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Visible Laser Absorption Spectroscopy of Gas-Phase YbCl, YbS, YbOH and CaS

by

Todd C. Melville

Submitted in partial fulfillment of
the requirements for the degree of
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at
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FACULTY OF GRADUATE STUDIES

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Abstract

High-resolution laser induced fluorescence and resolved fluorescence have been utilized to examine the $A^2\Pi - X^2\Sigma^+$ electronic transition of gaseous ^{174}Yb^{35}Cl and ^{172}Yb^{35}Cl. In total, more than 2600 line positions have been employed in least-squares fits of molecular parameters. The $A^2\Pi$ and $B^2\Sigma^+$ states are shown to act as a unique perturber pair. The interaction between the $A^2\Pi$ and $X^2\Sigma^+$ states has been investigated, and is shown to be the primary contributor to the spin-rotation splitting in the ground state.

In the first observation of YbS, the $A0^+ - X0^+$ and $B0^+ - X0^+$ transitions have been investigated at both low- and high-resolution using laser absorption spectroscopy. The $A0^+$ state experiences both vibrational and rotational perturbations. A partial deperturbation analysis has provided deperturbed parameters for both the $A0^+$ state and the perturbing state. The $B0^+$ state is subject to a strong predissociation in the $\upsilon = 0$ vibrational level. Molecular parameters for all of the observed levels are reported.

The $\tilde{A}^2\Pi$ – $\tilde{X}^2\Sigma^+$ transition in YbOH has been examined in the first reliable spectroscopic observation of a lanthanide monohydroxide. A vibrational analysis of this system has provided estimates for the vibrational frequencies of the Yb-O stretching and Yb-O-H bending modes. A rotational analysis of the (000) – (000) band indicates the molecule has a linear geometry in both electronic states. The unusual behaviour of the ground state spin-rotation parameter is discussed and compared to that of the isoelectronic YbF molecule.

Numerous bands in the CaS $A^1\Sigma^+$ – $X^1\Sigma^+$ transition have been investigated using high-resolution laser spectroscopy. The $A^1\Sigma^+$ state is extensively perturbed by at least three other electronic states (which may include spin-components of a triplet state). A deperturbation analysis of the nine observed level crossings has provided estimates of molecular parameters for the $A^1\Sigma^+$ and perturbing states. The identity of the perturbers, though not established unequivocally, is discussed in terms of the low-lying $a^3\Pi$ and $A'^1\Pi$ states.

List of Abbreviations and Symbols

α_e	Equilibrium vibration-rotation interaction constant
α	Homogeneous perturbation interaction constant
A	Spin-orbit coupling constant
A_D	Centrifugal distortion correction to the spin-orbit coupling
Å	Ångstrom unit (10^{-10} m)
B_υ	Rotational constant for the vibrational level υ
B_e	Equilibrium rotational constant
β	Heterogeneous perturbation interaction constant
CCD	Charge-coupled device
D_e	Equilibrium dissociation energy
D_υ	Centrifugal distortion constant for the vibrational level υ
e, f	Rotation-independent parity label
F	Rotational energy
$F_{1,2}$	Spin components
FC	Franck-Condon
γ_e	Equilibrium spin-rotation constant
G	Vibrational energy term value
H	Centrifugal distortion constant; coefficient of $[J(J+1)]^3$
J	Total angular momentum quantum number (exclusive of nuclear spin)
J_0	Non-integer crossing point of the vibration-rotation energy of two states
L	Centrifugal distortion constant; coefficient of $[J(J+1)]^4$

LIF	Laser induced fluorescence
ν_i	Vibrational mode (i = 1, 2, 3)
ν_0	Band origin
N	Total angular momentum quantum number (excluding spin)
Ω	Quantum number for Hund's case (c) projection of J onto internuclear axis
ω_e	Equilibrium vibrational frequency
$\omega_e x_e$	Anharmonicity constant to vibrational frequency
p_υ	Λ-type doubling constant
$p_{D\upsilon}$	Centrifugal distortion to the Λ-type doubling
P_i	Perturber (i)
PMT	Photomultiplier tube
ρ	Square-root of the ratio of reduced masses for a diatomic molecule
q_υ	Λ-type doubling constant
R	bond length
RKR	Rydberg-Klein-Rees
S/N	Signal-to-noise ratio
σ	Standard deviation
T	Term value energy
υ	Vibrational quantum number

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Chapter 1

Introduction

In the past twenty-five years, there has been a resurgence of interest in lanthanide chemistry and spectroscopy in an attempt to gain insight into the chemical properties, bonding and molecular structure of molecules that contain a lanthanide atom. Nevertheless, the state of work done on this class of molecules can be said to be in its infancy when compared to that accomplished for molecules that possess elements that are lighter than the lanthanides. One reason for this is that electronic configurations with an open 4*f* subshell exist in molecules that contain a lanthanide atom, creating a very dense manifold of excited electronic states.[1] Furthermore, lanthanide atoms are relatively heavy, and molecules with such an atom often have small rotational constants and therefore dense vibration-rotation structure. These factors, coupled with the presence of large hyperfine effects and numerous isotopes, render investigations of these molecules a challenge both for experimental spectroscopists, and for theoreticians attempting to calculate their electronic and molecular properties.

For the most part, very sparse information is available for small, gas-phase molecules that contain a lanthanide atom. A notable exception to this is the series of lanthanide monoxide molecules (CeO,[2] PrO,[3] NdO,[4] SmO,[5] GdO,[6] TbO,[7] DyO,[7] HoO,[7] ErO,[8] YbO[9] and LuO[10]), which have been studied experimentally and theoretically. There has also been work done on several ytterbium-containing molecules, largely at low-resolution. Ytterbium-containing molecules are of particular interest spectroscopically because they afford an ideal opportunity to study the properties of electronic states with both closed and open *f*-shells. Among the diatomic halides, only YbF has been studied in any detail. Past work on YbF includes spectroscopic studies at high-resolution,[11-14] as well as several theoretical studies.[15-18] The ground electronic state of the ytterbium atom is similar to that of an alkaline-earth atom, except that it has a filled 4*f* subshell. Therefore, it is possible to draw comparisons between the electronic structure of ytterbium containing molecules, and the analogous alkaline-earth molecules, which have been studied in considerably better detail. With single-frequency, tunable dye lasers, and careful selective detection schemes, these molecules can be examined in a systematic and thorough fashion.

The subject matter of the present thesis is the low- and high-resolution spectroscopic investigation of several small molecules that contain an ytterbium atom, YbCl, YbS and YbOH. In each of these studies, the present work represents the first high-resolution, rotational analysis of the molecule, and for YbS and YbOH, this is the first reliable experimental observation of any kind. The principal objective of this thesis has been to initiate a systematic investigation of the low-lying electronic states of several Yb-containing molecules, and to draw comparisons with the analogous alkaline-earth species. Further motivation comes from the opportunity to examine the role that *f* electrons play in the bonding in this class of molecules. However, because the majority of electronic states observed have closed 4*f* sub-shells, the information extracted from the work in this regard is limited. Nevertheless, we have gained considerable insight into the manifold of electronic states that exist in each of these molecules.

Also included in this thesis is a study of CaS, which complements the work done on YbS. The CaS project was undertaken to identify and examine perturbations in the

$A^1\Sigma^-$ excited state. Similar perturbations are found in the $A0^-$ state of YbS, and are the basis for a comparison of the two species.

A description of the experimental aspects of this thesis is presented in the following chapter. The first section describes the Broida oven production source for the molecules observed. Following that, a detailed account of the low-resolution laser excitation system and detection scheme is given. Lastly, a description is given of the high-resolution laser system used for absorption and fluorescence experiments.

In Chapter 3, several theoretical aspects of this thesis work are described. These include descriptions of the relevant Hund's coupling cases, energy level formulae and parity. In addition, Rydberg-Klein-Rees potential energy curves, the technique of least-squares merging, and the presence of perturbations in the spectra of diatomic molecules are discussed.

The fourth chapter is concerned with a rotational analysis of several bands of the $A^2\Pi - X^2\Sigma^-$ transition in YbCl. Doppler-limited laser excitation spectroscopy was employed to examine the A–X transition of ^{174}Yb^{35}Cl and ^{172}Yb^{35}Cl. Resolved fluorescence from selectively populated J-levels of the $A^2\Pi$ $\upsilon = 0$ level was used to access vibrational levels $\upsilon \leq 3$ of the ground state for both isotopomers. The interaction of the $A^2\Pi$ and $X^2\Sigma^-$ states has been studied and is shown to be the main contributor to the ground state spin-rotation splitting. Rotational, lambda-doubling, spin-orbit and spin-rotation parameters have been determined through least-squares fits of more than 2600 line positions.

Chapter 5 describes the investigation of the $A0^- - X0^-$ and $B0^- - X0^-$ transitions in YbS. This work represents the first spectroscopic observation of any kind for this molecule and includes both low and high-resolution analyses of these systems. The $A0^-$ state has been found to be both globally and rotationally perturbed, and a partial deperturbation analysis of the $A0^-$ ~ Perturber interaction is presented. The $B0^-$ state was found to exhibit a predissociation in the $\upsilon = 0$ level. Vibrational and rotational constants are reported for all of the observed levels.

An analysis of the $\tilde{A}^2\Pi - \tilde{X}\,^2\Sigma^-$ transition in YbOH is presented in Chapter 6. Vibrational parameters for the Yb-O stretching mode and the Yb-O-H bending mode are estimated from low-resolution laser excitation and resolved fluorescence spectra. High-resolution laser excitation experiments of the (000) – (000) and (000) – (100) bands (where v_1 is the Yb-O stretching mode) have established the geometries of the $\tilde{A}^2\Pi$ and $\tilde{X}^2\Sigma^-$ states as linear. The unusual behaviour of the spin-rotation parameter in the ground state is compared to that of the isoelectronic YbF molecule.

Chapter 7 concerns a rotational analysis of the $A^1\Sigma^- - X^1\Sigma^+$ electronic transition in CaS. The $A^1\Sigma^-$ state is extensively perturbed by at least three other states, which may include one or more spin-components of a triplet state. A deperturbation analysis of this system has allowed for the determination of a complete set of deperturbed molecular constants for both the $A^1\Sigma^-$ and perturbing states.

In Chapter 8, the electronic structures of the molecules examined are discussed in a broader sense by considering the role *f*-electrons have in their bonding. Finally, the perturbations observed in YbS and CaS are compared to the analogous perturbations in SrS and BaS.

Chapter 2

Experimental Arrangement

2.1 Broida Oven Production Source

Selection of an appropriate method for producing a novel molecule is the main prerequisite to observation of molecular spectra. To overcome this major obstacle, a number of production methods have been developed over the years. The most commonly used sources of small molecules in the gas-phase include laser ablation,[19] sputter sources,[20] heat pipes,[21] furnaces,[22] microwave discharges,[23] and ovens.[24] As would be expected, no single method is without deficiencies, and one must carefully choose a production method that is suitable for the project of interest.

For the production of gas phase molecules, the present work employs a Broida-type oven,[24] based on the design used by Professor Field's group at MIT. The Broida oven provides a source of gaseous metal atoms in a relatively low-temperature flow system. This is a substantial improvement over heat pipes and furnaces in that molecules produced in the Broida oven have temperatures on the order of 500 K, in a region where the total pressure is approximately 1 – 5 torr. The oven can be used for elements (or compounds) that have significant vapour pressure at temperatures below 1000 K, though it is unsatisfactory for the more refractory elements. It should be noted, however, that different models of Broida ovens have been successfully used for producing gas phase metal atoms of the more refractory elements.[25]

A schematic diagram of the Broida oven is given in Figure 2.1. A metal sample is placed in a small alumina crucible and resistively headed by a preformed, commercially

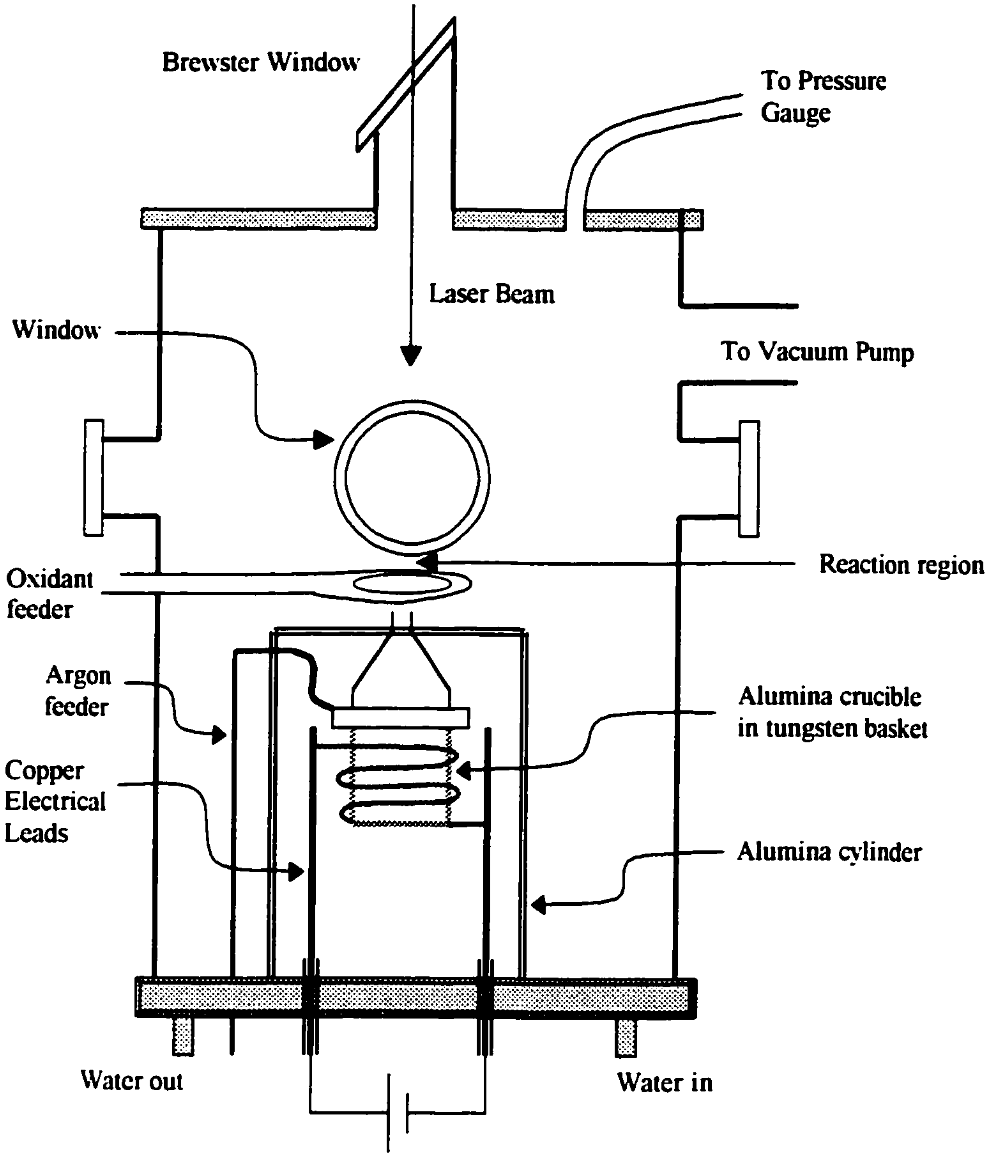


Figure 2.1: The Broida oven, based on the design of Professor Field's group at MIT; originally developed by West and coworkers (Ref. 24).

available, tungsten wire basket (R. D. Mathis Co., B10-4X.030W). The metal vapour is then entrained in a flow of argon gas (Praxair, 99.99%) that is fed in through 0.05 mm holes in a 1/16 inch-diameter stainless steel tube (Chromatographic Specialties, T30C40D) directly above the crucible. To optimize the flow of the metal atoms in the argon carrier gas, the steel tubing is bent such that it encircles the top of the crucible. The argon gas, which is controlled using a metered needle valve (Hoke, 1315G4B), also cools the gaseous metal atoms that flow up through the chimney to the region where the oxidant gas is introduced. The oxidant gas enters the oven through one of two different tubes: copper tubing, similar in design to the stainless steel tubing, or a quartz glass tube that is used for corrosive gases, such as chlorine. The flow of the oxidant gas can be controlled using a needle valve (Hoke, 1654G4BA). Typically, the oxidant gas made up a few mtorr of the total pressure, though this varied considerably depending on the species involved. Experimental details concerning the production of individual molecules are given in the relevant chapters.

Two copper rods, that also serve as electrical leads, support the tungsten wire basket and crucible. This entire assembly is contained inside the oven in a capped alumina cylinder that both minimizes the heating of the surroundings, and reduces radiation given off by the heated sample. In order to reduce the scattered laser light in the oven, the capped cylinder and chimney also serve as a convenient 'dump' for the laser beam, which enters the oven vertically through a quartz Brewster window. The window is set at the Brewster angle (55°) for radiation with wavelengths near 650 nm in order to minimize scattered light from the window. Laser induced fluorescence (LIF) can be viewed through 2″-diameter quartz windows on either side of the oven.

The body of the Broida oven is composed of an 8″-long, 4″-diameter segment of copper pipe. The base and lower portion of the oven are water-cooled. All ports, windows and end plates on the oven have flange end-mounts with O-ring grooves that enable the system to easily maintain reduced pressures of a few torr. During operation, the oven was continuously pumped by a dual stage rotary vane pump (Leybold-Heraeus, D4A). The power requirements of the Broida oven were supplied by two transformers (Hammond, 165X5) connected in parallel. Precise control of the heating was achieved using a variable transformer (Powerstat, 116B) to vary the primary voltage supplied to the transformers. Typically, the temperature in the oven was kept at just below the melting point of the metal employed.

Several different forms of ytterbium metal were tested, namely, pieces (Alfa Aesar, 99.9%), ingot (Aldrich, 99.9%) and chips (Strem, 99.9%), to determine which produced the most intense LIF. It was determined that the chips (which are essentially metal turnings) were most effective, probably because they possessed the largest surface area/mass ratio of the different forms tested. Conditions in the Broida oven were adjusted at the beginning of each experiment to attain the optimal LIF signal. This was achieved by slowly adjusting the argon partial pressure, the oxidant partial pressure and the operating temperature of the oven. In general, chemiluminescence was visible in the reaction region of the oven, though the colour varied depending on the molecule being studied. For the most part, it was found that a relatively intense chemiluminescence coincided with a strong LIF signal.

2.2 Low-Resolution Laser Excitation Spectroscopy

The low-resolution laser excitation experiments were carried out utilizing a Coherent 599 standing wave dye laser pumped by approximately 5 W of 514.5-nm radiation from an argon ion laser. The dye laser was operated in broadband mode (bandwidth of approximately 1 cm^{-1}), with typical output powers in the range 100 – 400 mW, depending on the dye and region selected. The output wavelength was varied using a three-plate birefringent filter (BRF) connected to a stepper motor. The speed of the stepper motor was continuously variable from one revolution every 3.41 seconds, to one revolution every 18 minutes, and was computer controlled. A schematic diagram of the low-resolution experimental setup is given in Fig. 2.2. Two types of low-resolution spectra were recorded: laser excitation and resolved fluorescence.

Laser excitation spectra were obtained by scanning the laser and recording the total laser induced fluorescence with a photomultiplier tube (RCA C31034/76) through a red-pass filter to remove scattered laser light. The cutoff wavelength of the filter used depended on the wavelength region and the molecule being studied. The estimated uncertainty of measurements of bandheads in the laser excitation spectra is approximately ± 5 cm^{-1}.

In separate experiments, the laser-induced fluorescence was dispersed with a 1.26-m f/9 monochromator (Spex Industries, model 1269) fitted with a 2400 groove/mm grating (Bausch and Lomb) blazed at 5000 Å, and detected with a CCD array detector (S.A. CCD-2000, 15-μm pixel size) cooled to −140°C. Dispersed fluorescence spectra were calibrated using a hollow cathode uranium lamp and the standard atlas of atomic uranium wavelengths.[26] Well-resolved spectra were obtained by tuning the laser to a

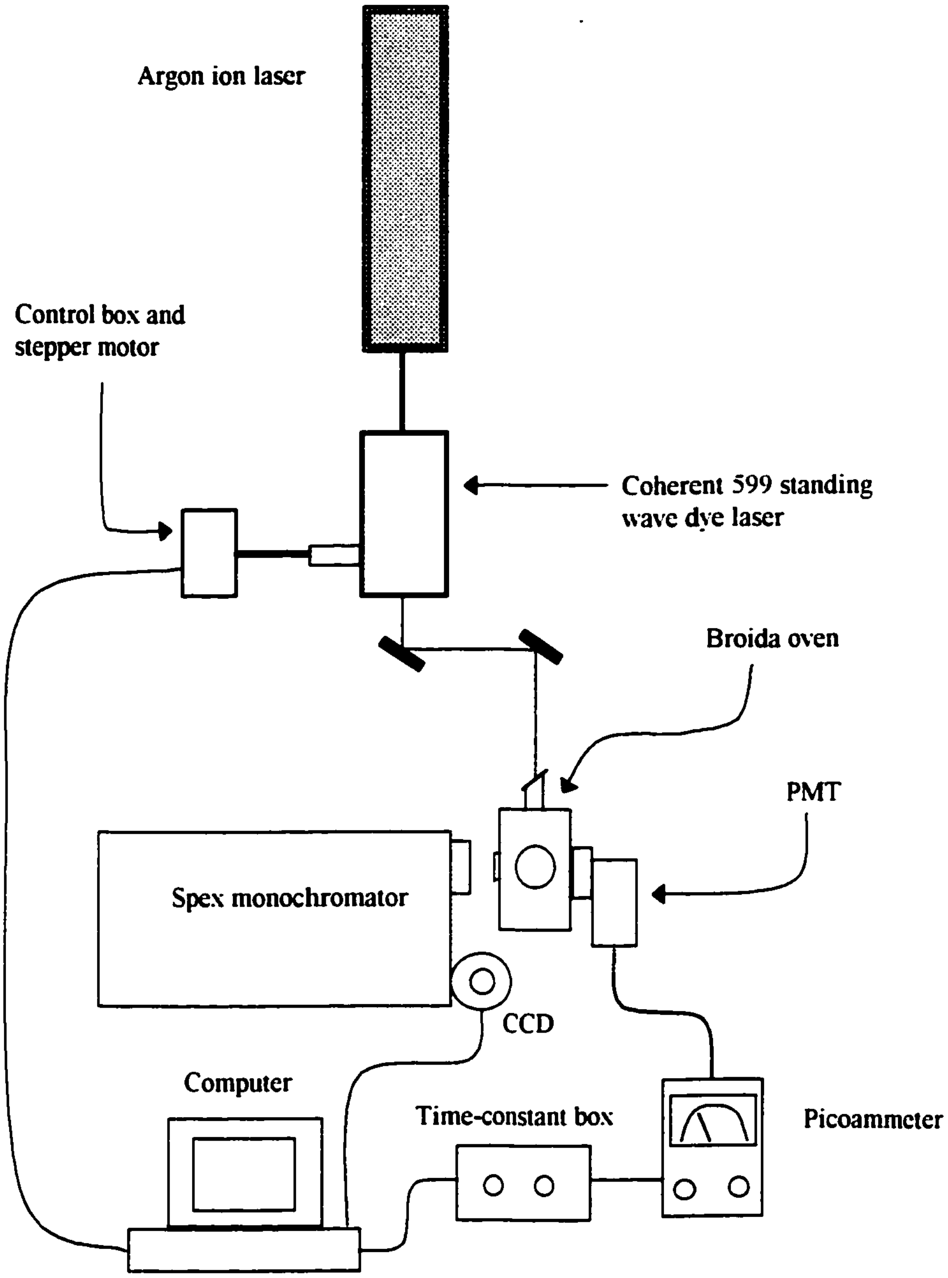


Figure 2.2: Experimental arrangement for low-resolution laser spectroscopy. For laser excitation spectroscopy, the PMT, picoammeter and computer are used to record the intensity of the total fluorescence. The monochromator and CCD array detector are used when performing resolved fluorescence experiments.

band-head, and recording fluorescence outside the region of the laser with monochromator slit-widths in the range 20 – 100 μm. The estimated uncertainty of measurements of band head positions in the resolved fluorescence spectra is about ± 2 cm^{-1}.

2.3 High-Resolution Laser Excitation Spectroscopy

In 1977, the first report appeared of single-frequency output from a ring dye laser.[27] Since then, ring lasers have been developed to oscillate at high powers throughout the visible region of the spectrum.[28] For this thesis work, high resolution laser excitation spectroscopy was performed with a Coherent 699-29 'Autoscan' computer controlled ring dye laser. The dye laser was pumped with 7 W of output from a Coherent Sabre (TSM-15) argon ion laser. Depending on the dye being pumped, either the 514.5 or 488.0 nm line was used. When operating in single mode, the effective bandwidth of the 699-29 laser beam is approximately 1 MHz, with output powers in the range 100 – 400 mW, depending on the dye and region being scanned. The laser beam was modulated by a mechanical chopper at 540 Hz and directed vertically down into the Broida oven. Laser-induced fluorescence (LIF) was imaged onto the entrance slit of the monochromator, and detected with a GaAs photomultiplier tube (RCA C31034). The output signal of the PMT was fed to a lock-in amplifier (EG&G Model 186A) for phase sensitive detection, effectively eliminating unwanted background radiation and suppressing the chemiluminescence signal. The spectrum obtained from the lock-in amplifier was then stored on a desktop computer. A schematic diagram of the system is given in Figure 2.3.

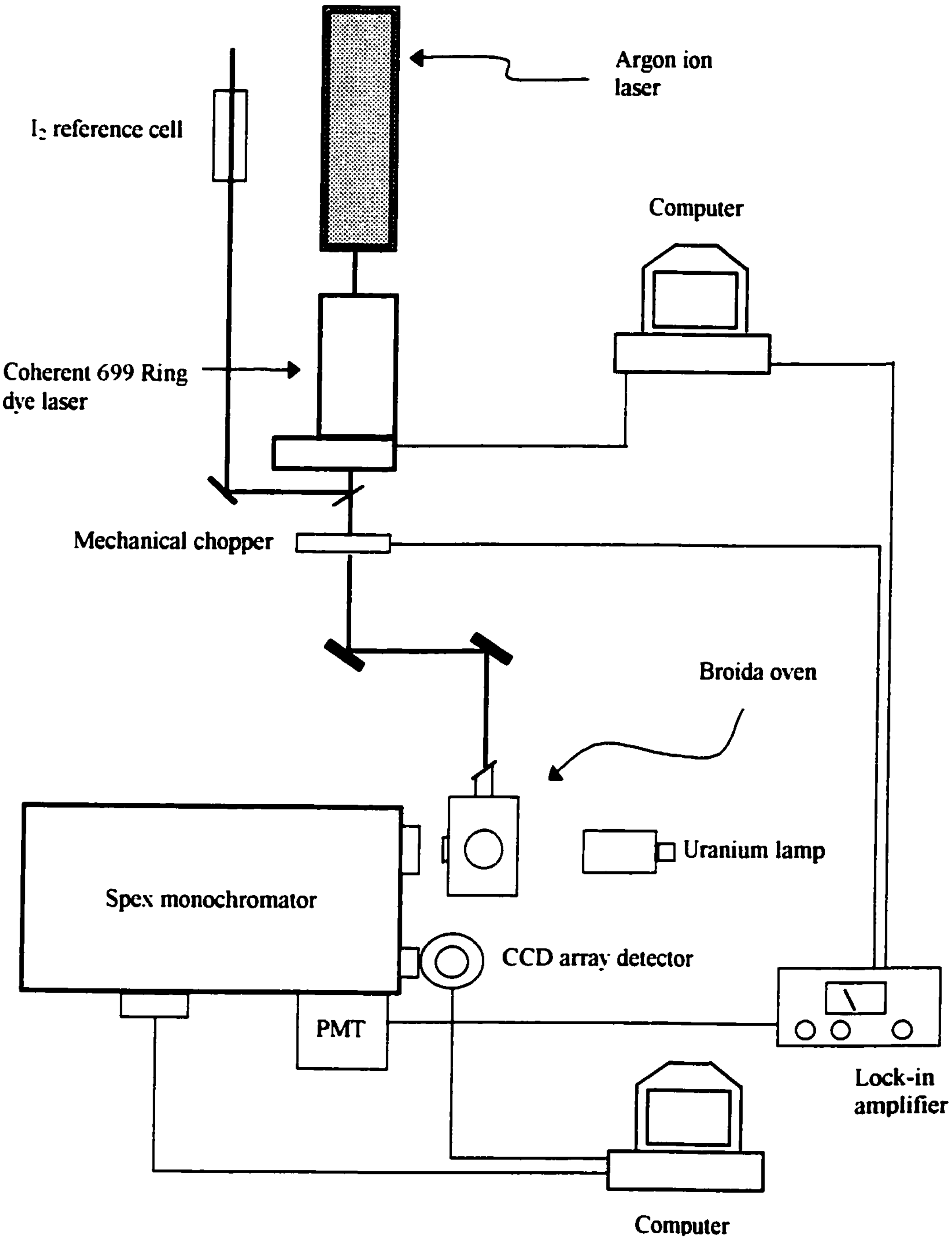


Figure 2.3: Experimental arrangement for high-resolution laser spectroscopy.

The spectral line width was dominated by Doppler broadening, which was typically 1.2 GHz for the present molecular source. Line positions in the excitation spectra were measured using the laser's internal wavemeter and the Autoscan software. The precision of measurements in similar previous work with this arrangement was typically 0.003 cm^{-1}. During all scans, a small portion of the laser beam (≈ 5 %) was directed into an evacuated I_2 cell to record a fluorescence spectrum. The I_2 spectrum was compared to the standard I_2 atlas[29] for verification of the calibration of the wavemeter.

When recording laser excitation spectra, the monochromator served as a narrow band-pass filter for selective detection of LIF. The detection scheme consisted of scanning the laser over the *R*-branch and detecting the LIF from the corresponding *P*-branch. By interchanging the laser and monochromator wavelengths, the opposite branch could be easily recorded. Selective detection completely suppressed overlapping branches and transitions, and was enormously useful for elucidating the branch structure of congested spectra.

Dispersion of laser-induced fluorescence (also referred to as resolved fluorescence) was employed for two purposes during experiments at high resolution: (1) to unambiguously assign the quantum number J (or N) to rotational lines in the excitation spectra, and (2) to investigate the vibration-rotation structure of the ground electronic state. The experimental arrangement for resolved fluorescence experiments was similar to that of the laser excitation work, which is illustrated in Fig. 2.3. The 699 was operated in single-frequency mode, but instead of being scanned, the laser wavelength was held fixed at a known rotational transition. The resulting fluorescence signal was detected with the CCD array detector, and calibrated with a uranium lamp in the same fashion as described above for the low-resolution work. The monochromator slit-width was held fixed at 17 μm and integration times varied depending on the observed LIF signal. This slit-width offered a reasonable balance between signal and resolution, the latter of which was typically about 0.2 cm^{-1}.

To establish assignments of the rotational quantum number (J) for a series of rotational lines, the P-R separation method was employed. This procedure involved taking resolved fluorescence spectra of several different rotational lines in a branch, effectively determining the rate of change of the separation of the P-R lines with J. This series of separations could then be plotted to establish an unequivocal assignment of J, which is crucial for a least-squares analysis that determines accurate molecular parameters. The traditional method of combination differences was also used for assigning J, most notably when the spectra being examined were perturbed.

Resolved fluorescence experiments have also been used to probe the vibration-rotation structure of the ground electronic state. These experiments are very similar to those described above for assigning quantum numbers, but were used to examine vibrational levels above $\upsilon = 0$ in the ground electronic state. By setting the laser frequency to a known rotational transition in the 0–0 band, fluorescence to higher vibrational levels in the ground state could be recorded by setting the monochromator to the appropriate wavelength region. These experiments offered a relatively quick and easy method of examining the ground states of the molecules studied.

Chapter 3

Theoretical Background

3.1 Hund's Coupling Cases

Neglecting nuclear spin, the different angular momenta in a molecule – electron spin **S**, electronic orbital angular momentum **L**, and angular momentum of rotation **R** – always form a resultant, total angular momentum that is designated **J**.[30] The simplest situation for an electronic state arises when the spin **S** and the component of orbital angular momentum Λ of the electrons are zero (as for a $^1\Sigma$ state), resulting in the angular momentum of rotation being equal to the total angular momentum, **J**. For all other cases, it is necessary to distinguish different modes of coupling of the angular momenta.

In Hund's case (a) it is assumed that the interactions of the angular momentum of rotation with the spin and orbital angular momenta are very weak, but the electronic motions (**S**, **L**) are coupled strongly along the internuclear axis. The projections of **S** and **L** onto the internuclear axis are designated Σ and Λ, respectively, and the sum of these is defined as $\mathbf{\Omega}$. A vector diagram of a Hund's case (a) diatomic molecule is given in Fig. 3.1(a). Development of the theory that gives rise to quantized levels for rotational energy in case (a) states can be found in Herzberg.[30]

When $\Lambda = 0$ and $S \neq 0$, the spin vector **S** is weakly coupled to the internuclear axis, if at all, and therefore $\mathbf{\Omega}$ is not defined. Hence, Hund's case (a) cannot apply, and this weak (or zero) coupling of **S** to the internuclear axis is referred to as Hund's case (b).[30] A vector diagram for a Hund's case (b) diatomic is given in Fig. 3.1(b). Because they have both $\Lambda = 0$ and $S \neq 0$, $^2\Sigma$ states always follow Hund's case (b) coupling.

Figure 3.1 (a): Vector diagram for Hund's coupling case (a) in a diatomic molecule

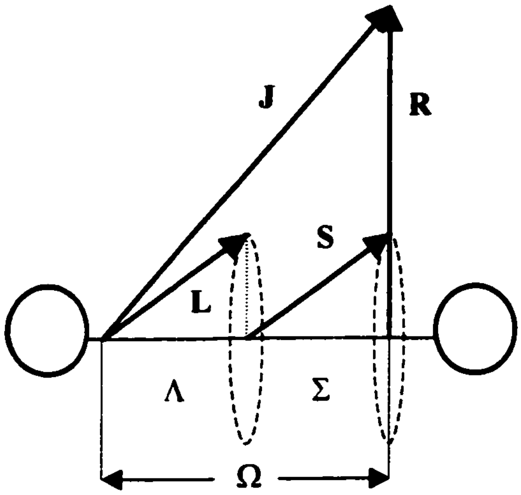


Figure 3.1 (b): Vector diagram for Hund's coupling case (b) in a diatomic molecule.

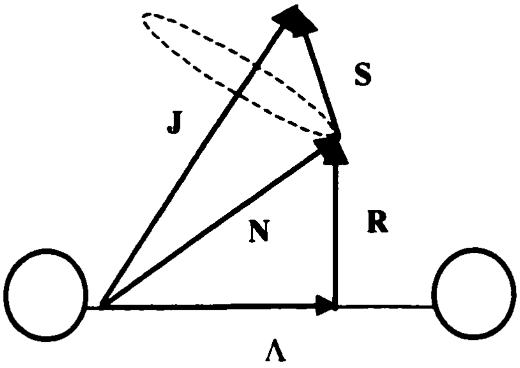
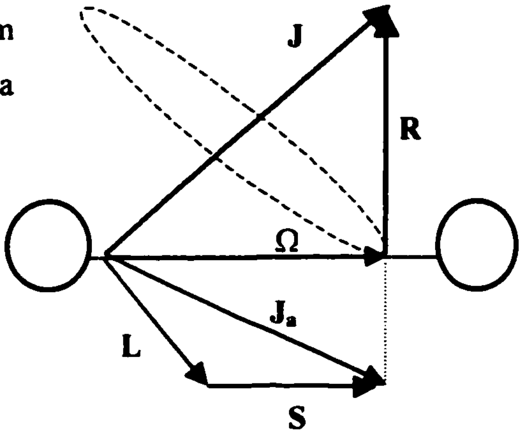


Figure 3.1 (c): Vector diagram for Hund's coupling case (c) in a diatomic molecule.



Another type of coupling that should be mentioned briefly is Hund's case (c), in which the interaction of **L** and **S**, particularly in heavy molecules, is stronger than the interaction with the internuclear axis. In this case Λ and Σ are not defined; rather, **L** and **S** form a resultant J_a, which is then coupled along the internuclear axis with a component Ω. A vector diagram for a Hund's case (c) diatomic is given in Fig. 3.1(c). Further details regarding the various Hund's coupling cases can be found in Herzberg.[30]

The consideration of Hund's cases is relevant in a number of different situations. For example, in a $^2\Pi$ state there are two limiting cases for the energy levels that depend on the extent of spin-orbit coupling. When A (the spin-orbit coupling constant) is large ($A \gg BJ$), the coupling is close to Hund's case (a), while when A is small ($A \ll BJ$), the coupling in the $^2\Pi$ state is very near Hund's case (b). If the $^2\Pi$ state belongs to case (a) there is a large separation between the $^2\Pi_{1/2}$ and $^2\Pi_{3/2}$ spin-orbit components, and we can divide each of the bands of a $^2\Pi$ – $^2\Sigma$ transition into two sub-bands, $^2\Pi_{1/2}$ – $^2\Sigma$ and $^2\Pi_{3/2}$ – $^2\Sigma$. This type of system exists in YbCl and YbOH, and is discussed in further detail below.

3.2 Empirical Energy Level Formulae

As mentioned above, the total angular momentum **J** in a $^1\Sigma$ state is equal to the angular momentum of rotation. Following Herzberg,[30] the usual expression for the rotational term values of a vibrational level υ in a $^1\Sigma$ state is,

$$F(J) = B_\upsilon J(J + 1) - D_\upsilon[J(J + 1)]^2 + \ldots \qquad (3.1)$$

Here, the parameters B_υ and D_υ are the familiar rotational and centrifugal distortion constants, respectively, and J is the rotational quantum number, $J = 0, 1, 2, \ldots$

With the exception of the degenerate bending vibrational levels, the rotational energy level expressions for linear triatomic molecules in a $^2\Sigma$ state are the same as those for diatomic molecules. Following Herzberg,[30] the usual case (b) expressions for a $^2\Sigma$ state are,

$$F_1(N) = B_\upsilon N(N+1) - D_\upsilon\,[N(N+1)]^2 + \tfrac{1}{2}\gamma_\upsilon N \tag{3.2}$$

$$F_2(N) = B_\upsilon N(N+1) - D_\upsilon[N(N+1)]^2 - \tfrac{1}{2}\gamma_\upsilon(N+1) \tag{3.3}$$

Here, F_1 and F_2 are the two spin-components in the $^2\Sigma$ state and γ_υ is the spin-rotation parameter. Details regarding the Hamiltonian matrix representation of $^2\Sigma$ states can be found in Kotlar *et al.*[31]

Transitions involving $^2\Pi$ states are of interest in the present work because they are found in both YbCl and YbOH. The branch structure of a case (a) $^2\Pi$ - case (b) $^2\Sigma^+$ transition is depicted in Fig. 3.2. Typical $^2\Pi_{1/2}$–$^2\Sigma^+$ transitions consist of two 'unblended' branches, R_{11} and P_{12}, and four 'blended' branches, $Q_{11} + R_{12}$ and $P_{11} + Q_{12}$. In the $^2\Pi_{3/2}$–$^2\Sigma^+$ sub-bands, the P_{22} and R_{21} branches are unblended while the $Q_{22} + P_{21}$ and $R_{22} + Q_{21}$ transitions are blended. The branches in pairs are only observed as separate branches if the spin-rotation splitting in the ground state is resolvable. The Hamiltonian matrix representation employed for $^2\Pi$ states in the present work is given in Table 3.1.[32]

For the present work, least squares fitting of transitions is performed using the approach of Zare *et al.*[33] In this non-linear fitting procedure, all measured line positions are iteratively compared with those calculated from numerically diagonalized Hamlitonians with adjustable molecular constants.

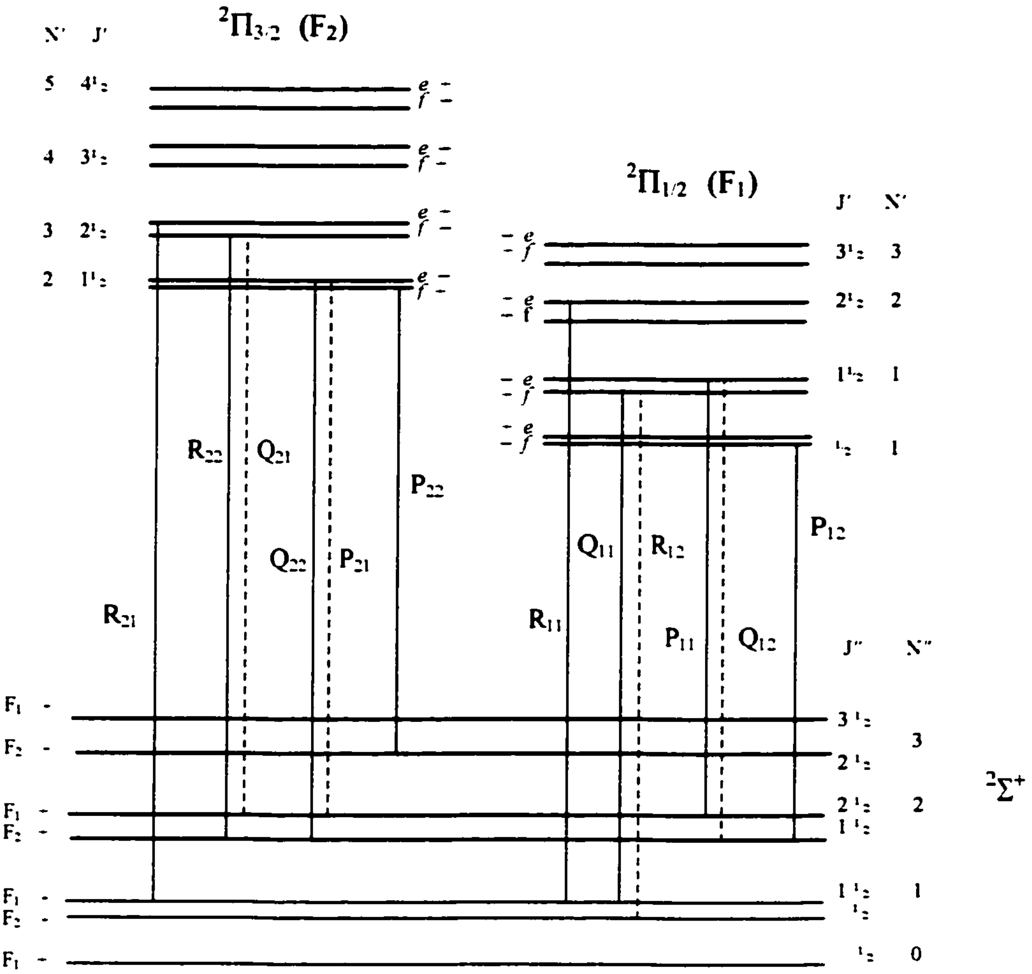


Figure 3.2: Energy level diagram for a case (a) $^2\Pi - {}^2\Sigma^+$ system. The broken lines are satellite branches and are only observed if the spin-rotation splitting in the $^2\Sigma^+$ state is resolvable.

