7	5*
6	13	7	26	41*	7	13	7	37	6*	8	13	7	21	26*
9	13	7	12	15*	10	13	7	5	26*	11	13	7	14	5*
0	14	7	44	24*	1	14	7	19	38*	2	14	7	8	22*
3	14	7	13	36*	4	14	7	7	6*	5	14	7	42	41*
6	14	7	31	6*	7	14	7	34	35*	8	14	7	5	8*
9	14	7	14	27*	10	14	7	16	2*	0	15	7	43	36*
1	15	7	45	6*	2	15	7	33	36*	3	15	7	7	11*
4	15	7	29	42*	5	15	7	12	2*	6	15	7	8	33*
7	15	7	5	12*	8	15	7	4	27*	0	16	7	68	4*
1	16	7	23	33*	2	16	7	28	3*	3	16	7	6	27*
4	16	7	23	6*	5	16	7	4	31*	6	16	7	18	7*
0	17	7	12	32*	1	17	7	6	3*	2	17	7	4	15*
3	17	7	4	4*	0	0	8	46	44*	0	1	8	83	88
1	1	8	57	48*	0	2	8	110	118	1	2	8	51	66*
2	2	8	80	89	0	3	8	7	45*	1	3	8	133	139
2	3	8	28	40*	3	3	8	101	119	0	4	8	140	150
1	4	8	27	44*	2	4	8	73	84	3	4	8	7	27*
4	4	8	105	108	0	5	8	35	27*	1	5	8	99	100
2	5	8	52	26*	3	5	8	98	85	4	5	8	43	17*
5	5	8	110	108	0	6	8	104	101	1	6	8	48	6*
2	6	8	84	82	3	6	8	41	36*	4	6	8	65	74
5	6	8	20	26*	6	6	8	71	81	0	7	8	28	5*
1	7	8	51	51*	2	7	8	7	6*	3	7	8	61	66
4	7	8	7	30*	5	7	8	49	64*	6	7	8	8	14*
7	7	8	79	62	0	8	8	8	15*	1	8	8	91	4*
2	8	8	57	77*	3	8	8	48	20*	4	8	8	76	68
5	8	8	39	5*	6	8	8	43	63*	7	8	8	33	8*
8	8	8	8	25*	0	9	8	33	44*	1	9	8	50	63*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60°C)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	9	8	39	24*	3	9	8	83	87	4	9	8	33	25*
5	9	8	63	64	6	9	8	29	6*	7	9	8	36	39*
8	9	8	18	22*	9	9	8	39	24*	0	10	8	56	39*
1	10	8	14	28*	2	10	8	73	74	3	10	8	42	22*
4	10	8	41	49*	5	10	8	28	10*	6	10	8	42	41*
7	10	8	25	21*	8	10	8	26	37*	9	10	8	38	7*
10	10	8	37	53*	0	11	8	21	24*	1	11	8	47	57*
2	11	8	74	49*	3	11	8	41	45*	4	11	8	7	3*
5	11	8	52	40	6	11	8	7	8*	7	11	8	32	42*
8	11	8	36	5*	9	11	8	40	41*	10	11	8	5	9*
11	11	8	4	35*	0	12	8	57	52*	1	12	8	38	23*
2	12	8	38	52*	3	12	8	26	23*	4	12	8	42	50*
5	12	8	32	5*	6	12	8	6	31*	7	12	8	35	15*
8	12	8	6	29*	9	12	8	5	14*	10	12	8	19	22*
0	13	8	35	18*	1	13	8	8	35*	2	13	8	8	15*
3	13	8	7	28*	4	13	8	22	4*	5	13	8	6	38*
6	13	8	14	13*	7	13	8	26	30*	8	13	8	17	9*
9	13	8	4	16*	0	14	8	38	27*	1	14	8	26	5*
2	14	8	21	19*	3	14	8	44	9*	4	14	8	29	32*
5	14	8	5	8*	6	14	8	11	28*	7	14	8	16	4*
0	15	8	35	7*	1	15	8	6	28*	2	15	8	9	10*
3	15	8	30	17*	4	15	8	42	4*	5	15	8	4	22*
0	1	9	57	33*	0	2	9	54	5*	1	2	9	99	106
0	3	9	8	24*	1	3	9	49	21*	2	3	9	84	89
0	4	9	30	18*	1	4	9	88	94	2	4	9	8	31*
3	4	9	91	94	0	5	9	46	52*	1	5	9	35	13*
2	5	9	89	88	3	5	9	42	31*	4	5	9	71	83
0	6	9	50	20*	1	6	9	43	30*	2	6	9	44	22*
3	6	9	54	54*	4	6	9	18	7*	5	6	9	37	50*
0	7	9	43	44*	1	7	9	51	18*	2	7	9	37	46*
3	7	9	37	9*	4	7	9	60	63*	5	7	9	8	20*
6	7	9	44	37*	0	8	9	45	15*	1	8	9	74	39
2	8	9	19	15*	3	8	9	52	48*	4	8	9	32	29*
5	8	9	7	38*	6	8	9	27	13*	7	8	9	9	15*
0	9	9	10	38*	1	9	9	9	17*	2	9	9	46	22*
3	9	9	8	8*	4	9	9	7	45*	5	9	9	21	21*
6	9	9	35	33*	7	9	9	22	16*	8	9	9	30	33*
0	10	9	9	24*	1	10	9	32	50*	2	10	9	50	18*
3	10	9	57	60*	4	10	9	7	5*	5	10	9	29	49*
6	10	9	36	16*	7	10	9	23	28*	8	10	9	6	16*
9	10	9	5	33*	0	11	9	61	59*	1	11	9	8	9*
2	11	9	50	46*	3	11	9	29	14*	4	11	9	33	51*
5	11	9	24	10*	6	11	9	30	37*	7	11	9	33	5*
8	11	9	4	20*	9	11	9	4	10*	0	12	9	8	5*
1	12	9	86	26*	2	12	9	7	4*	3	12	9	7	38*
4	12	9	6	6*	5	12	9	32	26*	6	12	9	17	4*
7	12	9	25	24*	0	13	9	7	27*	1	13	9	7	9*
2	13	9	6	28*	3	13	9	27	8*	4	13	9	5	20*
5	13	9	4	3*	6	13	9	14	26*	0	14	9	5	10*
1	14	9	13	18*	2	14	9	24	13*	3	14	9	4	27*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $GePh_4$ (-60°C)

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	0	10	34	44*	0	1	10	58	0*	1	1	10	62	43*
0	2	10	55	49*	1	2	10	40	19*	2	2	10	63	62*
0	3	10	9	26*	1	3	10	59	49*	2	3	10	48	6*
3	3	10	41	82*	0	4	10	21	20*	1	4	10	33	38*
2	4	10	32	45*	3	4	10	23	12*	4	4	10	8	64*
0	5	10	9	40*	1	5	10	47	27*	2	5	10	9	9*
3	5	10	17	54*	4	5	10	40	11*	5	5	10	8	55*
0	6	10	9	51*	1	6	10	41	16*	2	6	10	72	51
3	6	10	50	18*	4	6	10	47	52*	5	6	10	8	9*
6	6	10	8	19*	0	7	10	45	2*	1	7	10	54	47*
2	7	10	42	19*	3	7	10	8	30*	4	7	10	40	19*
5	7	10	35	27*	6	7	10	35	6*	7	7	10	7	21*
0	8	10	57	31*	1	8	10	23	6*	2	8	10	43	30*
3	8	10	37	10*	4	8	10	29	29*	5	8	10	28	25*
6	8	10	32	17*	7	8	10	14	18*	8	8	10	30	33*
0	9	10	30	5*	1	9	10	42	29*	2	9	10	29	16*
3	9	10	38	25*	4	9	10	40	13*	5	9	10	36	33*
6	9	10	13	10*	7	9	10	26	28*	8	9	10	20	1*
0	10	10	44	30*	1	10	10	34	7*	2	10	10	7	26*
3	10	10	41	13*	4	10	10	30	33*	5	10	10	5	14*
6	10	10	22	21*	7	10	10	3	4*	0	11	10	7	3*
1	11	10	7	32*	2	11	10	6	6*	3	11	10	27	31*
4	11	10	21	15*	5	11	10	4	30*	0	12	10	29	24*
1	12	10	5	6*	2	12	10	25	28*	0	1	11	29	25*
0	2	11	17	29*	1	2	11	37	47*	0	3	11	8	38*
1	3	11	43	21*	2	3	11	8	26*	0	4	11	39	3*
1	4	11	51	31*	2	4	11	15	16*	3	4	11	7	16*
0	5	11	8	42*	1	5	11	42	7*	2	5	11	7	29*
3	5	11	40	14*	4	5	11	7	19*	0	6	11	8	13*
1	6	11	9	36*	2	6	11	7	12*	3	6	11	30	29*
4	6	11	6	26*	5	6	11	37	29*	0	7	11	28	38*
1	7	11	36	9*	2	7	11	42	31*	3	7	11	37	17*
4	7	11	5	27*	5	7	11	21	20*	6	7	11	4	29*
0	8	11	7	5*	1	8	11	45	21*	2	8	11	35	16*
3	8	11	19	31*	4	8	11	29	11*	0	9	11	26	18*
1	9	11	5	5*	2	9	11	23	20*	0	0	12	38	59*
0	1	12	29	6*	1	1	12	6	30*	0	2	12	28	25*
1	2	12	37	7*	2	2	12	5	14*	0	3	12	22	8*
1	3	12	5	23*	2	3	12	12	6*	3	3	12	28	24*
0	4	12	23	22*	1	4	12	24	4*	2	4	12	4	16*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Sn$