Table 3.1

Matrix Representation of a Hund's Case (a) $^2\Pi$ State

$\vert\, ^2\Pi_{3/2}; J \pm \rangle$	$\vert\, ^2\Pi_{1/2}; J \pm \rangle$
$T_\upsilon + \tfrac{1}{2}\,[A_\upsilon + A_{D\upsilon}(z-2) + B_\upsilon(z-2)$ $- D_\upsilon[(z-2)^2 + z - 1]$	$-\,[\,B_\upsilon - 2\,D_\upsilon(z-1) \mp \tfrac{1}{2}\,q_\upsilon(J+\tfrac{1}{2})](z-1)^{1/2}$
$-\,[\,B_\upsilon - 2\,D_\upsilon(z-1) \mp \tfrac{1}{2}\,q_\upsilon(J+\tfrac{1}{2})](z-1)^{1/2}$	$T_\upsilon - \tfrac{1}{2}\,[A_\upsilon + A_{D\upsilon}\,z] + B_\upsilon\,z - D_\upsilon(z^2 + z - 1)$ $\mp \tfrac{1}{2}(p_\upsilon + 2q_\upsilon)(J+\tfrac{1}{2})$

$z = (J+\tfrac{1}{2})^2$; the upper/lower signs refer to the *e*/*f* parity levels.

3.3 Parity

Because there are several types of parity, such as *g*/*u*, *e*/*f*, and +/–, there is a great deal of confusion that surrounds the concept of parity.[34] The basic idea, however, is quite simple, and has been described in detail in the books of Herzberg,[30] Bernath,[34] and Lefebvre-Brion and Field.[35] The inversion operator $\hat{E}^*$ inverts the laboratory coordinates of all atoms in a molecule, and is used to divide all rovibronic energy levels into two groups by means of the equation

$$\hat{E}^* \psi = \hat{E}^*(\psi_{\mathrm{el}} \psi_{\mathrm{vib}} \psi_{\mathrm{rot}}) = \pm \psi. \tag{3.4}$$

All rovibronic energy states (ψ) for which the upper sign applies have positive (+) total parity, while all those states for which the lower sign applies have negative (–) total parity. The effects of $\hat{E}^*$ on the electronic, vibrational and rotational parts (ψ_{el}, ψ_{vib}, and ψ_{rot}, respectively) need to be determined individually, as discussed by Bernath.[34]

Although the alternation of the total parity with J is always present, it is useful to factor it out by defining *e* and *f* parity as[34]

$$\hat{E}^* \psi = +(-1)^J \psi \qquad \text{for } e, \tag{3.5}$$

and

$$\hat{E}^* \psi = -(-1)^J \psi \qquad \text{for } f, \tag{3.6}$$

for integer J in which ψ is the total rovibronic wavefunction. Notice that *e* and *f* parity is a residual parity, also called a rotationless parity, describing the total parity with the rotational part removed. Since the alternation of sign with J has been removed, *e*/*f* parity is more convenient to use than total parity. For example, all rotational energy levels of a $^1\Sigma^-$ state have *e* parity, but the total parity of each rovibronic level changes with J. Expressions analogous to Equations 3.5 and 3.6 for non-integer J-values, and a summary of the parity levels for the most common electronic states, have been described by Bernath.[34]

3.4 Rydberg-Klein-Rees Curves and Franck-Condon Factors

Interatomic potential energy curves that are accurate over a large radial range are desirable in a variety of spectroscopic problems.[35] In fact, numerous empirical representations of these potentials have been proposed, the earliest of which date back approximately 70 years.[36-38] It is worthwhile to emphasize that vibration-rotation data can be employed to yield accurate potential energy curves for bound electronic states. In particular, Rydberg[39] and Klein[40] have developed a method for calculating potential curves, which makes use of the experimental energy levels and does not depend on some derived formula for these levels. The difficulties associated with the earlier graphical procedures[39] were overcome by the introduction of analytical expressions for the turning points of a diatomic oscillator by Rees.[41] Rydberg-Klein-Rees (RKR) curves were an important development for the representation of spectroscopic data using a potential energy curve, but were not economical prior to the development of the modern computer. With today's computational power, it is trivial to calculate a potential energy curve for a diatomic molecule when data are available for a number of vibrational levels. A detailed description of this procedure has been described by Coxon.[42]

In 1925, Franck proposed an idea to explain the different cases of intensity distribution found in vibronic transitions,[43] corresponding to simultaneous changes in vibrational and electronic states. Condon later developed Franck's qualitative treatment mathematically on a quantum mechanical basis.[44] The quantum mechanical version of the Franck-Condon principle is based on the probability of a transition between two states, the measure of which is denoted the Franck-Condon factor ($q_{\upsilon'\upsilon''}$) for that transition. For a diatomic molecule,

$$q_{\upsilon'\upsilon''} = [\int \psi_{\upsilon'} \psi_{\upsilon''} dR]^2 \tag{3.7}$$

where $\int \psi_{\upsilon'} \psi_{\upsilon''} dR$ is the vibrational overlap integral. Franck-Condon factors have been determined for transitions in a variety of molecules, and can be calculated by standard numerical means employing RKR curves for the two electronic states involved in the transition.[45]

3.5 Least-Squares Merge Procedure

A method for merging the results of separate least-squares fits to obtain the most precise, single values for each of the molecular constants of a spectroscopic system was first described by Albritton *et al.*[46] In their paper, Albritton *et al.* demonstrated that the output molecular constants from individual band fits can be taken together as input to a correlated least-squares fit, which then yields the optimal, single values for the parameters. The resulting parameters are equivalent to a global, weighted least-squares fit employing the entire data set.

This technique is extremely valuable when many of the bands of a molecular band system share common upper or lower vibrational levels. For such a system, where the parameters obtained from separate band-fits are redundant, merging allows for the determination of the "best" single value for the molecular constants. For example, this procedure has been applied in the present thesis work to YbCl, where the 0–0, 1–0, 0–1, 0–2 and 0–3 bands have been investigated. The method of stepwise merging was later developed by Coxon.[47]

3.6 Perturbations in the Spectra of Diatomic Molecules

Examined in sufficient detail, the electronic spectrum of virtually every diatomic molecule will possess perturbations of some kind. In a spectroscopic sense, perturbations can be defined as deviations from an expected polynomial representation of the energy levels for an electronic state. In other words, perturbations may be viewed as a failure of a subset of observed υ, J levels to be accommodated by the empirical energy level expression defined by the majority of sampled levels.[48] There are, in fact, several different types of perturbations, though it is beyond the scope of the present work to discuss them all. A common type of perturbation, often referred to as a level crossing, was encountered in the spectra of YbS and CaS and is discussed below.

Level crossings can occur when the rotational energy levels of two different states (with $\Delta\Omega \leq 1$) cross one another. Only rotational energy levels with the same parity and rotational quantum number, J, can interact with one another, so, a noticeable perturbation will take place only if, for one and the same J and parity in both states, the levels have about the same energy.[30] The resultant energy levels are shifted from their expected energies by equal amounts and in opposite directions. A schematic of an energy level diagram for a level crossing is given in Fig. 3.3. The "strength" of the perturbation, or, more specifically, the strength of the interaction between the two states, dictates the magnitude of the shifts of the energy levels.

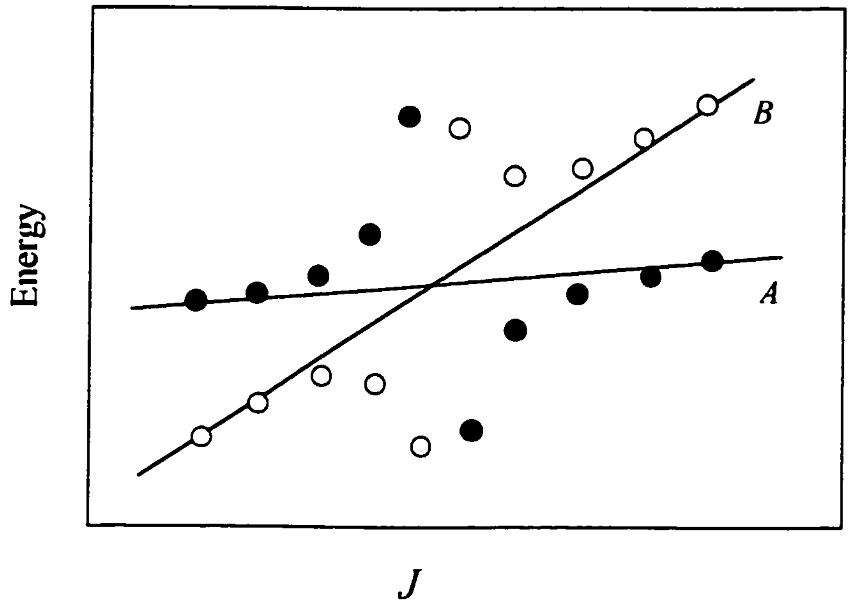


Figure 3.3: Schematic of a level crossing between two hypothetical states, *A* (filled circles) and *B* (hollow circles). As the levels get closer together, they repel one another further from their expected positions (along the straight lines).

After the presence of a level crossing perturbation is established with some confidence, an approximate position of the crossing point must first be determined. Following this, lines can be assigned by starting on either side of the crossing point and moving in towards it. Lines relatively far from the crossing will not be shifted much from their expected positions, provided good estimates of molecular constants are known *a priori*. Generally, the residuals of the lines follow a pattern that approaches an asymptote on either side of the level crossing (see Fig. 3.3). Of course, all branches must experience the perturbation in exactly the same fashion, though one of the branches is often easier to assign than the others. The unassigned branches can then serve as a check for the reliability of the initial assignments. In addition, it is very useful to have data from more than one band that samples the perturbed vibrational level. For the present thesis work, most perturbations were assigned in both branches, and all perturbed levels were examined in two different bands, providing strong support for the proposed assignments. Examples of perturbed spectra are given in Chapter 5 and 7 for the YbS and CaS systems, respectively, along with a procedure for fitting the perturbed bands in a non-linear, least-squares fashion. Thorough descriptions of perturbations can be found in the books of Herzberg,[30] Kovács,[49] and Lefebvre-Brion and Field.[48]

Chapter 4

The $A^2\Pi$ – $X^2\Sigma^+$ Transition of YbCl

4.1 Background

Although the general pattern of the manifold of electronic states is expected to be similar for the ytterbium halides, their energies will be different and, because of the high-density of electronic states, this could lead to significant differences in the interactions between the excited states of the different halides. It is therefore important, in order to increase our understanding of their electronic structure, to extend the experimental and theoretical investigation of the ytterbium halides beyond YbF.

Electronic transitions attributed to the YbCl radical in the visible region were first observed by Gatterer *et al.* about sixty years ago.[50] Since then, there have been several low-resolution, vibrational studies of gaseous YbCl.[51-53] These studies were all done in emission, and included observation of what are thought to be four electronic transitions in the region 380-600 nm. The first two systems, observed by Lee and Zare[51] and then later by Kramer,[52] were assigned as $A^2\Pi$-$X^2\Sigma^-$ and $B^2\Sigma^-$-$X^2\Sigma^-$, based on the ordering of the known electronic transitions in the alkaline-earth halide diatomics. These transitions were assigned in such a manner because the ground electronic state of the Yb atom is similar to that of an alkaline-earth atom, except that it has a filled 4*f*-subshell. Lee and Zare also observed two systems in the blue and violet region of the spectrum, which they classified as C-X and D-X, again by analogy with the alkaline-earth halides.[51] In 1997, Uttam *et al.* recorded the thermal emission spectrum of YbCl and reported band-head measurements for all four of the known electronic systems.[53] Recent high-resolution optical studies of YbCl have examined the $A^2\Pi$-$X^2\Sigma^-$ (Ref. 54) and $B^2\Sigma^-$-$X^2\Sigma^-$ (Ref. 55) transitions in detail. There has also been a microwave Fourier-transform study of the ground electronic state by Dickinson *et al.* that examined the $\upsilon = 0$ and 1 vibrational levels.[56] In addition to these experimental studies, Kaledin *et al.* have investigated the electronic structure of the lanthanide monohalides using ligand-field calculations.[15] Figure 4.1 summarizes the known electronic states in YbCl.

Ytterbium exists naturally in seven isotopes, and thus there are fourteen isotopomers present in the spectra of YbCl. The two principal isotopomers, ^{174}Yb^{35}Cl and ^{172}Yb^{35}Cl, which have natural abundances of 24.1 and 16.6%, respectively, are the subject of the present work. The results for the two isotopomers follow those expected from simple isotopomer relations within the uncertainty of the parameters.

4.2 Experimental Details

The basic experimental setup has been described in Chapter 2. Gas phase YbCl molecules were produced in a Broida oven in experiments at both Dalhousie University and the University of New Brunswick. At Dalhousie, Yb metal vapor, entrained in a flow of argon carrier gas, was reacted with Cl_2 gas to produce YbCl at total pressures near 1 torr. The $A^2\Pi_{1/2}$ -$X\,^2\Sigma^-$ sub-bands were probed with the output of a ring dye laser operating in single-frequency mode with Rhodamine 110 dye.

At UNB, YbCl radicals were produced by resistively heating a mixture of Yb metal and $AlCl_3$ in a Broida oven. Although the mechanism for formation of YbCl radicals under these conditions is not clear, it is suspected that the Yb metal first reacts

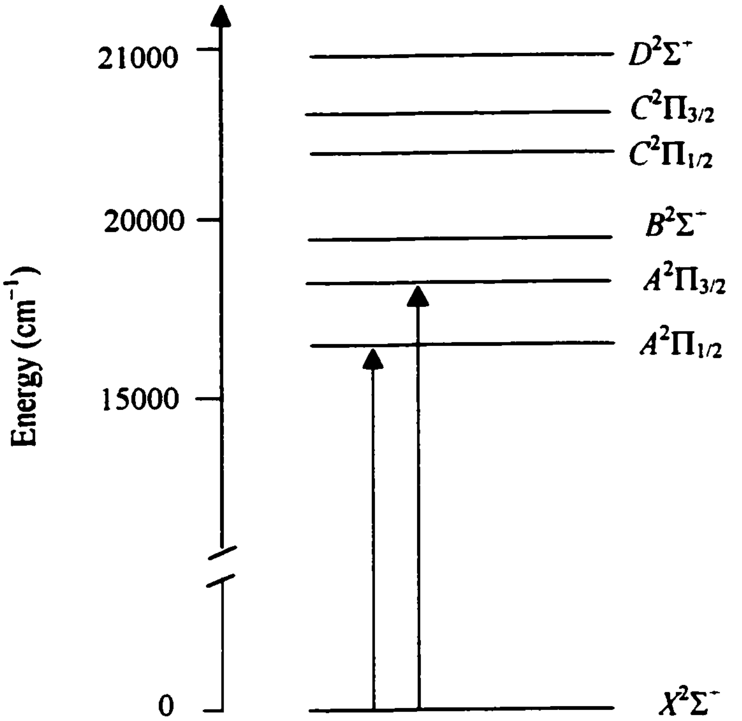


Figure 4.1: Energy level diagram of the known electronic states in YbCl. The transitions marked with vertical arrows were observed in the present work.

with the $AlCl_3$ forming a mixture of solid YbCl and other products, and the YbCl eventually sublimes or vapourizes to form gaseous YbCl. The products were entrained in a flow of argon carrier gas with total pressures in the oven near 0.2 torr. The $A^2\Pi_{3/2}-X^2\Sigma^-$ sub-bands were investigated using a Coherent 699-29 ring dye laser operating with Coumarin 521 dye. Total fluorescence was recorded with a Jarell Ash 0.5-m spectrometer fitted with a small PMT and set to selectively detect emission from excited YbCl molecules. Both sets of experiments (at Dalhousie and at UNB) produced Doppler-limited spectra with linewidths that were on the order of 0.03 cm^{-1}.

4.3 Results

The $A^2\Pi$ state of YbCl is very close in character to Hund's case (a), and thus there are twelve allowed branches in the $A^2\Pi-X^2\Sigma^-$ system. In addition to this, the presence of numerous isotopomers and a relatively small rotational constant ($\approx$ 0.1 cm^{-1}) lead to severely congested rotational structure. With Doppler-limited resolution, the only viable method of investigating the rotational structure of the $A-X$ system is by using very careful selective detection with narrow monochromator slit widths. In doing so, it is possible to isolate individual branches and to obtain spectra relatively free of overlap.

All twelve branches in the $A^2\Pi-X^2\Sigma^-$ system of YbCl are violet degraded and there are two heads in the sub-bands of each spin-orbit component. In the $A^2\Pi_{1/2}-X^2\Sigma^-$ transitions, the P_{12} branch reaches a head at low frequency and does not overlap the other branches in the main head region except at very high N. Near the band origin, the Q_{11} branch forms the main head in a spectral region where there are five overlapping branches. The P_{12} branch was recorded by setting the monochromator in the main head region and scanning from lower frequency. Rotational lines in this branch appear with shoulders due to the blending of the various isotopomers. By interchanging the monochromator and laser wavelengths, the $Q_{11} + R_{12}$ branches could be recorded without the overlap from the three other branches (R_{11} and $P_{11}+Q_{12}$) in the main head region. In contrast to YbF, in which spin-rotation splitting in $\upsilon'' = 0$ could be recorded only at sub-Doppler resolution,[13,14] the spin rotation splitting in YbCl was readily observable. The splitting was resolved for $N \geq 36$ and, by $N \approx 65$, it was comparable to the rotational spacing ($\approx$ 0.3 cm^{-1}), and very careful analysis of the blended branches was required. A portion of the $Q_{11} + R_{12}$ branches in this region (1–0 band) is shown in Fig. 4.2. The $A^2\Pi_{3/2}$–$X^2\Sigma^-$ sub-bands investigated at UNB were recorded in a similar fashion. In these bands, the P_{22} branch forms a head at low frequency while the $P_{21} + Q_{22}$ branches quickly form heads near the band origin. Careful selective detection, with monochromator slit widths between 30 and 120 μm, was used to record spectra for all six branches. Typically, line positions were recorded for N up to approximately 120.

To probe the $X^2\Sigma^-$ state further, the 0–1, 0–2 and 0–3 bands were investigated using the CCD array detector. By setting the laser frequency to a known rotational transition in the 0–0 band, fluorescence from the bands of interest could be quickly and easily recorded. A portion of a resolved fluorescence is shown in Fig. 4.3. Increasing integration times were required to obtain sufficient signal when recording fluorescence to the higher vibrational levels in the ground state. This is primarily due to the decreasing Franck-Condon overlap, as can be seen in Table 4.1, which lists Franck-Condon (FC) factors for transitions involving the low vibrational levels of the A and X states. To calculate FC factors, RKR potential curves were generated for the A and X states using

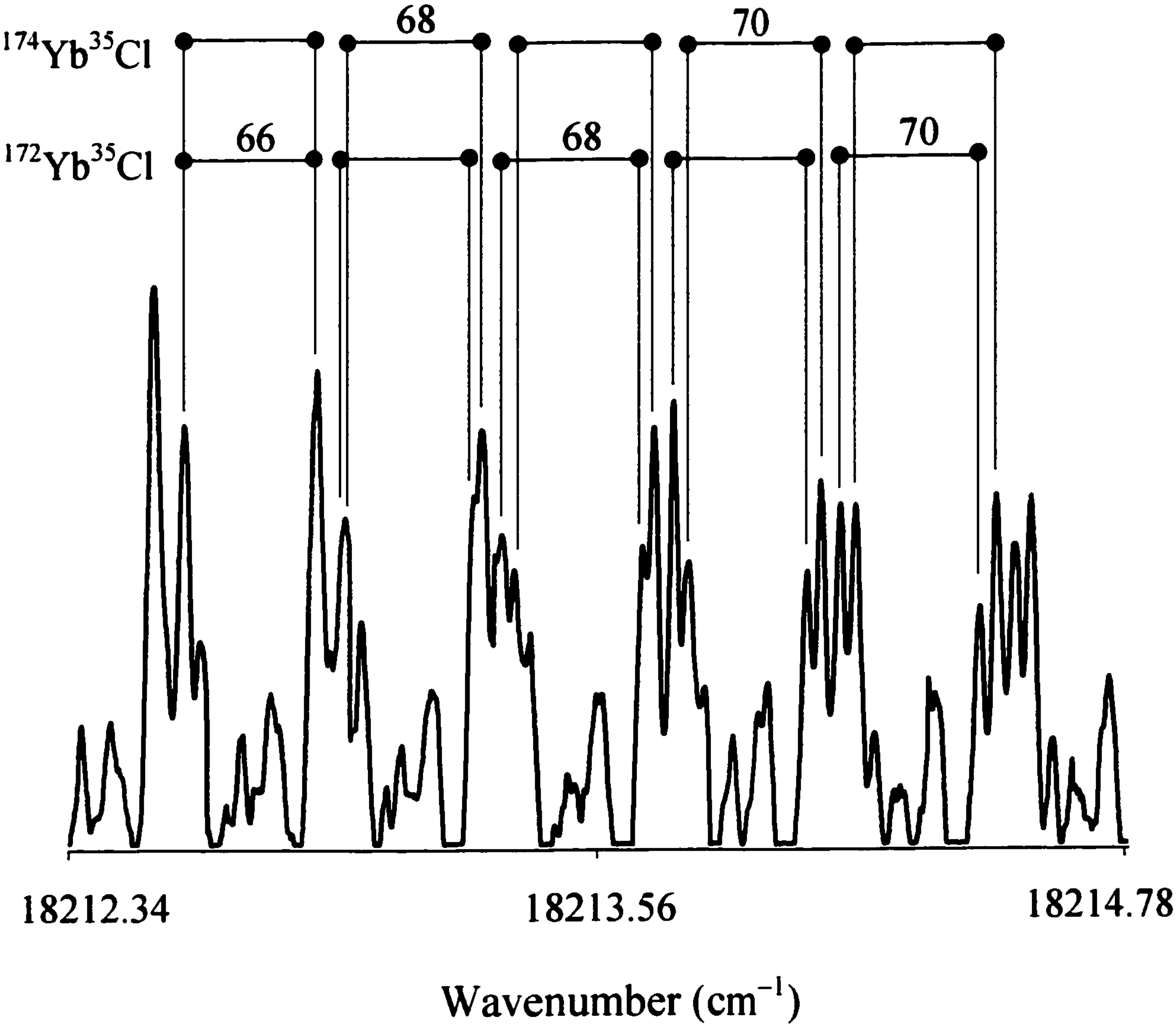


Figure 4.2: A portion of the $A^2\Pi$–$X^2\Sigma^+$ laser excitation spectrum of YbCl showing the effect of spin-rotation splitting in the Q_{11}+R_{12} branches of the 1–0 bands of $^{174}Yb^{35}Cl$ and $^{172}Yb^{35}Cl$. The branches are assigned with the $Q_{11}(N'')$ line at lower frequency and the $R_{12}(N'')$ line at higher frequency. The rotational quantum number N'' is shown above individual Q_{11} and R_{12} pairs.

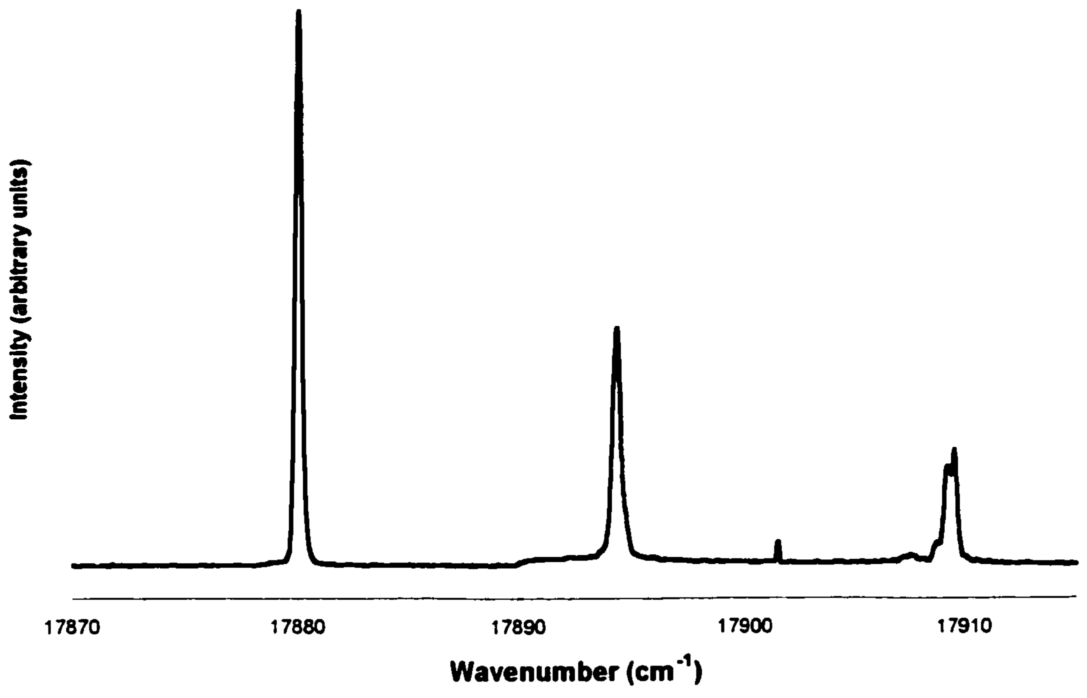


Figure 4.3: Resolved fluorescence spectrum of YbCl. The laser line is the most intense peak, corresponding to a P_{12} transition. The central peak corresponds to the fluorescence from a 'low J' Q_{11} line, and the high frequency peak a 'high J' line. The 'high J' line is split due to spin-rotation effects so that an R_{12} line and a Q_{11} line are resolvable.

Table 4.1

Franck-Condon Factors for the $A^2\Pi$–$X^2\Sigma^+$ system of YbCl

$\upsilon' \setminus \upsilon''$	0	1	2	3
0	0.792	0.181	0.024	0.003
1	0.188	0.463	0.278	0.061
2	0.019	0.301	0.243	0.314
3	0.001	0.051	0.355	0.107

experimental data for the $\upsilon = 0$ and 1 levels, and extrapolated values for higher vibrational levels. The FC factors could then be calculated using the wavefunctions obtained with a standard numerical algorithm,[45] as described in Chapter 3.

Once the spectra were recorded and measured, assignment of the rotational numbering, N, was achieved using both the resolved fluorescence spectra and the standard combination difference relations for the ground state. The data for individual bands were then employed in a weighted, nonlinear least-squares fitting program that contains the usual analytical expressions for the rotational terms in the $X^2\Sigma^-$ state.[31] For the $A^2\Pi$ state, a 2×2 Hamiltonian matrix for each J value and e/f parity component was employed.[31,32] The weighting feature was particularly useful since data for individual bands came from several different sources. For example, line positions measured using the Autoscan software were assigned accuracies of 0.003 cm^{-1}, whereas data recorded using the array detector were given an accuracy of 0.01 cm^{-1}. The corresponding weighting for a particular measurement accuracy is given as 1/(accuracy)^2. For the 0−0 and 1−0 bands, the fitted parameters were the band origin, ν_0, the rotational parameters, B_υ and D_υ for both states, the spin-orbit and lambda-doubling parameters, A_υ, $A_{D\upsilon}$, p_υ, $p_{D\upsilon}$ and q_υ, and the spin-rotation parameter, γ_υ, for the $X^2\Sigma^-$ state. For the 0−1, 0−2 and 0−3 bands, the constants for the upper state were held fixed at those determined in the 0−0 fit, while the band origin, ν_0, and the rotational parameters, B_υ and D_υ, and γ_υ for the ground state were allowed to vary. After fitting the five bands individually, the output parameters were then merged together in a fashion that is equivalent to a global fit of the entire data set to 25 single valued parameters (B_e'', α_e'', D_e'', β_e'', γ_e'', $\alpha_{\gamma e}''$, five band origins, and B_υ, D_υ, A_υ, $A_{D\upsilon}$, p_υ, $p_{D\upsilon}$ and q_υ for $\upsilon = 0$ and 1 in the A state). The ground state constants follow a regular trend with vibrational quantum number, and it was possible to calculate equilibrium values in the merge of the constants from the five bands. The band origins and parameters for the $X\,^2\Sigma^-$ and $A^2\Pi$ states obtained from the merge fit are given in Table 4.2. The constants for individual vibrational levels calculated from these parameters are listed in Table 4.3. All of the observed line positions used in the fits, lines calculated using the parameters in Table 4.3, and residuals between the observed and calculated lines are given in Appendix 1.

4.4 Discussion

The normalized standard deviations of all the weighted fits for individual bands were close to unity, indicating that the deviations between the calculated and measured line positions were consistent, on average, with the estimated measurement accuracy of the lines. Another indication of the reliability of the fits was the isotopic self-consistencies between the two isotopomers. The rotational constants, B_υ, for both the $A^2\Pi$ and $X\,^2\Sigma^-$ states, as well as the Λ–doubling parameters, p_υ', for the $\upsilon' = 0$ and 1 levels, all abide by the standard isotopic relations within their experimental errors. As an example, a comparison of ρ^2 with the ratio of the B_e'' values for the ^{174}Yb^{35}Cl and ^{172}Yb^{35}Cl isotopomers is given in Table 4.2.

Following the completion of the present work on YbCl, Dickinson *et al.* published a study examining the Fourier transform microwave spectrum of YbX (X = F, Cl, Br).[56] Because of the high accuracy of the constants obtained for the ground state of YbCl in the microwave work, the present data set was re-examined and refit, holding the ground state constants fixed at the microwave values. In these fits, large systematic errors were

Table 4.2[a]

Equilibrium parameters (cm^{-1}) for the $X^2\Sigma^-$ and $A^2\Pi$ states of YbCl and band origins for the A–X system

	^{174}Yb^{35}Cl	^{172}Yb^{35}Cl
$10^{-2}B_e''$	$9.3508_{78}(6)$	$9.3714_{25}(8)$
$10^{4}\alpha_e''$	$3.85_{41}(5)$	$3.89_{73}(5)$
$10^{3}\gamma_e''$	$4.58_6(2)$	$4.58_7(3)$
$10^{4}\alpha_{\gamma e}''$	$-1.1_7(3)$	$-0.97_9(44)$
ρ^2	1	1.0020
$B_e/B_e(174)$[b]	1	1.0022(1)
R_e'' (A)	2.4883(1)	2.4880(1)
$10^{-2}B_e'$	$9.6794_5(5)$	$9.7004_7(7)$
$10^{4}\alpha_e'$	3.79(5)	3.81(5)
A_e'	1491.494(2)	1491.502(2)
α_{Ae}'	1.843(2)	1.841(2)
R_e' (Å)	2.4457(1)	2.4455(1)
ν_0 (1–0)	18947.606(1)	18947.945(1)
ν_0 (0–0)	18636.341(1)	18636.377(1)
ν_0 (0–1)	$18346.67_9(1)$	$18346.53_1(2)$
ν_0 (0–2)	$18059.00_2(2)$	$18058.51_3(3)$
ν_0 (0–3)	$17772.98_6(3)$	$17772.22_4(4)$

[a] Values in parentheses are standard errors for the corresponding parameter in units of the least significant digit shown in regular type. Additional digits are given as subscripts to permit calculation of line positions to within the residuals of the fit.

[b] The ratio $B_e/B_e(174)$ is the ratio of equilibrium rotational constant for a particular isotopomer to that of the ^{174}Yb^{35}Cl isotopomer.

Table 4.3[a]

Parameters (cm^{-1}) for the observed $X^2\Sigma^+$ and $A^2\Pi$ levels of YbCl

	$\upsilon = 0$	$\upsilon = 1$	$\upsilon = 2$	$\upsilon = 3$
B_υ''	$0.093316_1(5)$ $0.093519_4(10)$	$0.092930_7(6)$ $0.093129_7(19)$	$0.092545_3(12)$ $0.092739_9(26)$	$0.092159_9(16)$ $0.092350_2(66)$
$10^8 D_\upsilon''$	$3.87_6(3)$ $3.96_5(5)$	$3.91_3(4)$ $4.00_3(12)$	$3.94_9(10)$ $4.04_1(16)$	$3.98_5(13)$ $4.07_9(62)$
$10^3 \gamma_\upsilon''$	$4.52_7(1)$ $4.53_8(2)$	$4.41_1(10)$ $4.44_0(20)$	$4.29_4(9)$ $4.34_2(21)$	$4.17_7(8)$ $4.24_4(24)$
B_υ'	$0.096605_{13}(5)$ $0.096814_{37}(7)$	$0.096225_{67}(5)$ $0.096433_{88}(8)$		
$10^8 D_\upsilon'$	$3.73_{58}(4)$ $3.81_{65}(5)$	$3.81_{65}(5)$ $3.81_{59}(4)$		
A_υ'	$1492.416_0(2)$ $1492.421_9(2)$	$1494.259_2(2)$ $1494.262_6(2)$		
$10^5 A'_{D\upsilon}$	$6.52_1(4)$ $6.52_5(5)$	$6.41_7(4)$ $6.42_3(5)$		
p_υ'	$-0.2174_8(1)$ $-0.2179_5(1)$	$-0.2168_2(1)$ $-0.2172_6(1)$		
$10^7 p'_{D\upsilon}$	$2.34_6(9)$ $2.37_7(10)$	$2.25_0(8)$ $2.27_4(10)$		
$10^4 q_\upsilon'$	$3.6_2(4)$ $3.6_8(5)$	$2.9_1(4)$ $3.2_8(5)$		

[a] The upper entry of each pair is for ^{174}Yb^{35}Cl while the lower entry is for ^{172}Yb^{35}Cl. Values in parentheses are the standard errors in units of the least significant digit of the corresponding parameter shown in regular type. Additional digits are given as subscripts to permit calculation of line positions to within the residuals of the fit.

apparent, particularly at high N-values. Tests determined the cause of the systematic errors to be the values of the centrifugal distortion constants determined in the microwave work. This result is not surprising when one considers the limited N-range sampled in the microwave study ($N \leq 4$). The extensive data set obtained in the present work extends up to $N \approx 125$, and it is believed that the reported centrifugal distortion constants herein are quite reliable. It is important to note, however, that the constants for both studies agree to within approximately two combined standard errors, as shown in Table 4.4. Also included in Table 4.4 are the results for the ground state from the optical study of the $B^2\Sigma^+ - X\,^2\Sigma^+$ transition by Linton and Adam.[55] Again, the parameters are found to be in agreement with the present work.

As discussed previously by other authors, the lanthanide halides all display ionic bonding (M^+X^-), with the electronic structure depending primarily on the configuration of the metal ion.[51,52] The $A^2\Pi$ and $B^2\Sigma^+$ states of YbCl are thought to arise primarily from the π and σ spin-orbitals of the $Yb^+(4f^{14}6p)$ configuration, respectively.[51,54] This idea comes from the known ordering of the manifold of electronic states in the alkaline-earth halides. Therefore, the A – X and B – X transitions involve promotion of an electron in the "metallic" $6s\sigma_{Yb}$ orbital to the $6p_{Yb}$ σ and π spin-orbitals.

A particularly interesting aspect of the current results is the behavior of γ, the spin-rotation parameter for the ground state. In preliminary analyses, satisfactory fits could be obtained for both positive and negative γ values by interchanging the assignments of the 'blended' branches. However, when the complete data sets were used in the final fits, large systematic errors were apparent for assignments that produced a negative γ value. The final positive values for γ are comparable in magnitude and of the

Table 4.4

Comparison of ground state constants (cm^{-1}) for ^{174}Yb^{35}Cl

Constant	Present Work[54]	Microwave Study[56]	Optical Study[55]
B_0	$0.093316_1(5)$	0.09331670(2)	[0.0933161]
10^8D_0	$3.87_6(3)$	4.07(7)	[3.876]
$10^3\gamma_0$	$4.52_7(1)$	4.5153(1)	[4.527]
B_1	$0.092930_7(6)$	0.09292478(5)	0.0929277(38)
10^8D_1	$3.91_3(4)$	4.38(17)	3.933(42)
$10^3\gamma_1$	$4.41_1(10)$	4.4307(3)	4.450(10)
R_e (Å)	2.4883(1)	2.488285(1)	–

Parameters in square brackets were held fixed in the fits. Digits in parentheses are standard errors for the last digit given in regular type.

same sign as those found for the alkaline-earth halide diatomics, which is in stark contrast to that observed in YbF.[13] Dunfield *et al.* found that γ was extremely small in the ground state of YbF, and that it had a strong vibrational dependence, giving rise to a negative value in the $\upsilon = 1$ and 2 levels.[13] In addition, Sauer *et al.* investigated γ for the $\upsilon = 0$ level of YbF using Doppler-free laser spectroscopy, finding that it had a strong rotational dependence and changed sign at $N \approx 60$.[14] Such anomalous behavior was not found during the current work on YbCl. γ varied smoothly and slowly with vibrational quanta and was positive in sign, indicative of normal behavior for an $X\,^2\Sigma^-$ state.

Another notable aspect of the present work is the lack of observation of any perturbations in the $A^2\Pi$ state of YbCl. Extensive perturbations have been observed in the $A^2\Pi$ state of YbF caused, at least in part, by a nearby state with $\Omega = ½$ that is labeled [18.6]0.5.[11-13] The $\upsilon = 0$ vibrational level of the [18.6]0.5 state was found to severely perturb the $\upsilon = 1$ level of the $A^2\Pi_{1/2}$ state, causing a downward shift in energy and an anomalously large effective rotational constant, B. In contrast, the $\upsilon = 0$ and 1 levels in the $A^2\Pi$ state of YbCl exhibited none of the perturbations observed in YbF.

The above perturbations in the $A^2\Pi_{1/2}$ state of YbF may, in fact, be the primary reason for the difference in the ground state spin-rotation constants of YbF and YbCl, and for the negative sign of γ in YbF. The main contribution to spin-rotation splitting in a ground $^2\Sigma^-$ state is usually interaction with an excited $^2\Pi$ state, in which both states arise from σ and π components of a single atomic configuration. Since the $A^2\Pi$ state in YbF is severely perturbed, there is likely a significant amount of mixing between the electronic configurations of the A state and perturbing state. Thus, the perturbing state could be interacting with the ground state through its interaction with the $A^2\Pi$ state, causing the anomalous spin-rotation parameter. This hypothesis is consistent with the results of the present work on YbCl in which the spin-rotation parameter in the ground state was found to behave normally, and the $A^2\Pi$ is unperturbed in its lowest vibrational levels.

The lambda doubling in the $A^2\Pi_{1/2}$ spin-orbit component is primarily a result of the interaction between the $A^2\Pi_{1/2}(6p\pi)$ and $B^2\Sigma^-(6p\sigma)$ states. In fact, the $A^2\Pi$ and $B^2\Sigma^-$ states act as a unique perturber pair with the Λ-doubling constant, p, of the A state extremely close in value to the spin-rotation constant, γ, of the B state. From the present work, and results from an investigation of the B–X transition at UNB,[55] we have $p(A^2\Pi, \upsilon = 0) = -0.2175(1)$ cm^{-1} and $\gamma(B^2\Sigma^+, \upsilon = 0) = -0.21615(2)$ cm^{-1}. Comparison of the molecular spin-orbit constant, $A_\Pi = 1492$ cm^{-1}, with the atomic spin-orbit parameter, $\xi(6p_{\mathrm{Yb}^+}) = 2200$ cm^{-1}, indicates that the $A^2\Pi$ state contains a maximum of 70% $6p\pi$ character. It may be more appropriate to describe the A and B state as strongly mixed $\Omega = \frac{1}{2}$ states, each with significant $^2\Sigma$ and $^2\Pi$ character. The fact that the spin-orbit parameter and separation of the A and B states are very similar also means that the usual second order perturbation theory approach is inappropriate in this case.

4.5 Concluding Remarks

This work provides the first high resolution spectroscopic study of YbCl, and the rotational analysis confirms the assignment of the transition as $A^2\Pi - X^2\Sigma^+$.[54] The results from the present work have been employed in two subsequent high-resolution studies of this molecule.[55,56] Results from both the optical study of the $B^2\Sigma^-$ state, and the Fourier-transform microwave study of the ground state, are in good agreement with the results from this work.

Five bands have been analyzed in the present work for each of the ^{174}Yb^{35}Cl and ^{172}Yb^{35}Cl isotopomers. In total, over 2600 line positions have been employed in nonlinear, least-squares fits of molecular parameters. Both the ground and excited states were found to be well behaved, and no indication of perturbations was observed. The $A^2\Pi$ and $B^2\Sigma^-$ states have been shown to act as a unique perturber pair.

Finally, it should be mentioned that a number of unsuccessful experiments were undertaken to examine the YbCl $C^2\Pi$–$X\,^2\Sigma^-$ transition at high-resolution in the blue region of the spectrum. This system has been examined at low-resolution, and accurate band-head measurements are available.[53] The experiments employed the same production source described above for the work done at UNB; however, it was not possible to attain sufficient signal/noise to conduct a proper laser excitation study of this transition. This is likely due to a smaller transition dipole for this system compared to the YbCl $A-X$ and $B-X$ transitions.

Chapter 5

The $A0^+ - X0^+$ and $B0^+ - X0^+$ Transitions in YbS

5.1 Background

Prior to recent reports,[57-59] the only spectroscopic information available for YbS was the density functional study of Liu *et al.*[60] This theoretical work concluded the ground state of YbS came primarily from the $Yb^{2+}(4f^{14})S^{2-}$ electronic configuration, which is interesting because of the controversy that surrounded the assignment of the YbO ground state configuration.

YbO is unique among the lanthanide monoxides in that both the f^{14} and $f^{13}s$ electronic configurations are low-lying in its manifold of states. As discussed elsewhere,[1,9,61] electronic states arising from the two configurations can be distinguished based on their vibrational frequencies. For example, vibrational frequencies from the f^{14} and $f^{13}s$ configurations are expected to be about 680 and 830 cm^{-1}, respectively.[9,61] The first reliable experimental report of YbO appeared in 1983, and tentatively assigned the ground state as arising from the $Yb^{2+}(4f^{14})O^{2-}$ configuration.[61] This conclusion was in agreement with ligand field theory predictions.[62,63] However, in 1989, Dolg and Stoll[64,65] reported density functional calculations predicting the $4f^{14}$ configuration to lie higher in energy than the $4f^{13}6s$ configuration, in complete disagreement with the earlier experimental work. This led Field and coworkers to reinvestigate the low-lying electronic states of YbO using laser spectroscopy, and to identify conclusively the low-lying $f^{13}s$ and f^{14} configurations.[9] They unequivocally assigned the ground electronic state as arising from the f^{14} configuration.

Later work published by Dolg and coworkers (in 1997) was in agreement with experimental observations, and concluded the ground states of both YbO and YbS arose primarily from the $4f^{14}$ configuration.[60] Because of the earlier controversy surrounding the YbO assignment, it seemed worthwhile to investigate the electronic spectrum of YbS to test the predictions of Dolg and coworkers. Like YbO, the states arising from the two different configurations in YbS can be distinguished by their vibrational frequencies. Expected frequencies for the f^{14} and $f^{13}s$ configurations in YbS are 370 and 460 cm^{-1}, respectively. Further motivation for the present work is the chance to extend the body of spectroscopic data on lanthanide-containing diatomics beyond the monoxides and monofluorides.

While sulfur exists naturally in four isotopes, ^{32}S (95.0%), ^{33}S (0.75%), ^{34}S(4.2%) and ^{36}S(0.02%), ytterbium is present in nature as a mixture of seven isotopes, 6 of which have greater than 1% abundance. This work is focused on the $^{172}Yb^{32}S$, $^{174}Yb^{32}S$, and $^{176}Yb^{32}S$ isotopomers, which have abundances of 21, 30, and 12%, respectively.

5.2 Experimental Details

The experimental setup for this work was described in Chapter 2. Gas-phase YbS was produced by the reaction of ytterbium metal vapour with either CS_2 or OCS. Though both oxidant gases produced a sufficient amount of YbS to study using laser spectroscopy, the most stable conditions, and best signal/noise, were found while using OCS. Total pressures in the oven were kept in the range 3 – 5 torr.

The low-resolution, survey work on the $A0^+ - X0^+$ transition was conducted at Dalhousie University employing the 599 laser system in broadband mode with

Rhodamine 110, Rhodamine 6G and Kiton Red dyes. High-resolution work on the $A-X$ system was performed at the University of New Brunswick with the ring dye laser operating in single frequency mode with Rhodamine 6G dye. The $B0^+ - X0^+$ transition in the blue region of the spectrum was also examined at UNB, with the dye laser operating with Coumarin 480 dye. In these experiments, the 699 was pumped by 4 W of the multi-line, UV output of a Coherent argon ion laser.

5.3 Low-resolution study of the $A0^+ - X0^+$ transition

Preliminary work on YbS consisted of two types of low-resolution, survey work. Laser excitation spectra were recorded for most of the visible region to search for electronic transitions. Following the identification of a band spectrum, assignments and vibrational frequencies were established using dispersed fluorescence spectra recorded with the CCD array detector. The resolution of these experiments was not sufficient to distinguish between the different Yb isotopes in the spectra.

The YbS low-resolution laser excitation spectra obtained in the present work consisted of a large number of red-degraded bands in the range 560 – 600 nm. Fig. 5.1 shows a portion of the spectrum containing the $\Delta\upsilon = 1$ sequence. Most of the 34 bands recorded were assigned to the principal isotopomer, $Yb^{32}S$, while a few heads of the minor isotopomers $Yb^{33}S$ and $Yb^{34}S$ were recorded for the 0–1 and 0–2 bands, confirming the carrier of the present spectra as YbS. Band head positions for the principal isotopomer, $Yb^{32}S$, are arranged in a Deslandres array in Table 5.1. As can be seen in Fig. 5.2, which was recorded with the CCD array detector, the characteristic R-head and P-branch structure is easily resolvable in the dispersed fluorescence spectra.

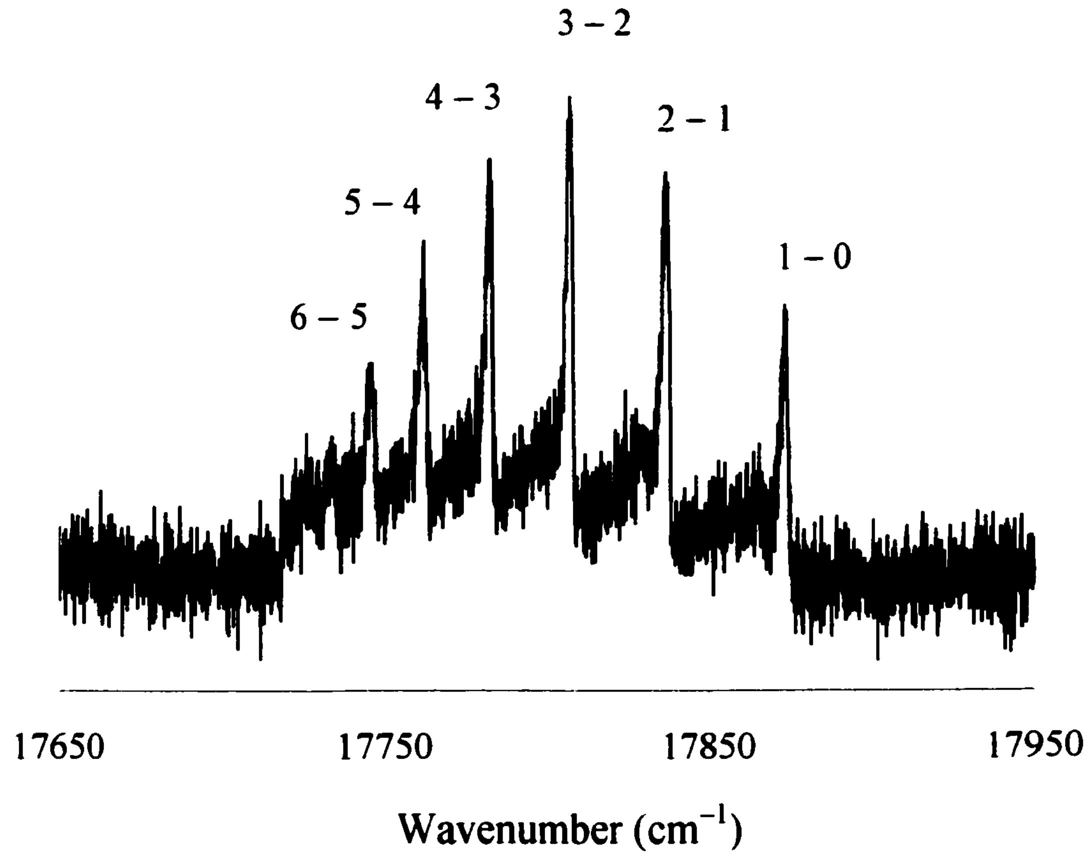


Figure 5.1: A portion of the low-resolution laser excitation spectrum of YbS showing the $\Delta\upsilon = 1$ sequence of the $A0^{-} - X0^{-}$ electronic transition.

Table 5.1

Deslandres table for the $A0^{+} - X0^{+}$ transition in Yb^{32}S (cm^{-1})

$\upsilon'\backslash\upsilon''$	0		1		2		3		4		5		6		7		8		9
0	17546	363	17183	361	16822	359	16463												
	324		324		324		323												
1	17870	363	17507	361	17146	360	16786												
	328		327		327		328												
2	18198	364	17834	361	17473	359	17114	355	16759										
			331		330		332		329										
3			18165	362	17803	357	17446	358	17088	353	16735								
					336		333		336		334								
4					18139	360	17779	355	17424	355	17069	352	16717	350	16367				
							338		336		337		337		338				
5							18117	357	17760	354	17406	352	17054	349	16705	348	16357		
													339		339		340		
6													17393	349	17044	347	16697	346	16351

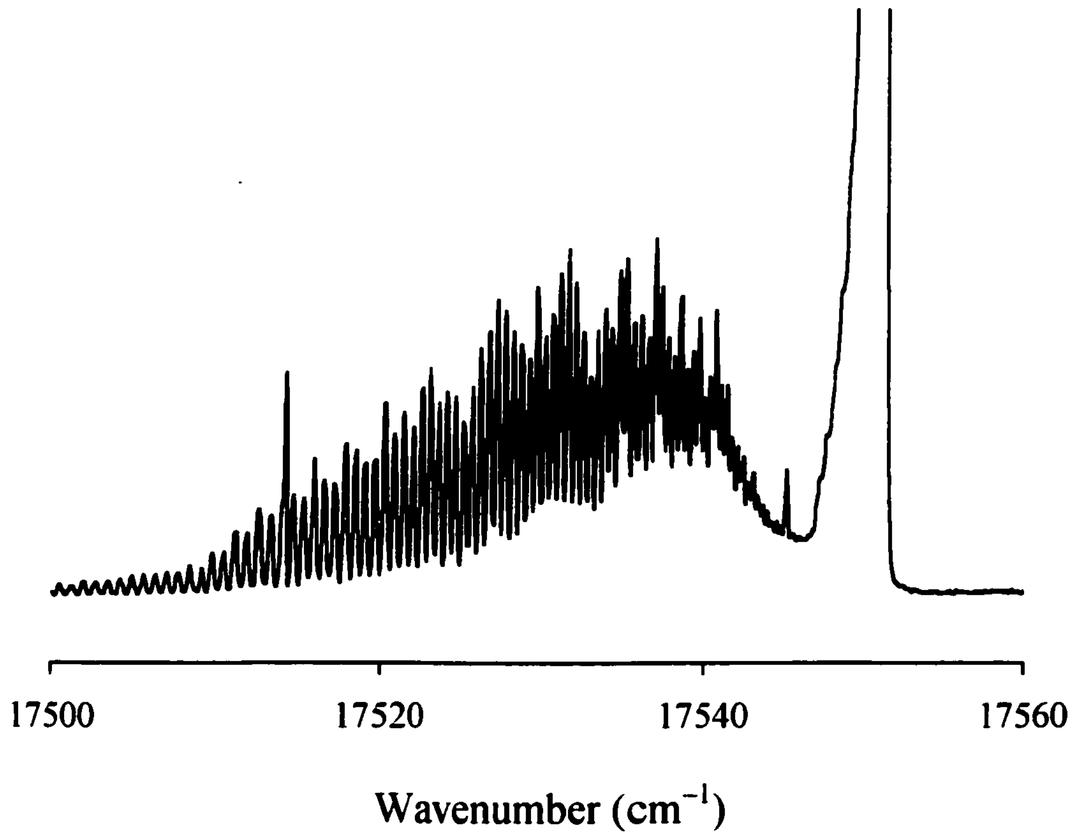


Figure 5.2: Resolved fluorescence spectrum showing the 0 – 0 band of the $A0^{-}$ – $X0^{-}$ electronic transition in YbS recorded with the laser tuned to the R-head of the 0 – 1 band.

This type of branch structure is indicative of an $\Omega = 0 - \Omega = 0$ electronic transition, in Hund's case (c) notation.

It is apparent from Table 5.1 that the vibrational intervals, $\Delta G_{\upsilon+1/2}$, in the excited state *increase* with increasing υ' (corresponding to a negative anharmonicity parameter, $\omega_e'x_e'$). This highly unusual result was also observed by Morbi and Bernath for the $A^1\Sigma^+$ state of BaS.[66] The vibrational intervals for the $A^1\Sigma^+$ state of BaS, and those obtained for the upper state of the new YbS system, are compared in Fig. 5.3. Clearly, the vibrational spacings in BaS are somewhat irregular, and it was concluded by Morbi and Bernath that the BaS $A^1\Sigma^+$ state experiences a global perturbation.[66] In view of the similar electronic structure of YbS and BaS, and hence also of the expected manifolds of electronic states, it seems likely that the perturbed upper state of YbS observed in the present work is the analogue of the $A^1\Sigma^+$ state of BaS.

A least-squares fit employing the band-head data in Table 5.1 was performed to obtain the vibrational constants, ω_e'' and $\omega_e''x_e''$, for the lower state and, because of the perturbations, term values (T_υ') for the upper state. Subsequent work on this system at high-resolution, however, has provided more accurate estimates for the vibrational parameters. These are given later in this chapter in Table 5.2. Based on the similarity of the vibrational parameters for YbS and BaS, the fact that the YbS transition is likely $\Omega = 0 - \Omega = 0$, and the similarity of the observed perturbations in YbS to those in BaS, it is reasonable to conclude that the electronic transition observed in the present work is analogous to the $A^1\Sigma^+ - X^1\Sigma^+$ transition in BaS. In addition, the observed ground state vibrational frequency is consistent with an electronic configuration that is primarily

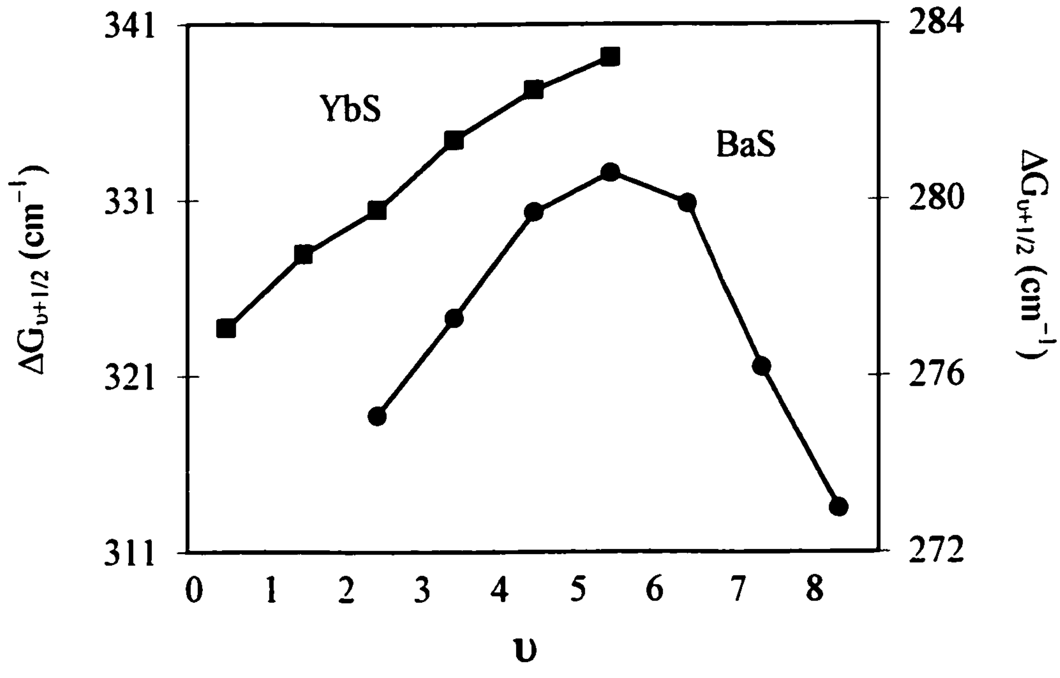


Figure 5.3: Vibrational intervals for the $A0^-$ state of YbS and the $A^1\Sigma^-$ state of BaS. Data for YbS (filled squares) are referred to the left ordinate; data for BaS (filled circles, from Ref. 66) are referred to the right ordinate.

$Yb^{2+}(4f^{14})S^{2-}$. Unfortunately, it was not possible to establish a linkage between the f^{14} and $f^{13}6s$ configurations because electronic states arising from the $4f^{13}6s$ configuration, which are also expected to be low-lying, have yet to be observed.

5.4 High-Resolution study of the $A0^+ - X0^+$ transition

The $A0^+$ – $X0^+$ 0–0, 0–1, 1–1, 1–2, 2–2 and 2–3 bands observed in the high-resolution work consist of red-degraded P and R branches. Typically, rotational lines for both branches were recorded, but because the R branch forms a head at mid-range J-values ($J \approx 45$), selective detection was used to record the low- and high-J rotational lines for this branch. Selective detection was performed by setting the monochromator wavelength to that of low- or high-J transitions in the P-branch, and recording the corresponding transition in the R-branch. Once the spectra were recorded and measured, assignment of the rotational numbering, J, was achieved using the standard combination differences. In addition, it was possible to observe the "first lines" of several bands. The data for individual bands were then employed in a least-squares fitting program that contains the usual analytical expression for $^1\Sigma^+$ states ($\Omega = 0^+$ in Hund's case (c) notation). For each band, the fitted parameters were the band origin T_υ, and the rotational parameters B_υ and D_υ for both the upper and lower states.

5.5 Perturbations

While the initial fits of the 0–0, 0–1, 1–1, and 1–2 bands had standard deviations on the order of 0.003 cm^{-1}, the fits of the 2–2 and 2–3 bands possessed anomalously large standard deviations, with many lines displaying large systematic errors. Further inspection of the 2–2 and 2–3 bands revealed a localized perturbation for all three isotopomers that appeared to be similar to a classic level crossing. Fig. 5.4 shows a portion of the P-branch of the 2–3 band in the region of the perturbation for ^{174}YbS. No extra lines were identified in any of the spectra. The crossing point was the same in both the 2–2 and 2–3 bands, signifying the crossing occurs in the $A0^+$ $\upsilon = 2$ level. Fig. 5.5 illustrates the residuals between the observed and expected line positions in the 2–3 band near the perturbation for ^{174}YbS. The divergent pattern of residuals that approaches an asymptote in this figure is indicative of a typical level crossing perturbation.

The band-fitting program was then modified to incorporate a perturbing state described by its term value (T_P), and rotational parameters, B_P and D_P. Interaction between the $A0^+$ state and the perturber could be modeled either as a homogenous ($\Delta\Omega = 0$ perturber, J-independent) or a heterogeneous ($\Delta\Omega = \pm 1$ perturber, J-dependent) perturbation. The modifications made to the program make it non-linear, and include solving a 2 × 2 matrix that describes the interaction between $A0^+$ and the perturbing state. The diagonal components of this matrix contain the standard expression for case (a) rotational energy in a $^1\Sigma$ state, while the interaction between the $A0^+$ and perturbing state is described in the off-diagonal matrix element by either α or $\beta[J(J+1)]^{1/2}$. To properly characterize the crossing of the $A0^+$ and perturbing state, very careful selection of the trial parameters was essential, and it was necessary to keep the centrifugal distortion constant for the perturbing state, D_P, fixed during the fits.

With no additional knowledge of the perturbing state, separate fits were performed for the perturbed bands assuming either a heterogeneous or homogeneous interaction. Interestingly, both models worked equally well; the deperturbed line

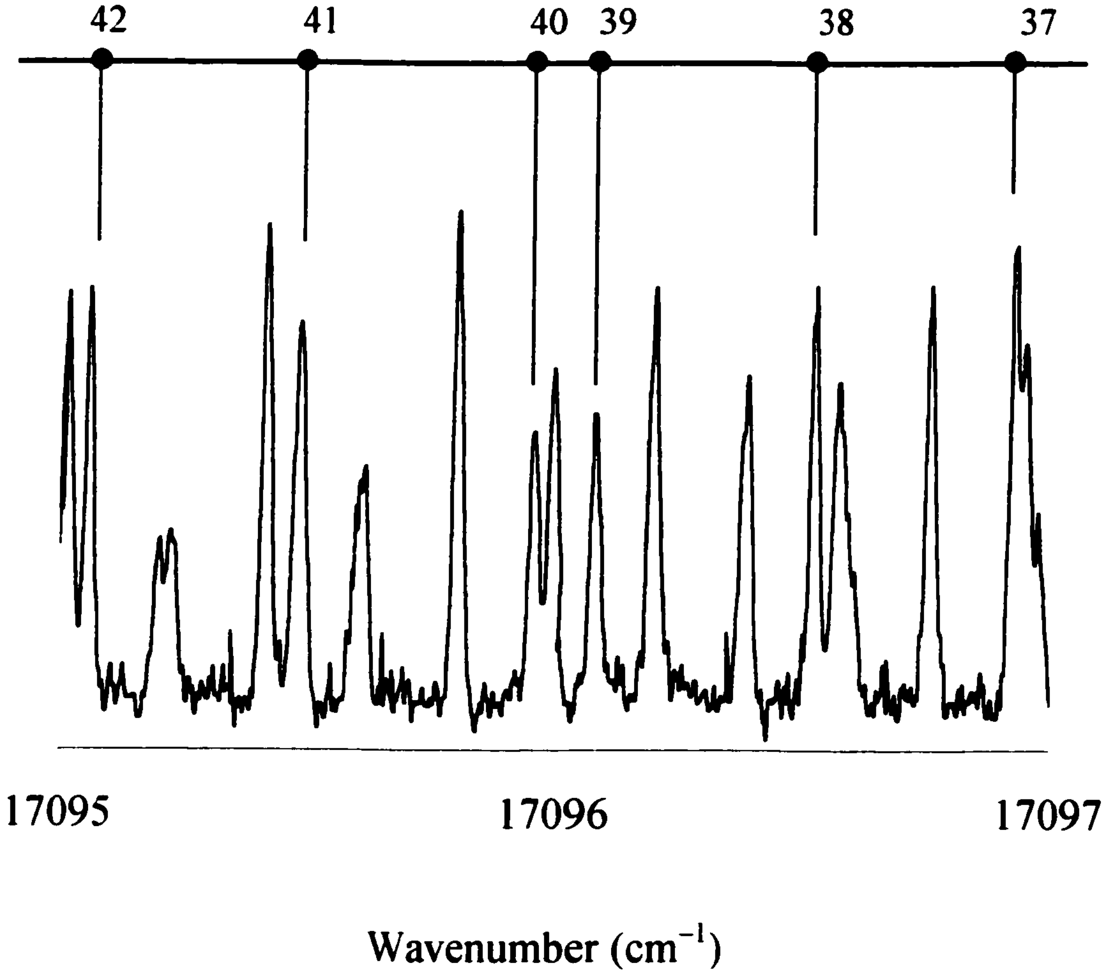


Figure 5.4: A portion of the YbS $A0^{+}$ – $X0^{+}$ 2–3 band in the region of the ^{174}YbS perturbation. The rotational assignment, J'', for the P-branch of ^{174}YbS is given above the spectrum.

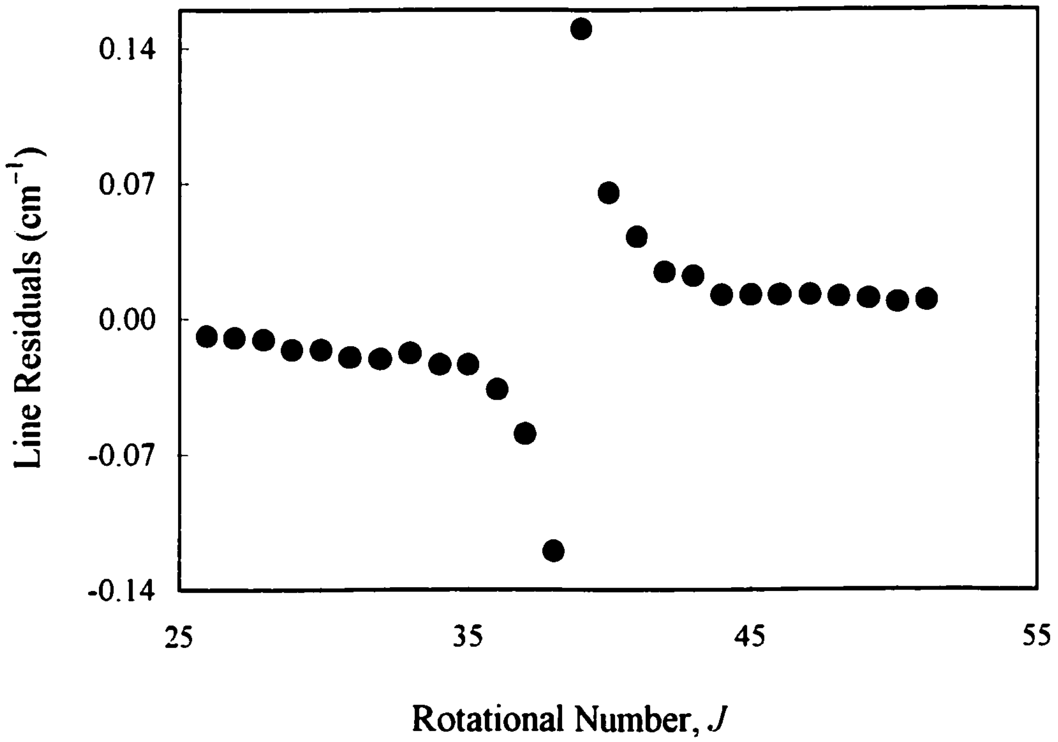


Figure 5.5: A plot of the residuals of the line positions near the crossing point of the 2–3 band for ^{174}YbS. The residuals represent the difference between the observed line positions and those expected if there were no perturbation.

positions displayed no systematic error, and the fits had standard deviations on the order of 0.003 cm^{-1}. The calculated crossing points for the ^{172}YbS, ^{174}YbS and ^{176}YbS isotopomers were $J' = 46.6$, 38.6 and 25.0, respectively.

After fitting the six bands for each isotopomer individually, the output parameters were then merged together to a set of 20 single valued parameters (B_e'', α_e'', ω_e'', $\omega_e''x_e''$, D_υ'' for $\upsilon = 0 - 3$, B_υ' and D_υ' for $\upsilon = 0 - 2$, B_P, α or β, T_2', T_1' and T_0' for the $A0^+$ state, and ΔT, the difference ($T_P - T_2'$) between the perturbing state term value (T_P) and the $A0^+$ $\upsilon = 2$ term (T_2')). The ground state constants follow a regular trend with vibrational quantum number, and it was possible to estimate equilibrium values in the merge of the constants from the six bands. The molecular parameters for the $X0^+$ state, which are in good agreement with the results of the Density Functional study,[60] are given in Table 5.2. Parameters for the $A0^+$ state obtained from the merge fit are given in Table 5.3. It was not possible to estimate equilibrium values for the $A0^+$ state parameters, most likely because of the perturbation affecting the $\upsilon = 2$ vibrational level. Constants for the perturbing state, together with the fitted interaction parameters, are given in Table 5.4. Because of a strong correlation between the fitted parameters T_P and B_P for the $A0^+ \sim P$ interaction, the reported values must be regarded as effective, and not necessarily physically meaningful. In all tables the standard errors (given in parentheses after the parameters in units of the last digit shown in regular type) take account of the estimated σ_M-values of the merge fits (typically $\sigma_M \approx 3.5$). Additional digits are given as subscripts to allow calculation of the line positions within the experimental uncertainty. All of the observed line positions, lines calculated using the parameters in Tables 5.2 – 5.4, and residuals are listed in Appendix 2.

Table 5.2

Parameters (cm^{-1}) for the $X0^-$ state of YbS

	^{172}YbS	^{174}YbS	^{176}YbS	DF Study[a]
B_e	$0.112358_2(8)$	$0.112151_9(9)$	$0.111969_7(15)$	
$10^4\alpha_e$	$4.106_1(13)$	$4.107_2(10)$	$4.152_9(30)$	
$B_e/B_e(^{174}\text{YbS})$	1.00184(10)	1	0.99838(15)	
ρ^2	1.00181	1	0.99823	
ω_e	367.042(3)	366.714(2)	366.408(4)	392(30)
$\omega_e x_e$	1.1671(6)	1.1656(5)	1.1665(8)	
$\omega_e/\omega_e(^{174}\text{YbS})$	1.00089(1)	1	0.99916(2)	
ρ	1.00090	1	0.99912	
$10^8 D_3$	$4.29_5(7)$	$4.22_7(14)$	$4.05_1(10)$	
$10^8 D_2$	$4.22_5(15)$	$4.17_7(13)$	$4.02_3(23)$	
$10^8 D_1$	$4.18_7(15)$	$4.15_0(13)$	$4.11_0(22)$	
$10^8 D_0$	$4.19_0(16)$	$4.16_9(13)$	$4.22_4(25)$	
R_e (Å)	$2.3590_9(1)$	$2.3591_5(1)$	$2.3589_6(2)$	2.32

[a] From the Density Function study of Liu *et al.* (Ref. 60). Note: the uncertainty in the bond length estimate was not given.

Table 5.3

Parameters (cm^{-1}) for the $A0^-$ state of YbS

	^{172}YbS	^{174}YbS	^{176}YbS
T_2	18378.021(4)	18377.258(3)	18376.538(7)
T_1	18049.556(3)	18049.095(3)	18048.665(5)
T_0	17724.621(2)	17724.456(2)	17724.315(3)
B_2	$0.108749_8(9)$	$0.108545_9(10)$	$0.108355_5(17)$
B_1	$0.109134_7(8)$	$0.108933_0(9)$	$0.108747_8(15)$
B_0	$0.109429_6(8)$	$0.109226_9(9)$	$0.109040_2(15)$
$10^8 D_2$	$4.32_5(12)$	$4.21_7(16)$	$4.16_9(14)$
$10^8 D_1$	$4.59_1(14)$	$4.55_6(13)$	$4.51_0(21)$
$10^8 D_0$	$4.85_0(15)$	$4.81_1(12)$	$4.74_9(23)$
R_0 (Å)	$2.3904_5(1)$	$2.3905_0(1)$	$2.3904_3(2)$

R_0 is the bond length of the $\upsilon = 0$ vibrational level.

Table 5.4

Parameters (cm^{-1}) for the $A0^{-} \sim P$ interaction in YbS

	B_P	$10^8 D_P$	α	$10^3 \beta$	$T_P - T_2'$
^{172}YbS					
Homogeneous model	0.10301(2)	[4.5][a]	$0.188_7(5)$	–	$12.79_6(6)$
Heterogeneous model	0.10293(7)	[4.5]	–	$4.05_5(10)$	$12.96_1(20)$
^{174}YbS					
Homogeneous model	$0.1020_6(7)$	[4.5]	$0.226_0(9)$	–	$9.92_3(11)$
Heterogeneous model	$0.1010_5(3)$	[4.5]	–	$6.19_1(21)$	$11.5_{14}(5)$
^{176}YbS					
Homogeneous model	0.10057(2)	[4.5]	$0.279_6(7)$	–	$4.98_3(4)$
Heterogeneous model	0.10105(4)	[4.5]	–	$10.97_3(21)$	$4.69_1(8)$

[a] Because it was not possible to float D_P in the least-squares fits, it was held fixed at 4.5×10^{-8}, similar to that found for the centrifugal distortion parameters of the $A0^{-}$ state.

5.6 Discussion

The standard deviations of all the individual band fits were on the order of 0.003 cm^{-1}, indicating that the deviations between the calculated and measured line positions were consistent, on average, with the estimated measurement precision of $\approx$ 0.003 cm^{-1}. Another indication of the reliability of the fits was the isotopic self-consistencies between the isotopomers for the $A0^-$ and $X0^-$ states. The fitted constants for both states abide by the standard isotopic relations within their experimental errors. For example, comparisons of ρ^2 with the ratio of the B_e'' values, and ρ with the ratio of the ω_e'' values, are given in Table 5.2 for the three isotopomers.

In the absence of any additional information on the perturbing state, beyond that deduced herein from the deperturbation, further discussion remains equivocal. One would expect that only one of the interaction types, homogenous or heterogeneous, would work properly, but in contrast both models were found to be equally satisfactory. Though somewhat unusual, this phenomenon has also been observed in the alkaline-earth monosulfides CaS[67] and SrS.[68]

It seems likely that the results in Table 5.4 point to a more complex interaction than that from a single homogeneous or heterogeneous perturbing level. It can be readily seen from this table that the interaction parameters, α and β, which are expected to be virtually the same for all three isotopomers, differ by as much as 60%, but at the same time follow a regular trend. Furthermore, the rotational constants, and probably the term values for the perturbing state, do not abide by standard isotopomer relations. Clearly, these parameters can only be regarded as effective and do not represent the "true" values for the perturber. Although the model used for the deperturbation analysis is probably too simple, it is difficult to see what might account for such significant variation between the interaction parameters for the different isotopomers. Very similar vibrational overlap between the $A0^-$ ($\upsilon' = 2$) and the perturber (P, υ) levels for the ^{172}YbS, ^{174}YbS and ^{176}YbS isotopomers is certainly expected. One plausible situation that could explain the unusual results for the perturbing state is that the perturber, P, is acting through a second perturber, P_2, and in this case, one would expect atypical behavior in the interaction between the $A0^-$ and P states. The perturber, P, could be considered an admixture of electronic configurations, causing the perturbation to be unlike the classic homogeneous or heterogeneous models. Furthermore, the possibility of two perturbation mechanisms operating simultaneously, as happens when a $^3\Pi$ state interacts with a $^3\Sigma$ state, could produce a situation where the interaction decreases at high J.[69] This would explain the unusually large decrease in the observed interaction parameters, α and β, for the three isotopomers, as the crossing points change from roughly 25 ~ 39 ~ 47, for the ^{176}YbS, ^{174}YbS and ^{172}YbS, respectively. It is interesting to note that the alkaline-earth monosulfides possess low lying $^3\Pi$, $^1\Pi$, and $^3\Sigma$ states, which, in the case of BaS, are known to perturb the $A^1\Sigma^-$ state.[70] Based on the similarities between the manifolds of electronic states in BaS and YbS, it is quite possible that the perturbing state(s) discussed above are analogous to one or more of those observed in BaS; e.g. the interacting $^3\Pi$ and $^3\Sigma$ states.

The present rotational analysis is further evidence that the observed electronic transition in YbS is the analogue of the $A^1\Sigma^-$–$X^1\Sigma^-$ transition in BaS,[66] and it can be concluded that the ground electronic state of YbS arises primarily from the $\mathrm{Yb}^{2+}(4f^{14})\mathrm{S}^{2-}$ configuration. At this point it appears further experimental and theoretical work that characterizes the manifold of electronic states in YbS may be necessary in order to better describe the perturber and its interaction with the $A0^-$ state.

5.7 High-Resolution study of the $B0^- - X0^-$ *transition*

In addition to the $A-X$ system, two bands were observed in the blue region of the YbS spectrum. The $B0^-$–$X0^-$ 0–0 and 0–1 bands consist of red-degraded P and R branches. Once the spectra were recorded and measured, assignment of the rotational numbering, J, was achieved using combination differences for the ground state. The most striking feature of both bands is the sudden truncation of rotational structure in the P and R branches at $J' = 50$, likely due to a predissociation of the $B0^-$ $\upsilon = 0$ level by a previously unknown dissociative state. Fig. 5.6 shows a portion of the YbS 0–1 band near the truncation point. Searches for bands involving excited vibrational levels in the $B0^-$ state were unsuccessful, suggesting that this state is indeed subject to a strong predissociation. At Doppler-limited resolution, it was not possible to observe any variation in linewidth that might characterize the predissociation in more detail.

As discussed by Herzberg[30] and Kovács,[49] there are a number of different types of predissociation, and it is beyond the scope of the present discussion to consider all of them. For diatomic molecules, the most common type of predissociation occurs when an electronic state overlaps the dissociation continuum of another electronic state.[30] In such cases, a radiationless transition into the dissociative state can take place, giving rise to a truncation in the vibrational and rotational structure of the observed electronic state. There are, in fact, different sub-cases of radiationless predissociations, as described in detail by Herzberg.[30] A schematic diagram of the potential energy curves for one of these

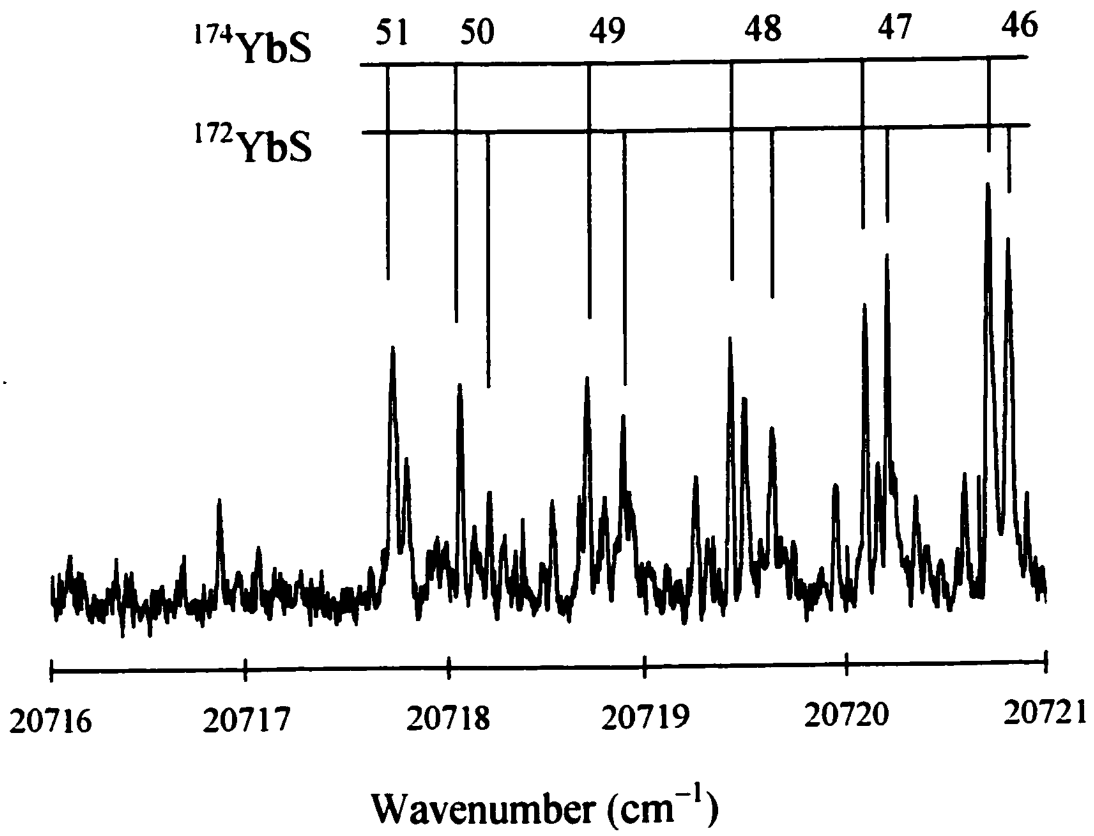


Figure 5.6: A portion of the YbS $B0^{-}$–$X0^{-}$ transition 0–1 band near the truncation of rotational structure in the P-branch. The rotational quantum number, *J*, for the P-branches of ^{174}YbS and ^{172}YbS is given above the spectrum.

cases is given in Fig. 5.7. Since predissociation is simply a special type of perturbation, the selection rules governing them are identical.

Analysis of the observed bands revealed large downward shifts in the rotational energy levels just prior to the predissociation, presumably due to the interaction between the $B0^-$ and dissociative states. Because of this, the last five lines in each branch were excluded from the least-squares fits of molecular parameters. Fig. 5.8 compares plots of $\Delta_2F(J)/(4J + 2)$ as a function of $(J + 1/2)^2$ for the $X0^-$ and $B0^-$ states, giving some indication of the perturbed structure of the rotational energy levels in the $B0^-$ state. Normal rotational structure, like that found in the $X0^-$ state, results in a relatively straight line, while the perturbed rotational structure of the $B0^-$ state gives rise to curvature in the plot, as well as an anomalously large slope even at $J = 0$. These results suggest there is a significant interaction between the $B0^-$ state and at least one other nearby electronic state.

The fitted parameters for both isotopomers were the band origins, ν_0, the rotational and centrifugal distortion constants B_0', D_0', H_0', and L_0' for the upper state and B_υ'' and D_υ'' for the ground state. The standard deviation for all the fits was ≈ 0.003 cm^{-1}, in accord with the estimated measurement precision. The output parameters of the individual band fits were then merged together to 10 single-valued parameters (B_0', D_0', H_0', L_0', B_υ'' and D_υ'' for $\upsilon'' = 0, 1$, and the two band origins). The results from the merge fit, which had an estimated $\hat{\sigma}_M \approx 1.2$, are given in Table 5.5 (where 1-σ uncertainties are given in parentheses after the parameters). Inspection of Table 5.5 reveals the fact that the centrifugal distortion constant D_0' for the $B0^-$ state is an order of magnitude larger than expected. Consequently, the bands are red-degraded when, under normal circumstances, a band with $B_0' > B_0''$ is violet degraded. For such a heavy molecule, the

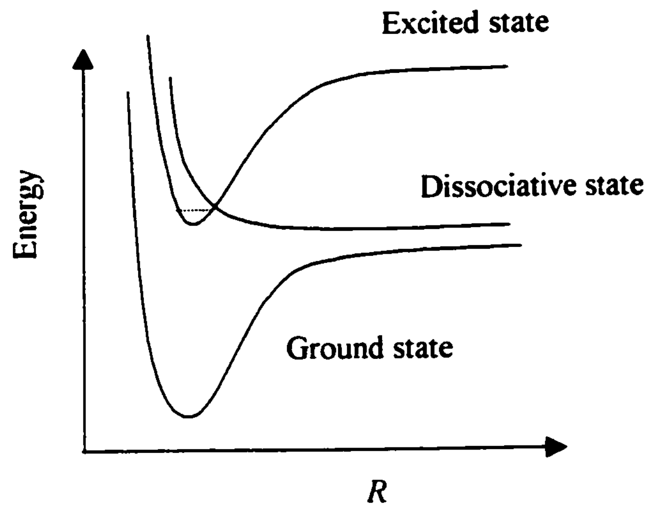


Figure 5.7: A hypothetical example of a predissociation in a diatomic molecule. After Herzberg (Ref. 30), pp.422, case I(c).

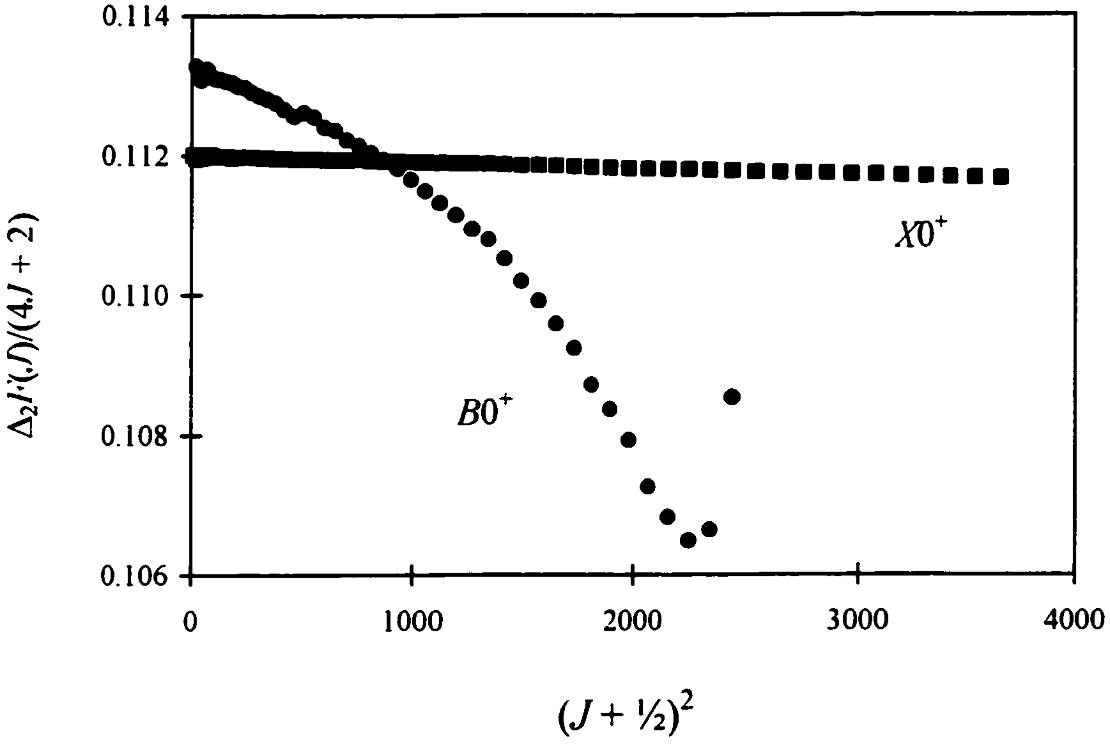


Figure 5.8: A plot of $\Delta_2F(J)/(4J+2)$ vs. $(J+1/2)^2$ for the $B0^+$ and $X0^+$ states of ^{174}YbS showing the perturbed rotational structure of the $B0^+$ state energy levels.