An * indicates weak or extinct reflections not used in the final refinements.

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	1	0	1060	990	0	2	0	970	936	1	2	0	120	118
2	2	0	130	128	1	3	0	754	748	2	3	0	143	142
3	3	0	1001	975	0	4	0	649	632	1	4	0	31	2*
2	4	0	637	636	3	4	0	209	201	4	4	0	348	341
1	5	0	609	598	2	5	0	86	84	3	5	0	620	631
4	5	0	163	157	5	5	0	426	436	0	6	0	695	674
1	6	0	100	97	2	6	0	827	811	3	6	0	248	244
4	6	0	582	590	5	6	0	65	60	6	6	0	483	494
1	7	0	611	597	2	7	0	29	25	3	7	0	429	434
4	7	0	18	18*	5	7	0	418	419	6	7	0	46	49
7	7	0	411	417	0	8	0	563	566	1	8	0	86	82
2	8	0	467	471	3	8	0	31	32	4	8	0	331	340
5	8	0	86	83	6	8	0	340	347	7	8	0	27	5*
8	8	0	330	350	1	9	0	545	546	2	9	0	37	45*
3	9	0	335	342	4	9	0	33	46	5	9	0	372	366
6	9	0	25	12*	7	9	0	303	309	8	9	0	42	7*
9	9	0	108	97	0	10	0	181	180	1	10	0	95	94
2	10	0	265	270	3	10	0	33	22	4	10	0	261	264
5	10	0	23	3*	6	10	0	265	267	7	10	0	26	9*
8	10	0	197	201	9	10	0	26	32*	10	10	0	135	130
1	11	0	210	210	2	11	0	106	112	3	11	0	159	163
4	11	0	25	19*	5	11	0	237	238	6	11	0	46	46
7	11	0	250	254	8	11	0	40	15*	9	11	0	136	135
10	11	0	26	31*	11	11	0	151	158	0	12	0	264	270
1	12	0	85	84	2	12	0	331	336	3	12	0	45	14*
4	12	0	195	195	5	12	0	38	46	6	12	0	173	180
7	12	0	22	22*	8	12	0	150	151	9	12	0	41	49
10	12	0	125	129	11	12	0	29	1*	1	13	0	248	246
2	13	0	31	40*	3	13	0	187	193	4	13	0	48	11*
5	13	0	156	163	6	13	0	26	10*	7	13	0	141	143
8	13	0	48	37	9	13	0	114	114	10	13	0	37	15*
0	14	0	118	116	1	14	0	39	28	2	14	0	182	188
3	14	0	35	12*	4	14	0	173	177	5	14	0	28	5*
6	14	0	125	129	7	14	0	53	17*	8	14	0	122	120
9	14	0	44	15*	1	15	0	147	151	2	15	0	42	2*
3	15	0	153	160	4	15	0	47	24*	5	15	0	142	143
6	15	0	37	21*	7	15	0	95	92	0	16	0	98	97
1	16	0	30	2*	2	16	0	94	91	3	16	0	56	14
4	16	0	110	117	5	16	0	28	15*	0	1	1	758	736
-1	2	1	1141	1158	0	2	1	1026	1040	1	2	1	1127	1148
-2	3	1	541	571	-1	3	1	446	442	0	3	1	682	696
1	3	1	440	442	2	3	1	563	543	-3	4	1	588	608
-2	4	1	102	99	-1	4	1	874	886	0	4	1	205	197
1	4	1	872	893	2	4	1	101	99	3	4	1	596	605
-4	5	1	596	594	-3	5	1	98	96	-2	5	1	613	613
-1	5	1	54	52	0	5	1	850	853	1	5	1	54	52
2	5	1	606	617	3	5	1	96	96	4	5	1	588	603
-5	6	1	457	442	-4	6	1	110	106	-3	6	1	406	419
-2	6	1	138	138	-1	6	1	568	564	0	6	1	192	182
1	6	1	554	577	2	6	1	140	138	3	6	1	414	418

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Sn$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	6	1	107	106	5	6	1	436	449	-6	7	1	477	469
-5	7	1	39	33	-4	7	1	442	449	-3	7	1	77	74
-2	7	1	553	563	-1	7	1	19	4*	0	7	1	529	528
1	7	1	57	4*	2	7	1	554	562	3	7	1	75	74
4	7	1	442	447	5	7	1	42	33	6	7	1	468	470
-7	8	1	292	295	-6	8	1	74	78	-5	8	1	379	386
-4	8	1	76	76	-3	8	1	522	537	-2	8	1	50	43
-1	8	1	453	459	0	8	1	39	34	1	8	1	460	458
2	8	1	45	43	3	8	1	538	528	4	8	1	75	76
5	8	1	380	382	6	8	1	81	78	7	8	1	292	295
-8	9	1	202	206	-7	9	1	78	84	-6	9	1	314	314
-5	9	1	20	34*	-4	9	1	263	262	-3	9	1	141	139
-2	9	1	395	404	-1	9	1	38	29	0	9	1	333	334
1	9	1	23	29*	2	9	1	398	398	3	9	1	133	139
4	9	1	263	261	5	9	1	48	34	6	9	1	311	315
7	9	1	90	84	8	9	1	211	203	-9	10	1	213	218
-8	10	1	45	40	-7	10	1	222	225	-6	10	1	38	28*
-5	10	1	237	228	-4	10	1	28	34*	-3	10	1	325	322
-2	10	1	102	104	-1	10	1	338	338	0	10	1	99	99
1	10	1	338	335	2	10	1	103	104	3	10	1	322	326
4	10	1	40	34	5	10	1	225	234	6	10	1	24	28*
7	10	1	223	227	8	10	1	44	40	9	10	1	217	215
-9	11	1	56	45	-8	11	1	170	171	-7	11	1	27	29*
-6	11	1	228	228	-5	11	1	26	24*	-4	11	1	242	229
-3	11	1	28	26*	-2	11	1	269	274	-1	11	1	123	122
0	11	1	292	290	1	11	1	122	122	2	11	1	273	270
3	11	1	24	26*	4	11	1	227	234	5	11	1	36	24
6	11	1	227	228	7	11	1	26	29*	8	11	1	175	166
9	11	1	46	45	10	11	1	140	138	-7	12	1	156	163
-6	12	1	34	13	-5	12	1	211	202	-4	12	1	33	16*
-3	12	1	235	233	-2	12	1	40	14*	-1	12	1	195	201
0	12	1	90	93	1	12	1	199	193	2	12	1	25	14*
3	12	1	232	233	4	12	1	21	16*	5	12	1	200	203
6	12	1	33	13*	7	12	1	162	161	8	12	1	49	4*
9	12	1	146	137	10	12	1	29	22*	11	12	1	114	116
-5	13	1	28	19*	-4	13	1	212	202	-3	13	1	47	17
-2	13	1	205	200	-1	13	1	46	49	0	13	1	249	247
1	13	1	49	49	2	13	1	198	196	3	13	1	26	17*
4	13	1	209	206	5	13	1	24	19*	6	13	1	175	176
7	13	1	29	2*	8	13	1	124	125	9	13	1	47	16*
10	13	1	92	85	-2	14	1	29	15*	-1	14	1	182	190
0	14	1	39	35	1	14	1	190	187	2	14	1	23	15*
3	14	1	158	164	4	14	1	21	11*	5	14	1	146	143
6	14	1	29	28*	7	14	1	124	126	8	14	1	32	19*
9	14	1	115	99	-1	15	1	41	31	0	15	1	135	133
1	15	1	28	31*	2	15	1	118	112	3	15	1	44	16*
4	15	1	113	111	5	15	1	38	8*	6	15	1	122	118
7	15	1	46	19*	-1	16	1	115	112	0	16	1	48	8*
1	16	1	117	111	2	16	1	15	8*	3	16	1	112	110
4	16	1	30	20*	5	16	1	103	98	0	0	2	411	429

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Sn$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-1	1	2	667	653	0	1	2	210	210	1	1	2	660	681
-1	2	2	319	317	0	2	2	576	574	1	2	2	322	317
2	2	2	897	931	-1	3	2	793	787	0	3	2	327	296
1	3	2	780	798	2	3	2	160	162	3	3	2	753	748
-1	4	2	94	94	0	4	2	704	710	1	4	2	96	95
2	4	2	773	768	3	4	2	250	247	4	4	2	429	430
-1	5	2	585	598	0	5	2	43	43	1	5	2	591	601
2	5	2	250	239	3	5	2	552	557	4	5	2	87	90
5	5	2	512	510	-1	6	2	163	163	0	6	2	370	405
1	6	2	169	163	2	6	2	470	469	3	6	2	43	36
4	6	2	507	514	5	6	2	86	88	6	6	2	400	403
-1	7	2	405	413	0	7	2	20	5*	1	7	2	414	405
2	7	2	36	27	3	7	2	437	438	4	7	2	146	148
5	7	2	388	391	6	7	2	57	58	7	7	2	259	256
-1	8	2	102	102	0	8	2	452	450	1	8	2	104	102
2	8	2	353	343	3	8	2	80	81	4	8	2	397	396
5	8	2	78	75	6	8	2	248	248	7	8	2	74	76
8	8	2	299	285	-1	9	2	338	336	0	9	2	38	42
1	9	2	336	339	2	9	2	84	84	3	9	2	343	349
4	9	2	47	47	5	9	2	286	292	6	9	2	88	84
7	9	2	235	233	8	9	2	49	35	9	9	2	247	241
-1	10	2	32	38*	0	10	2	346	335	1	10	2	31	38*
2	10	2	303	305	3	10	2	94	104	4	10	2	343	348
5	10	2	26	22*	6	10	2	215	218	7	10	2	40	30
8	10	2	198	198	9	10	2	29	18*	10	10	2	167	161
-1	11	2	294	298	0	11	2	34	12*	1	11	2	296	296
2	11	2	38	36	3	11	2	298	295	4	11	2	46	40
5	11	2	219	224	6	11	2	28	43*	7	11	2	171	171
8	11	2	29	18*	9	11	2	158	152	10	11	2	20	3*
11	11	2	109	112	-1	12	2	45	41	0	12	2	217	218
1	12	2	45	41	2	12	2	213	212	3	12	2	27	23*
4	12	2	178	184	5	12	2	41	40	6	12	2	175	178
7	12	2	29	6*	8	12	2	152	145	9	12	2	28	19*
10	12	2	129	119	11	12	2	32	13*	-1	13	2	155	158
0	13	2	14	2*	1	13	2	165	157	2	13	2	68	68
3	13	2	151	156	4	13	2	47	44	5	13	2	155	153
6	13	2	30	11*	7	13	2	143	144	8	13	2	42	23*
9	13	2	110	106	10	13	2	31	25*	-1	14	2	38	35*
0	14	2	144	142	1	14	2	39	35	2	14	2	148	144
3	14	2	36	24	4	14	2	127	128	5	14	2	17	17*
6	14	2	136	132	7	14	2	40	6*	8	14	2	98	86
-1	15	2	134	135	0	15	2	25	34*	1	15	2	137	131
2	15	2	30	16*	3	15	2	109	110	4	15	2	31	14*
5	15	2	95	101	6	15	2	33	8*	-1	16	2	34	14*
0	16	2	120	120	1	16	2	33	14*	2	16	2	116	103
3	16	2	31	4*	4	16	2	92	85	0	1	3	501	498
-1	2	3	651	657	0	2	3	77	75	1	2	3	655	652
-1	3	3	80	80	0	3	3	537	541	1	3	3	79	80
2	3	3	716	716	-1	4	3	376	393	0	4	3	160	159
1	4	3	391	377	2	4	3	145	146	3	4	3	711	700

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Sn$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-1	5	3	25	27*	0	5	3	367	378	1	5	3	30	27
2	5	3	454	459	3	5	3	102	108	4	5	3	536	540
-1	6	3	495	500	0	6	3	51	33	1	6	3	506	498
2	6	3	50	45	3	6	3	475	470	4	6	3	75	72
5	6	3	306	317	-1	7	3	65	61	0	7	3	413	416
1	7	3	64	61	2	7	3	366	367	3	7	3	56	61
4	7	3	344	336	5	7	3	192	193	6	7	3	221	214
-1	8	3	283	281	0	8	3	23	3*	1	8	3	288	280
2	8	3	65	73	3	8	3	288	291	4	8	3	68	73
5	8	3	311	319	6	8	3	89	92	7	8	3	225	223
-1	9	3	55	61	0	9	3	317	317	1	9	3	63	61
2	9	3	281	285	3	9	3	45	39*	4	9	3	325	317
5	9	3	36	34	6	9	3	272	270	7	9	3	27	13*
8	9	3	206	212	-1	10	3	309	316	0	10	3	37	23*
1	10	3	309	313	2	10	3	26	11*	3	10	3	258	256
4	10	3	28	11*	5	10	3	275	276	6	10	3	27	26*
7	10	3	199	197	8	10	3	26	12*	9	10	3	146	145
-1	11	3	40	28*	0	11	3	286	290	1	11	3	26	28*
2	11	3	239	241	3	11	3	21	25*	4	11	3	239	240
5	11	3	22	18*	6	11	3	176	178	7	11	3	29	6*
8	11	3	158	163	9	11	3	35	31*	10	11	3	104	102
-1	12	3	198	202	0	12	3	29	37*	1	12	3	198	202
2	12	3	22	9*	3	12	3	183	183	4	12	3	17	9*
5	12	3	177	175	6	12	3	30	19*	7	12	3	132	136
8	12	3	30	19*	9	12	3	123	123	10	12	3	32	29*
-1	13	3	30	23*	0	13	3	142	141	1	13	3	41	23*
2	13	3	135	132	3	13	3	45	21	4	13	3	154	143
5	13	3	30	9*	6	13	3	104	94	7	13	3	31	8*
8	13	3	122	122	9	13	3	32	19*	-1	14	3	120	119
0	14	3	31	5*	1	14	3	119	122	2	14	3	25	35*
3	14	3	129	119	4	14	3	30	12*	5	14	3	93	95
6	14	3	31	8*	7	14	3	90	88	-1	15	3	31	26*
0	15	3	109	106	1	15	3	36	26*	2	15	3	130	123
3	15	3	30	14*	4	15	3	100	108	5	15	3	32	13*
-1	16	3	98	90	0	16	3	45	3*	0	0	4	443	449
-1	1	4	431	433	0	1	4	120	116	1	1	4	439	438
-1	2	4	135	131	0	2	4	498	498	1	2	4	138	131
2	2	4	527	533	-1	3	4	510	509	0	3	4	121	113
1	3	4	511	511	2	3	4	59	64	3	3	4	436	443
-1	4	4	24	14*	0	4	4	456	440	1	4	4	21	14*
2	4	4	412	415	3	4	4	28	15*	4	4	4	383	389
-1	5	4	400	400	0	5	4	37	37	1	5	4	404	405
2	5	4	20	31*	3	5	4	347	352	4	5	4	136	137
5	5	4	426	407	-1	6	4	73	81	0	6	4	369	381
1	6	4	78	81	2	6	4	367	369	3	6	4	103	104
4	6	4	350	346	5	6	4	85	84	6	6	4	309	295
-1	7	4	345	341	0	7	4	43	39*	1	7	4	344	345
2	7	4	60	69	3	7	4	318	325	4	7	4	79	82
5	7	4	303	298	6	7	4	36	33	7	7	4	254	273
-1	8	4	56	59	0	8	4	276	270	1	8	4	62	59