Table 5.5

Parameters (cm^{-1}) from the YbS $B0^-$ – $X0^-$ transition[a]

Parameter	^{174}YbS	^{172}YbS
ν_{00}	21 096.067(1)	21 096.261(1)
ν_{01}	20 731.687(1)	20 731.551(1)
B_0'	0.113222(13)	0.113432(15)
R_0'(Å)	$2.3479_4(3)$	$2.3489_7(3)$
$10^7 D_0'$	6.65(16)	6.33(18)
$10^{11} H_0'$	6.2(13)	6.8(15)
$10^{13} L_0'$	−1.138(35)	−1.111(41)
B_1''	0.111566(12)	0.111747(13)
B_1'' (A–X)	0.111536(10)	0.111742(9)
B_0''	0.111966(12)	0.112159(13)
B_0'' (A–X)	0.111947(10)	0.112153(9)
$10^8 D_1''$	5.37(50)	4.12(57)
$10^8 D_0''$	4.75(49)	3.94(59)

[a] Rotational constants for the ground state of YbS obtained from the study of the $A - X$ system are given for comparison, and are labelled ($A - X$).

magnitudes of the centrifugal distortion parameters indicate that the constants obtained must be regarded as effective and do not represent physically meaningful values for the $B0^+$ state. It is possible that the large centrifugal distortion parameters are the result of the interaction between the $B0^+$ and dissociative state, although it is certainly feasible that the B state is perturbed by yet another unobserved state. A list of all observed and calculated line positions is provided in Appendix 2.

For comparison, the rotational parameters for the ground state of ^{172}YbS and ^{174}YbS from the analysis of the $A0^+$ – $X0^+$ transition are included in Table 5.5. The rotational constants, as well as the centrifugal distortion constants, agree within two standard errors of one another.

5.8 Concluding Remarks

The present work on YbS represents the first spectroscopic information available for this molecule of any kind. The $A0^+$–$X0^+$ and $B0^+$–$X0^+$ electronic transitions have been rotationally analyzed with high precision. The $A0^+$ state has been shown to experience both vibrational (global) and rotational perturbations, while the $B0^+$ state has been found to possess a predissociation in the $\upsilon = 0$ level. A partial deperturbation analysis of the $A - X$ system has allowed for the determination of deperturbed constants for the $A0^+$ state and effective molecular parameters for the perturbing state.

The investigation of the $A0^+$–$X0^+$ and $B0^+$–$X0^+$ systems of YbS indicates there is a large density of electronic states in the 2–3 eV region of this molecule. It is tempting to speculate that some of the unidentified states arise from the $Yb^{2+}(4f^{13}6s)S^{2-}$ electronic configuration, which have yet to be directly observed experimentally. As for YbO, it is expected that several low-lying electronic states in YbS arise from the $f^{13}s$ configuration, but despite extensive searching, none have been conclusively identified.

The very fact that none of the identified electronic states are from the $f^{13}s$ configuration sheds light on the electronic structure of YbS. The manifold of electronic states in YbS appears to be more like that found in the alkaline-earth monosulfides, and not like that of YbO. Careful resolved fluorescence experiments were performed to search for low-lying electronic states above the ground state, but were unsuccessful. However, it should be noted that selection rules governing electronic transitions ($\Delta\Omega = 0, \pm 1$ and $+ \leftrightarrow +, - \leftrightarrow -$) might prohibit observation of some low-lying electronic states.

Chapter 6

The $\tilde{A}^2\Pi - \tilde{X}^2\Sigma^+$ Transition in YbOH

6.1 Background

In recent years, there have been numerous spectroscopic studies of electronic transitions in gas-phase metal monohydroxides (MOH, where M is a metal atom) involving alkaline earth and transition metals. The use of lasers in this type of work is now ubiquitous, and has facilitated detailed studies of the electronic and vibrational structure of a variety of species in this class of molecules. The only spectroscopic information available for lanthanide monohydroxides, however, is from flame studies, in which YbOH and EuOH have been tentatively identified.[71,72] In these studies, conducted more than forty years ago, no assignments of electronic transitions or vibrational bands were proposed. Prior to the present work, there has never been a report of a laser spectroscopic study of a lanthanide monohydroxide.

The equilibrium geometries of the alkaline earth monohydroxides are chiefly dependant on the nature of their chemical bonding (i.e. covalent versus ionic).[73] If the bonding is primarily ionic in nature, a linear molecular structure results, and as the covalency of the bonding increases, the equilibrium structure becomes bent.[74] It is expected that YbOH possesses a linear geometry, given the similarity of Yb-ligand molecules with their alkaline earth analogs. The present work focuses on the visible absorption spectrum of YbOH, recorded using tunable dye lasers and standard spectroscopic techniques.

In accord with previous spectroscopic work on linear triatomic molecules,[73,75] the vibrational modes referred to herein are designated ν_1, ν_2, and ν_3, where ν_1 corresponds to the Yb-O stretch, ν_2 the doubly degenerate Yb-O-H bending mode and ν_3 the O-H stretch. The lowest frequency mode is the bending vibration, which is on the order of 340 cm^{-1}. The Yb-O stretching mode has a frequency of $\approx$ 530 cm^{-1}, and the O-H stretching mode is not observed in the present work. Jarman and Bernath have reported values of 3847(10) and 3766(10) cm^{-1} for the O-H stretching frequencies in CaOH and SrOH, respectively.[76] These estimates are somewhat large when compared with the free ion (OH^-) value of 3556 cm^{-1} from the work of Rosenbaum *et al.*[77]

The main YbOH isotopomers, ^{174}YbOH and ^{172}YbOH, which have abundances of 31 and 22%, respectively, are the subject of the present high-resolution work. It was not possible to resolve the different isotopomers of YbOH in the low-resolution, survey experiments.

6.2 Experimental Details

Gas-phase YbOH was produced in a Broida oven by the reaction of Yb metal vapour with H_2O_2. The oxidant was contained in a Pyrex sidearm tube and had a sufficiently high vapour pressure that adequate amounts of H_2O_2 vapour could be obtained by simply pumping off the liquid at room temperature. A whitish chemiluminescence was visible in the reaction region and total pressures in the oven were kept around 5 torr, with the oxidant gas making up a few percent of this pressure.

For the low-resolution, survey work, YbOH radicals were probed with the output of a Coherent 599 dye laser operating in broadband mode with Coumarin 521, Rhodamine 110 and Rhodamine 6G dyes. High-resolution spectra were recorded in experiments that employed the ring dye laser operating in single frequency mode with Rhodamine 6G dye.

6.3 Results: Vibrational Analysis

Preliminary survey experiments were performed at low resolution to establish vibrational assignments for the $\tilde{A}^2\Pi$ – $\tilde{X}\ ^2\Sigma^+$ system. The YbOH broadband laser excitation spectrum obtained in the present work consists of a number of blue-degraded bands in the range 520–580 nm. In addition to these, a red-degraded band near 580 nm attributed to YbO was identified.[61] The excitation spectrum was recorded in stages using different dyes, depending on the spectral region being examined. As discussed in Chapter 2, the total fluorescence was recorded through red-pass filters to remove scattered laser light. Tests were performed to establish the best filter for each spectral region examined, based on their cutoff wavelengths. Fig. 6.1 shows a portion of the low-resolution laser excitation spectrum, with assignments given for several vibrational bands of the $\tilde{A}^2\Pi_{1/2} - \tilde{X}^2\Sigma^+$ transition.

Resolved fluorescence experiments were employed to make assignments in the excitation spectrum, and to establish vibrational frequencies and band-head positions. Fig. 6.2 shows a portion of the resolved fluorescence spectrum of the (000) – (100) band, recorded with the broadband dye laser tuned to the main head of the $\tilde{A}^2\Pi_{1/2} - \tilde{X}^2\Sigma^+$ (000) – (000) band. The separation of the (000) – (100) and (000) – (000) bands is ≈ 540 cm^{-1}, and the branch structure of the bands (see Fig. 6.2) identifies them as arising from the Yb-O stretching mode.

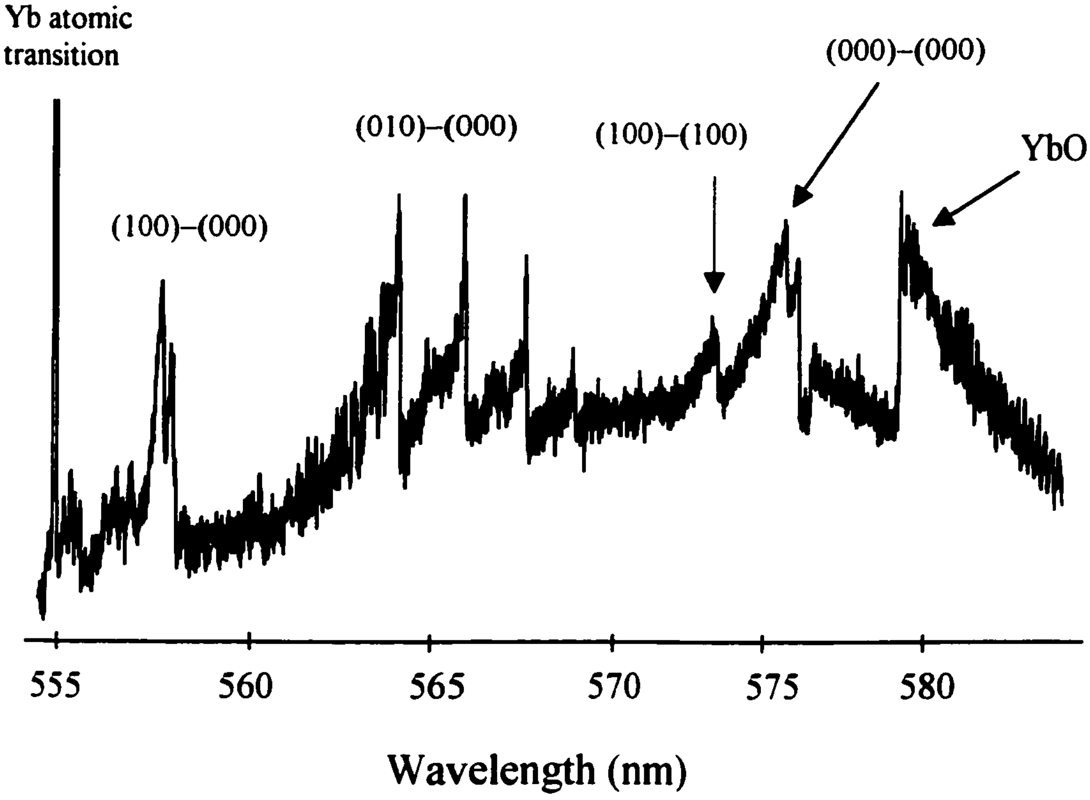


Figure 6.1: A portion of the $\tilde{A}\,^2\Pi - \tilde{X}\,^2\Sigma^-$ low-resolution (1 cm^{-1} bandwidth) laser excitation spectrum of YbOH. The total fluorescence was recorded through a red-pass filter to remove scattered laser light.

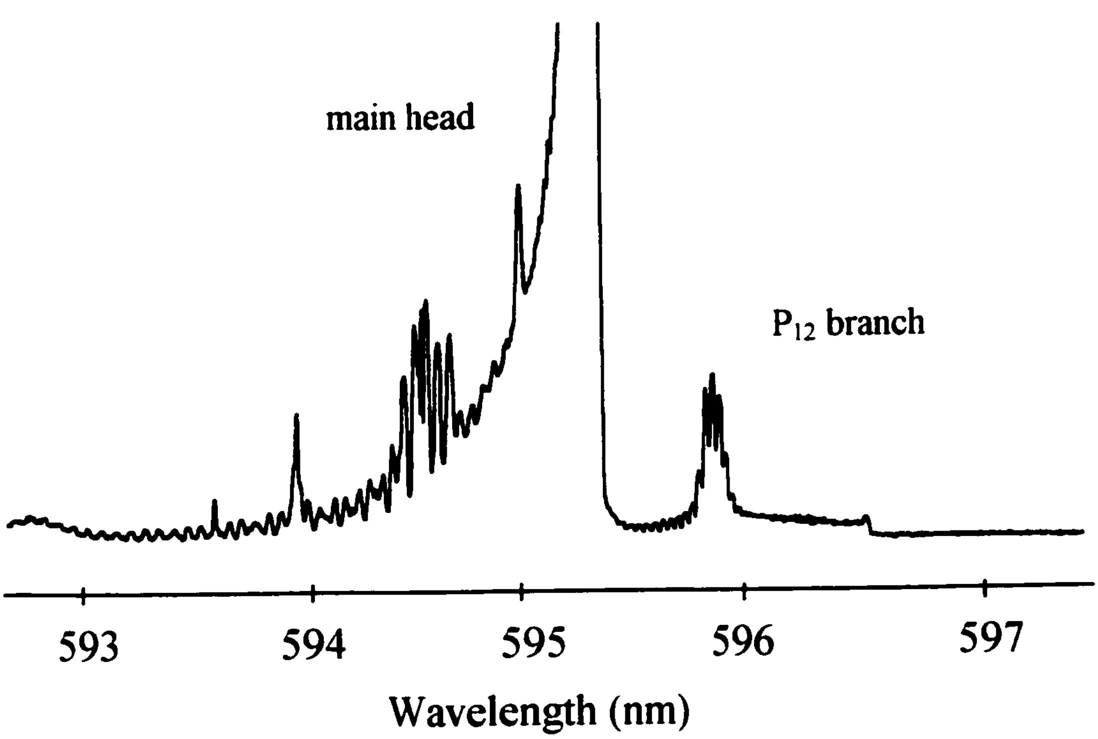


Figure 6.2: Resolved fluorescence spectrum of the $\tilde{A}\,^2\Pi_{1/2} - \tilde{X}\,^2\Sigma^-$ (000) – (100) transition in YbOH recorded with the CCD array detector. A broadband (1 cm^{-1} bandwidth) laser is tuned to the main head of the (000) – (000) band and the monochromator is set in the region of the (000) – (100) band.

The structure of the band shown in Fig. 6.2 is strong evidence that the electronic transition observed in YbOH is a $^2\Pi - {}^2\Sigma^-$ system. A very similar structure was observed in the $A^2\Pi - X^2\Sigma^-$ transition of YbCl,[54] and the separation of the two band-heads ($\approx$ 30 cm^{-1}) was the same as that found in the isoelectronic molecule YbF.[13]

The vibrational structure of the $\tilde{A}\ {}^2\Pi_{3/2} - \tilde{X}\ {}^2\Sigma^-$ transition was somewhat more complicated, and only four bands were tentatively identified in the excitation spectrum. This complexity may be due to overlapping transitions involving nearby electronic states, as discussed further below. All of the assigned band heads from the present work are listed in Table 6.1. The three heads listed in Table 6.1 for the $\tilde{A}\ {}^2\Pi_{1/2} - \tilde{X}\ {}^2\Sigma^-$ (010) – (000) band correspond to transitions to different vibronic components of the $v_2 = 1$ bending level in the excited state. Without a rotational analysis of these bands, however, this assignment must be regarded as tentative. The estimated value of $v_2(\tilde{A}\ {}^2\Pi)$ was obtained by finding the center of the two outer vibronic components observed in the laser excitation spectra.

Estimated vibrational parameters for the $\tilde{A}\ {}^2\Pi$ and $\tilde{X}\ {}^2\Sigma^-$ states of YbOH are given in Table 6.2, with the corresponding parameters for CaOH,[75] SrOH,[73] and BaOH[78] included for comparison. Uncertainties in the vibrational parameters take account of the experimental error, as well as the band head-origin separation. The separation of the (000) – (000) band heads provides an estimate for the spin-orbit constant of the $\tilde{A}\ {}^2\Pi$ state, $A \approx 1350$ cm^{-1}. As expected, this is very similar to that found for the $A^2\Pi$ state of YbF, $A = 1365.3$ cm^{-1}.[13]

Table 6.1

Vibrational assignments for the observed YbOH $\tilde{A}\,^2\Pi$ – $\tilde{X}^2\Sigma^-$ band heads (in cm^{-1}); the estimated accuracy is ± 5 cm^{-1}.

Band	$\tilde{A}\,^2\Pi_{1/2}-\tilde{X}\,^2\Sigma^-$	$\tilde{A}\,^2\Pi_{3/2}-\tilde{X}\,^2\Sigma^-$
(000)–(000)	17 327	18 677
(000)–(100)	16 794	18 155
(000)–(200)	16 271	–
(100)–(000)	17 898	19 250
(100)–(100)	17 380	–
(100)–(200)	16 855	–
(010)– (000)	17729 17681 17638	19 047
(010)– (010)	17 339	–

Table 6.2

Comparison of vibrational parameters (cm^{-1}) for the $\tilde{X}^2\Sigma^-$ and $\tilde{A}\,^2\Pi$ states of YbOH

	YbOH[a]	CaOH[b]	SrOH[c]	BaOH[d]
ν_1 ($\tilde{X}^2\Sigma^-$)	529.341(1)[e]	609.0	527.0	492
ν_2 ($\tilde{X}^2\Sigma^-$)	339(5)	352.9	360.6	342
ν_1 ($\tilde{A}^2\Pi$)	573(5)	628.5	542.6	458
ν_2 ($\tilde{A}^2\Pi$)	357(5)	361.3	381.4	352

[a] from the present work; ν_1 is the M–O stretch and ν_2 is the M–O–H bend.

[b] from Ref. 75

[c] from Ref. 73

[d] from Ref. 78

[e] from the separation of the (000)–(000) ~ (000)–(100) band origins for ^{174}YbOH, determined in the high-resolution work.

6.4 Results: Rotational Analysis

Three bands were rotationally analyzed: the $\tilde{A}\,^2\Pi_{1/2} - \tilde{X}\,^2\Sigma^+$ (000) – (000) and (000) – (100) bands of ^{174}YbOH, and the (000) – (000) band of ^{172}YbOH. The branch structure of all 3 bands was blue-degraded and characteristic of a typical Hund's case (a) $^2\Pi_{1/2} - {}^2\Sigma^+$ transition, the same as that for a diatomic molecule. While the P_{12} branch forms a head at low frequency, the other five branches in this transition are overlapped with one another. Details concerning this type of electronic transition are discussed in Chapter 3.

At Doppler-limited resolution, the only viable method of investigating the rotational structure of the $\tilde{A} - \tilde{X}$ system is by using selective detection, which has been described in Chapter 2. Employing this technique, it is possible to isolate individual branches and to obtain spectra relatively free of overlap. Fig. 6.3 shows a portion of the (000) – (000) R_{11} branch recorded at high-resolution, with transitions from the ^{176}YbOH, ^{174}YbOH and ^{172}YbOH isotopomers labelled in the figure.

Not at all unexpectedly, the ^{171}YbOH and ^{173}YbOH isotopomers were not observed in the present work, despite having natural abundances of 14 and 16%, respectively. In fact, these abundances are comparable to that of the ^{172}YbOH isotopomer, and even greater than that of ^{176}YbOH. The explanation for this is straightforward: the ^{171}Yb and ^{173}Yb nuclei have non-zero nuclear spins of 1/2 and 5/2, respectively. The nuclear spins couple to the spin of the unpaired electron, producing a multiplet of peaks for each rotational line. Of course, the integrated intensity of the split lines remains the same as if there were no splitting, effectively giving each hyperfine

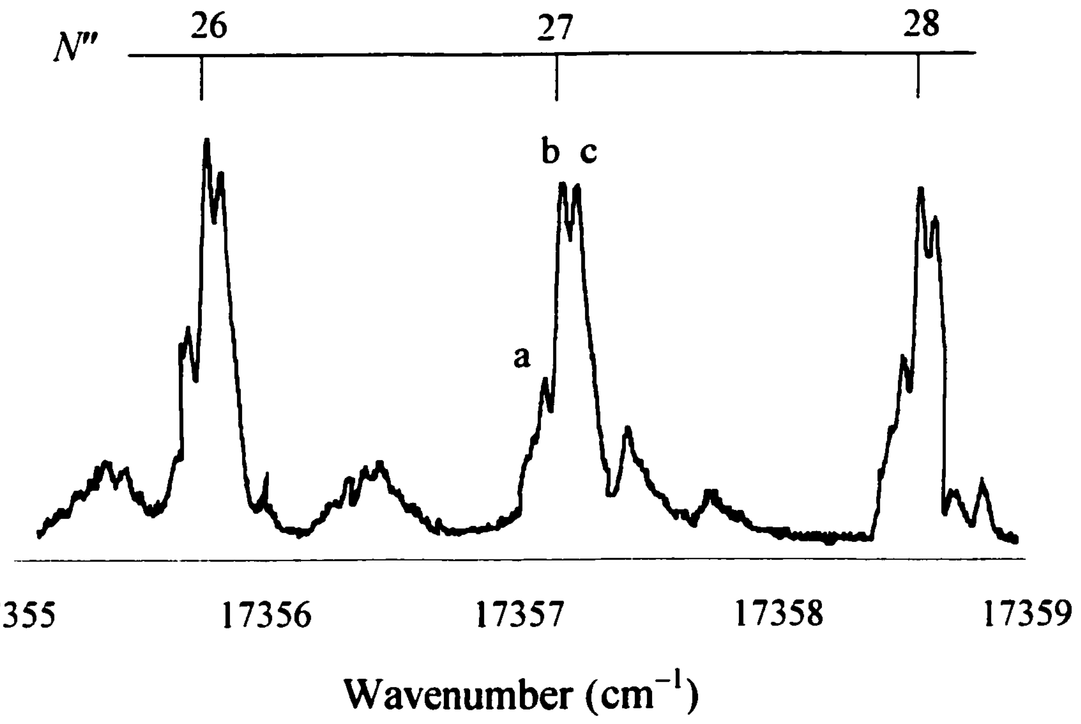


Figure 6.3: A portion of the $\tilde{A}\,^2\Pi_{1/2} - \tilde{X}\,^2\Sigma^+$ laser excitation spectrum of YbOH showing the R_{11} branch in the (000) – (000) band (a, b and c refer to the ^{176}YbOH, ^{174}YbOH and ^{172}YbOH isotopomers, respectively). The rotational quantum number N'' is shown above the lines.

component a significantly smaller signal/noise. The same situation exists for the $A^2\Pi - X^2\Sigma^-$ transition of YbCl.

Even at Doppler-limited resolution, the effect of the ground state spin-rotation splitting in the $Q_{11} + R_{12}$ branches of the (000) – (000) band was observable. A portion of the spectrum containing these branches is shown in Fig. 6.4. Because of the multiple isotopomers present in the spectra, assigning the rotational lines was not trivial. However, a similar spectral pattern was observed in the 0 – 0 and 1 – 0 bands of YbCl, giving some indication as to the correct assignments for these branches.

Because of a smaller signal/noise, the (000) – (100) band proved more difficult to investigate than the (000) – (000) band, and it was possible to record transitions involving only the 'unblended' branches, P_{12} and R_{11}. During these experiments the monochromator was set to detect fluorescence from the (000) – (000) band, which has a more favourable Franck-Condon factor then the (000) – (100) band. Nevertheless, attempts to record the other branches in this transition were met with frustration. The observed signal/noise was poor due to a smaller population in the ground state (100) vibrational level, when compared to the (000) vibrational level. A simple calculation using Boltzmann's relation, and assuming $T_{\mathrm{Broida}} \approx 500$ K, indicates the population of the (100) level is about 1/5 the population of the (000) level, effectively decreasing the observed signal by roughly a factor of five.

Once the spectra were recorded and measured, assignment of the rotational numbering, *N*, was achieved using resolved fluorescence spectra. This procedure, sometimes referred to as the *R*/*P* separation method, is described in detail in Chapter 2.

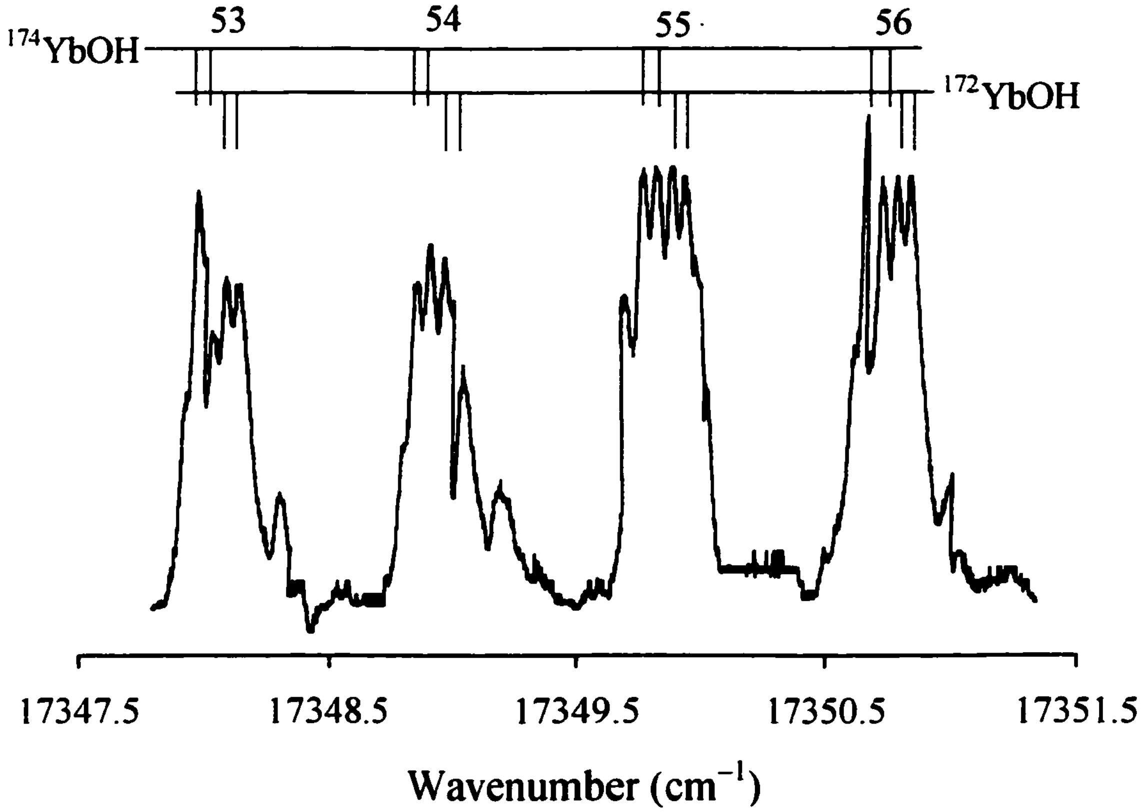


Figure 6.4: A portion of the $\tilde{A}\,^2\Pi_{1/2} - \tilde{X}\,^2\Sigma^+$ laser excitation spectrum of YbOH showing the effect of spin rotation in the Q_{11} + R_{12} branches of the (000) – (000) bands of ^{174}YbOH and ^{172}YbOH. The branches are assigned with the Q_{11} line at lower frequency and the R_{12} line at higher frequency. The rotational quantum number *N*″ is shown above the Q_{11} + R_{12} pairs.

The data for individual bands were then employed in a least-squares fit with the usual analytical expressions employed for the rotational terms in the $\tilde{X}^2\Sigma^+$ state.[31] For the $\tilde{A}\ ^2\Pi$ state, a 2 × 2 Hamiltonian matrix for each J value and *e/f* parity component was employed.[31,32]

The fitted parameters for the (000) – (000) band of ^{174}YbOH and ^{172}YbOH were the band origin, ν_0, the rotational parameters, B_υ and D_υ, for both states, the lambda-doubling parameters, p_υ and $p_{D\upsilon}$, for the $\tilde{A}\ ^2\Pi$ state, and the spin-rotation parameter γ_υ for the $\tilde{X}\ ^2\Sigma^+$ state. The spin-orbit coupling constant (A) for the $\tilde{A}^2\Pi$ state was held fixed at 1350 cm^{-1} (estimated using the low-resolution spectrum from the separation of the (000) – (000) heads of the two spin-orbit components). For the ^{174}YbOH (000) – (100) band, the parameters for the $\tilde{A}^2\Pi$ state were held fixed at those determined in the fit of the (000) – (000) band, while the band origin and the parameters B_υ, D_υ, and γ_υ for the $\tilde{X}^2\Sigma^+$ state were allowed to vary. The standard deviations of all the fits were on the order of 0.004 cm^{-1}, indicating that the deviations between the calculated and measured line positions were consistent, on average, with the estimated measurement accuracy. The estimated parameters for YbOH are summarized in Table 6.3. All of the observed line positions used in the fits, lines calculated using the parameters in Table 6.3, and residuals between the observed and calculated lines are given in Appendix 3.

In addition to the bands mentioned above, portions of the $\tilde{A}\ ^2\Pi_{1/2} - \tilde{X}\ ^2\Sigma^+$ (100) – (000) band near 17 900 cm^{-1} were also recorded. The rotational structure in the region of the (100) – (000) band was complicated by the presence of an overlapping band, and the density of lines in this region precluded the possibility of assigning the rotational transitions unequivocally. Furthermore, it is plausible that the (100) – (000) band is

Table 6.3

Rotational Parameters[a] (cm^{-1}) from least squares fits of the $\tilde{A}\,^2\Pi - \tilde{X}\,^2\Sigma^-$ transition in YbOH

	^{174}YbOH		^{172}YbOH
	(000) – (000)	(000) – (100)	(000) – (000)
ν_0	17998.616(1)	17469.275(1)	17998.628(1)
B'	0.253358(13)	[0.253358]	0.253996(21)
$10^7D'$	2.319(26)	[2.319]	2.506(40)
p'	-0.438925(57)	[-0.438925]	-0.43717(10)
$10^6p'_D$	2.552(19)	[2.552]	2.357(31)
A'	[1350.0]	[1350.0]	[1350.0]
B''	0.245434(13)	0.2439771(35)	0.246054(22)
D''	2.183(28)	2.168(19)	2.359(43)
$10^4\gamma''$	9.64(14)	-1.62(48)	10.01(19)
N	194	47	165
σ	0.0036	0.0035	0.0046

[a] Values in parentheses are standard errors for the corresponding parameter. N is the number of lines fit in each band, and σ is the standard deviation. Parameters in square brackets were held fixed in the fits.

perturbed by a nearby electronic state. A similar situation exists in YbF, where the $A^2\Pi$ state $\upsilon = 1$ and 2 vibrational levels are perturbed (see discussion below).[13]

A portion of one of the $\tilde{A}\,^2\Pi_{1/2} - \tilde{X}\,^2\Sigma^-$ (010) – (000) vibronic components near 17730 cm^{-1} was also partially investigated at high-resolution during the course of this work. Despite a sufficient signal/noise to record a satisfactory rotational spectrum, only a single, blue-degraded branch that forms the band head at 17730 cm^{-1}, was identified. Unfortunately, time constraints precluded an in-depth analysis of this transition, and no conclusive rotational assignments have been made.

6.5 Discussion

Despite careful searching, none of the features tentatively assigned to YbOH by Gilbert[71,72] were observed in the absorption spectrum of YbOH. Based on the results obtained in the present work, it appears that Gilbert's assignment of YbOH as the carrier of the bands observed in the flame spectra was either erroneous, or involves transitions terminating at an excited state.

During the course of their work on YbO, Linton *et al.* observed two excited electronic states which were tentatively attributed to the $Yb^{-}O^{-}$ electronic configuration.[61] This configuration should be very similar to the YbO moiety in YbOH, and, in fact, the estimated vibrational frequency of 540 cm^{-1} for the states observed in YbO[61] is similar to the observed frequencies of 573 and 529 cm^{-1} for the Yb-O stretching mode in the $\tilde{A}$ and $\tilde{X}$ states of YbOH, respectively.

It is clear from Table 6.2 that the estimated frequencies of the stretching and bending modes in YbOH are very similar to those determined previously for the alkaline earth monohydroxides. Upon examination of the rotational parameters for the four molecules, one also finds that the parameters for YbOH and the alkaline-earth monohydroxides are similar. The rotational analysis of the $\tilde{A}\,^2\Pi - \tilde{X}\,^2\Sigma^+$ transition in this work is consistent with a linear structure for YbOH, the same as that found in BaOH,[79] CaOH,[80] and SrOH.[81]

Despite careful searches at low-resolution, no transitions involving the O-H stretching mode were observed during the course of this work. Previous studies of the alkaline-earth monohydroxides have also been unsuccessful in identifying the O-H stretch. The explanation for this has been noted previously by several different authors.[73,75,79] Essentially, transitions involving the O-H stretching mode have extremely small Franck-Condon factors because the unpaired electron involved in the observed electronic transitions is centered on the metal atom, far away from the O-H center.

Despite the fact that reliable rotational parameters were obtained for two isotopomers of YbOH, ^{172}YbOH and ^{174}YbOH, it was not possible to calculate sensible estimates of the Yb-O and O-H bond lengths. This regrettable circumstance arises from a combination of two factors: the small difference in the reduced masses of the isotopomers, and the accuracy of the parameters. However, assuming the O-H bond length in YbOH is the same as that in BaOH, it is possible to obtain an estimate of the Yb-O bond length. From their work on BaOH/D, Bernath and coworkers were able to calculate an accurate estimate of the O-H bond length in BaOH, 0.923 Å.[79] Using this value, the Yb-O bond length in the $\tilde{X}\,^2\Sigma^+$ state of YbOH is found to be 2.15(1) Å. Considering the similarity in electronic structure between the ground states of Ba and Yb, it is not surprising that the derived Yb-O bond length is close to that for Ba-O in BaOH, 2.201 Å.[79]

Of interest in the present work is the variation of γ, the spin-rotation parameter, in the (000) and (100) vibrational levels of the ground state. For diatomic and linear polyatomic molecules with a $^2\Sigma^-$ ground state, γ values are most often positive. This is a result of the fact that the main contribution to γ is from second-order effects arising from interactions with excited $^2\Pi$ states in the manifold of states in the molecule. For a ground $^2\Sigma^-$ state, the contributions to γ are all positive when the $^2\Pi$ states that lie above it are regular (with the $^2\Pi_{3/2}$ spin-orbit component lying above the $^2\Pi_{1/2}$ component). However, negative γ values have been observed in the ground states of a variety of molecules including YO,[82] ZrN,[83,84] ScNH,[85] LaNH[86] and YbF.[13]

In the present work, γ was observed to change from a small and positive value in the (000) ground state level, to a small and negative value in the (100) level. A similar situation exists in the $X^2\Sigma^-$ state of the isoelectronic YbF molecule,[13] for which Dunfield *et al.* observed γ to be negative in $\upsilon = 1$ and 2. Dunfield *et al.* also observed perturbations in the $\upsilon = 1$ and 2 levels of the $A^2\Pi_{1/2}$ state of YbF as the result of an interaction with a nearby $\Omega = \frac{1}{2}$ state (labelled [18.6]0.5) that originates from the $Yb^+(4f^{13}6s^2)F^-$ configuration.[13] It is thought that configurational mixing of the $A^2\Pi_{1/2}$ state with the [18.6]0.5 state causes the unusual behaviour of γ in the ground state through the second order interaction of the nominal $A^2\Pi$ state with the $X^2\Sigma^-$ state.[13,54] Of relevance is the fact that no perturbations were observed in the $A^2\Pi$ state of YbCl, and that the ground state spin-rotation splitting in YbCl was found to behave normally (i.e. γ-values are positive with only a small vibrational dependence).[54] In the present work on YbOH, a negative spin-rotation parameter was observed in the ground $\tilde{X}\,^2\Sigma^+$ state (100) vibrational level. It is tempting to speculate that the mechanism that produces a negative value for γ in the ground state of the isoelectronic molecule YbF also gives rise to a negative value for the spin-rotation parameter in the (100) ground state level of YbOH. If that is the case, an unobserved state could be perturbing the (100) level of the $\tilde{A}\,^2\Pi$ state, thus producing a negative value for γ in the ground state (100) vibrational level. This situation would explain the complicated rotational structure observed in the $\tilde{A} - \tilde{X}$ (100) – (000) band. Further work on the $\tilde{A} - \tilde{X}$ system is required to draw any firm conclusions surrounding the unusual behaviour of the spin-rotation effect in the ground state of YbOH.

6.6 Concluding Remarks

The present work represents the first reliable spectroscopic observation of the YbOH radical. Low-resolution experiments were employed to establish vibrational frequencies for the Yb-O stretching and Yb-O-H bending modes in the $\tilde{A}^2\Pi$ and $\tilde{X}^2\Sigma^+$ states. A rotational analysis of the fundamental (000) – (000) band has established the molecular geometry of YbOH as linear in both states. The unusual behavior of the ground state spin-rotation parameter was discussed and compared to the isoelectronic YbF molecule.

Much like the alkaline-earth monohydroxides, the unpaired electron on YbOH is centered on the metal atom, effectively creating $Yb^+(4f^{14}6s)$ and OH^- centres. It is well known that the hydroxide ligand behaves much like a halide, and it is often referred to as a pseudo-halide. Not surprisingly, then, the observed transition in YbOH is found to be similar to that observed in YbCl, where an electron is excited out of a metal-centered 6sσ-orbital.

It should be noted that a number of unsuccessful experiments were performed in attempts to observe the deuterated species YbOD. Both D_2O and CH_3OD were employed as oxidants in separate experiments at both high and low-resolution. Regrettably, no spectra were recorded where the carrier could be identified conclusively as YbOD. It seems likely that the Broida oven source of YbOD was simply unable to produce a sufficient amount of YbOD to observe with our detection system using the aforementioned oxidants. D_2O_2, which would be a more promising oxidant, is not available commercially. It may be possible, however, to observe YbOD produced in a laser ablation system, which has significantly different production properties in terms of the species generated.

Chapter 7

The $A^1\Sigma^+$ - $X^1\Sigma^+$ Transition in CaS

7.1 Background

The alkaline-earth monosulfides CaS, SrS, and BaS have been the subject of a number of spectroscopic investigations.[66,68,70,87-94] However, their electronic structures, and, more specifically, their low-lying electronic states, are not as well characterized as those of the alkaline-earth monoxides (see, for example, Refs. 95 – 101, and references therein). With the exception of CaS,[87] all of the low-lying excited states of the alkaline earth monoxides and monosulfides are known to be extensively perturbed. In an effort to identify perturbations in CaS, and compare them to observed perturbations in YbS,[57,58] the $A^1\Sigma^+$ – $X^1\Sigma^+$ electronic transition in CaS has been reinvestigated in the present thesis work.

Blues and Barrow were the first to record the absorption spectrum of the $A^1\Sigma^+$ – $X^1\Sigma^+$ electronic transition of CaS in the red region of the spectrum.[87] These authors rotationally analyzed the 0–0, 1–0, 1–1, 0–1, 1–2 and 2–1 bands at high resolution to $J \approx 200$. They obtained equilibrium values for the vibrational and rotational parameters of the $A^1\Sigma^+$ and $X^1\Sigma^+$ states, but did not observe any perturbations.[87] Andersson and Davis also examined the $A^1\Sigma^+ - X^1\Sigma^+$ system (though they refer to it as the $B^1\Sigma^+ - X^1\Sigma^+$) using a Fourier Transform spectrometer and a carbon tube furnace.[94] In their work, Andersson and Davis recorded spectra involving the $\upsilon = 0 - 5$ vibrational levels in both states, though they did not report any perturbations. Other work on CaS includes a high-resolution laser study of three electronic transitions in the blue region of the spectrum by

Jarman, Hailey and Bernath,[88] a millimeter wave study in the ground electronic state by Takano, Yamamoto and Saito[89] and a study of CaS in a solid argon matrix by Martin and Schaber.[90] The previous high-resolution studies[87-89] were very helpful in the present work because they provided accurate constants for the ground $X^1\Sigma^+$ state up to $\upsilon = 7$, facilitating the use of ground state combination differences in assigning the $A^1\Sigma^+$ state perturbations.

In addition to the aforementioned experimental work, Partridge, Langhoff and Bauschlicher have performed *ab initio* calculations on the alkaline-earth monosulfides to determine the spectroscopic constants T_e, R_e, ω_e and D_e for the low-lying $X^1\Sigma^+$, $a^3\Pi$ and $A'^1\Pi$ states.[91] These calculations predict the $a^3\Pi$ and $A'^1\Pi$ states to lie in the infrared region with $T \approx 7000$ cm^{-1}, significantly below the $A^1\Sigma^+$ state (with $T \approx 15\ 000$ cm^{-1}). The predicted position of the $A'^1\Pi$ state is in good agreement with a tentative observation of this state by Jarman, Hailey and Bernath,[88] who observed low-lying states with $T \approx 7500$ cm^{-1} above the ground state in fluorescence from electronic states in the blue.

The present work is the first high-resolution laser study of the $A^1\Sigma^+ - X^1\Sigma^+$ electronic transition in CaS. The investigation of the $A - X$ system has resulted in the identification of a number of level crossings in the $A^1\Sigma^+$ state, and effective parameters for the perturbing states are determined from a partial deperturbation analysis.

7.2 Experimental Details

CaS was produced in the oven by the reaction of OCS with Ca metal vapour, with total pressures in the range 3 – 5 torr. Carbon disulfide, CS_2, was also tested as a possible oxidant, but the resulting signal was not as strong as that obtained for OCS. The $A^1\Sigma^+$ –

$X^1\Sigma^+$ bands were probed with the ring dye laser operating in single-frequency mode with DCM laser dye. An I_2 fluorescence spectrum was recorded simultaneously and compared to the standard I_2 atlas[29] for calibration, without the suggested 0.0056 cm^{-1} offset.[102]

7.3 Results and Deperturbation Analysis

The $A^1\Sigma^+ - X^1\Sigma^+$ 0–0, 1–0, 1–1, 2–1, 3–1, 3–2, 4–2, 4–3, 5–3, 5–4, 6–4, and 6–5 bands observed in the present work consist of red-degraded P- and R-branches. Typically, we were able to record rotational lines for both branches up to $J \approx 90$, with the R-branch forming a head at relatively low J ($\approx$ 15). Fig. 7.1 shows a portion of the 1–0 band R-branch in the region of the band head. Once the spectra were recorded and measured, assignment of the rotational numbering, J, was achieved using the standard combination differences. In addition, it was possible to observe the "first lines" of several bands. The data for individual bands were then employed in a least-squares fitting program that contains the usual analytical expression for the term values of $^1\Sigma^+$ states. For each band, the fitted parameters were the band origin ν_0, and the rotational parameters B_υ and D_υ for both the upper and lower states.

While the initial fits of the 0–0, 1–0, 1–1 and 2–1 bands had standard deviations on the order of 0.003 cm^{-1}, the remainder of the bands possessed anomalously large standard deviations, with many lines exhibiting systematically large residuals. It was immediately obvious that the $A^1\Sigma^+$ state υ = 3, 4, 5 and 6 levels are extensively perturbed. Careful inspection revealed no perturbations in the υ = 0, 1 and 2 vibrational levels up to $J \approx 90$, confirming Blues and Barrow's work on this system.[87] Fig. 7.2 shows a portion of the 6–4 band in the region of a perturbation in the P-branch. Some of the theoretical

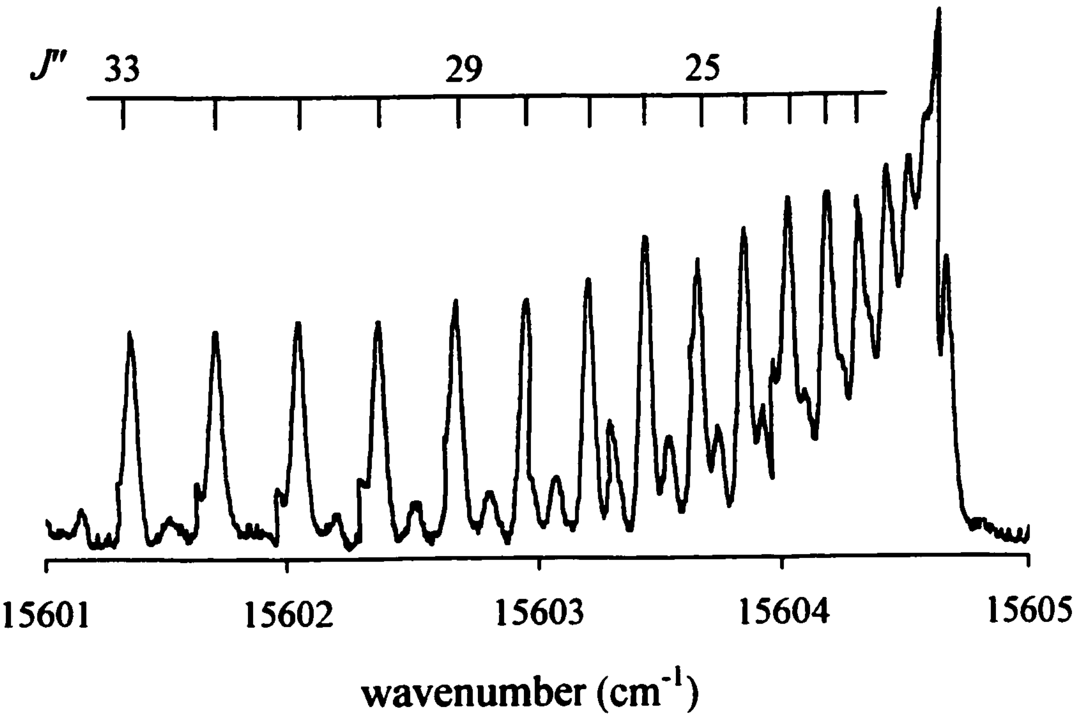


Figure 7.1: A portion of the 1 – 0 band of the CaS $A^1\Sigma^- - X^1\Sigma^-$ transition near the R-branch head.

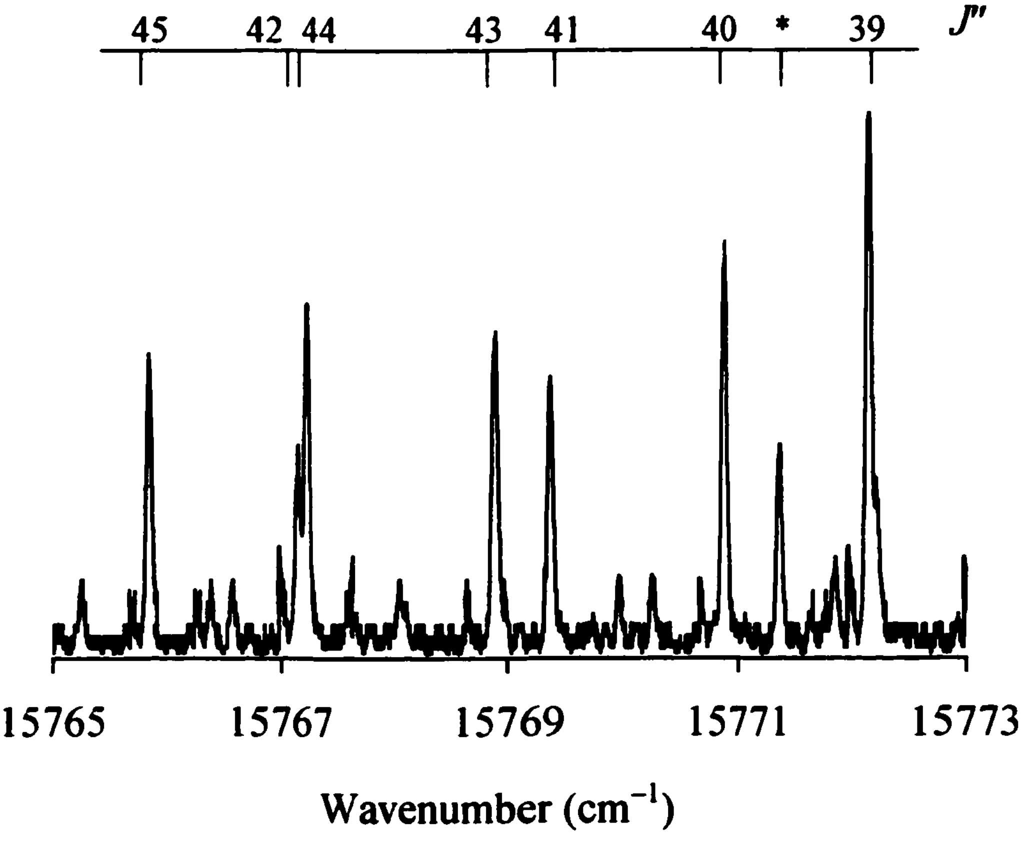


Figure 7.2: A portion of the P-branch of the CaS $A^1\Sigma^+ - X^1\Sigma^+$ 6 – 4 band. The spectrum is shown near the $A^1\Sigma^- \sim P_7$ level crossing. The line labelled with an asterisk is an 'extra line' assigned as P(42).

considerations regarding level crossings were discussed in Chapter 3. Assignment of the rotational lines near several of the perturbations (like the one shown in Fig. 7.2) was not trivial because lines on both sides of the crossing were shifted by up to ≈ 2 cm^{-1}. A plot of the residuals of the line positions in the 6–4 band before deperturbation is given in Fig. 7.3.

To determine accurate positions of the crossing points, and to obtain more information about the nature of the perturbers, the band-fitting program was modified to incorporate perturbing states described by their term values (T_P) and rotational parameters, B_P and D_P. Interaction between the $A^1\Sigma^+$ state and a perturber (P_i) could be modeled either as a homogeneous ($\Delta\Omega = 0$, J-independent) perturbation or a heterogeneous ($\Delta\Omega = \pm 1$, J-dependent) perturbation. To properly represent the crossings of the $A^1\Sigma^+$ and perturbing states, very careful selection of the trial parameters was essential, and it was necessary to keep the centrifugal distortion constants for the perturbing states, D_P, fixed during the deperturbation fits. Because no additional information about the perturbing states was available, separate fits of all the perturbed bands were performed assuming either a heterogeneous or homogeneous interaction. In all cases, both models worked equally well, as discussed further below.

7.3.1 $A^1\Sigma^+$ state $\upsilon = 3$ level:

Analysis of the 3–1 and 3–2 bands revealed two level crossings in the $\upsilon' = 3$ level, at $J' = 67.2$ and 77.3. The band-fitting program was modified to fit both crossings simultaneously by solving a 3×3 matrix for each J-value that describes the interactions between the $A^1\Sigma^+$ state and the perturbing states (referred to hereafter as P_1 and P_2 for the

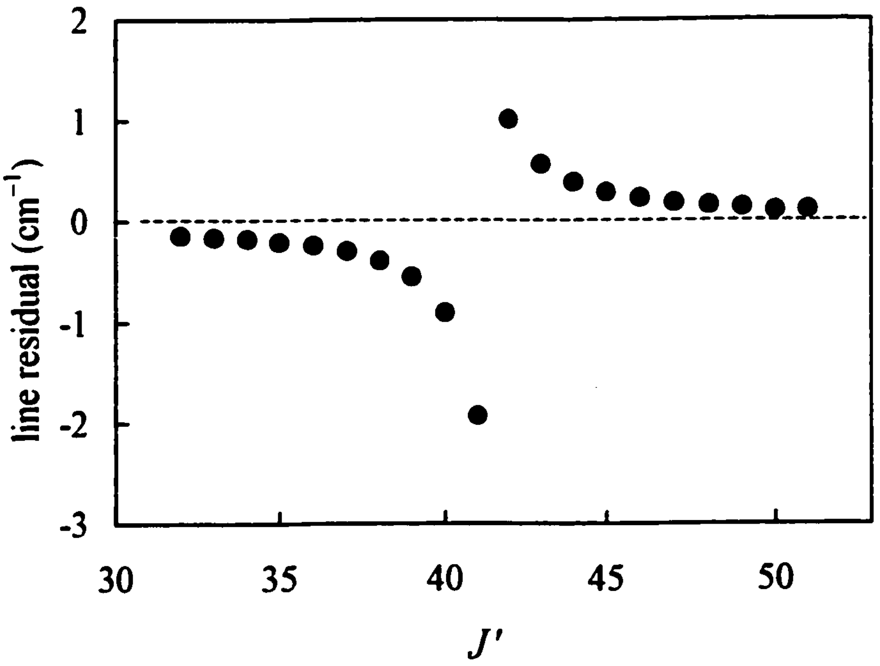


Figure 7.3: A plot of the residuals of the line positions near the $A^1\Sigma^+ \sim P_7$ crossing point in the 6 – 4 band of CaS. The residuals represent the differences between the observed line positions and those calculated before deperturbation.

J = 67.2 and 77.3 crossings, respectively). The diagonal components of each matrix contain the standard expressions for Hund's case (a) rotational energy, while the interactions between the $A^1\Sigma^+$ and perturbing states are described in the off-diagonal matrix elements by either α (homogeneous interaction) or $\beta[J(J+1)]^{1/2}$ (heterogeneous interaction). The matrix elements are summarized in Table 7.1(A). The fitted parameters for the 3–1 and 3–2 bands were the band origins, ν_0, the parameters B_υ and D_υ for the $X^1\Sigma$ and $A^1\Sigma$ states, the perturber term values, T_{P1} and T_{P2}, and B_{P1}, B_{P2}, and either α or β for each crossing. No extra lines associated with either perturbation were identified in these bands, indicating relatively weak interactions of $A^1\Sigma^+$ with both P_1 and P_2.

7.3.2 $A^1\Sigma^+$ state υ = 4 level:

Similar to the υ′ = 3 level, two perturbations were identified in υ′ = 4 in the 4–2 and 4–3 bands, with crossing points at J' = 37.3 and 50.6 (referred to later as P_3 and P_4, respectively). The program employed to fit the perturbations was the same as that for the 3–1 and 3–2 bands, and analogous sets of parameters were determined in the band fits. Despite the fact that the $A^1\Sigma^+ \sim P_3$ and $A^1\Sigma^+ \sim P_4$ interactions were significantly larger (by about a factor of 2) than the $A^1\Sigma^+ \sim P_1$ and $A^1\Sigma^+ \sim P_2$ interactions, it was not possible to identify any extra lines in the spectra.

7.3.3 $A^1\Sigma^+$ state υ = 5 level:

Analysis of the 5–3 and 5–4 bands revealed the presence of one perturbation in υ′ = 5 with a crossing point at J' = 69.6 (P_6). In addition to this, the least-squares fits displayed

Table 7.1

Hamiltonian Matrix Elements

(A)	$^1\Sigma$	P_1	P_2
$^1\Sigma$	E_A	α_{P1}	α_{P2}
P_1	α_{P1}	E_{P1}	0
P_2	α_{P2}	0	E_{P2}

(B)	$^1\Sigma$	P_1
$^1\Sigma$	E_A	α_{P1}
P_1	α_{P1}	E_{P1}

(C)	$^1\Sigma$	P_1	P_2	P_3
$^1\Sigma$	E_A	α_{P1}	α_{P2}	α_{P3}
P_1	α_{P1}	E_{P1}	0	0
P_2	α_{P2}	0	E_{P2}	0
P_3	α_{P3}	0	0	E_{P3}

$E_A = \nu_0 + B_\upsilon J(J+1) - D_\upsilon[J(J+1)]^2$

$E_P = \nu_P + B_P J(J+1) - D_P[J(J+1)]^2$

ν_0 is the band origin of the $A - X$ band; ν_P is the band origin of the perturber; B_υ, B_P are the rotational constants for the A and perturbing states; D_υ, D_P are the centrifugal distortion constants and α_{Pi} is the $A^1\Sigma^+ \sim P_i$ interaction parameter.

systematic residuals at low J, suggesting a second "crossing" occurs at $J < 0$ (P_5). However, because only one side of this level crossing was observed, it was not possible to obtain estimates of the parameters for P_5 in the deperturbation analysis. In order to obtain the best deperturbed estimates for the fitted parameters, the low-J lines involved in the $A^1\Sigma^+ \sim P_5$ interaction were excluded from the fit. The fitting program for the 5–3 and 5–4 bands treated a single level crossing by solving a 2×2 matrix that describes the interaction between the $A^1\Sigma^+$ and P_6 states. The elements for this matrix are given in Table 7.1(B). No extra lines were observed in either band.

7.3.4 $A^1\Sigma^+$ state $\upsilon = 6$ level:

The $\upsilon' = 6$ level is the most extensively perturbed $A^1\Sigma^+$ vibrational level observed in the present work. Level crossings at $J' = 41.1$, 73.4 and 77.4 have been identified unequivocally, and are labelled P_7, P_8, and P_9, respectively. In addition, residual systematic error at high J present after deperturbation suggests the possibility of a fourth crossing at $J > 86$. For the $A^1\Sigma^+ \sim P_7$ interaction ($J' = 41.1$ crossing), several 'extra lines' were identified in the 6–4 (5 lines) and 6–5 (2 lines) bands. Following the method of Gerö,[102] the perturbations in $\upsilon' = 6$ are illustrated in Fig. 7.4 by plotting $T/4J$ as a function of J, where $T/4J$ is defined as

$$T/4J = [\mathrm{R}(J-2) - \mathrm{R}(J-1) + \mathrm{P}(J) - \mathrm{P}(J+1)]/4J \approx B'' - B' + 6D'' - 2J^2(D'' - D'). \quad [1]$$

In unperturbed regions, the plot of $T/4J$ against J is approximately horizontal, with changes occurring in regions of perturbations, as illustrated in Fig. 7.4. The least-squares program for the 6–4 and 6–5 bands involved fitting all three crossings simultaneously,

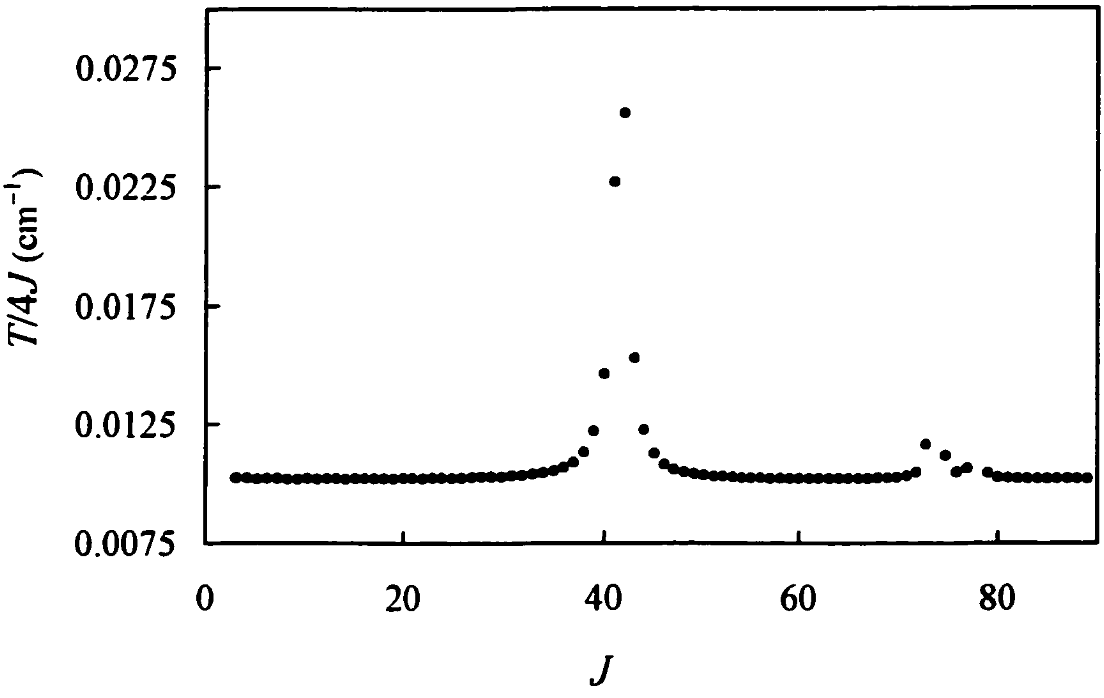


Figure 7.4: A Gerö plot (Ref. 102) of $T/4J$ against J for the 6 – 4 band of CaS $A - X$. The plot shows the perturbations in the $\upsilon = 6$ level of the $A^1\Sigma^+$ state (see text for the definition of $T/4J$). Perturbations appear as deviations from the horizontal.

with the extra lines included in the fit. Matrix elements for each 4×4 matrix employed in the fits are given in Table 7.1(C).

As can be seen in Table 7.1, it was assumed that the various perturbers did not interact with each other. To properly fit interactions between the perturbing states, which could be significant, data that directly sample the perturbing states would be required. Unfortunately, attempts to observe these states directly have been unsuccessful.

In all of the individual deperturbation band fits, the standard deviations of the fits were on the order of 0.003 cm^{-1}, indicating that the deviations between the calculated and measured line positions were consistent, on average, with the estimated measurement precision of 0.003 cm^{-1}. After fitting the twelve bands individually, the output parameters were then merged together. Parameters for the $A^1\Sigma^+$ and $X^1\Sigma^+$ states obtained from the merge fit (which had a $\hat{\sigma} \approx 2.4$) are given in Table 7.2 and constants for the perturbing states together with the fitted interaction parameters are given in Table 7.3. Additional digits beyond those required by the associated standard deviations are given as subscripts to permit calculation of line positions to within the residuals of the fit. As mentioned above, both models (homogeneous and heterogeneous) worked equally well in the deperturbation fits, and in all cases $\alpha_i \approx [J_0(J_0 + 1)]^{1/2}\beta_i$, where J_0 is the non-integer crossing point of P_i. For simplicity, only the α_i's are reported in Table 7.3.

The rotational parameters, B_υ, for the $X^1\Sigma^+$ and $A^1\Sigma^+$ states follow regular trends with increasing vibrational quantum number, and it was possible in the merge fit to estimate equilibrium values of the constants from the twelve bands. The results of the global merge fit are given in Table 7.4. Included in this table for comparison are the results from the previous study of this system by Blues and Barrow,[87] Andersson and

Table 7.2

Molecular parameters (cm^{-1}) for the $A^1\Sigma^+$ and $X^1\Sigma^+$ states of CaS

	υ	T_υ	B_υ	$10^7 D_\upsilon$
$X^1\Sigma^+$	0	0.0000	0.1762501(65)	1.025(0)
	1	458.6662(26)	0.1754171(65)	1.027(8)
	2	913.7663(34)	0.1745834(62)	1.037(8)
	3	1365.2921(40)	0.1737439(62)	1.048(8)
	4	1813.2205(72)	0.1729083(77)	1.073(12)
	5	2257.5644(79)	0.1720552(91)	1.068(22)
$A^1\Sigma^+$	0	15194.4337(18)	0.1663642(70)	1.087(14)
	1	15601.8705(15)	0.1657578(65)	1.092(9)
	2	16007.6364(35)	0.1651530(65)	1.086(8)
	3	16411.7859(30)	0.1645420(62)	1.075(8)
	4	16814.2626(38)	0.1639436(60)	1.080(8)
	5	17215.1383(53)	0.1633341(65)	1.076(8)
	6	17614.3096(74)	0.1627397(79)	1.098(13)

Values in parentheses are standard errors for the corresponding parameters.

Table 7.3

Effective parameters (cm^{-1}) for the $A^1\Sigma^+ \sim P_i$ interactions in CaS

$A^1\Sigma^+(\upsilon)$	P_i	T_{Pi}	B_{Pi}	$10^7 D_{Pi}$	α_{Pi}	J_0	Label
3	P_1	$16546._{40}(34)$	$0.1351_{72}(72)$	[1.0]	0.296(36)	67.2	$I(\upsilon)$
3	P_2	$16627._{26}(46)$	$0.1288_{43}(74)$	[1.0]	0.229(36)	77.3	$II(\upsilon')$
4	P_3	$16850._{680}(6)$	$0.1383_{88}(38)$	[1.0]	0.520(34)	37.3	$I(\upsilon+1)$
4	P_4	$16890._{20}(6)$	$0.1348_{79}(22)$	[1.0]	0.483(18)	50.6	$II(\upsilon'+1)$
5	P_5	–	–	–	–	< 0	
5	P_6	17373.23(6)	0.131152(13)	[1.0]	1.0640(52)	69.6	$III(\upsilon'')$
6	P_7	$17691.45_{8}(11)$	0.118133(67)	[1.0]	2.1051(22)	41.1	
6	P_8	$17950._{22}(50)$	$0.1012_{1}(94)$	[1.0]	1.125(79)	73.4	
6	P_9	$17719._{40}(65)$	$0.145_{37}(11)$	[1.0]	0.305(85)	77.4	

Values in parentheses are standard errors for the corresponding parameter in units of the least significant digit shown in regular type. Additional digits are given as subscripts to permit calculation of line positions to within the residuals of the fit. Values in square brackets were held fixed in the fits.

Table 7.4

Molecular parameters (cm^{-1}) for the $A^1\Sigma^+$ and $X^1\Sigma^+$ states of CaS

	Present Work	Ref. 87[a]	Ref. 94[b]	Ref. 89[c]
T_{00} (A–X)	15194.434(2)	15194.44	–	–
B_e''	0.176683(21)	0.17667	0.176673(4)	0.17667566(5)
$10^4\alpha_e''$	8.393(34)	8.37	8.251(2)	8.2697(7)
ω_e''	462.273(12)	462.23	462.263(2)	–
$\omega_e x_e''$	1.7926(17)	1.78	1.7907(3)	–
R_e'' (Å)	2.31770(14)	2.3178	–	2.317751(1)
B_e'	0.166676(22)	0.16666	0.166680(4)	–
$10^4\alpha_e'$	6.070(28)	6.05	6.071(2)	–
ω_e'	409.077(9)	409.04	409.062(2)	–
$\omega_e x_e'$	0.8231(12)	0.818	0.8200(3)	–
R_e' (Å)	2.38626(16)	2.3864	–	–

[a] Error estimates were not given by Blues and Barrow (Ref. 87).

[b] From the optical study of Andersson and Davis (Ref. 94).

[c] From the microwave study of Takano *et al.* (Ref. 89).

Davis,[94] and the microwave study by Takano *et al.*[89] It is clear from Table 7.4 that the results of the different studies are in good agreement with one another. A complete list of all 1200 line positions used in the fits, as well as residuals between the measured lines and line positions calculated using the parameters in Tables 7.2 and 7.3, is given in Appendix 4.

7.4 Discussion

As mentioned above, all of the perturbations (except P_5) were fit assuming either a homogeneous or heterogeneous model, and in all cases the fits were equally satisfactory. One possible explanation for this result is that the current measurement accuracy is not sufficient to distinguish between the two models. Similar situations have been observed for perturbations in SrS[68] and YbS.[58]

In the absence of any additional information about the perturbing states, beyond that deduced herein from the deperturbation analyses, further discussion remains equivocal. Based on the known electronic structure of the alkaline-earth monoxides,[95-101] it seems reasonable that the perturbations can be tentatively attributed to the low-lying $a^3\Pi$ and $A'^1\Pi$ states. These states have been identified in CaS in the infrared ($T \approx 7500$ cm^{-1}),[88] but no rotational analysis has been attempted. Because of mixing between the basis functions of the $^3\Pi$ state (nominally $^3\Pi_0$, $^3\Pi_1$ and $^3\Pi_2$), all three substates can interact with the $A^1\Sigma^+$ state.[95] Accordingly, four states, $A'^1\Pi$, $a^3\Pi_0$, $a^3\Pi_1$ and $a^3\Pi_2$, can perturb the $A^1\Sigma^+$ state, with the $A^1\Sigma^+ \sim a^3\Pi_2$ interaction likely being the weakest.

In the present work, nine perturbations in the $A^1\Sigma^+$ state $\upsilon = 3 - 6$ vibrational levels have been identified unequivocally. As a first step in understanding the identity of the perturbing states, the vibration-rotation energies of the $A^1\Sigma^+$ and perturbing states are plotted as a function of $J(J+1)$ in Fig. 7.5. It seems reasonable, based on Figure 7.5, to assume that the pairs of perturbers that cross the $A^1\Sigma^+$ $\upsilon = 3$ and 4 levels (P_1/P_2 and P_3/P_4) arise from two states. In other words, P_1 and P_3 are successive vibrational levels from the same perturbing state (*I*), and P_2 and P_4 are successive vibrational levels from a second perturbing state (*II*). It would be expected that the perturbing states have approximately the same vibrational spacing, and, indeed, $\omega^I \approx \omega^{II} \approx 330$ cm^{-1} (with an estimated uncertainty of ≈ 10 cm^{-1}). Values for the vibrational spacings were obtained from the separation of the vibrational levels near the perturbations, thereby reducing the error associated with extrapolation to $J = 0$. It should be noted that the relative strengths of the perturbations are consistent with the above assignments. If the two states (*I* and *II*) arise from the low-lying $a^3\Pi$ and $A'^1\Pi$ states in the infrared, then the quantum number of the perturbing vibrational levels would be quite high ($\approx 25 - 30$). This situation is plausible despite the fact that no perturbations were observed in $A^1\Sigma^+$ $\upsilon = 0 - 2$. Crossings in these vibrational levels may have energy shifts that are too small to observe with the current measurement accuracy, or that of the previous work by Blues and Barrow,[87] because of the small interaction between the *A* state and perturbing state. The $A \sim P$ interaction was observed to decrease with decreasing vibrational level from $A^1\Sigma^+$ $\upsilon = 6 - 3$. The change in interaction strength of the perturbations is almost certainly due to the change in the vibrational overlap between the *A* state levels and the perturbing levels.

Unfortunately, an understanding of the perturbations in $\upsilon = 5$ and 6 is not as obvious as for $P_1 - P_4$. By extrapolation of the perturbing states *I* and *II* by the estimated vibrational frequency $\omega_P \approx 330$ cm^{-1}, it is found that the vibrational levels above those

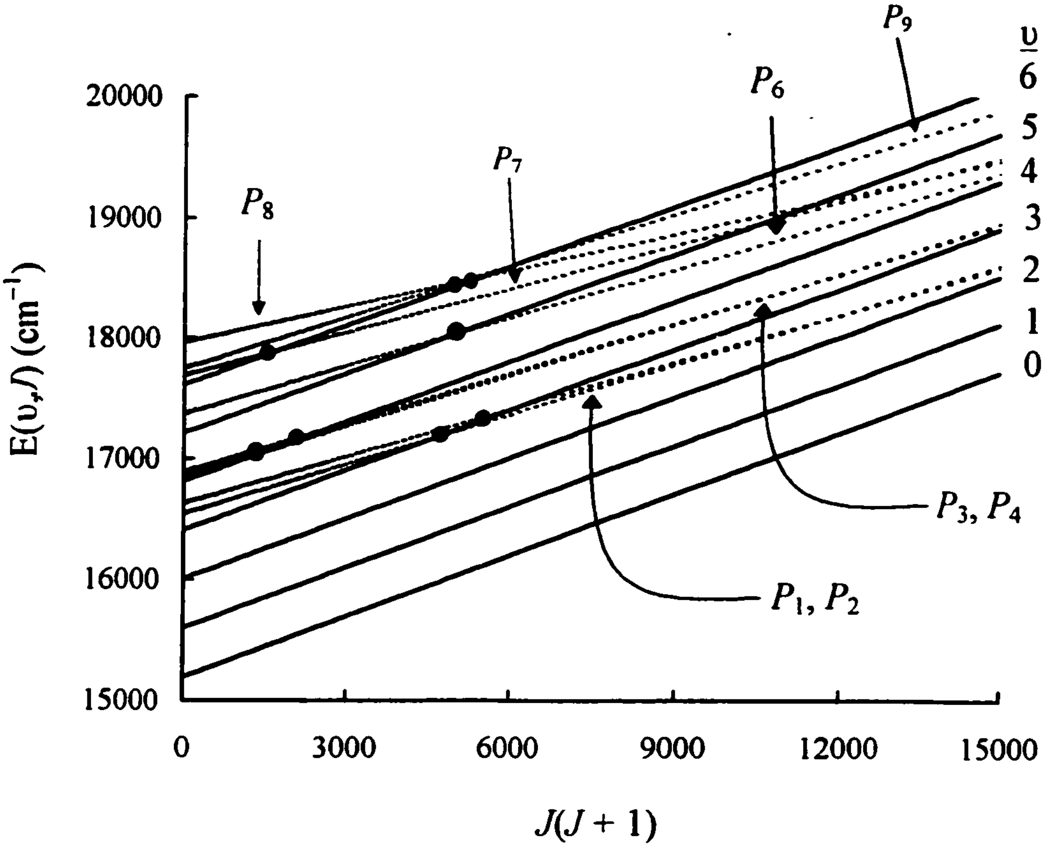


Figure 7.5: The dependence of vibration-rotation energy on $J(J + 1)$ for the $A^1\Sigma^-$ state of CaS (solid lines) and the perturbers P_1 - P_9 (dashed lines). Note: P_5 occurs at $J < 0$ and is therefore not shown. Observed level crossings are indicated by •.

responsible for P_3/P_4 would cross in the energy region below the $J = 0$ level in $A^1\Sigma^+$ $\upsilon = 5$. These level(s) could be responsible for P_5, which crosses $\upsilon = 5$ at $J < 0$, though this interpretation should be regarded as tentative.

Based on Fig. 7.5, P_6 does not appear to arise from either perturber *I* or *II*, and therefore it is assumed to arise from a third state (*III*). Furthermore, from the rotationless energy separation of P_6 and P_7 ($\approx$ 320 cm^{-1}), it is tempting to presume that both perturbations arise from the same electronic state (*III*). However, the rotational constants for the two perturbing levels are significantly different (Table 7.3) and it is not prudent to draw any firm conclusions about the identity of these perturbers. It is unclear at the present time why some of the fitted parameters vary to such a degree, since all the perturbing levels are expected to have similar rotational constants.

With relatively little data sampling the P_8 and P_9 perturbations, and their close proximity to one another, least-squares fitting of these level crossings was difficult. In fact, these factors likely contribute to the inconsistency in the fitted rotational parameters for these two perturbing levels (Table 7.3). It is important to note that the model employed assumes no interactions between the perturbers, and that this may cause the model to be inadequate for properly fitting perturbations so close to one another. Considering the above discussion, the parameters for the P_8 and P_9 perturbations should probably be regarded as effective, and not necessarily the true, physically meaningful, molecular parameters.

It is somewhat surprising to note that in their recent work on the $A^1\Sigma^+ - X^1\Sigma^+$ transition in CaS, Andersson and Davis did not report any perturbations, despite the fact they observed vibrational levels that experience level crossings. Inspection of their data set reveals a number of incorrectly assigned lines near the perturbations in $\upsilon = 4$ and 5 of the $A^1\Sigma^+$ state. These misassignments should serve as a warning to those who employ software (such as the Loomis-Wood program) to pick out lines and branches, since the presence of perturbations makes assigning lines in this fashion a rather precarious practice.

7.5 Concluding Remarks

In summary, high-resolution laser spectroscopic techniques have been employed to investigate the $A^1\Sigma^+ - X^1\Sigma^+$ transition in CaS. Nine perturbations have been observed in the $\upsilon = 3 - 6$ levels of the $A^1\Sigma^+$ state, and through a partial deperturbation analysis of the perturbed bands, molecular parameters for the perturbing levels have been obtained.

The present investigation provides an important first step in understanding the low-lying electronic states of CaS. However, further work that directly samples the other low-lying states in CaS is required to better understand the manifold of electronic states in this molecule, and to unequivocally assign the perturbations observed. With data that sample the perturbing levels, it would be possible to carry out a complete, global deperturbation analysis of the low-lying $a^3\Pi$, $A'^1\Pi$ and $A^1\Sigma^+$ states, like that carried out for the analogous states in BaS by Cummins *et al.*[70]

Chapter 8

General Conclusions and Discussion

This thesis work has concerned the low-lying electronic states of YbCl, YbS, YbOH and CaS. By employing visible laser absorption spectroscopy and resolved fluorescence, electronic transitions in each of the above molecules have been extensively examined. Rotational analyses of the observed systems have allowed for the determination of vibrational frequencies and molecular geometries for the observed electronic states. For YbS and YbOH, the present work represents the first observation of any kind for these molecules.

The $A^2\Pi - X^2\Sigma^+$ transition in YbCl has been rotationally analyzed, and found to be very much like the $A^2\Pi - X^2\Sigma^+$ transitions in the alkaline-earth monochlorides CaCl, SrCl, and BaCl. This work, along with a complementary rotational study of the $B^2\Sigma^+$ – $X^2\Sigma^+$ transition at the University of New Brunswick, has revealed the fact that the $A^2\Pi$ and $B^2\Sigma^+$ states are a unique perturber pair, by virtue of the fact that the lambda doubling constant for the $A^2\Pi_{1/2}$ state is very close in value to the spin-rotation parameter in the $B^2\Sigma^+$ state. Again, this behaviour is very much like that found in the alkaline-earth monohalides. All of the observed electronic states in YbCl arise from electronic configurations that possess a closed 4*f* subshell (as mentioned above, electronic states with open *f*-configurations would have markedly different vibrational frequencies). Based on the current information for the known electronic states in YbCl, it appears that the 4*f* subshell does not contribute much to the bonding, and is localized on the Yb center.

Two electronic systems have been observed in YbS in this thesis work, namely the $A0^+ - X0^+$ and $B0^+ - X0^+$ transitions. The $A0^+ - X0^+$ transition has been shown to be analogous to the $A^1\Sigma^+ - X^1\Sigma^+$ transition in BaS, with the $A0^+$ and $A^1\Sigma^+$ states possessing the same unusual global perturbations in their vibrational structure. A rotational analysis of the $A0^+ - X0^+$ system has revealed a level crossing perturbation in the $\upsilon' = 2$ vibrational level. A deperturbation analysis has provided effective constants for the perturbing state, and deperturbed molecular parameters for the $A0^+$ state. The $B0^+$ state was found to experience a strong predissociation in the $\upsilon' = 0$ level, and no higher vibrational levels were observed. At present, there are no known electronic transitions in the alkaline-earth monosulfides that are analogous to the $B0^+ - X0^+$ transition in YbS.

Somewhat disappointingly, no electronic states with open *f*-subshell configurations were identified in YbS. It appears that the manifold of electronic states in YbS is similar to that in CaS, SrS and BaS, but unlike that of YbO. Perhaps other spectroscopic techniques, such as Fourier transform spectroscopy, may be able to identify states with open *f*-subshell configurations in the infrared region of the spectrum.

The $\tilde{A}^2\Pi - \tilde{X}^2\Sigma^+$ transition in YbOH has been both vibrationally and rotationally analyzed in the present work. Like the alkaline-earth monohydroxides, the geometries of both electronic states are linear. In fact, the observed transition appears to be analogous to the well-studied $\tilde{A}^2\Pi - \tilde{X}^2\Sigma^+$ transitions in CaOH, SrOH and BaOH. The spin-orbit coupling constant for the $\tilde{A}^2\Pi$ state, 1350 cm^{-1}, is essentially the same as that found in the isoelectronic YbF molecule, and the unusual behaviour of γ is discussed and compared to that in YbF. Estimates for the Yb-O stretching and Yb-O-H bending mode frequencies are obtained for both the $\tilde{A}^2\Pi$ and $\tilde{X}^2\Sigma^+$ states.

The $A^1\Sigma^-$ – $X^1\Sigma^-$ transition in CaS has been reinvestigated in order to examine perturbations in the $A^1\Sigma^-$ state. A deperturbation analysis has provided molecular parameters for the perturbing states, and deperturbed parameters for the $A^1\Sigma^-$ state. The perturbations observed in CaS are similar to those observed in YbS, SrS and BaS. Heterogeneous and homogeneous deperturbation models worked equally well for both CaS and YbS, indicating that the current measurement accuracy is insufficient to distinguish between the two. Further work on CaS and YbS that directly samples the perturbing levels is necessary to unequivocally identify the states involved in the perturbations. Possible experimental methods that could be utilized to do this would be double-resonance techniques, like that used for BaO.[95] Only when a complete data set is obtained can a proper, global deperturbation analysis of all the low-lying states be performed.

Appendix 1

YbCl Line Positions

Rotational transitions in the $A^2\Pi - X^2\Sigma^-$ system of $^{174}Yb^{35}Cl$ and $^{172}Yb^{35}Cl$. For each transition, the tables show the assigned rotational quantum number J, the measured line position in cm^{-1} and the residual between the observed and calculated values. Lines marked with ** were excluded in the least-squares fit.