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Sn$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
2	8	4	260	257	3	8	4	26	21*	4	8	4	266	272
5	8	4	18	17*	6	8	4	207	206	7	8	4	22	30*
8	8	4	216	213	-1	9	4	268	264	0	9	4	30	48*
1	9	4	263	271	2	9	4	26	10*	3	9	4	236	235
4	9	4	33	35*	5	9	4	225	223	6	9	4	27	11*
7	9	4	169	172	8	9	4	30	17*	9	9	4	174	170
-1	10	4	41	40	0	10	4	238	244	1	10	4	48	40
2	10	4	229	228	3	10	4	42	51	4	10	4	224	227
5	10	4	31	21*	6	10	4	148	148	7	10	4	37	23*
8	10	4	151	154	9	10	4	29	10*	10	10	4	121	118
-1	11	4	198	191	0	11	4	39	0*	1	11	4	197	195
2	11	4	35	46*	3	11	4	187	183	4	11	4	33	13*
5	11	4	164	167	6	11	4	32	19*	7	11	4	137	133
8	11	4	55	12*	9	11	4	109	115	10	11	4	33	5*
-1	12	4	29	11*	0	12	4	165	167	1	12	4	26	11*
2	12	4	161	160	3	12	4	27	2*	4	12	4	147	156
5	12	4	30	11*	6	12	4	121	124	7	12	4	47	11*
8	12	4	117	113	9	12	4	32	6*	-1	13	4	140	137
0	13	4	49	13*	1	13	4	136	140	2	13	4	31	7*
3	13	4	128	130	4	13	4	40	37*	5	13	4	122	125
6	13	4	31	5*	7	13	4	102	106	8	13	4	39	9*
-1	14	4	31	11*	0	14	4	109	109	1	14	4	24	11*
2	14	4	114	108	3	14	4	34	34*	4	14	4	110	104
5	14	4	28	23*	6	14	4	98	101	-1	15	4	110	104
0	15	4	30	6*	1	15	4	110	105	2	15	4	32	9*
0	1	5	431	435	-1	2	5	383	387	0	2	5	28	6*
1	2	5	378	385	-1	3	5	119	117	0	3	5	390	383
1	3	5	114	117	2	3	5	295	310	-1	4	5	374	374
0	4	5	59	50	1	4	5	377	370	2	4	5	86	89
3	4	5	235	227	-1	5	5	53	54	0	5	5	381	379
1	5	5	54	54	2	5	5	314	307	3	5	5	61	58
4	5	5	248	243	-1	6	5	298	302	0	6	5	27	3*
1	6	5	303	300	2	6	5	31	28*	3	6	5	268	260
4	6	5	63	65	5	6	5	265	265	-1	7	5	51	57
0	7	5	282	283	1	7	5	27	57*	2	7	5	272	269
3	7	5	46	8*	4	7	5	236	240	5	7	5	112	116
6	7	5	251	248	-1	8	5	266	266	0	8	5	33	31*
1	8	5	267	267	2	8	5	35	27*	3	8	5	251	254
4	8	5	84	87	5	8	5	188	198	6	8	5	59	56
7	8	5	183	185	-1	9	5	36	53*	0	9	5	205	200
1	9	5	51	53	2	9	5	211	207	3	9	5	29	12*
4	9	5	165	166	5	9	5	27	42*	6	9	5	152	155
7	9	5	33	26*	8	9	5	128	122	-1	10	5	152	149
0	10	5	31	19*	1	10	5	155	147	2	10	5	36	23*
3	10	5	158	153	4	10	5	41	33	5	10	5	122	119
6	10	5	64	47	7	10	5	121	127	8	10	5	31	25*
9	10	5	112	108	-1	11	5	29	24*	0	11	5	147	144
1	11	5	29	24*	2	11	5	148	154	3	11	5	27	13*
4	11	5	114	119	5	11	5	30	10*	6	11	5	122	120
7	11	5	33	21*	8	11	5	83	96	9	11	5	55	28*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Sn$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
-1	12	5	136	129	0	12	5	22	29*	1	12	5	134	132
2	12	5	31	4*	3	12	5	121	124	4	12	5	32	3*
5	12	5	119	113	6	12	5	32	11*	7	12	5	109	103
-1	13	5	32	28*	0	13	5	122	120	1	13	5	52	28*
2	13	5	114	117	3	13	5	31	6*	4	13	5	114	113
5	13	5	43	12*	-1	14	5	122	116	0	14	5	52	22*
1	14	5	109	119	2	14	5	48	29*	0	0	6	384	384
-1	1	6	380	384	0	1	6	82	73	1	1	6	387	386
-1	2	6	58	35*	0	2	6	296	295	1	2	6	30	35*
2	2	6	231	227	-1	3	6	199	200	0	3	6	73	71
1	3	6	202	198	2	3	6	46	45	3	3	6	190	182
-1	4	6	51	48	0	4	6	245	242	1	4	6	43	48
2	4	6	239	238	3	4	6	61	68	4	4	6	270	268
-1	5	6	248	256	0	5	6	26	21*	1	5	6	257	254
2	5	6	68	76	3	5	6	239	236	4	5	6	34	25*
5	5	6	182	184	-1	6	6	27	19*	0	6	6	214	211
1	6	6	41	19*	2	6	6	210	205	3	6	6	26	39*
4	6	6	161	158	5	6	6	29	26*	6	6	6	176	181
-1	7	6	238	243	0	7	6	32	8*	1	7	6	249	237
2	7	6	52	27	3	7	6	212	201	4	7	6	29	35*
5	7	6	159	161	6	7	6	22	3*	7	7	6	164	174
-1	8	6	34	43*	0	8	6	212	207	1	8	6	55	43
2	8	6	219	216	3	8	6	52	34*	4	8	6	134	138
5	8	6	56	39*	6	8	6	160	176	7	8	6	27	23*
8	8	6	85	93	-1	9	6	150	151	0	9	6	54	29
1	9	6	150	150	2	9	6	45	31*	3	9	6	130	136
4	9	6	51	13*	5	9	6	121	125	6	9	6	31	27*
7	9	6	126	128	8	9	6	17	19*	9	9	6	90	77
-1	10	6	32	13*	0	10	6	130	135	1	10	6	38	13*
2	10	6	125	126	3	10	6	63	33	4	10	6	85	91
5	10	6	40	10*	6	10	6	128	142	7	10	6	52	9*
8	10	6	75	83	-1	11	6	95	101	0	11	6	36	4*
1	11	6	95	100	2	11	6	31	30*	3	11	6	103	102
4	11	6	17	24*	5	11	6	94	101	6	11	6	36	22*
-1	12	6	57	33	0	12	6	106	102	1	12	6	44	33
2	12	6	98	94	3	12	6	44	12*	4	12	6	83	86
0	1	7	222	222	-1	2	7	144	147	0	2	7	95	100
1	2	7	153	140	-1	3	7	61	58	0	3	7	254	259
1	3	7	43	58*	2	3	7	220	218	-1	4	7	187	187
0	4	7	31	1*	1	4	7	187	188	2	4	7	31	22*
3	4	7	176	178	-1	5	7	48	33*	0	5	7	155	150
1	5	7	38	33*	2	5	7	162	161	3	5	7	33	9*
4	5	7	144	140	-1	6	7	166	164	0	6	7	31	14*
1	6	7	165	168	2	6	7	32	8*	3	6	7	157	169
4	6	7	38	22*	5	6	7	154	158	-1	7	7	28	19*
0	7	7	101	112	1	7	7	30	19*	2	7	7	131	126
3	7	7	26	31*	4	7	7	117	125	5	7	7	36	25*
6	7	7	104	105	-1	8	7	121	127	0	8	7	33	11*
1	8	7	122	127	2	8	7	59	15*	3	8	7	111	109
4	8	7	31	16*	5	8	7	98	106	6	8	7	47	14*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Sn$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
7	8	7	97	101	-1	9	7	33	12*	0	9	7	124	132
1	9	7	56	12*	2	9	7	153	149	3	9	7	49	18
4	9	7	135	127	5	9	7	52	12*	6	9	7	75	82
-1	10	7	96	101	0	10	7	44	40*	1	10	7	106	98
2	10	7	25	16*	3	10	7	93	95	4	10	7	31	19*
0	0	8	44	9*	-1	1	8	123	119	0	1	8	45	35*
1	1	8	125	124	-1	2	8	55	20*	0	2	8	133	135
1	2	8	47	20*	2	2	8	167	178	-1	3	8	141	144
0	3	8	31	4*	1	3	8	149	146	2	2	8	43	35*
3	3	8	116	136	-1	4	8	36	13*	0	4	8	134	136
1	4	8	34	13*	2	4	8	133	137	3	4	8	37	10*
4	4	8	149	157	-1	5	8	123	126	0	5	8	29	28*
1	5	8	130	128	2	5	8	31	12*	3	5	8	120	123
4	5	8	44	24*	5	5	8	108	115	-1	6	8	51	3*
0	6	8	90	94	1	6	8	43	3*	2	6	8	93	87
3	6	8	35	32*	4	6	8	101	96	5	6	8	32	13*
-1	7	8	87	83	0	7	8	40	9*	1	7	8	91	83
2	7	8	28	19*	3	7	8	112	100	4	7	8	32	8*
-1	8	8	26	4*	0	8	8	75	70	1	8	8	30	4*
2	8	8	104	92	0	1	9	103	94	-1	2	9	103	94
0	2	9	34	34*	1	2	9	92	95	-1	3	9	35	39*
0	3	9	58	66	1	3	9	27	39*					

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Pb$

M160

An * indicates weak or extinct reflections not used in the final refinements.

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
1	1	0	1593	1536	0	2	0	1518	1509	1	2	0	136	132
2	2	0	705	677	1	3	0	1291	1290	2	3	0	159	156
3	3	0	1459	1466	0	4	0	1186	1139	1	4	0	24	11*
2	4	0	1129	1117	3	4	0	214	209	4	4	0	801	790
1	5	0	1089	1079	2	5	0	96	89	3	5	0	1063	1066
4	5	0	152	150	5	5	0	813	848	0	6	0	1160	1106
1	6	0	110	109	2	6	0	1250	1232	3	6	0	236	229
4	6	0	976	967	5	6	0	84	72	6	6	0	838	821
1	7	0	975	983	2	7	0	25	32*	3	7	0	777	779
4	7	0	40	49*	5	7	0	725	736	6	7	0	61	54*
7	7	0	690	687	0	8	0	897	892	1	8	0	95	82
2	8	0	799	811	3	8	0	54	42*	4	8	0	643	657
5	8	0	104	94	6	8	0	616	624	7	8	0	50	4*
8	8	0	551	552	1	9	0	827	830	2	9	0	29	26*
3	9	0	619	627	4	9	0	73	35*	5	9	0	618	628
6	9	0	32	12*	7	9	0	524	525	8	9	0	35	14*
9	9	0	273	262	0	10	0	433	430	1	10	0	97	110
2	10	0	505	516	3	10	0	31	42*	4	10	0	496	497
5	10	0	38	5*	6	10	0	473	473	7	10	0	35	6*
8	10	0	383	373	9	10	0	73	32*	10	10	0	290	284
1	11	0	450	459	2	11	0	103	114	3	11	0	385	390
4	11	0	7	24*	5	11	0	436	432	6	11	0	52	53*
7	11	0	420	422	8	11	0	38	25*	9	11	0	289	275
10	11	0	40	28*	11	11	0	251	266	0	12	0	478	493
1	12	0	93	87	2	12	0	520	544	3	12	0	35	22*
4	12	0	393	385	5	12	0	53	44*	6	12	0	325	333
7	12	0	59	8*	8	12	0	279	276	9	12	0	71	54*
10	12	0	234	234	11	12	0	13	2*	12	12	0	133	131
1	13	0	403	408	2	13	0	37	41*	3	13	0	339	351
4	13	0	38	8*	5	13	0	305	308	6	13	0	39	14*
7	13	0	266	268	8	13	0	61	46*	9	13	0	228	217
10	13	0	43	7*	11	13	0	172	177	12	13	0	42	22*
13	13	0	126	123	0	14	0	247	253	1	14	0	44	28*
2	14	0	323	323	3	14	0	39	1*	4	14	0	307	303
5	14	0	47	5*	6	14	0	253	245	7	14	0	42	13*
8	14	0	237	221	9	14	0	26	9*	10	14	0	214	200
11	14	0	44	26*	12	14	0	80	120*	13	14	0	12	14*
1	15	0	269	266	2	15	0	75	1*	3	15	0	271	270
4	15	0	41	34*	5	15	0	238	237	6	15	0	43	25*
7	15	0	184	178	8	15	0	41	8*	9	15	0	156	157
10	15	0	44	1*	11	15	0	78	114*	12	15	0	71	21*
0	16	0	156	182	1	16	0	40	5*	2	16	0	174	180
3	16	0	42	7*	4	16	0	214	199	5	16	0	43	13*
6	16	0	122	141	7	16	0	31	8*	8	16	0	132	136
9	16	0	44	3*	10	16	0	120	112	11	16	0	92	5*
1	17	0	148	147	2	17	0	9	12*	3	17	0	43	152*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Pb$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
4	17	0	43	3*	5	17	0	145	144	6	17	0	44	1*
7	17	0	93	116*	8	17	0	44	3*	9	17	0	55	103*
0	18	0	155	154	1	18	0	39	13*	2	18	0	119	132
3	18	0	42	7*	4	18	0	138	138	5	18	0	43	3*
6	18	0	74	97*	7	18	0	42	2*	1	19	0	88	104*
2	19	0	40	14*	3	19	0	90	100*	4	19	0	45	5*
0	1	1	1270	1261	0	2	1	1054	1039	1	2	1	1651	1677
0	3	1	1233	1210	1	3	1	459	440	2	3	1	1006	963
0	4	1	207	199	1	4	1	1364	1398	2	4	1	79	82
3	4	1	1077	1074	0	5	1	1321	1318	1	5	1	63	47
2	5	1	1067	1056	3	5	1	77	72	4	5	1	976	1013
0	6	1	204	197	1	6	1	983	992	2	6	1	138	134
3	6	1	778	807	4	6	1	133	110	5	6	1	803	804
0	7	1	895	915	1	7	1	9	15*	2	7	1	927	920
3	7	1	73	73*	4	7	1	788	782	5	7	1	29	26*
6	7	1	770	764	0	8	1	27	22*	1	8	1	792	780
2	8	1	60	55*	3	8	1	829	817	4	8	1	46	82*
5	8	1	669	653	6	8	1	97	81	7	8	1	518	521
0	9	1	635	635	1	9	1	29	31*	2	9	1	669	667
3	9	1	137	134	4	9	1	508	522	5	9	1	65	31*
6	9	1	527	549	7	9	1	54	83*	8	9	1	404	399
0	10	1	67	106*	1	10	1	602	594	2	10	1	105	114
3	10	1	585	582	4	10	1	33	18*	5	10	1	448	469
6	10	1	35	35*	7	10	1	399	410	8	10	1	37	36*
9	10	1	377	367	0	11	1	508	515	1	11	1	103	107
2	11	1	497	486	3	11	1	52	26*	4	11	1	432	443
5	11	1	35	26*	6	11	1	398	407	7	11	1	37	27*
8	11	1	324	304	9	11	1	46	49*	10	11	1	262	255
0	12	1	121	118	1	12	1	379	368	2	12	1	36	22*
3	12	1	423	420	4	12	1	23	18*	5	12	1	375	373
6	12	1	38	14*	7	12	1	293	301	8	12	1	40	4*
9	12	1	254	253	10	12	1	68	28*	11	12	1	201	213
0	13	1	415	414	1	13	1	47	48*	2	13	1	369	356
3	13	1	38	18*	4	13	1	357	363	5	13	1	39	14*
6	13	1	299	311	7	13	1	66	5*	8	13	1	237	236
9	13	1	76	14*	10	13	1	165	171	11	13	1	37	6*
12	13	1	141	155	0	14	1	38	27*	1	14	1	313	311
2	14	1	24	18*	3	14	1	282	294	4	14	1	71	10*
5	14	1	268	260	6	14	1	41	36*	7	14	1	238	225
8	14	1	58	21*	9	14	1	183	175	10	14	1	44	5*
11	14	1	118	137*	12	14	1	41	20*	13	14	1	56	97*
0	15	1	249	243	1	15	1	40	29*	2	15	1	221	215
3	15	1	41	13*	4	15	1	234	211	5	15	1	77	12*
6	15	1	219	205	7	15	1	43	18*	8	15	1	164	174
9	15	1	44	11*	10	15	1	122	133	11	15	1	43	13*
12	15	1	78	110*	0	16	1	41	15*	1	16	1	208	205
2	16	1	56	13*	3	16	1	216	200	4	16	1	43	24*
5	16	1	194	175	6	16	1	53	12*	7	16	1	148	146