$^{174}Yb^{35}Cl$

0-0 Band

	$P_{11}(ee)$			$Q_{12}(ef)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
33.5	17894.102	17894.096	.006	-	17894.483	
34.5	17894.314	17894.327	-.013**	-	17894.725	
35.5	17894.575	17894.564	.011**	-	17894.973	
36.5	17894.811	17894.808	.003	17895.230	17895.228	.002
37.5	17895.058	17895.058	.000	17895.489	17895.489	.000
38.5	17895.319	17895.315	.004	17895.755	17895.757	-.002
39.5	17895.579	17895.578	.001	17896.026	17896.032	-.006
40.5	17895.845	17895.848	-.003	17896.316	17896.312	.004
41.5	17896.126	17896.125	.001	17896.599	17896.600	-.001
42.5	17896.403	17896.407	-.004	17896.893	17896.894	-.001
43.5	17896.689	17896.697	-.008	17897.193	17897.194	-.001
44.5	17896.992	17896.993	-.001	17897.497	17897.501	-.004
45.5	17897.294	17897.295	-.001	17897.813	17897.815	-.002
46.5	17897.602	17897.604	-.002	17898.136	17898.135	.001
47.5	17897.917	17897.920	-.003	17898.459	17898.461	-.002
48.5	17898.244	17898.242	.002	17898.794	17898.795	-.001
49.5	17898.574	17898.570	.004	17899.135	17899.134	.001
50.5	17898.907	17898.906	.001	17899.486	17899.480	.006
51.5	17899.248	17899.247	.001	-	17899.833	

	$Q_{11}(ef)$			$R_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
25.5	-	17891.883		17892.155	17892.158	-.003
26.5	-	17892.038		17892.320	17892.325	-.005
27.5	17892.196	17892.200	-.004	17892.496	17892.497	-.001
28.5	17892.363	17892.368	-.005	17892.678	17892.676	.002
29.5	17892.536	17892.543	-.007	17892.865	17892.862	.003
30.5	17892.720	17892.724	-.004	17893.057	17893.054	.003
31.5	17892.907	17892.912	-.005	17893.254	17893.253	.001
32.5	17893.100	17893.106	-.006	17893.464	17893.458	.006
33.5	17893.307	17893.306	.001	17893.671	17893.670	.001
34.5	17893.521	17893.514	.007	17893.885	17893.888	-.003
35.5	17893.727	17893.727	.000	17894.109	17894.113	-.004
36.5	17893.946	17893.948	-.002	17894.343	17894.344	-.001
37.5	17894.163	17894.174	-.011**	17894.581	17894.582	-.001
38.5	17894.411	17894.408	.003	17894.827	17894.827	.000
39.5	17894.647	17894.648	-.001	17895.076	17895.077	-.001
40.5	17894.895	17894.894	.001	17895.330	17895.335	-.005
41.5	17895.147	17895.147	.000	17895.598	17895.599	-.001
42.5	17895.412	17895.406	.006	17895.857	17895.869	-.012**
43.5	17895.674	17895.672	.002	17896.149	17896.146	.003
44.5	17895.945	17895.945	.000	17896.431	17896.430	.001
45.5	-	17896.224		17896.720	17896.720	.000
46.5	17896.512	17896.510	.002	17897.018	17897.017	.001
47.5	17896.804	17896.802	.002	17897.326	17897.320	.006
48.5	17897.104	17897.101	.003	17897.633	17897.630	.003
49.5	17897.404	17897.406	-.002	17897.950	17897.946	.004

50.5	17897.717	17897.718	-.001	17898.275	17898.269	.006
51.5	17898.034	17898.036	-.002	17898.604	17898.598	.006
52.5	17898.362	17898.361	.001	17898.944	17898.934	.010
53.5	17898.692	17898.692	.000	17899.271	17899.277	-.006
54.5	17899.038	17899.030	.008	17899.637	17899.626	.011**
55.5	17899.367	17899.375	-.008	-	17899.982	
56.5	17899.731	17899.726	.005	-	17900.344	
57.5	-	17900.084		17900.716	17900.713	.003
58.5	17900.450	17900.448	.002	17901.092	17901.088	.004
59.5	17900.822	17900.819	.003	17901.474	17901.470	.004
60.5	17901.199	17901.196	.003	17901.861	17901.858	.003
61.5	17901.583	17901.580	.003	17902.256	17902.253	.003
62.5	17901.963	17901.970	-.007	17902.658	17902.655	.003
63.5	17902.365	17902.368	-.003	17903.062	17903.063	-.001
64.5	17902.769	17902.771	-.002	-	17903.478	
65.5	17903.175	17903.181	-.006	17903.902	17903.899	.003
66.5	17903.594	17903.598	-.004	17904.333	17904.327	.006
67.5	-	17904.022		17904.765	17904.762	.003
68.5	17904.454	17904.452	.002	17905.205	17905.203	.002
69.5	17904.889	17904.888	.001	17905.653	17905.651	.002
70.5	17905.339	17905.331	.008	17906.106	17906.105	.001
71.5	17905.777	17905.781	-.004	17906.564	17906.566	-.002
72.5	17906.235	17906.237	-.002	17907.025	17907.033	-.008**
73.5	-	17906.700		17907.508	17907.507	.001
74.5	17907.172	17907.170	.002	17907.992	17907.988	.004
75.5	17907.643	17907.646	-.003	17908.477	17908.475	.002
76.5	17908.125	17908.129	-.004	17908.972	17908.969	.003
77.5	17908.613	17908.618	-.005	17909.469	17909.470	-.001
78.5	17909.112	17909.114	-.002	17909.974	17909.977	-.003
79.5	17909.613	17909.617	-.004	17910.489	17910.490	-.001
80.5	17910.124	17910.126	-.002	17911.021	17911.011	.010
81.5	17910.641	17910.642	-.001	17911.541	17911.538	.003
82.5	17911.164	17911.164	.000	17912.073	17912.071	.002
83.5	17911.695	17911.693	.002	17912.612	17912.611	.001
84.5	17912.230	17912.229	.001	17913.157	17913.158	-.001
85.5	17912.773	17912.771	.002	17913.711	17913.712	-.001
86.5	17913.318	17913.320	-.002	17914.272	17914.272	.000
87.5	17913.871	17913.876	-.005	17914.837	17914.839	-.002
88.5	17914.439	17914.438	.001	17915.419	17915.412	.007
89.5	17915.001	17915.007	-.006	17915.990	17915.992	-.002
90.5	17915.578	17915.582	-.004	17916.576	17916.579	-.003
91.5	17916.163	17916.165	-.002	17917.169	17917.172	-.003
92.5	17916.756	17916.753	.003	17917.775	17917.772	.003
93.5	17917.344	17917.349	-.005	17918.382	17918.379	.003
94.5	17917.952	17917.951	.001	17918.997	17918.992	.005
95.5	17918.556	17918.560	-.004	17919.614	17919.612	.002
96.5	17919.173	17919.175	-.002	17920.240	17920.239	.001
97.5	17919.795	17919.797	-.002	17920.873	17920.872	.001
98.5	17920.431	17920.426	.005	17921.514	17921.512	.002
99.5	17921.057	17921.062	-.005	17922.159	17922.159	.000
100.5	17921.703	17921.704	-.001	17922.815	17922.812	.003
101.5	17922.355	17922.352	.003	17923.479	17923.472	.007
102.5	17923.007	17923.008	-.001	17924.144	17924.139	.005
103.5	17923.662	17923.670	-.008	17924.820	17924.812	.008
104.5	17924.371	17924.339	.032**	17925.487	17925.492	-.005
105.5	17925.009	17925.015	-.006	17926.172	17926.179	-.007
106.5	17925.690	17925.697	-.007	17926.890	17926.873	.017

107.5	17926.382	17926.386	-.004	17927.562	17927.573	-.011
108.5	17927.083	17927.082	.001	17928.287	17928.280	.007
109.5	17927.777	17927.784	-.007	17928.985	17928.993	-.008
110.5	17928.478	17928.493	-.015	17929.719	17929.714	.005
111.5	17929.191	17929.209	-.018	17930.452	17930.441	.011
112.5	17929.920	17929.932	-.012	-	17931.175	

	$R_{11}(ee)$			$P_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
6.5	17893.250	17893.248	.002	-	17887.752	
7.5	17893.689	17893.689	.000	-	17887.408	
8.5	17894.140	17894.137	.003	-	17887.071	
9.5	17894.596	17894.591	.005	17886.740	17886.740	.000
10.5	17895.052	17895.052	.000	17886.411	17886.416	-.005
11.5	17895.523	17895.519	.004	17886.094	17886.099	-.005
12.5	17895.996	17895.993	.003	17885.784	17885.787	-.003
13.5	17896.473	17896.473	.000	17885.478	17885.483	-.005
14.5	17896.959	17896.959	.000	17885.184	17885.185	-.001
15.5	-	17897.452		17884.891	17884.893	-.002
16.5	-	17897.952		17884.608	17884.608	.000
17.5	-	17898.458		17884.328	17884.330	-.002
18.5	-	17898.971		-	17884.058	
19.5	-	17899.489		17883.791	17883.792	-.001
20.5	-	17900.015		17883.532	17883.533	-.001
21.5	-	17900.547		17883.278	17883.281	-.003
22.5	-	17901.085		17883.028	17883.035	-.007
23.5	-	17901.630		17882.794	17882.796	-.002
24.5	-	17902.181		17882.558	17882.563	-.005
25.5	-	17902.739		17882.338	17882.337	.001
26.5	-	17903.303		17882.116	17882.118	-.002
27.5	17903.871	17903.874	-.003	17881.905	17881.905	.000
28.5	17904.451	17904.451	.000	17881.696	17881.698	-.002
29.5	17905.027	17905.035	-.008	17881.490	17881.498	-.008
30.5	17905.626	17905.625	.001	17881.300	17881.305	-.005
31.5	17906.222	17906.221	.001	17881.119	17881.118	.001
32.5	17906.826	17906.824	.002	17880.938	17880.938	.000
33.5	-	17907.434		17880.764	17880.765	-.001
34.5	17908.055	17908.050	.005	17880.598	17880.598	.000
35.5	17908.675	17908.672	.003	17880.441	17880.437	.004
36.5	17909.305	17909.301	.004	-	17880.284	
37.5	17909.938	17909.936	.002	17880.142	17880.136	.006
38.5	17910.578	17910.578	.000	17879.997	17879.996	.001
39.5	17911.229	17911.226	.003	17879.858	17879.862	-.004
40.5	17911.877	17911.880	-.003	17879.734	17879.734	.000
41.5	17912.537	17912.541	-.004	17879.616	17879.614	.002
42.5	17913.213	17913.209	.004	17879.500	17879.500	.000
43.5	17913.885	17913.883	.002	17879.393	17879.392	.001
44.5	17914.563	17914.563	.000	17879.289	17879.291	-.002
45.5	17915.249	17915.250	-.001	17879.195	17879.197	-.002
46.5	17915.943	17915.943	.000	17879.106	17879.109	-.003
47.5	17916.646	17916.643	.003	17879.027	17879.028	-.001
48.5	17917.346	17917.349	-.003	17878.951	17878.953	-.002
49.5	17918.059	17918.062	-.003	17878.886	17878.886	.000
50.5	17918.778	17918.781	-.003	17878.826	17878.825	.001

51.5	17919.507	17919.506	.001	17878.770	17878.770	.000
52.5	17920.242	17920.238	.004	17878.722	17878.722	.000
53.5	17920.974	17920.976	-.002	-	17878.681	
54.5	17921.723	17921.721	.002	-	17878.646	
55.5	17922.470	17922.473	-.003	-	17878.618	
56.5	17923.235	17923.230	.005	-	17878.597	
57.5	17924.000	17923.994	.006	-	17878.582	
58.5	17924.763	17924.765	-.002	-	17878.575	
59.5	17925.542	17925.542	.000	-	17878.573	
60.5	17926.329	17926.325	.004	-	17878.579	
61.5	17927.117	17927.115	.002	-	17878.591	
62.5	17927.911	17927.912	-.001	-	17878.610	
63.5	17928.714	17928.715	-.001	-	17878.635	
64.5	17929.523	17929.524	-.001	-	17878.667	
65.5	17930.339	17930.340	-.001	-	17878.706	
66.5	17931.160	17931.162	-.002	-	17878.752	
67.5	17931.991	17931.990	.001	-	17878.804	
68.5	17932.825	17932.825	.000	-	17878.863	
69.5	17933.668	17933.667	.001	-	17878.928	
70.5	17934.511	17934.515	-.004	-	17879.001	
71.5	17935.367	17935.369	-.002	-	17879.080	
72.5	17936.232	17936.230	.002	-	17879.166	
73.5	17937.095	17937.097	-.002	-	17879.258	
74.5	17937.975	17937.971	.004	-	17879.358	
75.5	17938.852	17938.851	.001	-	17879.464	
76.5	17939.734	17939.738	-.004	17879.573	17879.577	-.004
77.5	17940.631	17940.631	.000	17879.698	17879.696	.002
78.5	17941.530	17941.530	.000	17879.822	17879.822	.000
79.5	17942.437	17942.436	.001	17879.959	17879.955	.004
80.5	17943.346	17943.349	-.003	17880.090	17880.095	-.005
81.5	17944.269	17944.268	.001	17880.242	17880.242	.000
82.5	17945.194	17945.193	.001	17880.400	17880.395	.005
83.5	17946.124	17946.125	-.001	17880.554	17880.555	-.001
84.5	17947.062	17947.063	-.001	17880.720	17880.722	-.002
85.5	17948.010	17948.008	.002	17880.892	17880.896	-.004
86.5	17948.957	17948.959	-.002	17881.079	17881.076	.003
87.5	17949.918	17949.916	.002	17881.262	17881.263	-.001
88.5	17950.883	17950.880	.003	17881.460	17881.457	.003
89.5	-	17951.851		17881.660	17881.658	.002
90.5	-	17952.828		17881.876	17881.866	.010**
91.5	17953.808	17953.811	-.003	17882.073	17882.080	-.007
92.5	17954.800	17954.801	-.001	17882.296	17882.302	-.006
93.5	17955.797	17955.798	-.001	17882.528	17882.530	-.002
94.5	17956.808	17956.801	.007	17882.765	17882.765	.000
95.5	17957.812	17957.810	.002	17883.008	17883.007	.001
96.5	17958.832	17958.826	.006	17883.255	17883.255	.000
97.5	17959.850	17959.848	.002	17883.513	17883.511	.002
98.5	17960.876	17960.877	-.001	17883.778	17883.773	.005
99.5	17961.910	17961.912	-.002	17884.047	17884.042	.005
100.5	17962.946	17962.953	-.007	17884.322	17884.318	.004
101.5	17963.992	17964.002	-.010	17884.597	17884.601	-.004
102.5	17965.057	17965.056	.001	17884.888	17884.891	-.003
103.5	-	17966.117		17885.184	17885.188	-.004
104.5	-	17967.185		17885.486	17885.491	-.005
105.5	-	17968.259		17885.799	17885.801	-.002
106.5	-	17969.340		17886.114	17886.119	-.005
107.5	-	17970.427		17886.438	17886.443	-.005

108.5	-	17971.520		17886.775	17886.774	.001
109.5	-	17972.620		17887.110	17887.112	-.002
110.5	-	17973.727		17887.454	17887.457	-.003
111.5	-	17974.840		17887.807	17887.809	-.002
112.5	-	17975.959		17888.165	17888.168	-.003
113.5	-	17977.085		17888.533	17888.533	.000
114.5	-	17978.217		17888.907	17888.906	.001
115.5	-	17979.356		17889.287	17889.286	.001
116.5	-	17980.502		17889.671	17889.672	-.001
117.5	-	17981.654		17890.067	17890.066	.001
118.5	-	17982.812		17890.466	17890.466	.000
119.5	-	17983.977		17890.875	17890.873	.002
120.5	-	17985.149		17891.290	17891.288	.002

	P_{22}(*ff*)			R_{21}(*ee*)		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
3.5	19381.371	19381.371	.000	-	19383.646	
4.5	19381.118	19381.117	.001	-	19383.960	
5.5	19380.870	19380.869	.001	-	19384.281	
6.5	19380.627	19380.628	-.001	-	19384.608	
7.5	19380.394	19380.394	.000	-	19384.943	
8.5	19380.168	19380.166	.002	-	19385.284	
9.5	19379.949	19379.945	.004	-	19385.631	
10.5	19379.729	19379.730	-.001	-	19385.985	
11.5	19379.526	19379.523	.003	-	19386.346	
12.5	19379.321	19379.322	-.001	-	19386.713	
13.5	19379.127	19379.127	.000	-	19387.088	
14.5	19378.938	19378.940	-.002	-	19387.468	
15.5	19378.759	19378.759	.000	-	19387.856	
16.5	19378.585	19378.584	.001	-	19388.250	
17.5	19378.418	19378.417	.001	-	19388.650	
18.5	19378.256	19378.256	.000	-	19389.057	
19.5	19378.100	19378.102	-.002	-	19389.471	
20.5	19377.956	19377.954	.002	-	19389.892	
21.5	19377.812	19377.813	-.001	19390.321	19390.319	.002
22.5	19377.674	19377.679	-.005	19390.755	19390.753	.002
23.5	19377.546	19377.552	-.006	19391.196	19391.193	.003
24.5	19377.428	19377.431	-.003	19391.649	19391.640	.009
25.5	19377.315	19377.317	-.002	19392.097	19392.094	.003
26.5	19377.207	19377.210	-.003	19392.558	19392.554	.004
27.5	19377.106	19377.109	-.003	19393.026	19393.021	.005
28.5	19377.014	19377.015	-.001	19393.497	19393.495	.002
29.5	19376.926	19376.928	-.002	19393.976	19393.975	.001
30.5	19376.844	19376.847	-.003	19394.470	19394.462	.008
31.5	19376.772	19376.774	-.002	19394.957	19394.955	.002
32.5	19376.705	19376.706	-.001	19395.458	19395.455	.003
33.5	19376.643	19376.646	-.003	19395.962	19395.962	.000
34.5	19376.591	19376.593	-.002	19396.477	19396.475	.002
35.5	19376.542	19376.546	-.004	19396.996	19396.995	.001
36.5	19376.503	19376.506	-.003	19397.523	19397.521	.002
37.5	19376.478	19376.472	.006	19398.056	19398.055	.001
38.5	-	19376.445		19398.594	19398.594	.000
39.5	-	19376.426		19399.140	19399.141	-.001
40.5	-	19376.412		19399.695	19399.694	.001

41.5	-	19376.406		19400.254	19400.253	.001
42.5	-	19376.406		19400.821	19400.820	.001
43.5	-	19376.413		19401.394	19401.393	.001
44.5	-	19376.427		19401.969	19401.972	-.003
45.5	19376.449	19376.448	.001	19402.553	19402.558	-.005
46.5	19376.477	19376.475	.002	19403.151	19403.151	.000
47.5	19376.505	19376.509	-.004	19403.750	19403.751	-.001
48.5	-	19376.550		19404.358	19404.357	.001
49.5	-	19376.598		19404.970	19404.969	.001
50.5	19376.646	19376.652	-.006	19405.588	19405.588	.000
51.5	19376.709	19376.713	-.004	19406.211	19406.214	-.003
52.5	19376.776	19376.781	-.005	19406.846	19406.847	-.001
53.5	19376.850	19376.856	-.006	19407.485	19407.486	-.001
54.5	19376.933	19376.937	-.004	19408.130	19408.132	-.002
55.5	19377.018	19377.026	-.008	19408.782	19408.784	-.002
56.5	19377.115	19377.121	-.006	19409.442	19409.443	-.001
57.5	19377.217	19377.223	-.006	19410.105	19410.109	-.004
58.5	19377.325	19377.331	-.006	19410.779	19410.781	-.002
59.5	19377.442	19377.447	-.005	19411.459	19411.460	-.001
60.5	19377.564	19377.569	-.005	19412.144	19412.145	-.001
61.5	19377.688	19377.698	-.010	19412.836	19412.838	-.002
62.5	19377.828	19377.834	-.006	19413.534	19413.536	-.002
63.5	19377.973	19377.977	-.004	19414.240	19414.242	-.002
64.5	19378.125	19378.127	-.002	19414.953	19414.954	-.001
65.5	19378.280	19378.283	-.003	19415.669	19415.672	-.003
66.5	19378.440	19378.446	-.006	19416.397	19416.398	-.001
67.5	19378.611	19378.616	-.005	19417.129	19417.130	-.001
68.5	19378.788	19378.793	-.005	19417.868	19417.868	.000
69.5	19378.971	19378.977	-.006	19418.613	19418.613	.000
70.5	19379.163	19379.168	-.005	19419.362	19419.365	-.003
71.5	19379.361	19379.365	-.004	19420.122	19420.124	-.002
72.5	19379.566	19379.569	-.003	19420.888	19420.889	-.001
73.5	19379.775	19379.780	-.005	19421.660	19421.660	.000
74.5	19379.996	19379.998	-.002	19422.437	19422.439	-.002
75.5	19380.220	19380.223	-.003	19423.224	19423.224	.000
76.5	19380.452	19380.455	-.003	19424.015	19424.015	.000
77.5	19380.693	19380.694	-.001	19424.817	19424.814	.003
78.5	19380.936	19380.939	-.003	19425.619	19425.619	.000
79.5	19381.190	19381.191	-.001	19426.433	19426.430	.003
80.5	19381.450	19381.451	-.001	19427.251	19427.248	.003
81.5	19381.716	19381.717	-.001	19428.075	19428.073	.002
82.5	19381.990	19381.990	.000	19428.907	19428.905	.002
83.5	19382.268	19382.270	-.002	19429.745	19429.743	.002
84.5	19382.556	19382.557	-.001	19430.589	19430.588	.001
85.5	19382.854	19382.850	.004	19431.445	19431.439	.006
86.5	19383.153	19383.151	.002	19432.302	19432.297	.005
87.5	19383.461	19383.458	.003	-	19433.162	
88.5	19383.775	19383.773	.002	-	19434.033	
89.5	19384.096	19384.094	.002	-	19434.911	
90.5	19384.425	19384.423	.002	-	19435.796	
91.5	19384.766	19384.758	.008	-	19436.688	
92.5	19385.108	19385.100	.008	-	19437.586	
93.5	19385.454	19385.449	.005	-	19438.490	
94.5	19385.809	19385.805	.004	-	19439.402	
95.5	19386.173	19386.168	.005	-	19440.320	
96.5	19386.546	19386.538	.008	-	19441.244	

	Q$_{22}$(*fe*)			P$_{21}$(*ee*)		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
38.5	19383.879	19383.876	.003	-	19383.536	
39.5	19384.045	19384.048	-.003	-	19383.697	
40.5	19384.227	19384.228	-.001	19383.879	19383.865	.014**
41.5	19384.415	19384.413	.002	19384.045	19384.040	.005
42.5	19384.607	19384.606	.001	19384.227	19384.221	.006
43.5	19384.803	19384.805	-.002	19384.415	19384.409	.006
44.5	19385.009	19385.011	-.002	19384.607	19384.604	.003
45.5	19385.225	19385.224	.001	19384.803	19384.805	-.002
46.5	19385.446	19385.443	.003	19385.009	19385.013	-.004
47.5	19385.673	19385.669	.004	19385.225	19385.228	-.003
48.5	19385.908	19385.902	.006	19385.446	19385.450	-.004
49.5	19386.148	19386.142	.006	19385.673	19385.678	-.005
50.5	19386.394	19386.388	.006	19385.908	19385.913	-.005
51.5	-	19386.641		19386.148	19386.155	-.007
52.5	19386.912	19386.901	.011	19386.394	19386.403	-.009
53.5	19387.171	19387.167	.004	19386.653	19386.658	-.005
54.5	19387.443	19387.440	.003	-	19386.920	
55.5	19387.720	19387.720	.000	-	19387.189	
56.5	19388.007	19388.006	.001	-	19387.464	
57.5	19388.301	19388.300	.001	19387.743	19387.746	-.003
58.5	19388.598	19388.600	-.002	19388.030	19388.035	-.005
59.5	19388.905	19388.906	-.001	-	19388.330	
60.5	19389.218	19389.220	-.002	-	19388.633	
61.5	19389.532	19389.540	-.008	19388.953	19388.942	.011**
62.5	19389.864	19389.867	-.003	19389.265	19389.257	.008
63.5	19390.200	19390.201	-.001	19389.587	19389.580	.007
64.5	19390.540	19390.541	-.001	19389.916	19389.909	.007
65.5	19390.889	19390.889	.000	19390.251	19390.245	.006
66.5	19391.240	19391.243	-.003	19390.591	19390.588	.003
67.5	19391.604	19391.603	.001	19390.941	19390.937	.004
68.5	19391.971	19391.971	.000	19391.292	19391.293	-.001
69.5	19392.346	19392.345	.001	19391.657	19391.656	.001
70.5	19392.726	19392.726	.000	19392.022	19392.026	-.004
71.5	19393.117	19393.114	.003	19392.397	19392.402	-.005
72.5	19393.510	19393.508	.002	19392.780	19392.786	-.006
73.5	19393.911	19393.910	.001	19393.174	19393.176	-.002
74.5	19394.322	19394.318	.004	19393.570	19393.572	-.002
75.5	19394.737	19394.733	.004	19393.971	19393.976	-.005
76.5	19395.161	19395.154	.007	19394.382	19394.386	-.004
77.5	19395.586	19395.583	.003	19394.798	19394.803	-.005
78.5	19396.021	19396.018	.003	19395.223	19395.227	-.004
79.5	19396.460	19396.460	.000	19395.651	19395.658	-.007
80.5	19396.909	19396.909	.000	19396.087	19396.095	-.008
81.5	19397.368	19397.364	.004	-	19396.540	
82.5	-	19397.827		-	19396.991	
83.5	19398.304	19398.296	.008	-	19397.449	

	R$_{22}$(*ff*)			Q$_{21}$(*fe*)		
J	OBS	CALC	DIFF	OBS	CALC	DIFF

13.5	19384.537	19384.539	-.002	-	19384.285	
14.5	19384.740	19384.737	.003	19384.475	19384.473	.002
15.5	19384.946	19384.943	.003	19384.670	19384.667	.003
16.5	19385.161	19385.155	.006	19384.868	19384.868	.000
17.5	19385.378	19385.373	.005	19385.080	19385.076	.004
18.5	19385.603	19385.599	.004	19385.292	19385.290	.002
19.5	19385.835	19385.831	.004	19385.514	19385.511	.003
20.5	19386.072	19386.070	.002	19385.742	19385.738	.004
21.5	19386.317	19386.315	.002	19385.976	19385.972	.004
22.5	19386.567	19386.567	.000	19386.216	19386.213	.003
23.5	19386.825	19386.825	.000	19386.462	19386.460	.002
24.5	19387.089	19387.091	-.002	19386.717	19386.715	.002
25.5	19387.359	19387.363	-.004	19386.978	19386.975	.003
26.5	19387.639	19387.641	-.002	19387.246	19387.243	.003
27.5	19387.925	19387.927	-.002	19387.518	19387.517	.001
28.5	19388.219	19388.219	.000	19387.801	19387.798	.003
29.5	19388.517	19388.517	.000	19388.086	19388.085	.001
30.5	19388.827	19388.822	.005	19388.380	19388.379	.001
31.5	19389.136	19389.134	.002	19388.676	19388.680	-.004
32.5	19389.454	19389.453	.001	19388.985	19388.987	-.002
33.5	19389.778	19389.778	.000	19389.301	19389.301	.000
34.5	19390.108	19390.110	-.002	19389.622	19389.622	.000
35.5	19390.447	19390.449	-.002	19389.949	19389.949	.000
36.5	19390.795	19390.794	.001	19390.283	19390.283	.000
37.5	19391.143	19391.146	-.003	19390.621	19390.624	-.003
38.5	19391.503	19391.504	-.001	19390.974	19390.972	.002
39.5	19391.866	19391.870	-.004	19391.328	19391.326	.002
40.5	19392.239	19392.242	-.003	19391.685	19391.686	-.001
41.5	19392.617	19392.620	-.003	19392.055	19392.054	.001
42.5	19393.005	19393.006	-.001	19392.429	19392.428	.001
43.5	19393.395	19393.397	-.002	19392.813	19392.809	.004
44.5	19393.796	19393.796	.000	19393.200	19393.196	.004
45.5	19394.200	19394.201	-.001	19393.602	19393.590	.012
46.5	19394.611	19394.613	-.002	19393.994	19393.991	.003
47.5	19395.027	19395.032	-.005	19394.401	19394.398	.003
48.5	19395.453	19395.457	-.004	19394.818	19394.812	.006
49.5	19395.883	19395.889	-.006	19395.235	19395.233	.002
50.5	19396.324	19396.328	-.004	19395.661	19395.661	.000
51.5	19396.768	19396.774	-.006	19396.096	19396.095	.001
52.5	19397.218	19397.226	-.008	19396.538	19396.536	.002
53.5	19397.681	19397.684	-.003	19396.985	19396.983	.002
54.5	19398.145	19398.150	-.005	19397.440	19397.438	.002
55.5	19398.623	19398.622	.001	19397.902	19397.899	.003
56.5	19399.103	19399.101	.002	19398.369	19398.366	.003
57.5	19399.586	19399.586	.000	19398.842	19398.840	.002
58.5	19400.079	19400.079	.000	19399.320	19399.321	-.001
59.5	19400.577	19400.577	.000	19399.811	19399.809	.002
60.5	19401.084	19401.083	.001	19400.304	19400.304	.000
61.5	19401.595	19401.595	.000	19400.805	19400.805	.000
62.5	19402.117	19402.114	.003	19401.318	19401.312	.006
63.5	-	19402.640		19401.830	19401.827	.003
64.5	19403.178	19403.173	.005	19402.350	19402.348	.002
65.5	-	19403.712		19402.870	19402.876	-.006
66.5	-	19404.258		19403.406	19403.411	-.005

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	$Q_{11}(ef)$			$R_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
34.5	-	18203.402		18203.747	18203.750	-.003
35.5	-	18203.589		18203.940	18203.947	-.007
36.5	18203.784	18203.782	.002	18204.149	18204.150	-.001
37.5	18203.981	18203.980	.001	18204.350	18204.359	-.009
38.5	18204.189	18204.185	.004	18204.575	18204.574	.001
39.5	18204.400	18204.395	.005	18204.795	18204.794	.001
40.5	18204.611	18204.611	.000	18205.020	18205.021	-.001
41.5	18204.830	18204.833	-.003	18205.257	18205.253	.004
42.5	18205.058	18205.060	-.002	18205.489	18205.491	-.002
43.5	18205.294	18205.294	.000	18205.734	18205.734	.000
44.5	18205.534	18205.533	.001	18205.988	18205.984	.004
45.5	18205.777	18205.778	-.001	18206.240	18206.239	.001
46.5	18206.023	18206.028	-.005	18206.502	18206.500	.002
47.5	18206.286	18206.285	.001	18206.762	18206.767	-.005
48.5	18206.552	18206.547	.005	18207.035	18207.039	-.004
49.5	18206.814	18206.815	-.001	18207.315	18207.317	-.002
50.5	18207.088	18207.089	-.001	18207.602	18207.602	.000
51.5	18207.370	18207.368	.002	18207.893	18207.891	.002
52.5	18207.651	18207.654	-.003	18208.189	18208.187	.002
53.5	18207.948	18207.945	.003	18208.488	18208.489	-.001
54.5	18208.242	18208.242	.000	18208.794	18208.796	-.002
55.5	18208.540	18208.545	-.005	18209.107	18209.109	-.002
56.5	18208.845	18208.853	-.008	18209.428	18209.428	.000
57.5	18209.160	18209.168	-.008	18209.742	18209.753	-.011**
58.5	18209.494	18209.488	.006	18210.078	18210.083	-.005
59.5	18209.814	18209.814	.000	18210.430	18210.420	.010**
60.5	18210.127	18210.146	-.019**	18210.762	18210.762	.000
61.5	18210.464	18210.483	-.019**	18211.112	18211.110	.002
62.5	18210.812	18210.827	-.015**	18211.463	18211.464	-.001
63.5	18211.179	18211.176	.003	18211.824	18211.823	.001
64.5	18211.531	18211.531	.000	18212.185	18212.189	-.004
65.5	18211.894	18211.892	.002	18212.556	18212.560	-.004
66.5	18212.257	18212.259	-.002	18212.933	18212.937	-.004
67.5	18212.627	18212.631	-.004	18213.324	18213.320	.004
68.5	18213.003	18213.010	-.007	18213.712	18213.709	.003
69.5	18213.394	18213.394	.000	18214.108	18214.103	.005
70.5	18213.791	18213.784	.007	18214.506	18214.504	.002
71.5	18214.187	18214.180	.007	18214.914	18214.910	.004
72.5	18214.585	18214.582	.003	18215.327	18215.322	.005
73.5	18214.994	18214.989	.005	18215.741	18215.740	.001
74.5	18215.404	18215.403	.001	18216.164	18216.164	.000
75.5	18215.820	18215.822	-.002	18216.594	18216.594	.000
76.5	18216.245	18216.247	-.002	18217.033	18217.029	.004
77.5	18216.675	18216.678	-.003	18217.473	18217.470	.003
78.5	18217.114	18217.115	-.001	18217.921	18217.918	.003
79.5	18217.557	18217.558	-.001	18218.372	18218.371	.001
80.5	18218.008	18218.006	.002	18218.829	18218.830	-.001
81.5	18218.463	18218.461	.002	18219.294	18219.294	.000
82.5	18218.924	18218.921	.003	18219.761	18219.765	-.004
83.5	18219.392	18219.387	.005	18220.235	18220.242	-.007

84.5	18219.864	18219.859	.005	18220.720	18220.724	-.004
85.5	18220.333	18220.337	-.004	18221.205	18221.212	-.007
86.5	18220.818	18220.821	-.003	18221.713	18221.707	.006
87.5	18221.308	18221.311	-.003	18222.219	18222.207	$.012^{**}$
88.5	18221.809	18221.806	.003	-	18222.713	
89.5	18222.309	18222.308	.001	18223.226	18223.225	.001
90.5	18222.818	18222.815	.003	18223.744	18223.742	.002
91.5	18223.332	18223.328	.004	18224.263	18224.266	-.003
92.5	18223.850	18223.847	.003	18224.794	18224.796	-.002
93.5	18224.371	18224.372	-.001	18225.332	18225.331	.001
94.5	18224.902	18224.903	-.001	18225.873	18225.872	.001
95.5	18225.439	18225.440	-.001	18226.421	18226.420	.001
96.5	18225.985	18225.983	.002	18226.976	18226.973	.003
97.5	18226.531	18226.532	-.001	18227.536	18227.532	.004
98.5	18227.087	18227.086	.001	18228.099	18228.097	.002
99.5	18227.650	18227.647	.003	18228.671	18228.668	.003
100.5	18228.215	18228.213	.002	18229.247	18229.245	.002
101.5	18228.785	18228.785	.000	18229.828	18229.828	.000
102.5	18229.363	18229.364	-.001	18230.418	18230.417	.001
103.5	18229.944	18229.948	-.004	18231.012	18231.011	.001
104.5	18230.535	18230.538	-.003	18231.614	18231.612	.002
105.5	18231.131	18231.134	-.003	18232.222	18232.219	.003
106.5	18231.734	18231.736	-.002	-	18232.831	
107.5	18232.340	18232.344	-.004	-	18233.450	

		$R_{11}(ee)$			$P_{12}(ff)$	
J	OBS	CALC	DIFF	OBS	CALC	DIFF
7.5	-	18203.999		18197.728	18197.735	-.007
8.5	-	18204.440		18197.391	18197.392	-.001
9.5	-	18204.886		18197.055	18197.055	.000
10.5	18205.341	18205.337	.004	18196.729	18196.724	.005
11.5	18205.794	18205.795	-.001	18196.400	18196.399	.001
12.5	18206.257	18206.258	-.001	18196.079	18196.079	.000
13.5	18206.726	18206.727	-.001	18195.760	18195.765	-.005
14.5	18207.198	18207.201	-.003	18195.452	18195.457	-.005
15.5	18207.678	18207.682	-.004	18195.154	18195.155	-.001
16.5	18208.166	18208.168	-.002	18194.860	18194.858	.002
17.5	18208.659	18208.660	-.001	18194.568	18194.568	.000
18.5	18209.156	18209.157	-.001	18194.286	18194.283	.003
19.5	18209.663	18209.660	.003	18194.004	18194.003	.001
20.5	18210.168	18210.169	-.001	18193.728	18193.730	-.002
21.5	18210.682	18210.684	-.002	18193.459	18193.462	-.003
22.5	18211.209	18211.204	.005	18193.200	18193.201	-.001
23.5	18211.732	18211.730	.002	18192.942	18192.945	-.003
24.5	18212.265	18212.262	.003	18192.690	18192.694	-.004
25.5	18212.801	18212.799	.002	18192.447	18192.450	-.003
26.5	18213.348	18213.342	.006	18192.211	18192.211	.000
27.5	18213.890	18213.891	-.001	18191.977	18191.979	-.002
28.5	18214.446	18214.446	.000	18191.746	18191.752	-.006
29.5	18215.005	18215.006	-.001	18191.528	18191.530	-.002
30.5	18215.573	18215.572	.001	18191.318	18191.315	.003
31.5	18216.144	18216.143	.001	18191.107	18191.106	.001
32.5	18216.719	18216.721	-.002	18190.903	18190.902	.001
33.5	18217.306	18217.304	.002	18190.699	18190.704	-.005

34.5	18217.891	18217.893	-.002	18190.512	18190.512	.000
35.5	18218.487	18218.487	.000	18190.329	18190.326	.003
36.5	18219.088	18219.087	.001	18190.147	18190.145	.002
37.5	18219.692	18219.693	-.001	18189.971	18189.971	.000
38.5	18220.304	18220.304	.000	18189.800	18189.802	-.002
39.5	18220.920	18220.922	-.002	18189.646	18189.639	.007
40.5	18221.544	18221.544	.000	18189.487	18189.482	.005
41.5	18222.175	18222.173	.002	18189.332	18189.331	.001
42.5	18222.808	18222.807	.001	18189.185	18189.185	.000
43.5	18223.447	18223.447	.000	18189.042	18189.046	-.004
44.5	18224.093	18224.093	.000	18188.911	18188.912	-.001
45.5	18224.750	18224.744	.006	18188.783	18188.784	-.001
46.5	18225.402	18225.401	.001	18188.664	18188.663	.001
47.5	18226.064	18226.064	.000	18188.548	18188.547	.001
48.5	18226.731	18226.732	-.001	18188.439	18188.436	.003
49.5	18227.405	18227.407	-.002	18188.331	18188.332	-.001
50.5	18228.085	18228.086	-.001	18188.239	18188.234	.005
51.5	18228.772	18228.772	.000	18188.134	18188.141	-.007
52.5	18229.463	18229.463	.000	-	18188.055	
53.5	18230.158	18230.160	-.002	-	18187.974	
54.5	18230.861	18230.862	-.001	-	18187.899	
55.5	18231.571	18231.571	.000	-	18187.830	
56.5	18232.286	18232.284	.002	-	18187.767	
57.5	18233.006	18233.004	.002	-	18187.710	
58.5	18233.730	18233.729	.001	-	18187.659	
59.5	18234.463	18234.460	.003	-	18187.613	
60.5	18235.197	18235.197	.000	-	18187.574	
61.5	18235.938	18235.939	-.001	-	18187.541	
62.5	18236.684	18236.687	-.003	-	18187.513	
63.5	18237.443	18237.441	.002	-	18187.491	
64.5	18238.204	18238.201	.003	-	18187.476	
65.5	18238.965	18238.966	-.001	-	18187.466	
66.5	18239.735	18239.737	-.002	-	18187.462	
67.5	18240.514	18240.513	.001	-	18187.465	
68.5	18241.297	18241.295	.002	-	18187.473	
69.5	18242.086	18242.083	.003	-	18187.487	
70.5	18242.876	18242.877	-.001	-	18187.507	
71.5	18243.682	18243.676	.006	-	18187.533	
72.5	18244.480	18244.481	-.001	-	18187.565	
73.5	18245.293	18245.291	.002	-	18187.603	
74.5	18246.108	18246.108	.000	-	18187.647	
75.5	18246.934	18246.930	.004	-	18187.697	
76.5	18247.758	18247.758	.000	-	18187.753	
77.5	18248.593	18248.591	.002	18187.818	18187.814	.004
78.5	18249.429	18249.430	-.001	18187.883	18187.882	.001
79.5	18250.278	18250.275	.003	18187.959	18187.956	.003
80.5	18251.123	18251.125	-.002	18188.020	18188.036	-.016**
81.5	18251.983	18251.982	.001	18188.124	18188.122	.002
82.5	18252.843	18252.844	-.001	18188.218	18188.214	.004
83.5	18253.710	18253.711	-.001	18188.317	18188.312	.005
84.5	18254.588	18254.585	.003	18188.422	18188.416	.006
85.5	18255.465	18255.464	.001	18188.532	18188.526	.006
86.5	18256.346	18256.348	-.002	18188.646	18188.642	.004
87.5	18257.240	18257.239	.001	18188.765	18188.764	.001
88.5	18258.134	18258.135	-.001	18188.893	18188.892	.001
89.5	18259.028	18259.037	-.009	18189.021	18189.026	-.005
90.5	18259.943	18259.944	-.001	18189.166	18189.167	-.001

91.5	18260.857	18260.858	-.001	18189.308	18189.313	-.005
92.5	18261.775	18261.776	-.001	18189.475	18189.465	.010
93.5	18262.698	18262.701	-.003	18189.622	18189.624	-.002
94.5	18263.629	18263.632	-.003	18189.785	18189.788	-.003
95.5	-	18264.568		18189.956	18189.959	-.003
96.5	-	18265.510		18190.136	18190.136	.000
97.5	-	18266.457		18190.318	18190.318	.000
98.5	-	18267.410		18190.507	18190.507	.000
99.5	-	18268.369		18190.702	18190.702	.000
100.5	-	18269.334		18190.903	18190.903	.000
101.5	-	18270.304		18191.110	18191.111	-.001
102.5	-	18271.281		18191.320	18191.324	-.004
103.5	-	18272.263		18191.540	18191.543	-.003
104.5	-	18273.250		18191.767	18191.769	-.002
105.5	-	18274.243		18191.998	18192.001	-.003
106.5	-	18275.243		18192.236	18192.238	-.002
107.5	-	18276.247		18192.479	18192.482	-.003
108.5	-	18277.258		18192.731	18192.733	-.002
109.5	-	18278.274		-	18192.989	
110.5	-	18279.296		-	18193.251	
111.5	-	18280.324		18193.518	18193.520	-.002
112.5	-	18281.357		18193.793	18193.795	-.002
113.5	-	18282.397		18194.075	18194.076	-.001
114.5	-	18283.442		18194.361	18194.363	-.002

		$P_{22}(ff)$			$R_{21}(ee)$	
J	OBS	CALC	DIFF	OBS	CALC	DIFF
6.5	-	19692.801		19696.772	19696.771	.001
7.5	-	19692.562		19697.107	19697.099	.008
8.5	-	19692.329		19697.438	19697.433	.005
9.5	-	19692.101		19697.779	19697.772	.007
10.5	-	19691.880		19698.123	19698.118	.005
11.5	19691.666	19691.664	.002	19698.470	19698.469	.001
12.5	19691.461	19691.454	.007	19698.827	19698.826	.001
13.5	19691.253	19691.250	.003	19699.184	19699.189	-.005
14.5	19691.054	19691.052	.002	19699.557	19699.558	-.001
15.5	19690.862	19690.860	.002	19699.934	19699.933	.001
16.5	19690.654	19690.674	-.020**	19700.317	19700.314	.003
17.5	19690.493	19690.494	-.001	19700.705	19700.700	.005
18.5	19690.323	19690.320	.003	19701.096	19701.093	.003
19.5	19690.157	19690.152	.005	19701.493	19701.491	.002
20.5	19689.992	19689.989	.003	19701.897	19701.895	.002
21.5	19689.835	19689.833	.002	19702.303	19702.305	-.002
22.5	19689.682	19689.682	.000	19702.723	19702.721	.002
23.5	19689.536	19689.538	-.002	19703.145	19703.143	.002
24.5	19689.400	19689.399	.001	19703.572	19703.570	.002
25.5	19689.268	19689.266	.002	19704.007	19704.004	.003
26.5	19689.140	19689.140	.000	19704.446	19704.443	.003
27.5	19689.019	19689.019	.000	19704.892	19704.889	.003
28.5	19688.908	19688.904	.004	19705.341	19705.340	.001
29.5	19688.796	19688.795	.001	19705.796	19705.797	-.001
30.5	19688.693	19688.692	.001	19706.262	19706.260	.002
31.5	19688.590	19688.595	-.005	19706.728	19706.728	.000
32.5	19688.505	19688.504	.001	19707.204	19707.203	.001

33.5	19688.413	19688.419	-.006	19707.682	19707.684	-.002
34.5	19688.320	19688.340	-.020**	19708.171	19708.170	.001
35.5	19688.269	19688.267	.002	19708.663	19708.662	.001
36.5	19688.199	19688.200	-.001	19709.162	19709.160	.002
37.5	19688.138	19688.139	-.001	19709.663	19709.664	-.001
38.5	19688.084	19688.084	.000	19710.173	19710.174	-.001
39.5	19688.034	19688.034	.000	19710.689	19710.690	-.001
40.5	19687.992	19687.991	.001	19711.209	19711.211	-.002
41.5	19687.952	19687.954	-.002	19711.737	19711.738	-.001
42.5	19687.928	19687.923	.005	19712.272	19712.272	.000
43.5	-	19687.898		19712.810	19712.811	-.001
44.5	-	19687.878		19713.353	19713.356	-.003
45.5	-	19687.865		19713.908	19713.907	.001
46.5	-	19687.858		19714.462	19714.463	-.001
47.5	-	19687.856		19715.024	19715.026	-.002
48.5	-	19687.861		19715.595	19715.594	.001
49.5	-	19687.872		19716.169	19716.169	.000
50.5	19687.886	19687.889	-.003	19716.750	19716.749	.001
51.5	19687.907	19687.911	-.004	19717.334	19717.335	-.001
52.5	19687.938	19687.940	-.002	19717.925	19717.927	-.002
53.5	19687.974	19687.975	-.001	19718.522	19718.525	-.003
54.5	19688.012	19688.016	-.004	19719.125	19719.128	-.003
55.5	19688.063	19688.063	.000	19719.735	19719.738	-.003
56.5	19688.114	19688.116	-.002	19720.351	19720.353	-.002
57.5	19688.174	19688.175	-.001	19720.969	19720.974	-.005
58.5	19688.236	19688.240	-.004	19721.598	19721.602	-.004
59.5	19688.306	19688.311	-.005	19722.233	19722.234	-.001
60.5	19688.388	19688.388	.000	19722.870	19722.873	-.003
61.5	19688.471	19688.471	.000	19723.517	19723.518	-.001
62.5	19688.552	19688.560	-.008	19724.167	19724.169	-.002
63.5	19688.655	19688.655	.000	19724.823	19724.825	-.002
64.5	19688.756	19688.757	-.001	19725.486	19725.487	-.001
65.5	19688.864	19688.864	.000	19726.154	19726.156	-.002
66.5	19688.979	19688.977	.002	19726.831	19726.830	.001
67.5	19689.088	19689.097	-.009	19727.507	19727.510	-.003
68.5	19689.224	19689.222	.002	19728.193	19728.196	-.003
69.5	19689.350	19689.354	-.004	19728.886	19728.887	-.001
70.5	19689.493	19689.492	.001	19729.582	19729.585	-.003
71.5	19689.624	19689.636	-.012	19730.287	19730.288	-.001
72.5	19689.785	19689.786	-.001	19730.998	19730.998	.000
73.5	19689.944	19689.942	.002	19731.713	19731.713	.000
74.5	19690.111	19690.104	.007	19732.435	19732.434	.001
75.5	19690.274	19690.272	.002	19733.162	19733.161	.001
76.5	19690.442	19690.446	-.004	19733.892	19733.894	-.002
77.5	19690.626	19690.627	-.001	19734.633	19734.633	.000
78.5	19690.815	19690.813	.002	19735.376	19735.377	-.001
79.5	19691.007	19691.006	.001	19736.129	19736.128	.001
80.5	-	19691.205		19736.884	19736.884	.000
81.5	-	19691.410		19737.646	19737.647	-.001
82.5	-	19691.621		19738.414	19738.415	-.001
83.5	-	19691.838		19739.188	19739.189	-.001
84.5	-	19692.061		19739.970	19739.969	.001
85.5	-	19692.291		19740.755	19740.755	.000
86.5	-	19692.526		19741.548	19741.547	.001
87.5	-	19692.768		19742.346	19742.344	.002
88.5	-	19693.016		19743.152	19743.148	.004
89.5	-	19693.270		19743.960	19743.957	.003

90.5	-	19693.530		19744.775	19744.773	.002
91.5	-	19693.797		19745.596	19745.594	.002
92.5	-	19694.070		19746.426	19746.421	.005
93.5	-	19694.348		19747.258	19747.255	.003
94.5	-	19694.633		19748.100	19748.094	.006
95.5	-	19694.925		19748.942	19748.939	.003
96.5	-	19695.222		19749.797	19749.789	.008
97.5	-	19695.526		19750.653	19750.646	.007

	$Q_{22}(fe)$			$P_{21}(ee)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
25.5	19694.176	19694.173	.003	-	19693.998	
26.5	-	19694.238		-	19694.053	
27.5	-	19694.310		-	19694.114	
28.5	-	19694.387		-	19694.181	
29.5	19694.478	19694.470	.008	-	19694.253	
30.5	19694.561	19694.559	.002	-	19694.332	
31.5	19694.649	19694.654	-.005	19694.420	19694.417	.003
32.5	19694.757	19694.755	.002	19694.511	19694.507	.004
33.5	19694.864	19694.862	.002	19694.604	19694.603	.001
34.5	19694.976	19694.975	.001	19694.710	19694.706	.004
35.5	19695.076	19695.094	-.018**	19694.814	19694.814	.000
36.5	19695.216	19695.218	-.002	19694.929	19694.928	.001
37.5	19695.347	19695.349	-.002	19695.048	19695.048	.000
38.5	19695.487	19695.485	.002	19695.170	19695.175	-.005
39.5	19695.629	19695.628	.001	19695.308	19695.307	.001
40.5	19695.776	19695.776	.000	19695.441	19695.445	-.004
41.5	19695.930	19695.931	-.001	19695.589	19695.588	.001
42.5	19696.093	19696.091	.002	19695.739	19695.738	.001
43.5	19696.268	19696.257	.011	19695.898	19695.894	.004
44.5	19696.429	19696.429	.000	19696.059	19696.056	.003
45.5	19696.606	19696.608	-.002	19696.240	19696.223	.017**
46.5	19696.787	19696.792	-.005	19696.399	19696.397	.002
47.5	-	19696.982		19696.569	19696.577	-.008
48.5	19697.176	19697.178	-.002	19696.760	19696.762	-.002
49.5	19697.377	19697.380	-.003	19696.951	19696.954	-.003
50.5	19697.583	19697.587	-.004	19697.141	19697.151	-.010
51.5	19697.798	19697.801	-.003	19697.348	19697.354	-.006
52.5	19698.020	19698.021	-.001	-	19697.564	
53.5	19698.244	19698.247	-.003	-	19697.779	
54.5	19698.475	19698.479	-.004	-	19698.000	
55.5	19698.711	19698.716	-.005	-	19698.227	
56.5	19698.952	19698.960	-.008	-	19698.461	
57.5	19699.201	19699.210	-.009	19698.710	19698.700	.010
58.5	19699.459	19699.465	-.006	19698.943	19698.945	-.002
59.5	19699.722	19699.727	-.005	19699.197	19699.196	.001
60.5	19699.992	19699.995	-.003	19699.457	19699.453	.004
61.5	19700.264	19700.268	-.004	19699.721	19699.716	.005
62.5	19700.544	19700.548	-.004	19699.992	19699.985	.007
63.5	19700.830	19700.833	-.003	19700.264	19700.260	.004
64.5	19701.119	19701.125	-.006	19700.544	19700.541	.003
65.5	19701.418	19701.422	-.004	19700.829	19700.828	.001
66.5	-	19701.726		19701.118	19701.121	-.003

	$R_{22}(ff)$			$Q_{21}(fe)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
11.5	19696.282	19696.284	-.002	19696.063	19696.063	.000
12.5	19696.465	19696.459	.006	19696.230	19696.227	.003
13.5	19696.646	19696.640	.006	19696.411	19696.398	.013
14.5	19696.834	19696.827	.007	19696.567	19696.575	-.008
15.5	19697.028	19697.020	.008	19696.760	19696.757	.003
16.5	19697.210	19697.219	-.009	19696.943	19696.945	-.002
17.5	19697.424	19697.423	.001	19697.141	19697.140	.001
18.5	19697.641	19697.634	.007	19697.344	19697.340	.004
19.5	19697.852	19697.850	.002	19697.557	19697.546	.011
20.5	19698.073	19698.073	.000	19697.760	19697.758	.002
21.5	19698.311	19698.301	.010	19697.972	19697.975	-.003
22.5	19698.541	19698.535	.006	19698.197	19698.199	-.002
23.5	19698.774	19698.775	-.001	19698.432	19698.429	.003
24.5	19699.019	19699.021	-.002	19698.665	19698.664	.001
25.5	19699.270	19699.273	-.003	19698.907	19698.905	.002
26.5	19699.529	19699.530	-.001	19699.154	19699.153	.001
27.5	19699.792	19699.794	-.002	19699.402	19699.406	-.004
28.5	19700.063	19700.064	-.001	19699.665	19699.665	.000
29.5	19700.340	19700.339	.001	19699.930	19699.930	.000
30.5	19700.622	19700.620	.002	19700.200	19700.201	-.001
31.5	19700.906	19700.907	-.001	19700.479	19700.478	.001
32.5	19701.202	19701.201	.001	19700.760	19700.760	.000
33.5	19701.498	19701.500	-.002	19701.053	19701.049	.004
34.5	19701.802	19701.805	-.003	19701.344	19701.343	.001
35.5	19702.118	19702.115	.003	19701.643	19701.644	-.001
36.5	19702.431	19702.432	-.001	19701.950	19701.950	.000
37.5	19702.751	19702.755	-.004	19702.260	19702.262	-.002
38.5	19703.078	19703.083	-.005	19702.579	19702.580	-.001
39.5	19703.418	19703.418	.000	19702.902	19702.904	-.002
40.5	19703.758	19703.758	.000	19703.234	19703.234	.000
41.5	19704.105	19704.104	.001	19703.569	19703.570	-.001
42.5	19704.457	19704.457	.000	19703.911	19703.912	-.001
43.5	19704.812	19704.815	-.003	19704.260	19704.260	.000
44.5	19705.176	19705.179	-.003	19704.614	19704.613	.001
45.5	19705.542	19705.549	-.007	19704.975	19704.973	.002
46.5	19705.918	19705.925	-.007	19705.339	19705.338	.001
47.5	19706.304	19706.306	-.002	19705.705	19705.710	-.005
48.5	19706.690	19706.694	-.004	19706.083	19706.087	-.004
49.5	19707.083	19707.088	-.005	19706.467	19706.470	-.003
50.5	19707.487	19707.487	.000	19706.858	19706.859	-.001
51.5	19707.890	19707.893	-.003	19707.253	19707.254	-.001
52.5	19708.302	19708.304	-.002	19707.654	19707.655	-.001
53.5	19708.721	19708.721	.000	19708.062	19708.062	.000
54.5	19709.144	19709.145	-.001	19708.476	19708.475	.001
55.5	19709.572	19709.574	-.002	19708.891	19708.893	-.002
56.5	19710.007	19710.009	-.002	19709.316	19709.318	-.002
57.5	19710.450	19710.450	.000	19709.745	19709.749	-.004
58.5	19710.893	19710.897	-.004	19710.186	19710.185	.001
59.5	19711.347	19711.350	-.003	19710.627	19710.628	-.001
60.5	19711.808	19711.809	-.001	19711.076	19711.076	.000
61.5	19712.271	19712.274	-.003	19711.531	19711.530	.001
62.5	19712.744	19712.744	.000	19711.989	19711.991	-.002

63.5	19713.219	19713.221	-.002	19712.457	19712.457	.000
64.5	19713.701	19713.704	-.003	19712.927	19712.929	-.002
65.5	19714.192	19714.192	.000	19713.408	19713.407	.001
66.5	19714.689	19714.687	.002	19713.891	19713.891	.000
67.5	19715.189	19715.187	.002	19714.382	19714.381	.001
68.5	19715.696	19715.694	.002	19714.878	19714.877	.001
69.5	19716.207	19716.206	.001	19715.379	19715.379	.000
70.5	19716.726	19716.725	.001	19715.888	19715.887	.001
71.5	19717.248	19717.249	-.001	19716.401	19716.401	.000
72.5	19717.779	19717.779	.000	19716.920	19716.921	-.001
73.5	19718.317	19718.315	.002	19717.449	19717.446	.003
74.5	19718.858	19718.858	.000	19717.979	19717.978	.001
75.5	19719.405	19719.406	-.001	19718.516	19718.516	.000
76.5	19719.964	19719.960	.004	19719.060	19719.059	.001
77.5	19720.523	19720.520	.003	19719.612	19719.609	.003
78.5	19721.094	19721.086	.008	19720.166	19720.165	.001
79.5	19721.663	19721.658	.005	19720.731	19720.726	.005
80.5	19722.236	19722.236	.000	19721.295	19721.294	.001
81.5	19722.828	19722.820	.008	19721.873	19721.867	.006
82.5	-	19723.410		19722.449	19722.447	.002

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	$P_{11}(ee)$			$Q_{12}(ef)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
41.5	-	17607.129		17607.642	17607.632	.010
42.5	17607.441	17607.444	-.003	-	17607.959	
43.5	-	17607.767		-	17608.293	
44.5	-	17608.097		17608.621	17608.635	-.014
45.5	17608.416	17608.434	-.018	-	17608.984	
46.5	-	17608.779		-	17609.340	
47.5	-	17609.131		17609.702	17609.704	-.002
48.5	17609.479	17609.490	-.011	-	17610.075	
49.5	-	17609.857		-	17610.453	
50.5	-	17610.231		-	17610.839	
51.5	-	17610.612		17611.257	17611.232	.025
52.5	17611.016	17611.000	.016	-	17611.632	
53.5	-	17611.396		17612.046	17612.040	.006
54.5	17611.799	17611.800	-.001	-	17612.455	
55.5	-	17612.210		-	17612.877	
56.5	-	17612.628		17613.338	17613.307	.031
57.5	17613.072	17613.053	.019	-	17613.744	
58.5	-	17613.486		-	17614.188	
59.5	-	17613.925		17614.675	17614.639	.036
60.5	17614.395	17614.373	.022	-	17615.098	
61.5	-	17614.827		-	17615.565	
62.5	-	17615.289		17616.073	17616.038	.035
63.5	17615.781	17615.758	.023	-	17616.519	
64.5	-	17616.235		-	17617.008	
65.5	-	17616.719		17617.533	17617.503	.030
66.5	17617.226	17617.210	.016	-	17618.006	
67.5	-	17617.709		-	17618.517	
68.5	-	17618.215		17619.062	17619.035	.027

69.5	17618.741	17618.728	.013	-	17619.560	
70.5	-	17619.249		-	17620.092	
71.5	-	17619.777		17620.667	17620.632	.035
72.5	17620.340	17620.312	.028	-	17621.179	
73.5	-	17620.855		-	17621.734	
74.5	-	17621.405		17622.331	17622.296	.035
75.5	17621.990	17621.963	.027	-	17622.865	
76.5	-	17622.528		17623.483	17623.442	.041
77.5	17623.129	17623.100	.029	-	17624.026	
78.5	-	17623.680		17624.662	17624.618	.044
79.5	17624.301	17624.267	.034	-	17625.217	
80.5	-	17624.862		17625.868	17625.823	.045
81.5	17625.503	17625.463	.040	-	17626.437	
82.5	-	17626.073		-	17627.058	
83.5	-	17626.690		17627.739	17627.686	.053
84.5	17627.369	17627.314	.055	-	17628.322	
85.5	-	17627.945		17629.012	17628.966	.046
86.5	17628.626	17628.584	.042	-	17629.617	
87.5	-	17629.231		17630.327	17630.275	.052
88.5	17629.934	17629.884	.050	-	17630.940	
89.5	-	17630.546		17631.665	17631.613	.052
90.5	17631.256	17631.214	.042	-	17632.294	
91.5	-	17631.890		-	17632.982	
92.5	-	17632.574		17633.733	17633.677	.056
93.5	17633.308	17633.265	.043	-	17634.380	
94.5	-	17633.963		17635.147	17635.090	.057
95.5	17634.712	17634.669	.043	-	17635.808	
96.5	-	17635.383		17636.581	17636.533	.048
97.5	17636.134	17636.103	.031	-	17637.266	
98.5	-	17636.832		17638.057	17638.006	.051
99.5	17637.592	17637.567	.025**	-	17638.754	
100.5	-	17638.310		17639.556	17639.509	.047
101.5	17639.087	17639.061	.026**	-	17640.271	
102.5	-	17639.819		17641.086	17641.041	.045
103.5	17640.625	17640.585	.040	-	17641.819	

	Q_{11}(*ef*)			R_{12}(*ff*)		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
77.5	-	17621.288		17622.090	17622.191	-.101**
78.5	17621.714	17621.844	-.130**	-	17622.759	
79.5	-	17622.409		17623.293	17623.335	-.042**
80.5	17622.923	17622.980	-.057**	-	17623.919	
81.5	-	17623.559		17624.501	17624.510	-.009**
82.5	17624.123	17624.146	-.023**	-	17625.108	
83.5	-	17624.740		17625.699	17625.714	-.015**
84.5	17625.323	17625.341	-.018**	-	17626.327	
85.5	-	17625.950		17626.998	17626.948	.050
86.5	17626.608	17626.566	.042	-	17627.576	
87.5	-	17627.190		17628.186	17628.211	-.025**
88.5	17627.782	17627.821	-.039**	-	17628.854	
89.5	-	17628.460		17629.576	17629.505	.071
90.5	17629.171	17629.106	.065	-	17630.163	
91.5	-	17629.759		17630.911	17630.828	.083
92.5	17630.500	17630.420	.080	-	17631.501	

93.5	-	17631.088		17632.188	17632.181	.007**
94.5	17631.758	17631.764	-.006**	-	17632.869	
95.5	-	17632.447		17633.610	17633.564	.046
96.5	17633.211	17633.138	.073	-	17634.267	
97.5	-	17633.837		17634.981	17634.977	.004**
98.5	17634.531	17634.542	-.011**	-	17635.694	
99.5	-	17635.256		17636.499	17636.420	.079
100.5	17636.049	17635.976	.073	-	17637.152	
101.5	-	17636.704		17637.969	17637.892	.077
102.5	17637.515	17637.440	.075	-	17638.640	
103.5	-	17638.183		17639.471	17639.395	.076
104.5	17639.004	17638.934	.070	-	17640.158	
105.5	-	17639.692		17641.005	17640.928	.077
106.5	17640.538	17640.458	.080	-	17641.706	
107.5	-	17641.232		17642.567	17642.491	.076
108.5	17642.092	17642.012	.080	-	17643.284	
109.5	-	17642.801		17644.155	17644.084	.071
110.5	17643.666	17643.597	.069	-	17644.892	
111.5	-	17644.400		17645.773	17645.707	.066
112.5	17645.277	17645.211	.066	-	17646.530	

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	$P_{11}(ee)$			$Q_{12}(ef)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
50.5	-	17323.542		17324.193	17324.184	.009
51.5	17323.972	17323.963	.009	-	17324.617	
52.5	-	17324.392		17325.073	17325.059	.014
53.5	17324.843	17324.829	.014	-	17325.508	
54.5	-	17325.274		17325.987	17325.965	.022
55.5	17325.743	17325.727	.016	-	17326.431	
56.5	-	17326.188		17326.924	17326.905	.019
57.5	17326.675	17326.658	.017	-	17327.387	
58.5	-	17327.135		17327.840	17327.877	-.037**
59.5	17327.635	17327.621	.014	-	17328.375	
60.5	-	17328.115		17328.896	17328.881	.015
61.5	17328.635	17328.617	.018	-	17329.395	
62.5	-	17329.127		17329.927	17329.918	.009
63.5	17329.671	17329.645	.026	-	17330.448	
64.5	-	17330.171		17331.013	17330.987	.026
65.5	17330.737	17330.706	.031	-	17331.534	
66.5	-	17331.249		17332.149	17332.089	.060
67.5	17331.845	17331.799	.046	-	17332.652	
68.5	-	17332.358		17333.261	17333.224	.037
69.5	17332.958	17332.925	.033	-	17333.803	
70.5	-	17333.501		17334.228	17334.391	-.163**
71.5	17333.890	17334.084	-.194**	-	17334.987	
72.5	-	17334.676		17335.624	17335.591	.033
73.5	17335.314	17335.275	.039	-	17336.203	
74.5	-	17335.883		17336.856	17336.823	.033
75.5	17336.537	17336.499	.038	-	17337.452	
76.5	-	17337.123		17338.118	17338.089	.029
77.5	17337.820	17337.756	.064	-	17338.734	
78.5	-	17338.396		17339.434	17339.387	.047

79.5	17339.103	17339.045	.058	-	17340.048	
80.5	-	17339.702		17340.745	17340.717	.028
81.5	17340.423	17340.367	.056	17341.440	17341.395	.045
82.5	17341.095	17341.041	.054	17342.123	17342.081	.042
83.5	17341.768	17341.722	.046	17342.815	17342.775	.040
84.5	17342.466	17342.412	.054	17343.515	17343.477	.038
85.5	17343.168	17343.110	.058	17344.231	17344.188	.043
86.5	17343.860	17343.817	.043	-	17344.907	
87.5	-	17344.531		17345.673	17345.634	.039
88.5	17345.294	17345.254	.040	17346.411	17346.369	.042
89.5	17346.044	17345.985	.059	17347.158	17347.112	.046
90.5	17346.778	17346.724	.054	-	17347.864	
91.5	-	17347.471		-	17348.624	
92.5	-	17348.227		17349.432	17349.392	.040
93.5	17349.042	17348.991	.051	17350.220	17350.169	.051
94.5	17349.822	17349.763	.059	-	17350.953	

	$Q_{11}(ef)$			$R_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
74.5	-	17334.139		17335.087	17335.057	.030
75.5	-	17334.733		-	17335.662	
76.5	-	17335.334		17336.300	17336.276	.024
77.5	-	17335.943		-	17336.898	
78.5	-	17336.561		17337.567	17337.528	.039
79.5	-	17337.187		-	17338.167	
80.5	-	17337.821		-	17338.813	
81.5	-	17338.463		-	17339.468	
82.5	-	17339.114		17340.167	17340.131	.036
83.5	-	17339.773		-	17340.803	
84.5	-	17340.440		17341.489	17341.482	.007**
85.5	-	17341.115		-	17342.170	
86.5	-	17341.799		17342.645	17342.866	-.221**
87.5	-	17342.490		-	17343.570	
88.5	-	17343.190		-	17344.283	
89.5	-	17343.898		-	17345.004	
90.5	-	17344.615		-	17345.733	
91.5	-	17345.340		17346.505	17346.470	.035
92.5	-	17346.073		-	17347.216	
93.5	-	17346.814		17348.005	17347.969	.036
94.5	-	17347.564		-	17348.732	

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	$P_{11}(ee)$			$Q_{12}(ef)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
55.5	-	17040.905		17041.683	17041.646	.037
56.5	17041.437	17041.410	.027	-	17042.164	
57.5	-	17041.924		17042.735	17042.691	.044
58.5	17042.474	17042.446	.028	-	17043.226	
59.5	-	17042.978		17043.802	17043.771	.031
60.5	17043.542	17043.518	.024	-	17044.324	
61.5	-	17044.068		17044.915	17044.887	.028

62.5	17044.648	17044.626	.022	-	17045.458	
63.5	-	17045.193		17046.065	17046.039	.026
64.5	17045.790	17045.769	.021	17046.651	17046.628	.023
65.5	17046.373	17046.354	.019	17047.255	17047.226	.029
66.5	17046.972	17046.948	.024	17047.861	17047.833	.028
67.5	17047.576	17047.551	.025	17048.534	17048.449	.085**
68.5	17048.194	17048.163	.031	17049.108	17049.074	.034
69.5	17048.816	17048.784	.032	17049.751	17049.708	.043
70.5	17049.442	17049.413	.029	17050.386	17050.351	.035
71.5	17050.080	17050.052	.028	17051.027	17051.003	.024
72.5	17050.728	17050.700	.028	17051.696	17051.663	.033
73.5	17051.387	17051.356	.031	17052.367	17052.333	.034
74.5	17052.054	17052.022	.032	-	17053.012	
75.5	-	17052.696		17053.733	17053.700	.033
76.5	17053.425	17053.380	.045	-	17054.396	
77.5	-	17054.073		17055.138	17055.102	.036
78.5	17054.793	17054.774	.019	-	17055.817	
79.5	-	17055.484		17056.578	17056.540	.038
80.5	17056.242	17056.204	.038	-	17057.273	
81.5	-	17056.932		17058.061	17058.014	.047
82.5	17057.706	17057.670	.036	-	17058.765	
83.5	-	17058.416		17059.560	17059.525	.035
84.5	17059.213	17059.172	.041	-	17060.293	
85.5	-	17059.936		17061.120	17061.071	.049
86.5	17060.747	17060.710	.037	-	17061.858	
87.5	-	17061.492		17062.686	17062.654	.032
88.5	17062.332	17062.284	.048	-	17063.458	
89.5	-	17063.084		17064.346	17064.272	.074
90.5	17063.938	17063.894	.044	-	17065.095	
91.5	-	17064.713		-	17065.927	
92.5	-	17065.541		17066.811	17066.768	.043
93.5	17066.425	17066.377	.048	-	17067.618	

Observed and Calculated Line Positions for $^{172}Yb^{35}Cl$

0-0 Band

	$P_{11}(ee)$			$Q_{12}(ef)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
34.5	-	17894.367		17894.768	17894.766	.002
35.5	-	17894.605		17895.015	17895.015	.000
36.5	17894.853	17894.849	.004	17895.273	17895.270	.003
37.5	17895.103	17895.100	.003	17895.534	17895.532	.002
38.5	17895.355	17895.357	-.002	17895.800	17895.800	.000
39.5	17895.624	17895.621	.003	17896.075	17896.075	.000
40.5	17895.891	17895.891	.000	17896.354	17896.357	-.003
41.5	17896.166	17896.168	-.002	17896.643	17896.645	-.002
42.5	17896.450	17896.452	-.002	17896.941	17896.939	.002
43.5	17896.741	17896.742	-.001	17897.237	17897.240	-.003
44.5	17897.032	17897.038	-.006	17897.547	17897.548	-.001
45.5	17897.329	17897.341	-.012	17897.862	17897.862	.000
46.5	17897.645	17897.651	-.006	17898.177	17898.182	-.005
47.5	17897.967	17897.967	.000	17898.509	17898.510	-.001

48.5	17898.288	17898.290	-.002	17898.848	17898.843	.005
49.5	17898.623	17898.619	.004	17899.190	17899.184	.006
50.5	17898.959	17898.955	.004	17899.534	17899.531	.003
51.5	-	17899.297		17899.872	17899.884	-.012

	$Q_{11}(ef)$			$R_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
27.5	17892.239	17892.237	.002	-	17892.534	
28.5	17892.411	17892.405	.006	-	17892.714	
29.5	17892.590	17892.580	.010	-	17892.900	
30.5	17892.762	17892.761	.001	-	17893.092	
31.5	17892.953	17892.949	.004	-	17893.291	
32.5	17893.145	17893.144	.001	-	17893.497	
33.5	17893.342	17893.345	-.003	-	17893.709	
34.5	17893.559	17893.553	.006	-	17893.928	
35.5	17893.765	17893.767	-.002	-	17894.153	
36.5	17893.986	17893.987	-.001	17894.384	17894.385	-.001
37.5	17894.218	17894.215	.003	17894.619	17894.623	-.004
38.5	17894.447	17894.448	-.001	17894.866	17894.868	-.002
39.5	17894.684	17894.689	-.005	17895.115	17895.119	-.004
40.5	17894.932	17894.936	-.004	17895.384	17895.377	.007
41.5	17895.184	17895.189	-.005	17895.641	17895.642	-.001
42.5	17895.447	17895.449	-.002	17895.909	17895.913	-.004
43.5	17895.711	17895.716	-.005	17896.227	17896.191	.036**
44.5	17895.984	17895.989	-.005	17896.473	17896.475	-.002
45.5	17896.265	17896.268	-.003	17896.763	17896.765	-.002
46.5	17896.555	17896.554	.001	17897.061	17897.063	-.002
47.5	17896.847	17896.847	.000	17897.364	17897.366	-.002
48.5	17897.145	17897.146	-.001	17897.674	17897.677	-.003
49.5	17897.432	17897.452	-.020**	17897.993	17897.994	-.001
50.5	17897.755	17897.765	-.010**	17898.320	17898.317	.003
51.5	17898.056	17898.083	-.027**	17898.649	17898.647	.002
52.5	17898.403	17898.409	-.006	17898.989	17898.984	.005
53.5	17898.737	17898.741	-.004	17899.332	17899.327	.005
54.5	17899.085	17899.080	.005	17899.681	17899.677	.004
55.5	17899.412	17899.425	-.013**	-	17900.033	
56.5	17899.778	17899.777	.001	17900.397	17900.396	.001
57.5	-	17900.135		17900.771	17900.766	.005
58.5	17900.501	17900.500	.001	17901.146	17901.142	.004
59.5	17900.877	17900.872	.005	17901.528	17901.524	.004
60.5	17901.252	17901.250	.002	17901.915	17901.914	.001
61.5	17901.637	17901.634	.003	17902.317	17902.309	.008
62.5	17902.020	17902.026	-.006	17902.712	17902.712	.000
63.5	17902.420	17902.424	-.004	17903.118	17903.121	-.003
64.5	17902.829	17902.828	.001	17903.544	17903.536	.008
65.5	17903.235	17903.239	-.004	17903.961	17903.959	.002
66.5	17903.661	17903.657	.004	17904.401	17904.387	.014**
67.5	-	17904.081		17904.828	17904.823	.005
68.5	17904.512	17904.512	.000	17905.269	17905.265	.004
69.5	17904.954	17904.949	.005	17905.712	17905.713	-.001
70.5	17905.399	17905.393	.006	17906.170	17906.169	.001
71.5	-	17905.844		17906.630	17906.630	.000
72.5	17906.305	17906.301	.004	17907.099	17907.099	.000
73.5	17906.786	17906.765	.021**	17907.579	17907.574	.005

74.5	17907.248	17907.236	.012**	17908.057	17908.055	.002
75.5	17907.717	17907.713	.004	17908.546	17908.544	.002
76.5	17908.201	17908.197	.004	17909.043	17909.039	.004
77.5	17908.689	17908.687	.002	17909.543	17909.540	.003
78.5	17909.186	17909.184	.002	17910.051	17910.048	.003
79.5	17909.687	17909.688	-.001	17910.566	17910.563	.003
80.5	17910.199	17910.198	.001	17911.093	17911.085	.008
81.5	17910.715	17910.715	.000	17911.623	17911.613	.010
82.5	17911.242	17911.238	.004	17912.159	17912.147	.012**
83.5	17911.771	17911.768	.003	17912.693	17912.689	.004
84.5	17912.306	17912.305	.001	17913.235	17913.237	-.002
85.5	17912.845	17912.849	-.004	17913.791	17913.791	.000
86.5	17913.401	17913.399	.002	17914.353	17914.353	.000
87.5	17913.950	17913.956	-.006	17914.918	17914.921	-.003
88.5	17914.500	17914.519	-.019**	17915.494	17915.495	-.001
89.5	17915.090	17915.089	.001	17916.076	17916.077	-.001
90.5	17915.660	17915.666	-.006	17916.661	17916.665	-.004
91.5	17916.248	17916.249	-.001	17917.257	17917.259	-.002
92.5	17916.843	17916.839	.004	17917.864	17917.861	.003
93.5	17917.436	17917.436	.000	17918.468	17918.469	-.001
94.5	-	17918.040		17919.080	17919.083	-.003
95.5	17918.636	17918.650	-.014**	17919.701	17919.705	-.004
96.5	17919.247	17919.267	-.020**	17920.331	17920.333	-.002
97.5	17919.886	17919.890	-.004	17920.965	17920.967	-.002
98.5	17920.525	17920.520	.005	17921.612	17921.609	.003
99.5	17921.158	17921.157	.001	17922.253	17922.257	-.004
100.5	17921.799	17921.801	-.002	17922.901	17922.912	-.011**
101.5	17922.461	17922.451	.010**	17923.572	17923.573	-.001
102.5	17923.099	17923.108	-.009	-	17924.242	
103.5	17923.772	17923.772	.000	-	17924.917	

	$R_{11}(ee)$			$P_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
6.5	17893.290	17893.287	.003	-	17887.780	
7.5	17893.725	17893.729	-.004	-	17887.435	
8.5	17894.181	17894.178	.003	-	17887.097	
9.5	17894.639	17894.633	.006	17886.764	17886.766	-.002
10.5	17895.095	17895.095	.000	17886.439	17886.441	-.002
11.5	17895.568	17895.563	.005	17886.125	17886.122	.003
12.5	17896.037	17896.038	-.001	17885.812	17885.811	.001
13.5	17896.522	17896.519	.003	17885.505	17885.505	.000
14.5	-	17897.006		17885.210	17885.206	.004
15.5	-	17897.501		17884.918	17884.914	.004
16.5	-	17898.001		17884.634	17884.629	.005
17.5	-	17898.508		17884.350	17884.349	.001
18.5	-	17899.022		-	17884.077	
19.5	-	17899.542		17883.819	17883.811	.008
20.5	-	17900.068		17883.559	17883.551	.008
21.5	-	17900.601		17883.302	17883.298	.004
22.5	-	17901.141		17883.052	17883.052	.000
23.5	-	17901.687		17882.813	17882.812	.001
24.5	-	17902.239		17882.581	17882.579	.002
25.5	-	17902.798		17882.342	17882.353	-.011**
26.5	-	17903.364		17882.135	17882.132	.003

27.5	-	17903.935		17881.920	17881.919	.001
28.5	17904.515	17904.514	.001	17881.713	17881.712	.001
29.5	17905.095	17905.098	-.003	17881.513	17881.512	.001
30.5	-	17905.690		17881.323	17881.318	.005
31.5	17906.291	17906.287	.004	17881.135	17881.131	.004
32.5	17906.895	17906.892	.003	17880.954	17880.950	.004
33.5	-	17907.502		17880.781	17880.776	.005
34.5	17908.123	17908.119	.004	17880.604	17880.609	-.005
35.5	17908.747	17908.743	.004	17880.441	17880.448	-.007
36.5	17909.374	17909.373	.001	17880.292	17880.294	-.002
37.5	17910.009	17910.010	-.001	17880.143	17880.147	-.004
38.5	17910.652	17910.652	.000	17879.997	17880.006	-.009
39.5	17911.301	17911.302	-.001	17879.858	17879.871	-.013**
40.5	17911.956	17911.958	-.002	17879.734	17879.744	-.010
41.5	17912.616	17912.620	-.004	17879.616	17879.622	-.006
42.5	17913.291	17913.289	.002	17879.501	17879.508	-.007
43.5	17913.966	17913.964	.002	17879.393	17879.400	-.007
44.5	17914.647	17914.646	.001	17879.289	17879.299	-.010
45.5	17915.336	17915.334	.002	17879.195	17879.204	-.009
46.5	17916.027	17916.029	-.002	17879.106	17879.116	-.010
47.5	17916.729	17916.730	-.001	17879.027	17879.035	-.008
48.5	17917.435	17917.437	-.002	17878.951	17878.961	-.010
49.5	17918.148	17918.151	-.003	17878.886	17878.893	-.007
50.5	17918.868	17918.872	-.004	17878.826	17878.831	-.005
51.5	17919.601	17919.599	.002	17878.770	17878.777	-.007
52.5	17920.330	17920.332	-.002	17878.722	17878.729	-.007
53.5	17921.069	17921.072	-.003	-	17878.687	
54.5	17921.812	17921.818	-.006	-	17878.653	
55.5	17922.572	17922.571	.001	-	17878.625	
56.5	17923.330	17923.330	.000	-	17878.603	
57.5	17924.096	17924.096	.000	-	17878.589	
58.5	17924.870	17924.868	.002	-	17878.581	
59.5	17925.645	17925.647	-.002	-	17878.579	
60.5	17926.434	17926.432	.002	-	17878.585	
61.5	17927.223	17927.223	.000	-	17878.597	
62.5	17928.021	17928.021	.000	-	17878.616	
63.5	17928.824	17928.826	-.002	-	17878.641	
64.5	17929.633	17929.636	-.003	-	17878.673	
65.5	17930.452	17930.454	-.002	-	17878.712	
66.5	17931.276	17931.278	-.002	-	17878.758	
67.5	-	17932.108		-	17878.810	
68.5	17932.945	17932.945	.000	-	17878.870	
69.5	17933.788	17933.788	.000	-	17878.935	
70.5	17934.635	17934.637	-.002	-	17879.008	
71.5	17935.490	17935.493	-.003	-	17879.087	
72.5	17936.359	17936.356	.003	-	17879.173	
73.5	17937.221	17937.225	-.004	-	17879.266	
74.5	17938.098	17938.100	-.002	-	17879.366	
75.5	17938.986	17938.982	.004	-	17879.472	
76.5	17939.871	17939.871	.000	17879.590	17879.585	.005
77.5	17940.767	17940.766	.001	17879.698	17879.705	-.007
78.5	17941.672	17941.667	.005	17879.822	17879.832	-.010
79.5	17942.576	17942.575	.001	17879.959	17879.965	-.006
80.5	17943.491	17943.489	.002	17880.110	17880.105	.005
81.5	17944.416	17944.410	.006	17880.242	17880.252	-.010
82.5	17945.338	17945.337	.001	17880.409	17880.406	.003
83.5	17946.275	17946.271	.004	17880.571	17880.566	.005

84.5	17947.212	17947.211	.001	17880.736	17880.734	.002
85.5	17948.163	17948.157	.006	17880.906	17880.908	-.002
86.5	17949.118	17949.110	.008	17881.079	17881.089	-.010
87.5	17950.073	17950.070	.003	17881.262	17881.277	-.015**
88.5	17951.039	17951.036	.003	17881.460	17881.471	-.011**
89.5	-	17952.008		17881.660	17881.673	-.013**
90.5	17952.991	17952.987	.004	17881.896	17881.881	.015**
91.5	17953.975	17953.973	.002	17882.099	17882.096	.003
92.5	17954.967	17954.965	.002	17882.321	17882.318	.003
93.5	17955.959	17955.963	-.004	17882.552	17882.547	.005
94.5	17956.966	17956.968	-.002	17882.788	17882.782	.006
95.5	17957.978	17957.979	-.001	17883.036	17883.025	.011**
96.5	17958.997	17958.997	.000	17883.281	17883.274	.007
97.5	17960.018	17960.022	-.004	17883.538	17883.531	.007
98.5	17961.050	17961.053	-.003	17883.805	17883.794	.011**
99.5	17962.086	17962.090	-.004	17884.075	17884.064	.011**
100.5	17963.130	17963.134	-.004	17884.341	17884.341	.000
101.5	17964.179	17964.184	-.005	17884.623	17884.624	-.001
102.5	17965.227	17965.241	-.014**	17884.915	17884.915	.000
103.5	-	17966.304		17885.210	17885.213	-.003
104.5	-	17967.374		17885.519	17885.517	.002
105.5	-	17968.450		17885.831	17885.828	.003
106.5	-	17969.533		17886.148	17886.147	.001
107.5	-	17970.622		17886.473	17886.472	.001
108.5	-	17971.718		17886.806	17886.804	.002
109.5	-	17972.820		17887.145	17887.143	.002
110.5	-	17973.929		17887.487	17887.489	-.002
111.5	-	17975.045		17887.844	17887.842	.002
112.5	-	17976.166		17888.199	17888.202	-.003
113.5	-	17977.295		17888.568	17888.569	-.001
114.5	-	17978.430		17888.943	17888.943	.000
115.5	-	17979.571		17889.324	17889.324	.000
116.5	-	17980.719		17889.706	17889.711	-.005
117.5	-	17981.873		17890.104	17890.106	-.002
118.5	-	17983.034		17890.506	17890.508	-.002
119.5	-	17984.202		17890.916	17890.917	-.001
120.5	-	17985.376		17891.330	17891.333	-.003

	$P_{22}(ff)$			$R_{21}(ee)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
4.5	19381.153	19381.152	.001	-	19384.002	
5.5	19380.908	19380.904	.004	-	19384.323	
6.5	19380.667	19380.662	.005	-	19384.652	
7.5	19380.430	19380.427	.003	-	19384.986	
8.5	19380.200	19380.199	.001	-	19385.328	
9.5	19379.978	19379.978	.000	-	19385.676	
10.5	19379.762	19379.763	-.001	-	19386.031	
11.5	19379.557	19379.555	.002	-	19386.393	
12.5	19379.352	19379.353	-.001	-	19386.761	
13.5	19379.155	19379.158	-.003	-	19387.136	
14.5	19378.970	19378.970	.000	-	19387.517	
15.5	19378.791	19378.789	.002	-	19387.905	
16.5	19378.618	19378.614	.004	-	19388.300	
17.5	19378.452	19378.446	.006	-	19388.702	

18.5	19378.287	19378.285	.002	-	19389.110	
19.5	19378.130	19378.130	.000	-	19389.524	
20.5	19377.985	19377.982	.003	-	19389.946	
21.5	19377.842	19377.841	.001	19390.377	19390.374	.003
22.5	19377.706	19377.707	-.001	19390.810	19390.808	.002
23.5	19377.580	19377.579	.001	19391.252	19391.250	.002
24.5	19377.458	19377.458	.000	19391.697	19391.698	-.001
25.5	-	19377.343		19392.153	19392.152	.001
26.5	19377.235	19377.236	-.001	19392.613	19392.613	.000
27.5	19377.131	19377.135	-.004	19393.084	19393.081	.003
28.5	-	19377.041		19393.556	19393.556	.000
29.5	19376.952	19376.953	-.001	19394.036	19394.037	-.001
30.5	19376.872	19376.873	-.001	19394.523	19394.525	-.002
31.5	19376.800	19376.799	.001	19395.019	19395.019	.000
32.5	19376.734	19376.731	.003	19395.521	19395.520	.001
33.5	19376.673	19376.671	.002	19396.027	19396.028	-.001
34.5	19376.618	19376.617	.001	19396.538	19396.542	-.004
35.5	-	19376.570		19397.060	19397.063	-.003
36.5	-	19376.530		19397.589	19397.591	-.002
37.5	-	19376.496		19398.125	19398.125	.000
38.5	-	19376.469		19398.667	19398.666	.001
39.5	-	19376.449		19399.211	19399.213	-.002
40.5	-	19376.436		19399.767	19399.767	.000
41.5	-	19376.430		19400.329	19400.328	.001
42.5	-	19376.430		19400.897	19400.896	.001
43.5	-	19376.437		19401.473	19401.470	.003
44.5	-	19376.451		19402.051	19402.050	.001
45.5	-	19376.471		19402.631	19402.638	-.007
46.5	-	19376.499		19403.232	19403.232	.000
47.5	-	19376.533		19403.833	19403.832	.001
48.5	-	19376.574		19404.441	19404.439	.002
49.5	-	19376.621		19405.054	19405.053	.001
50.5	-	19376.676		19405.674	19405.674	.000
51.5	-	19376.737		19406.299	19406.301	-.002
52.5	-	19376.805		19406.934	19406.935	-.001
53.5	-	19376.880		19407.575	19407.575	.000
54.5	-	19376.962		19408.222	19408.222	.000
55.5	19377.050	19377.050	.000	19408.874	19408.876	-.002
56.5	19377.143	19377.145	-.002	19409.535	19409.536	-.001
57.5	19377.245	19377.248	-.003	19410.202	19410.203	-.001
58.5	19377.353	19377.356	-.003	19410.877	19410.877	.000
59.5	19377.474	19377.472	.002	19411.556	19411.557	-.001
60.5	19377.596	19377.595	.001	19412.246	19412.244	.002
61.5	19377.721	19377.724	-.003	19412.938	19412.937	.001
62.5	19377.856	19377.860	-.004	19413.638	19413.637	.001
63.5	19378.003	19378.003	.000	19414.343	19414.344	-.001
64.5	19378.150	19378.153	-.003	19415.059	19415.057	.002
65.5	19378.308	19378.310	-.002	19415.778	19415.778	.000
66.5	19378.472	19378.474	-.002	19416.506	19416.504	.002
67.5	19378.642	19378.644	-.002	19417.238	19417.238	.000
68.5	19378.821	19378.821	.000	19417.977	19417.978	-.001
69.5	19379.005	19379.005	.000	19418.727	19418.724	.003
70.5	19379.196	19379.196	.000	19419.478	19419.478	.000
71.5	19379.396	19379.394	.002	19420.241	19420.238	.003
72.5	19379.600	19379.599	.001	19421.005	19421.004	.001
73.5	19379.810	19379.811	-.001	19421.778	19421.777	.001
74.5	19380.030	19380.029	.001	19422.554	19422.557	-.003

75.5	19380.253	19380.254	-.001	19423.345	19423.344	.001
76.5	19380.486	19380.487	-.001	19424.137	19424.137	.000
77.5	19380.728	19380.726	.002	19424.937	19424.937	.000
78.5	19380.972	19380.972	.000	19425.746	19425.743	.003
79.5	19381.226	19381.225	.001	19426.556	19426.557	-.001
80.5	19381.488	19381.485	.003	19427.379	19427.377	.002
81.5	19381.754	19381.752	.002	19428.204	19428.203	.001
82.5	19382.026	19382.025	.001	19429.041	19429.036	.005
83.5	19382.303	19382.306	-.003	19429.881	19429.876	.005
84.5	19382.587	19382.593	-.006	19430.731	19430.723	.008
85.5	19382.890	19382.888	.002	19431.580	19431.576	.004
86.5	19383.192	19383.189	.003	19432.432	19432.436	-.004
87.5	19383.499	19383.497	.002	-	19433.302	
88.5	19383.813	19383.813	.000	-	19434.175	
89.5	19384.135	19384.135	.000	-	19435.055	
90.5	19384.464	19384.464	.000	-	19435.942	
91.5	19384.804	19384.800	.004	-	19436.835	
92.5	19385.148	19385.143	.005	-	19437.735	
93.5	19385.498	19385.493	.005	-	19438.641	
94.5	19385.854	19385.850	.004	-	19439.555	
95.5	19386.219	19386.214	.005	-	19440.474	