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Pb$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
8	16	1	44	11*	9	16	1	98	119*	10	16	1	43	12*
11	16	1	64	97*	0	17	1	180	168	1	17	1	54	19*
2	17	1	164	169	3	17	1	43	14*	4	17	1	132	147
5	17	1	94	13*	6	17	1	152	125	7	17	1	44	1*
8	17	1	15	102*	9	17	1	42	10*	0	18	1	80	5*
1	18	1	156	120	2	18	1	43	13*	3	18	1	123	124
4	18	1	62	9*	5	18	1	92	115*	6	18	1	62	4*
7	18	1	80	95*	0	19	1	81	102*	1	19	1	42	2*
2	19	1	87	106*	3	19	1	63	7*	4	19	1	117	109
0	0	2	955	997	0	1	2	220	218	1	1	2	1141	1164
0	2	2	1087	1072	1	2	2	346	329	2	2	2	1429	1441
0	3	2	303	279	1	3	2	1276	1284	2	3	2	150	155
3	3	2	1217	1170	0	4	2	1147	1117	1	4	2	102	98
2	4	2	1212	1194	3	4	2	261	248	4	4	2	817	822
0	5	2	39	58*	1	5	2	944	995	2	5	2	265	252
3	5	2	957	944	4	5	2	69	91*	5	5	2	844	871
0	6	2	771	784	1	6	2	173	169	2	6	2	844	837
3	6	2	25	26*	4	6	2	845	867	5	6	2	91	88
6	6	2	686	682	0	7	2	26	5*	1	7	2	748	737
2	7	2	27	28*	3	7	2	752	756	4	7	2	135	148
5	7	2	674	674	6	7	2	31	33*	7	7	2	491	492
0	8	2	767	765	1	8	2	121	102	2	8	2	641	627
3	8	2	78	74*	4	8	2	667	680	5	8	2	47	68*
6	8	2	481	480	7	8	2	34	84*	8	8	2	483	472
0	9	2	30	38*	1	9	2	636	623	2	9	2	63	102*
3	9	2	615	617	4	9	2	45	39*	5	9	2	507	535
6	9	2	56	86*	7	9	2	444	433	8	9	2	36	46*
9	9	2	401	394	0	10	2	573	592	1	10	2	32	44*
2	10	2	541	540	3	10	2	110	104	4	10	2	564	577
5	10	2	35	20*	6	10	2	389	412	7	10	2	58	39*
8	10	2	370	362	9	10	2	39	18*	10	10	2	272	276
0	11	2	33	13*	1	11	2	510	503	2	11	2	35	32*
3	11	2	486	477	4	11	2	33	51*	5	11	2	402	401
6	11	2	58	43*	7	11	2	322	332	8	11	2	76	15*
9	11	2	286	274	10	11	2	41	7*	11	11	2	199	204
0	12	2	378	386	1	12	2	36	43*	2	12	2	378	370
3	12	2	37	22*	4	12	2	341	346	5	12	2	60	41*
6	12	2	316	322	7	12	2	39	13*	8	12	2	263	269
9	12	2	41	26*	10	12	2	218	213	11	12	2	42	12*
12	12	2	155	167	0	13	2	37	3*	1	13	2	299	303
2	13	2	30	68*	3	13	2	302	300	4	13	2	39	47*
5	13	2	290	286	6	13	2	40	17*	7	13	2	265	257
8	13	2	12	25*	9	13	2	200	195	10	13	2	43	21*
11	13	2	167	156	12	13	2	21	21*	13	13	2	88	123*
0	14	2	257	278	1	14	2	39	33*	2	14	2	272	276
3	14	2	40	30*	4	14	2	251	247	5	14	2	41	22*
6	14	2	232	230	7	14	2	44	10*	8	14	2	191	164
9	14	2	49	4*	10	14	2	118	134	11	14	2	73	25*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Pb$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
12	14	2	41	116*	13	14	2	37	5*	0	15	2	64	32*
1	15	2	240	236	2	15	2	41	17*	3	15	2	218	213
4	15	2	42	17*	5	15	2	182	193	6	15	2	43	12*
7	15	2	160	168	8	15	2	44	15*	9	15	2	144	131
10	15	2	44	17*	11	15	2	109	110*	12	15	2	20	14*
0	16	2	187	208	1	16	2	42	23*	2	16	2	198	186
3	16	2	43	2*	4	16	2	168	168	5	16	2	44	8*
6	16	2	168	161	7	16	2	87	2*	8	16	2	124	136
9	16	2	43	7*	10	16	2	42	104*	0	17	2	44	12*
1	17	2	139	164	2	17	2	43	5*	3	17	2	123	152
4	17	2	44	13*	5	17	2	121	141	6	17	2	26	17*
7	17	2	99	124*	8	17	2	42	10*	0	18	2	111	125*
1	18	2	44	12*	2	18	2	68	120*	3	18	2	43	18*
4	18	2	75	118*	5	18	2	45	9*	6	18	2	101	110*
0	19	2	49	3*	1	19	2	15	97*	2	19	2	20	8*
0	1	3	955	944	0	2	3	51	29*	1	2	3	1098	1082
0	3	3	938	945	1	3	3	99	96	2	3	3	1130	1110
0	4	3	150	146	1	4	3	743	730	2	4	3	168	165
3	4	3	1067	1049	0	5	3	753	756	1	5	3	24	15*
2	5	3	814	821	3	5	3	126	126	4	5	3	842	849
0	6	3	53	0*	1	6	3	846	835	2	6	3	38	38*
3	6	3	776	774	4	6	3	70	51*	5	6	3	557	584
0	7	3	702	710	1	7	3	52	58*	2	7	3	668	677
3	7	3	30	73*	4	7	3	612	594	5	7	3	205	220
6	7	3	449	439	0	8	3	50	11*	1	8	3	550	553
2	8	3	31	76*	3	8	3	551	562	4	8	3	33	76*
5	8	3	551	568	6	8	3	49	72*	7	8	3	427	437
0	9	3	566	567	1	9	3	44	53*	2	9	3	533	541
3	9	3	68	30*	4	9	3	545	534	5	9	3	30	40*
6	9	3	450	460	7	9	3	37	19*	8	9	3	375	376
0	10	3	37	16*	1	10	3	523	527	2	10	3	34	19*
3	10	3	452	458	4	10	3	18	23*	5	10	3	452	450
6	10	3	37	31*	7	10	3	345	344	8	10	3	60	8*
9	10	3	262	264	0	11	3	452	467	1	11	3	55	32*
2	11	3	408	423	3	11	3	37	25*	4	11	3	401	407
5	11	3	38	24*	6	11	3	324	328	7	11	3	39	9*
8	11	3	286	290	9	11	3	73	45*	10	11	3	197	204
0	12	3	36	18*	1	12	3	360	360	2	12	3	49	13*
3	12	3	327	330	4	12	3	55	12*	5	12	3	291	306
6	12	3	40	15*	7	12	3	245	251	8	12	3	51	20*
9	12	3	228	216	10	12	3	50	20*	11	12	3	134	162
0	13	3	278	287	1	13	3	53	29*	2	13	3	274	258
3	13	3	40	18*	4	13	3	267	256	5	13	3	41	9*
6	13	3	194	196	7	13	3	42	15*	8	13	3	222	210
9	13	3	43	20*	10	13	3	188	168	11	13	3	43	4*
12	13	3	121	122	0	14	3	40	3*	1	14	3	235	244
2	14	3	41	45*	3	14	3	238	228	4	14	3	42	10*
5	14	3	178	199	6	14	3	43	9*	7	14	3	174	180

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Pb$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
8	14	3	44	9*	9	14	3	135	159	10	14	3	85	6*
11	14	3	106	120*	12	14	3	72	10*	0	15	3	226	210
1	15	3	42	24*	2	15	3	229	219	3	15	3	43	10*
4	15	3	188	201	5	15	3	74	21*	6	15	3	168	161
7	15	3	44	20*	8	15	3	87	134*	9	15	3	44	1*
10	15	3	103	105*	11	15	3	41	11*	0	16	3	43	1*
1	16	3	166	172	2	16	3	43	10*	3	16	3	157	168
4	16	3	44	38*	5	16	3	154	151	6	16	3	66	26*
7	16	3	153	134	8	16	3	43	5*	9	16	3	99	96*
0	17	3	134	133	1	17	3	44	12*	2	17	3	74	143*
3	17	3	44	8*	4	17	3	162	124	5	17	3	44	7*
6	17	3	120	133	7	17	3	43	12*	0	18	3	45	3*
1	18	3	129	130	2	18	3	43	15*	3	18	3	94	105*
4	18	3	42	3*	5	18	3	111	95	0	0	4	869	887
0	1	4	116	111	1	1	4	805	806	0	2	4	847	844
1	2	4	143	139	2	2	4	842	810	0	3	4	138	117
1	3	4	857	854	2	3	4	28	42*	3	3	4	740	749
0	4	4	795	793	1	4	4	66	6*	2	4	4	743	742
3	4	4	39	28*	4	4	4	619	644	0	5	4	29	44*
1	5	4	718	727	2	5	4	50	36*	3	5	4	627	635
4	5	4	102	122	5	5	4	638	598	0	6	4	650	652
1	6	4	49	76*	2	6	4	635	641	3	6	4	91	94*
4	6	4	596	597	5	6	4	92	79	6	6	4	517	526
0	7	4	31	21*	1	7	4	605	600	2	7	4	80	68*
3	7	4	557	576	4	7	4	51	73*	5	7	4	518	510
6	7	4	35	15*	7	7	4	446	481	0	8	4	510	527
1	8	4	60	68*	2	8	4	502	491	3	8	4	53	26*
4	8	4	474	474	5	8	4	55	21*	6	8	4	394	389
7	8	4	38	27*	8	8	4	360	362	0	9	4	34	27*
1	9	4	466	486	2	9	4	35	15*	3	9	4	429	433
4	9	4	36	36*	5	9	4	385	378	6	9	4	48	15*
7	9	4	325	327	8	9	4	40	13*	9	9	4	292	295
0	10	4	408	409	1	10	4	36	46*	2	10	4	390	401
3	10	4	37	53*	4	10	4	389	387	5	10	4	39	16*
6	10	4	286	293	7	10	4	40	22*	8	10	4	268	275
9	10	4	42	12*	10	10	4	203	217	0	11	4	58	5*
1	11	4	349	358	2	11	4	39	43*	3	11	4	337	330
4	11	4	39	7*	5	11	4	288	295	6	11	4	50	23*
7	11	4	251	241	8	11	4	42	10*	9	11	4	217	210
10	11	4	43	6*	11	11	4	142	161	0	12	4	302	306
1	12	4	73	9*	2	12	4	309	308	3	12	4	43	12*
4	12	4	282	279	5	12	4	41	15*	6	12	4	240	233
7	12	4	42	8*	8	12	4	223	200	9	12	4	44	5*
10	12	4	140	158	11	12	4	71	8*	12	12	4	122	114
0	13	4	40	20*	1	13	4	260	260	2	13	4	41	7*
3	13	4	248	243	4	13	4	42	43*	5	13	4	195	227
6	13	4	66	4*	7	13	4	166	193	8	13	4	44	10*
9	13	4	156	157	10	13	4	44	12*	11	13	4	123	116

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
12	13	4	40	2*	0	14	4	191	208	1	14	4	42	8*
2	14	4	214	207	3	14	4	43	28*	4	14	4	189	186
5	14	4	44	14*	6	14	4	187	178	7	14	4	44	8*
8	14	4	175	146	9	14	4	44	11*	10	14	4	109	113*
11	14	4	42	5*	0	15	4	43	6*	1	15	4	184	189
2	15	4	80	5*	3	15	4	157	168	4	15	4	52	8*
5	15	4	121	153*	6	15	4	45	9*	7	15	4	74	136*
8	15	4	44	8*	9	15	4	74	113*	10	15	4	42	10*
0	16	4	166	155	1	16	4	44	2*	2	16	4	145	158
3	16	4	44	16*	4	16	4	89	128*	5	16	4	44	15*
6	16	4	58	120*	7	16	4	82	11*	8	16	4	115	108
0	17	4	45	2*	1	17	4	84	120*	2	17	4	44	5*
3	17	4	70	109*	4	17	4	68	20*	5	17	4	43	96*
6	17	4	26	4*	0	18	4	89	97*	1	18	4	42	3*
2	18	4	103	98*	0	1	5	728	741	0	2	5	30	18*
1	2	5	663	667	0	3	5	648	640	1	3	5	90	95*
2	3	5	562	567	0	4	5	63	48*	1	4	5	638	622
2	4	5	33	73*	3	4	5	476	485	0	5	5	625	624
1	5	5	54	59*	2	5	5	540	528	3	5	5	72	83*
4	5	5	479	472	0	6	5	33	18*	1	6	5	521	513
2	6	5	38	28*	3	6	5	476	468	4	6	5	65	75*
5	6	5	450	459	0	7	5	494	505	1	7	5	18	46*
2	7	5	479	489	3	7	5	66	21*	4	7	5	420	426
5	7	5	138	113	6	7	5	423	410	0	8	5	22	21*
1	8	5	441	455	2	8	5	62	19*	3	8	5	430	436
4	8	5	38	78*	5	8	5	348	360	6	8	5	39	44*
7	8	5	305	313	0	9	5	356	355	1	9	5	84	50*
2	9	5	373	366	3	9	5	39	17*	4	9	5	295	297
5	9	5	40	34*	6	9	5	311	300	7	9	5	41	16*
8	9	5	248	231	0	10	5	48	10*	1	10	5	297	294
2	10	5	20	16*	3	10	5	292	291	4	10	5	41	34*
5	10	5	248	240	6	10	5	58	38*	7	10	5	237	242
8	10	5	73	19*	9	10	5	204	199	0	11	5	276	274
1	11	5	40	22*	2	11	5	290	284	3	11	5	42	8*
4	11	5	232	230	5	11	5	42	4*	6	11	5	236	235
7	11	5	43	25*	8	11	5	178	184	9	11	5	86	32*
10	11	5	126	154	0	12	5	83	23*	1	12	5	244	246
2	12	5	75	10*	3	12	5	229	234	4	12	5	43	5*
5	12	5	215	212	6	12	5	44	9*	7	12	5	179	188
8	12	5	45	15*	9	12	5	142	146	10	12	5	45	13*
11	12	5	113	107*	0	13	5	224	229	1	13	5	47	34*
2	13	5	209	220	3	13	5	44	5*	4	13	5	217	201
5	13	5	72	15*	6	13	5	182	180	7	13	5	45	8*
8	13	5	135	136	9	13	5	57	12*	10	13	5	85	109*
11	13	5	42	3*	0	14	5	43	15*	1	14	5	207	200
2	14	5	67	32*	3	14	5	163	178	4	14	5	45	12*
5	14	5	180	161	6	14	5	23	5*	7	14	5	111	129*
8	14	5	45	10*	9	14	5	44	112*	10	14	5	74	4*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Pb$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	15	5	137	144	1	15	5	27	18*	2	15	5	159	137
3	15	5	45	14*	4	15	5	45	135*	5	15	5	45	16*
6	15	5	126	114	7	15	5	44	15*	8	15	5	43	107*
0	16	5	51	0*	1	16	5	119	116	2	16	5	44	5*
3	16	5	136	112	4	16	5	44	26*	5	16	5	123	103
6	16	5	37	16*	0	17	5	64	95*	1	17	5	34	10*
2	17	5	122	94	0	0	6	624	621	0	1	6	33	67*
1	1	6	572	585	0	2	6	498	505	1	2	6	34	31*
2	2	6	425	432	0	3	6	100	100	1	3	6	421	421
2	3	6	36	46*	3	3	6	411	395	0	4	6	450	440
1	4	6	69	43*	2	4	6	441	439	3	4	6	56	70*
4	4	6	431	439	0	5	6	36	19*	1	5	6	434	438
2	5	6	37	70*	3	5	6	420	420	4	5	6	38	12*
5	5	6	341	352	0	6	6	387	383	1	6	6	37	26*
2	6	6	382	387	3	6	6	59	31*	4	6	6	336	327
5	6	6	40	21*	6	6	6	313	318	0	7	6	62	25*
1	7	6	387	378	2	7	6	77	27*	3	7	6	353	341
4	7	6	40	47*	5	7	6	303	303	6	7	6	58	9*
7	7	6	285	284	0	8	6	347	344	1	8	6	39	42*
2	8	6	335	348	3	8	6	41	29*	4	8	6	263	276
5	8	6	42	38*	6	8	6	279	282	7	8	6	43	25*
8	8	6	212	196	0	9	6	28	27*	1	9	6	298	288
2	9	6	41	43*	3	9	6	247	259	4	9	6	71	17*
5	9	6	244	247	6	9	6	43	41*	7	9	6	212	216
8	9	6	45	23*	9	9	6	178	151	0	10	6	246	242
1	10	6	15	15*	2	10	6	234	234	3	10	6	43	30*
4	10	6	211	209	5	10	6	31	10*	6	10	6	224	229
7	10	6	45	9*	8	10	6	176	162	9	10	6	46	6*
10	10	6	141	124	0	11	6	42	18*	1	11	6	217	203
2	11	6	44	27*	3	11	6	210	196	4	11	6	61	21*
5	11	6	181	197	6	11	6	45	25*	7	11	6	173	172
8	11	6	35	3*	9	11	6	133	129	10	11	6	55	7*
11	11	6	97	110*	0	12	6	212	198	1	12	6	16	31*
2	12	6	216	189	3	12	6	45	4*	4	12	6	196	172
5	12	6	46	14*	6	12	6	123	154	7	12	6	48	4*
8	12	6	130	126	9	12	6	45	18*	10	12	6	44	107*
0	13	6	76	3*	1	13	6	204	179	2	13	6	45	34*
3	13	6	187	174	4	13	6	46	7*	5	13	6	139	136
6	13	6	56	7*	7	13	6	106	117*	8	13	6	60	15*
9	13	6	58	102*	0	14	6	153	139	1	14	6	45	24*
2	14	6	159	141	3	14	6	49	12*	4	14	6	120	133*
5	14	6	46	3*	6	14	6	96	114*	7	14	6	84	5*
0	15	6	44	10*	1	15	6	114	99*	2	15	6	45	9*
3	15	6	92	117*	4	15	6	44	9*	5	15	6	141	104
0	16	6	79	90*	1	16	6	42	4*	0	1	7	346	352
0	2	7	73	117*	1	2	7	313	309	0	3	7	403	407
1	3	7	38	34*	2	3	7	380	379	0	4	7	39	16*
1	4	7	340	335	2	4	7	32	32*	3	4	7	299	317

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Pb$

M167

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
0	5	7	312	295	1	5	7	40	31*	2	5	7	317	295
3	5	7	41	10*	4	5	7	266	278	0	6	7	54	153
1	6	7	292	300	2	6	7	41	10*	3	6	7	286	285
4	6	7	54	34*	5	6	7	252	271	0	7	7	235	239
1	7	7	42	4*	2	7	7	236	235	3	7	7	76	29*
4	7	7	242	234	5	7	7	44	9*	6	7	7	189	192
0	8	7	42	14*	1	8	7	225	230	2	8	7	67	163
3	8	7	193	210	4	8	7	44	9*	5	8	7	214	204
6	8	7	47	11*	7	8	7	179	178	0	9	7	238	229
1	9	7	43	9*	2	9	7	226	233	3	9	7	45	21*
4	9	7	215	224	5	9	7	45	11*	6	9	7	164	164
7	9	7	46	24*	8	9	7	29	144*	0	10	7	43	41*
1	10	7	180	188	2	10	7	45	23*	3	10	7	198	191
4	10	7	46	12*	5	10	7	150	169	6	10	7	37	55
7	10	7	116	140*	8	10	7	46	11*	9	10	7	46	111*
0	11	7	144	149	1	11	7	73	22*	2	11	7	171	170
3	11	7	47	11*	4	11	7	167	157	5	11	7	155	7*
6	11	7	145	127	7	11	7	65	13*	8	11	7	148	117
9	11	7	59	12*	0	12	7	77	32*	1	12	7	146	150
2	12	7	46	21*	3	12	7	150	139	4	12	7	10	1*
5	12	7	119	129*	6	12	7	23	10*	7	12	7	53	110*
8	12	7	44	9*	0	13	7	117	103*	1	13	7	45	20*
2	13	7	109	114*	3	13	7	46	1*	4	13	7	101	111*
5	13	7	46	10*	6	13	7	89	103*	0	14	7	43	11*
1	14	7	44	96*	2	14	7	39	4*	3	14	7	44	89*
4	14	7	75	11*	0	0	8	131	128	0	1	8	67	6*
1	1	8	266	259	0	2	8	265	254	1	2	8	42	18*
2	2	8	282	295	0	3	8	43	5*	1	3	8	247	254
2	3	8	27	30*	3	3	8	225	236	0	4	8	242	232
1	4	8	43	2*	2	4	8	240	237	3	4	8	89	15*
4	4	8	241	256	0	5	8	43	29*	1	5	8	221	224
2	5	8	22	16*	3	5	8	226	221	4	5	8	45	19*
5	5	8	177	190	0	6	8	183	191	1	6	8	44	7*
2	6	8	164	180	3	6	8	67	31*	4	6	8	174	183
5	6	8	54	16*	6	6	8	126	149*	0	7	8	44	10*
1	7	8	163	170	2	7	8	46	17*	3	7	8	209	189
4	7	8	46	12*	5	7	8	157	159	6	7	8	24	17*
7	7	8	65	123*	0	8	8	167	154	1	8	8	46	3*
2	8	8	172	165	3	8	8	62	5*	4	8	8	155	164
5	8	8	37	23*	6	8	8	123	133*	7	8	8	17	1*
8	8	8	72	102*	0	9	8	45	37*	1	9	8	148	147
2	9	8	47	5*	3	9	8	137	155	4	9	8	47	13*
5	9	8	128	132*	6	9	8	47	5*	7	9	8	109	108*
8	9	8	84	4*	9	9	8	58	117*	0	10	8	106	169*
1	10	8	46	26*	2	10	8	130	149	3	10	8	47	11*
4	10	8	149	136	5	10	8	47	10*	6	10	8	104	115*
7	10	8	45	6*	0	11	8	44	7*	1	11	8	120	131*
2	11	8	20	22*	3	11	8	23	127*	4	11	8	49	6*

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $(C_6H_5)_4Pb$

H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc	H	K	L	10Fo	10Fc
5	11	8	64	110*	6	11	8	45	10*	0	12	8	67	102*
1	12	8	75	14*	2	12	8	105	86*	3	12	8	42	7*
4	12	8	93	97*	0	1	9	205	186	0	2	9	46	30*
1	2	9	154	165	0	3	9	175	152	1	3	9	46	36*
2	3	9	190	184	0	4	9	82	40*	1	4	9	83	154*
2	4	9	47	2*	3	4	9	135	155	0	5	9	110	135*
1	5	9	46	10*	2	5	9	44	158*	3	5	9	71	8*
4	5	9	139	135	0	6	9	33	5*	1	6	9	92	144*
2	6	9	47	20*	3	6	9	126	142*	4	6	9	47	14*
5	6	9	137	123	0	7	9	23	143*	1	7	9	47	2*
2	7	9	127	129*	3	7	9	47	12*	4	7	9	33	121*
5	7	9	47	10*	6	7	9	104	91*	0	8	9	78	0*
1	8	9	150	126	2	8	9	47	10*	3	8	9	81	104*
4	8	9	47	18*	5	8	9	76	99*	6	8	9	57	16*
0	9	9	44	113*	1	9	9	45	3*	2	9	9	46	93*
3	9	9	49	14*	4	9	9	46	106*	0	10	9	46	2*
1	10	9	74	96*	0	0	10	75	116*	0	1	10	44	4*
1	1	10	126	121	0	2	10	57	130*	1	2	10	46	18*
2	2	10	43	107*	0	3	10	46	13*	1	3	10	115	110*
2	3	10	85	6*	3	3	10	46	95*	0	4	10	63	113*
1	4	10	50	3*	2	4	10	46	89*	3	4	10	46	9*
4	4	10	60	97*	0	5	10	45	1*	1	5	10	70	104*
2	5	10	45	14*	3	5	10	107	92*	0	6	10	99	116*
1	6	10	57	12*										