	$Q_{22}(fe)$			$P_{21}(ee)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
38.5	19383.905	19383.916	-.011	-	19383.575	
39.5	19384.084	19384.089	-.005	-	19383.737	
40.5	19384.261	19384.268	-.007	19383.905	19383.905	.000
41.5	19384.452	19384.454	-.002	19384.084	19384.080	.004
42.5	19384.646	19384.647	-.001	19384.261	19384.261	.000
43.5	19384.846	19384.847	-.001	19384.452	19384.450	.002
44.5	19385.053	19385.053	.000	19384.646	19384.645	.001
45.5	19385.270	19385.266	.004	19384.846	19384.847	-.001
46.5	19385.489	19385.486	.003	19385.053	19385.055	-.002
47.5	19385.717	19385.712	.005	19385.270	19385.270	.000
48.5	19385.950	19385.946	.004	19385.489	19385.492	-.003
49.5	19386.192	19386.186	.006	19385.717	19385.721	-.004
50.5	19386.439	19386.432	.007	19385.950	19385.956	-.006
51.5	19386.690	19386.686	.004	19386.192	19386.199	-.007
52.5	19386.950	19386.946	.004	19386.439	19386.448	-.009
53.5	19387.218	19387.213	.005	19386.690	19386.703	-.013**
54.5	19387.489	19387.486	.003	19386.950	19386.965	-.015**
55.5	19387.770	19387.767	.003	19387.218	19387.235	-.017**
56.5	19388.051	19388.054	-.003	19387.489	19387.510	-.021**
57.5	19388.344	19388.348	-.004	-	19387.793	
58.5	19388.648	19388.648	.000	19388.076	19388.082	-.006
59.5	19388.953	19388.956	-.003	19388.373	19388.378	-.005
60.5	19389.265	19389.270	-.005	19388.677	19388.681	-.004
61.5	19389.587	19389.591	-.004	19388.991	19388.991	.000
62.5	19389.916	19389.918	-.002	19389.309	19389.307	.002
63.5	19390.251	19390.253	-.002	19389.631	19389.630	.001
64.5	19390.591	19390.594	-.003	19389.969	19389.960	.009
65.5	19390.941	19390.942	-.001	19390.300	19390.297	.003
66.5	19391.292	19391.296	-.004	19390.644	19390.640	.004
67.5	19391.657	19391.658	-.001	19390.974	19390.990	-.016**

68.5	19392.022	19392.026	-.004	19391.342	19391.347	-.005
69.5	19392.397	19392.401	-.004	19391.708	19391.711	-.003
70.5	19392.780	19392.783	-.003	19392.074	19392.081	-.007
71.5	19393.174	19393.171	.003	19392.453	19392.458	-.005
72.5	19393.570	19393.567	.003	19392.831	19392.842	-.011
73.5	19393.971	19393.969	.002	19393.225	19393.233	-.008
74.5	19394.381	19394.378	.003	-	19393.631	
75.5	19394.798	19394.794	.004	19394.033	19394.035	-.002
76.5	19395.223	19395.216	.007	19394.444	19394.446	-.002
77.5	19395.651	19395.645	.006	19394.862	19394.864	-.002
78.5	19396.087	19396.082	.005	19395.286	19395.289	-.003
79.5	19396.528	19396.525	.003	19395.723	19395.721	.002
80.5	19396.977	19396.974	.003	19396.155	19396.159	-.004
81.5	19397.434	19397.431	.003	19396.599	19396.604	-.005
82.5	19397.900	19397.894	.006	19397.050	19397.056	-.006
83.5	19398.373	19398.364	.009	19397.511	19397.515	-.004
84.5	19398.848	19398.841	.007	19397.981	19397.981	.000
85.5	-	19399.325		19398.452	19398.453	-.001
86.5	-	19399.816		19398.931	19398.933	-.002

	$R_{22}(ff)$			$Q_{21}(fe)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
20.5	19386.121	19386.115	.006	19385.788	19385.783	.005
21.5	19386.365	19386.361	.004	19386.019	19386.018	.001
22.5	19386.620	19386.614	.006	19386.265	19386.259	.006
23.5	19386.878	19386.873	.005	19386.513	19386.507	.006
24.5	19387.143	19387.138	.005	19386.770	19386.761	.009
25.5	19387.414	19387.411	.003	19387.028	19387.023	.005
26.5	19387.695	19387.690	.005	19387.300	19387.291	.009
27.5	19387.980	19387.976	.004	19387.571	19387.565	.006
28.5	19388.270	19388.268	.002	19387.854	19387.847	.007
29.5	19388.570	19388.568	.002	19388.139	19388.135	.004
30.5	19388.872	19388.873	-.001	19388.432	19388.429	.003
31.5	19389.187	19389.186	.001	19388.732	19388.731	.001
32.5	19389.505	19389.505	.000	19389.039	19389.039	.000
33.5	19389.830	19389.831	-.001	19389.348	19389.353	-.005
34.5	19390.160	19390.164	-.004	19389.673	19389.675	-.002
35.5	19390.505	19390.503	.002	19390.000	19390.003	-.003
36.5	19390.848	19390.849	-.001	19390.333	19390.337	-.004
37.5	19391.200	19391.201	-.001	19390.674	19390.679	-.005
38.5	19391.558	19391.561	-.003	19391.018	19391.027	-.009
39.5	19391.925	19391.927	-.002	19391.373	19391.381	-.008
40.5	19392.298	19392.299	-.001	19391.739	19391.743	-.004
41.5	19392.681	19392.679	.002	19392.107	19392.111	-.004
42.5	19393.068	19393.065	.003	19392.481	19392.486	-.005
43.5	19393.459	19393.457	.002	19392.865	19392.867	-.002
44.5	19393.856	19393.857	-.001	19393.252	19393.255	-.003
45.5	19394.268	19394.263	.005	19393.649	19393.650	-.001
46.5	19394.678	19394.676	.002	19394.054	19394.052	.002
47.5	19395.094	19395.095	-.001	19394.459	19394.460	-.001
48.5	19395.520	19395.521	-.001	19394.878	19394.875	.003
49.5	19395.949	19395.954	-.005	19395.296	19395.297	-.001
50.5	19396.391	19396.394	-.003	19395.720	19395.725	-.005
51.5	19396.841	19396.840	.001	19396.158	19396.160	-.002

52.5	19397.288	19397.293	-.005	19396.600	19396.602	-.002
53.5	19397.752	19397.753	-.001	19397.050	19397.050	.000
54.5	19398.219	19398.219	.000	19397.504	19397.505	-.001
55.5	19398.690	19398.692	-.002	19397.965	19397.967	-.002
56.5	19399.171	19399.172	-.001	19398.438	19398.436	.002
57.5	19399.656	19399.658	-.002	19398.906	19398.911	-.005
58.5	19400.148	19400.152	-.004	19399.395	19399.393	.002
59.5	19400.651	19400.652	-.001	19399.878	19399.882	-.004
60.5	19401.158	19401.158	.000	19400.374	19400.377	-.003
61.5	19401.667	19401.672	-.005	19400.878	19400.879	-.001
62.5	19402.188	19402.192	-.004	19401.386	19401.388	-.002
63.5	19402.722	19402.718	.004	19401.899	19401.903	-.004
64.5	-	19403.252		19402.421	19402.426	-.005
65.5	-	19403.792		19402.950	19402.955	-.005

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	$Q_{11}(ef)$			$R_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
32.5	-	18203.388		18203.712	18203.716	-.004
33.5	-	18203.564		18203.900	18203.902	-.002
34.5	18203.747	18203.745	.002	18204.092	18204.094	-.002
35.5	18203.940	18203.933	.007	18204.290	18204.292	-.002
36.5	18204.122	18204.126	-.004	18204.494	18204.495	-.001
37.5	18204.323	18204.325	-.002	18204.703	18204.705	-.002
38.5	18204.530	18204.530	.000	18204.917	18204.920	-.003
39.5	18204.736	18204.741	-.005	18205.143	18205.141	.002
40.5	18204.955	18204.957	-.002	18205.363	18205.367	-.004
41.5	18205.183	18205.179	.004	18205.599	18205.600	-.001
42.5	18205.403	18205.407	-.004	18205.836	18205.838	-.002
43.5	18205.641	18205.641	.000	18206.078	18206.082	-.004
44.5	18205.882	18205.880	.002	18206.331	18206.332	-.001
45.5	18206.125	18206.126	-.001	18206.587	18206.588	-.001
46.5	18206.380	18206.377	.003	18206.839	18206.849	-.010
47.5	18206.638	18206.634	.004	18207.109	18207.116	-.007
48.5	18206.893	18206.896	-.003	18207.387	18207.390	-.003
49.5	18207.161	18207.165	-.004	18207.665	18207.668	-.003
50.5	18207.437	18207.439	-.002	18207.948	18207.953	-.005
51.5	18207.717	18207.719	-.002	18208.242	18208.243	-.001
52.5	18208.006	18208.005	.001	18208.540	18208.540	.000
53.5	18208.296	18208.297	-.001	18208.845	18208.842	.003
54.5	18208.596	18208.594	.002	18209.145	18209.150	-.005
55.5	18208.898	18208.898	.000	18209.462	18209.463	-.001
56.5	18209.206	18209.207	-.001	18209.791	18209.783	.008
57.5	18209.520	18209.522	-.002	18210.100	18210.108	-.008
58.5	18209.814	18209.843	-.029**	18210.430	18210.439	-.009
59.5	18210.143	18210.169	-.026**	18210.762	18210.776	-.014**
60.5	18210.478	18210.502	-.024**	18211.112	18211.119	-.007
61.5	18210.812	18210.840	-.028**	18211.463	18211.468	-.005
62.5	18211.179	18211.184	-.005	18211.824	18211.822	.002
63.5	18211.531	18211.534	-.003	18212.185	18212.182	.003
64.5	18211.894	18211.890	.004	18212.556	18212.549	.007
65.5	18212.257	18212.251	.006	18212.933	18212.921	.012**

66.5	18212.627	18212.619	.008	18213.300	18213.298	.002
67.5	18213.003	18212.992	.011**	18213.684	18213.682	.002
68.5	18213.361	18213.371	-.010**	18214.073	18214.071	.002
69.5	18213.757	18213.756	.001	18214.465	18214.467	-.002
70.5	18214.150	18214.147	.003	18214.870	18214.868	.002
71.5	18214.547	18214.543	.004	18215.275	18215.275	.000
72.5	18214.946	18214.946	.000	18215.689	18215.688	.001
73.5	18215.355	18215.354	.001	18216.108	18216.106	.002
74.5	18215.774	18215.768	.006	18216.530	18216.531	-.001
75.5	18216.192	18216.188	.004	18216.961	18216.961	.000
76.5	18216.609	18216.614	-.005	18217.397	18217.398	-.001
77.5	18217.033	18217.046	-.013**	18217.839	18217.840	-.001
78.5	18217.473	18217.484	-.011**	18218.288	18218.288	.000
79.5	18217.921	18217.927	-.006	18218.743	18218.742	.001
80.5	18218.372	18218.377	-.005	18219.201	18219.202	-.001
81.5	18218.829	18218.832	-.003	18219.667	18219.667	.000
82.5	18219.294	18219.293	.001	18220.136	18220.139	-.003
83.5	18219.761	18219.760	.001	18220.616	18220.616	.000
84.5	18220.235	18220.233	.002	18221.097	18221.100	-.003
85.5	18220.720	18220.712	.008	18221.590	18221.589	.001
86.5	18221.205	18221.196	.009	18222.082	18222.084	-.002
87.5	18221.690	18221.687	.003	18222.585	18222.585	.000
88.5	18222.182	18222.183	-.001	18223.092	18223.092	.000
89.5	-	18222.686		18223.605	18223.605	.000
90.5	18223.196	18223.194	.002	18224.121	18224.123	-.002
91.5	18223.708	18223.708	.000	18224.646	18224.648	-.002
92.5	18224.227	18224.228	-.001	18225.179	18225.179	.000
93.5	18224.751	18224.754	-.003	18225.714	18225.715	-.001
94.5	18225.286	18225.286	.000	18226.257	18226.257	.000
95.5	18225.825	18225.824	.001	18226.807	18226.806	.001
96.5	18226.362	18226.368	-.006	18227.361	18227.360	.001
97.5	18226.919	18226.918	.001	18227.920	18227.920	.000
98.5	18227.475	18227.473	.002	18228.486	18228.486	.000
99.5	18228.034	18228.035	-.001	18229.059	18229.058	.001
100.5	18228.602	18228.602	.000	18229.636	18229.636	.000
101.5	18229.189	18229.176	.013**	18230.220	18230.220	.000
102.5	18229.751	18229.755	-.004	18230.809	18230.810	-.001
103.5	18230.341	18230.340	.001	18231.406	18231.406	.000
104.5	18230.933	18230.932	.001	18232.005	18232.008	-.003
105.5	18231.530	18231.529	.001	18232.615	18232.615	.000
106.5	18232.135	18232.132	.003	-	18233.229	
107.5	18232.741	18232.741	.000	-	18233.849	

$R_{11}(ee)$ $P_{12}(ff)$

J	OBS	CALC	DIFF	OBS	CALC	DIFF
9.5	18205.236	18205.231	.005	-	18197.385	
10.5	18205.685	18205.684	.001	-	18197.053	
11.5	18206.141	18206.142	-.001	-	18196.727	
12.5	18206.604	18206.606	-.002	18196.402	18196.407	-.005
13.5	18207.072	18207.076	-.004	18196.079	18196.092	-.013**
14.5	18207.549	18207.552	-.003	18195.779	18195.784	-.005
15.5	18208.028	18208.033	-.005	18195.481	18195.481	.000
16.5	18208.520	18208.520	.000	18195.188	18195.184	.004
17.5	18209.014	18209.013	.001	18194.895	18194.892	.003

18.5	18209.512	18209.511	.001	18194.609	18194.607	.002
19.5	18210.014	18210.015	-.001	18194.330	18194.327	.003
20.5	18210.525	18210.525	.000	18194.054	18194.053	.001
21.5	18211.037	18211.041	-.004	18193.786	18193.785	.001
22.5	18211.566	18211.562	.004	18193.523	18193.522	.001
23.5	18212.090	18212.089	.001	18193.268	18193.266	.002
24.5	18212.624	18212.622	.002	18193.016	18193.015	.001
25.5	18213.161	18213.160	.001	18192.769	18192.770	-.001
26.5	18213.699	18213.705	-.006	18192.531	18192.531	.000
27.5	18214.253	18214.255	-.002	18192.300	18192.298	.002
28.5	18214.809	18214.810	-.001	18192.070	18192.070	.000
29.5	18215.369	18215.371	-.002	18191.850	18191.849	.001
30.5	18215.941	18215.938	.003	18191.634	18191.633	.001
31.5	18216.513	18216.511	.002	18191.427	18191.423	.004
32.5	18217.093	18217.090	.003	18191.220	18191.218	.002
33.5	18217.676	18217.674	.002	18191.018	18191.020	-.002
34.5	18218.263	18218.264	-.001	18190.831	18190.828	.003
35.5	18218.858	18218.859	-.001	18190.643	18190.641	.002
36.5	18219.459	18219.460	-.001	18190.460	18190.460	.000
37.5	18220.067	18220.067	.000	18190.289	18190.285	.004
38.5	18220.680	18220.680	.000	18190.118	18190.116	.002
39.5	18221.299	18221.298	.001	18189.951	18189.953	-.002
40.5	18221.923	18221.922	.001	18189.800	18189.795	.005
41.5	18222.552	18222.552	.000	18189.646	18189.644	.002
42.5	18223.188	18223.188	.000	18189.498	18189.498	.000
43.5	18223.831	18223.829	.002	18189.358	18189.358	.000
44.5	18224.476	18224.476	.000	18189.228	18189.224	.004
45.5	18225.127	18225.128	-.001	18189.098	18189.096	.002
46.5	18225.787	18225.787	.000	18188.975	18188.974	.001
47.5	18226.453	18226.450	.003	18188.868	18188.858	.010
48.5	18227.119	18227.120	-.001	18188.741	18188.747	-.006
49.5	18227.795	18227.795	.000	-	18188.643	
50.5	18228.475	18228.477	-.002	-	18188.544	
51.5	18229.162	18229.163	-.001	-	18188.451	
52.5	18229.853	18229.856	-.003	-	18188.364	
53.5	18230.554	18230.554	.000	-	18188.283	
54.5	18231.253	18231.258	-.005	-	18188.208	
55.5	18231.966	18231.967	-.001	-	18188.139	
56.5	18232.684	18232.683	.001	-	18188.076	
57.5	18233.411	18233.404	.007	-	18188.019	
58.5	18234.132	18234.130	.002	-	18187.967	
59.5	18234.864	18234.862	.002	-	18187.922	
60.5	18235.602	18235.601	.001	-	18187.882	
61.5	18236.344	18236.344	.000	-	18187.849	
62.5	18237.095	18237.094	.001	-	18187.821	
63.5	18237.851	18237.849	.002	-	18187.800	
64.5	18238.611	18238.610	.001	-	18187.784	
65.5	18239.372	18239.376	-.004	-	18187.774	
66.5	18240.150	18240.148	.002	-	18187.770	
67.5	18240.930	18240.926	.004	-	18187.772	
68.5	18241.711	18241.710	.001	-	18187.781	
69.5	18242.499	18242.499	.000	-	18187.795	
70.5	18243.296	18243.294	.002	-	18187.815	
71.5	18244.097	18244.095	.002	-	18187.841	
72.5	18244.902	18244.902	.000	-	18187.873	
73.5	18245.714	18245.714	.000	-	18187.911	
74.5	18246.532	18246.532	.000	-	18187.955	

75.5	18247.360	18247.355	.005	-	18188.005	
76.5	18248.179	18248.184	-.005	-	18188.061	
77.5	18249.016	18249.019	-.003	-	18188.123	
78.5	18249.859	18249.860	-.001	-	18188.191	
79.5	18250.700	18250.706	-.006	-	18188.265	
80.5	18251.559	18251.559	.000	-	18188.345	
81.5	18252.415	18252.416	-.001	-	18188.431	
82.5	18253.283	18253.280	.003	18188.532	18188.523	.009
83.5	18254.148	18254.149	-.001	18188.626	18188.621	.005
84.5	18255.024	18255.024	.000	18188.726	18188.725	.001
85.5	18255.909	18255.905	.004	18188.839	18188.836	.003
86.5	18256.795	18256.791	.004	18188.951	18188.952	-.001
87.5	18257.683	18257.683	.000	18189.075	18189.074	.001
88.5	18258.587	18258.581	.006	18189.204	18189.203	.001
89.5	18259.485	18259.484	.001	18189.338	18189.337	.001
90.5	18260.392	18260.394	-.002	18189.475	18189.478	-.003
91.5	18261.306	18261.309	-.003	18189.622	18189.624	-.002
92.5	18262.228	18262.229	-.001	18189.785	18189.777	.008
93.5	18263.146	18263.156	-.010	18189.936	18189.936	.000
94.5	-	18264.088		18190.103	18190.101	.002
95.5	-	18265.026		18190.272	18190.271	.001
96.5	-	18265.969		18190.448	18190.449	-.001
97.5	-	18266.919		18190.631	18190.632	-.001
98.5	-	18267.874		18190.823	18190.821	.002
99.5	-	18268.834		18191.014	18191.016	-.002
100.5	-	18269.801		18191.220	18191.218	.002
101.5	-	18270.773		18191.427	18191.426	.001
102.5	-	18271.751		18191.637	18191.639	-.002
103.5	-	18272.735		18191.858	18191.859	-.001
104.5	-	18273.724		18192.085	18192.086	-.001
105.5	-	18274.720		18192.316	18192.318	-.002
106.5	-	18275.720		18192.554	18192.556	-.002
107.5	-	18276.727		18192.800	18192.801	-.001
108.5	-	18277.740		-	18193.051	
109.5	-	18278.758		-	18193.308	
110.5	-	18279.782		18193.571	18193.571	.000
111.5	-	18280.811		18193.838	18193.841	-.003
112.5	-	18281.847		18194.113	18194.116	-.003

$P_{22}(ff)$ $R_{21}(ee)$

J	OBS	CALC	DIFF	OBS	CALC	DIFF
5.5	-	19693.383		19696.772	19696.794	-.022**
6.5	-	19693.138		19697.107	19697.116	-.009
7.5	-	19692.898		19697.438	19697.445	-.007
8.5	-	19692.664		19697.779	19697.779	.000
9.5	-	19692.436		19698.123	19698.119	.004
10.5	-	19692.214		19698.470	19698.465	.005
11.5	-	19691.997		19698.827	19698.817	.010
12.5	-	19691.787		19699.184	19699.175	.009
13.5	-	19691.583		19699.546	19699.539	.007
14.5	-	19691.384		19699.906	19699.909	-.003
15.5	-	19691.192		19700.285	19700.284	.001
16.5	19691.011	19691.005	.006	19700.669	19700.666	.003
17.5	19690.827	19690.825	.002	19701.053	19701.053	.000

18.5	19690.654	19690.650	.004	19701.448	19701.446	.002
19.5	19690.493	19690.482	.011	19701.847	19701.845	.002
20.5	19690.321	19690.319	.002	19702.251	19702.250	.001
21.5	19690.159	19690.162	-.003	19702.663	19702.661	.002
22.5	-	19690.011		19703.082	19703.078	.004
23.5	-	19689.866		19703.501	19703.501	.000
24.5	19689.728	19689.727	.001	19703.931	19703.929	.002
25.5	19689.594	19689.594	.000	19704.364	19704.363	.001
26.5	19689.469	19689.467	.002	19704.806	19704.804	.002
27.5	19689.341	19689.346	-.005	19705.250	19705.250	.000
28.5	19689.233	19689.231	.002	19705.701	19705.702	-.001
29.5	-	19689.122		19706.158	19706.160	-.002
30.5	-	19689.019		19706.624	19706.624	.000
31.5	-	19688.921		19707.091	19707.093	-.002
32.5	-	19688.830		19707.568	19707.569	-.001
33.5	-	19688.745		19708.048	19708.050	-.002
34.5	-	19688.665		19708.534	19708.537	-.003
35.5	-	19688.592		19709.028	19709.031	-.003
36.5	-	19688.525		19709.527	19709.530	-.003
37.5	-	19688.463		19710.031	19710.034	-.003
38.5	-	19688.408		19710.543	19710.545	-.002
39.5	-	19688.359		19711.060	19711.062	-.002
40.5	-	19688.315		19711.581	19711.584	-.003
41.5	-	19688.278		19712.112	19712.113	-.001
42.5	-	19688.246		19712.647	19712.647	.000
43.5	-	19688.221		19713.186	19713.187	-.001
44.5	-	19688.202		19713.725	19713.733	-.008
45.5	-	19688.188		19714.284	19714.285	-.001
46.5	-	19688.181		19714.840	19714.843	-.003
47.5	-	19688.180		19715.406	19715.406	.000
48.5	-	19688.184		19715.975	19715.976	-.001
49.5	19688.195	19688.195	.000	19716.550	19716.551	-.001
50.5	-	19688.212		19717.130	19717.133	-.003
51.5	19688.234	19688.235	-.001	19717.716	19717.720	-.004
52.5	19688.263	19688.263	.000	19718.310	19718.313	-.003
53.5	19688.300	19688.298	.002	19718.908	19718.912	-.004
54.5	19688.341	19688.339	.002	19719.512	19719.516	-.004
55.5	19688.385	19688.386	-.001	19720.125	19720.127	-.002
56.5	19688.441	19688.439	.002	19720.741	19720.744	-.003
57.5	19688.494	19688.498	-.004	19721.365	19721.366	-.001
58.5	19688.558	19688.563	-.005	19721.994	19721.994	.000
59.5	19688.630	19688.634	-.004	19722.625	19722.628	-.003
60.5	19688.709	19688.711	-.002	19723.265	19723.268	-.003
61.5	19688.797	19688.794	.003	19723.912	19723.914	-.002
62.5	19688.881	19688.884	-.003	19724.565	19724.566	-.001
63.5	19688.979	19688.979	.000	19725.223	19725.224	-.001
64.5	19689.081	19689.081	.000	19725.884	19725.887	-.003
65.5	19689.194	19689.188	.006	19726.554	19726.557	-.003
66.5	19689.306	19689.302	.004	19727.230	19727.232	-.002
67.5	19689.421	19689.422	-.001	19727.909	19727.913	-.004
68.5	19689.540	19689.547	-.007	19728.595	19728.600	-.005
69.5	19689.681	19689.679	.002	19729.291	19729.293	-.002
70.5	19689.827	19689.817	.010	19729.989	19729.992	-.003
71.5	19689.950	19689.961	-.011**	19730.695	19730.697	-.002
72.5	19690.108	19690.112	-.004	19731.403	19731.407	-.004
73.5	-	19690.268		19732.121	19732.124	-.003
74.5	-	19690.430		19732.842	19732.846	-.004

75.5	19690.583	19690.599	-.016**	19733.569	19733.575	-.006
76.5	-	19690.774		19734.305	19734.309	-.004
77.5	-	19690.954		19735.046	19735.049	-.003
78.5	-	19691.141		19735.793	19735.795	-.002
79.5	-	19691.334		19736.545	19736.547	-.002
80.5	-	19691.534		19737.302	19737.305	-.003
81.5	-	19691.739		19738.067	19738.068	-.001
82.5	-	19691.950		19738.837	19738.838	-.001
83.5	-	19692.168		19739.611	19739.613	-.002
84.5	-	19692.392		19740.396	19740.395	.001
85.5	-	19692.622		19741.183	19741.182	.001
86.5	-	19692.858		19741.976	19741.975	.001
87.5	-	19693.100		19742.775	19742.775	.000
88.5	-	19693.349		19743.581	19743.580	.001
89.5	-	19693.604		19744.393	19744.391	.002
90.5	-	19693.864		19745.210	19745.207	.003
91.5	-	19694.132		19746.033	19746.030	.003
92.5	-	19694.405		19746.863	19746.859	.004
93.5	-	19694.684		19747.696	19747.694	.002
94.5	-	19694.970		19748.540	19748.534	.006
95.5	-	19695.262		19749.385	19749.381	.004
96.5	-	19695.560		19750.236	19750.233	.003

	$Q_{22}(fe)$			$P_{21}(ee)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
25.5	19694.511	19694.511	.000	-	19694.336	
26.5	-	19694.577		-	19694.391	
27.5	19694.652	19694.648	.004	-	19694.452	
28.5	-	19694.725		19694.527	19694.519	.008
29.5	19694.815	19694.809	.006	-	19694.591	
30.5	19694.893	19694.898	-.005	19694.675	19694.670	.005
31.5	-	19694.993		19694.759	19694.755	.004
32.5	19695.096	19695.094	.002	19694.861	19694.845	.016**
33.5	19695.216	19695.201	.015**	-	19694.942	
34.5	19695.308	19695.314	-.006	19695.048	19695.045	.003
35.5	19695.441	19695.433	.008	19695.159	19695.153	.006
36.5	19695.559	19695.558	.001	-	19695.267	
37.5	19695.688	19695.689	-.001	19695.397	19695.388	.009
38.5	19695.827	19695.825	.002	-	19695.514	
39.5	19695.968	19695.968	.000	-	19695.646	
40.5	19696.121	19696.117	.004	19695.776	19695.784	-.008
41.5	19696.268	19696.271	-.003	19695.930	19695.928	.002
42.5	19696.427	19696.432	-.005	-	19696.078	
43.5	19696.599	19696.598	.001	19696.240	19696.234	.006
44.5	19696.760	19696.771	-.011	19696.399	19696.396	.003
45.5	19696.951	19696.949	.002	19696.569	19696.564	.005
46.5	19697.141	19697.133	.008	-	19696.738	
47.5	19697.323	19697.324	-.001	19696.920	19696.918	.002
48.5	19697.518	19697.520	-.002	19697.106	19697.104	.002
49.5	19697.721	19697.722	-.001	19697.298	19697.295	.003
50.5	19697.926	19697.930	-.004	19697.494	19697.493	.001
51.5	19698.144	19698.145	-.001	-	19697.697	
52.5	19698.366	19698.365	.001	19697.904	19697.906	-.002
53.5	19698.590	19698.591	-.001	-	19698.122	

54.5	19698.820	19698.823	-.003	19698.348	19698.344	.004
55.5	19699.063	19699.061	.002	-	19698.571	
56.5	19699.302	19699.305	-.003	19698.820	19698.805	.015**
57.5	19699.549	19699.555	-.006	19699.040	19699.044	-.004
58.5	19699.809	19699.811	-.002	19699.287	19699.290	-.003
59.5	19700.070	19700.073	-.003	19699.549	19699.541	.008
60.5	19700.344	19700.341	.003	19699.809	19699.799	.010
61.5	19700.619	19700.615	.004	19700.070	19700.062	.008
62.5	19700.898	19700.896	.002	19700.344	19700.332	.012
63.5	19701.182	19701.182	.000	19700.611	19700.607	.004
64.5	19701.471	19701.474	-.003	19700.898	19700.889	.009
65.5	-	19701.772		19701.182	19701.176	.006
66.5	-	19702.076		19701.471	19701.470	.001

	$R_{22}(ff)$			$Q_{21}(fe)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
13.5	-	19696.984		19696.743	19696.742	.001
14.5	-	19697.172		-	19696.919	
15.5	-	19697.365		-	19697.101	
16.5	19697.567	19697.564	.003	-	19697.290	
17.5	19697.763	19697.769	-.006	-	19697.485	
18.5	19697.982	19697.980	.002	-	19697.685	
19.5	19698.200	19698.197	.003	19697.898	19697.892	.006
20.5	19698.426	19698.420	.006	19698.097	19698.104	-.007
21.5	19698.661	19698.648	.013**	19698.318	19698.322	-.004
22.5	-	19698.883		19698.541	19698.546	-.005
23.5	19699.123	19699.123	.000	19698.778	19698.776	.002
24.5	19699.372	19699.370	.002	19699.009	19699.012	-.003
25.5	19699.620	19699.622	-.002	19699.252	19699.254	-.002
26.5	19699.880	19699.880	.000	19699.502	19699.502	.000
27.5	19700.140	19700.144	-.004	19699.761	19699.755	.006
28.5	19700.413	19700.414	-.001	19700.013	19700.015	-.002
29.5	19700.687	19700.690	-.003	19700.282	19700.280	.002
30.5	19700.968	19700.972	-.004	19700.553	19700.552	.001
31.5	19701.254	19701.260	-.006	19700.828	19700.829	-.001
32.5	-	19701.554		19701.115	19701.112	.003
33.5	-	19701.853		19701.403	19701.401	.002
34.5	19702.159	19702.159	.000	19701.694	19701.697	-.003
35.5	19702.467	19702.470	-.003	19701.994	19701.997	-.003
36.5	19702.790	19702.787	.003	19702.302	19702.304	-.002
37.5	19703.111	19703.111	.000	19702.620	19702.617	.003
38.5	19703.423	19703.440	-.017**	19702.937	19702.936	.001
39.5	19703.771	19703.775	-.004	19703.263	19703.261	.002
40.5	19704.105	19704.116	-.011	-	19703.591	
41.5	19704.457	19704.463	-.006	19703.911	19703.928	-.017**
42.5	19704.815	19704.816	-.001	19704.260	19704.270	-.010
43.5	19705.176	19705.174	.002	19704.614	19704.618	-.004
44.5	19705.543	19705.539	.004	19704.971	19704.972	-.001
45.5	19705.916	19705.910	.006	19705.341	19705.333	.008
46.5	19706.284	19706.286	-.002	19705.705	19705.699	.006
47.5	19706.665	19706.669	-.004	19706.073	19706.071	.002
48.5	19707.054	19707.057	-.003	19706.449	19706.449	.000
49.5	19707.447	19707.452	-.005	19706.831	19706.833	-.002
50.5	19707.852	19707.852	.000	19707.220	19707.222	-.002

51.5	19708.261	19708.258	.003	19707.615	19707.618	-.003
52.5	19708.669	19708.670	-.001	19708.017	19708.020	-.003
53.5	19709.087	19709.088	-.001	19708.425	19708.428	-.003
54.5	19709.508	19709.513	-.005	19708.840	19708.841	-.001
55.5	19709.945	19709.942	.003	19709.259	19709.261	-.002
56.5	19710.378	19710.378	.000	19709.683	19709.686	-.003
57.5	19710.817	19710.820	-.003	19710.120	19710.117	.003
58.5	19711.268	19711.268	.000	19710.552	19710.555	-.003
59.5	19711.720	19711.722	-.002	19710.995	19710.998	-.003
60.5	19712.179	19712.182	-.003	19711.448	19711.447	.001
61.5	19712.647	19712.647	.000	19711.903	19711.903	.000
62.5	19713.118	19713.119	-.001	19712.363	19712.364	-.001
63.5	19713.595	19713.597	-.002	19712.830	19712.831	-.001
64.5	19714.080	19714.080	.000	19713.302	19713.304	-.002
65.5	19714.570	19714.570	.000	19713.781	19713.783	-.002
66.5	19715.067	19715.065	.002	19714.268	19714.268	.000
67.5	19715.565	19715.567	-.002	19714.759	19714.759	.000
68.5	19716.073	19716.074	-.001	19715.256	19715.256	.000
69.5	19716.585	19716.587	-.002	19715.758	19715.759	-.001
70.5	19717.106	19717.107	-.001	19716.267	19716.267	.000
71.5	19717.633	19717.632	.001	19716.781	19716.782	-.001
72.5	19718.160	19718.163	-.003	19717.303	19717.303	.000
73.5	19718.697	19718.701	-.004	19717.830	19717.830	.000
74.5	19719.242	19719.244	-.002	19718.362	19718.363	-.001
75.5	19719.794	19719.793	.001	19718.902	19718.901	.001
76.5	19720.349	19720.348	.001	19719.448	19719.446	.002
77.5	19720.914	19720.910	.004	19719.999	19719.997	.002
78.5	19721.481	19721.477	.004	19720.555	19720.553	.002
79.5	19722.057	19722.050	.007	19721.121	19721.116	.005
80.5	19722.632	19722.629	.003	19721.684	19721.685	-.001
81.5	-	19723.214		19722.259	19722.259	.000
82.5	-	19723.806		19722.839	19722.840	-.001

0-1 Band

	$P_{11}(ee)$			$Q_{12}(ef)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
50.5	-	17610.107		17610.730	17610.718	.012
51.5	17610.487	17610.489	-.002	-	17611.112	
52.5	-	17610.879		-	17611.514	
53.5	-	17611.276		17611.934	17611.922	.012
54.5	17611.679	17611.680	-.001	-	17612.339	
55.5	-	17612.092		-	17612.762	
56.5	-	17612.511		17613.191	17613.193	-.002
57.5	17612.932	17612.938	-.006	-	17613.631	
58.5	-	17613.371		-	17614.077	
59.5	-	17613.813		17614.535	17614.530	.005
60.5	17614.254	17614.261	-.007	-	17614.990	
61.5	-	17614.717		-	17615.458	
62.5	-	17615.180		17615.933	17615.933	.000
63.5	17615.633	17615.651	-.018	-	17616.415	
64.5	-	17616.129		17616.901	17616.905	-.004
65.5	17616.587	17616.614	-.027	-	17617.402	
66.5	-	17617.107		17617.906	17617.907	-.001

67.5	17617.579	17617.607	-.028	-	17618.419	
68.5	-	17618.115		-	17618.938	
69.5	-	17618.629		17619.448	17619.465	-.017
70.5	17619.107	17619.152	-.045	-	17619.999	
71.5	-	17619.681		17620.551	17620.540	.011
72.5	17620.390	17620.219	.171**	-	17621.089	
73.5	-	17620.763		17621.622	17621.646	-.024
74.5	17621.248	17621.315	-.067**	-	17622.209	
75.5	-	17621.874		17622.770	17622.781	-.011
76.5	17622.376	17622.441	-.065**	-	17623.359	
77.5	-	17623.015		17623.925	17623.945	-.020
78.5	17623.512	17623.597	-.085**	-	17624.538	
79.5	-	17624.185		17625.105	17625.139	-.034
80.5	17624.686	17624.782	-.096**	-	17625.748	
81.5	-	17625.386		17626.336	17626.363	-.027
82.5	17625.905	17625.997	-.092**	-	17626.986	
83.5	-	17626.616		17627.597	17627.617	-.020
84.5	17627.152	17627.242	-.090**	-	17628.255	
85.5	-	17627.875		17628.880	17628.900	-.020
86.5	17628.425	17628.516	-.091**	-	17629.553	
87.5	-	17629.165		17630.182	17630.213	-.031
88.5	17629.696	17629.820	-.124**	-	17630.881	
89.5	-	17630.484		17631.535	17631.556	-.021
90.5	17631.044	17631.155	-.111**	-	17632.239	
91.5	-	17631.833		17632.905	17632.929	-.024
92.5	17632.400	17632.519	-.119**	-	17633.627	
93.5	-	17633.212		17634.316	17634.332	-.016
94.5	17633.768	17633.912	-.144**	-	17635.045	

$\mathrm{Q}_{11}(ef)$ $\mathrm{R}_{12}(ff)$

J	OBS	CALC	DIFF	OBS	CALC	DIFF
89.5	-	17628.394		17629.442	17629.444	-.002
90.5	17629.038	17629.042	-.004	-	17630.104	
91.5	-	17629.697		17630.768	17630.771	-.003
92.5	17630.347	17630.360	-.013	-	17631.446	
93.5	-	17631.031		-	17632.128	
94.5	-	17631.709		-	17632.818	
95.5	-	17632.394		-	17633.516	
96.5	-	17633.087		-	17634.221	
97.5	-	17633.788		-	17634.933	
98.5	-	17634.496		17635.645	17635.653	-.008
99.5	17635.204	17635.212	-.008	-	17636.381	
100.5	-	17635.935		17637.115	17637.116	-.001
101.5	17636.661	17636.665	-.004	-	17637.859	
102.5	-	17637.404		17638.609	17638.609	.000
103.5	17638.141	17638.149	-.008	17639.367	17639.367	.000
104.5	17638.862	17638.903	-.041	17640.127	17640.132	-.005
105.5	17639.655	17639.663	-.008	17640.896	17640.905	-.009
106.5	17640.420	17640.432	-.012	17640.920	17641.685	-.765**
107.5	17640.272	17641.208	-.936**	17642.463	17642.473	-.010
108.5	17641.974	17641.991	-.017	-	17643.268	

0-2 Band

$\mathrm{P}_{11}(ee)$ $\mathrm{Q}_{12}(ef)$

J	OBS	CALC	DIFF	OBS	CALC	DIFF
55.5	-	17325.281		17326.012	17325.989	.023
56.5	-	17325.744		-	17326.465	
57.5	-	17326.215		17326.967	17326.948	.019
58.5	-	17326.694		-	17327.440	
59.5	-	17327.182		17327.995	17327.940	.055**
60.5	-	17327.678		-	17328.448	
61.5	-	17328.181		17328.977	17328.965	.012
62.5	-	17328.693		-	17329.489	
63.5	-	17329.214		17330.017	17330.022	-.005
64.5	-	17329.742		-	17330.563	
65.5	-	17330.278		17331.112	17331.112	.000
66.5	-	17330.823		-	17331.669	
67.5	-	17331.376		17332.173	17332.234	-.061**
68.5	-	17331.937		-	17332.808	
69.5	-	17332.506		17333.640	17333.390	.250**
70.5	-	17333.084		-	17333.980	
71.5	-	17333.669		17334.571	17334.578	-.007
72.5	-	17334.263		-	17335.184	
73.5	-	17334.865		17335.782	17335.799	-.017
74.5	-	17335.475		-	17336.422	
75.5	-	17336.094		17337.027	17337.052	-.025
76.5	-	17336.720		-	17337.692	
77.5	-	17337.355		17338.320	17338.339	-.019
78.5	-	17337.998		-	17338.995	
79.5	-	17338.650		17339.641	17339.659	-.018
80.5	-	17339.309		-	17340.331	
81.5	-	17339.977		17340.942	17341.011	-.069**
82.5	-	17340.653		-	17341.700	
83.5	-	17341.337		17342.331	17342.397	-.066**
84.5	-	17342.030		-	17343.102	
85.5	-	17342.731		17343.778	17343.815	-.037
86.5	-	17343.440		17344.483	17344.537	-.054**
87.5	-	17344.157		17345.206	17345.267	-.061**
88.5	-	17344.882		17345.941	17346.005	-.064**
89.5	-	17345.616		17346.683	17346.751	-.068**
90.5	-	17346.358		-	17347.506	
91.5	-	17347.109		17348.214	17348.269	-.055**
92.5	-	17347.867		17349.159	17349.040	.119**
93.5	-	17348.634		17349.761	17349.820	-.059**
94.5	-	17349.410		17350.569	17350.608	-.039
95.5	-	17350.193		17351.361	17351.404	-.043

$Q_{11}(ef)$ $R_{12}(ff)$

J	OBS	CALC	DIFF	OBS	CALC	DIFF
89.5	-	17343.526		17344.628	17344.638	-.010
90.5	17344.235	17344.245	-.010	17345.354	17345.370	-.016
91.5	17344.973	17344.973	.000	17346.091	17346.111	-.020
92.5	17345.702	17345.709	-.007	17347.150	17346.859	.291**
93.5	17346.446	17346.453	-.007	-	17347.616	
94.5	-	17347.206		17348.367	17348.382	-.015
95.5	17347.955	17347.967	-.012	-	17349.155	

96.5	-	17348.736		-	17349.937	
97.5	-	17349.514		-	17350.727	
98.5	-	17350.300		17351.500	17351.526	-.026
99.5	17351.080	17351.094	-.014	17352.319	17352.333	-.014
100.5	17351.880	17351.897	-.017	17353.122	17353.148	-.026
101.5	17352.692	17352.708	-.016	17353.946	17353.972	-.026
102.5	17353.510	17353.527	-.017	17354.775	17354.804	-.029
103.5	17354.332	17354.355	-.023	17355.647	17355.644	.003
104.5	17355.203	17355.191	.012	17356.501	17356.493	.008
105.5	17356.043	17356.035	.008	17357.345	17357.350	-.005
106.5	17356.880	17356.888	-.008	17358.206	17358.216	-.010
107.5	17357.730	17357.749	-.019	17359.050	17359.090	-.040
108.5	17358.593	17358.619	-.026	-	17359.972	

0-3 Band

	$P_{11}(ee)$			$Q_{12}(ef)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
55.5	-	17040.198		17040.930	17040.945	-.015
56.5	17040.682	17040.705	-.023	-	17041.465	
57.5	-	17041.221		17041.977	17041.995	-.018
58.5	17041.735	17041.746	-.011	-	17042.533	
59.5	-	17042.280		17043.068	17043.080	-.012
60.5	17042.811	17042.823	-.012	-	17043.636	
61.5	-	17043.375		17044.191	17044.201	-.010
62.5	17043.921	17043.935	-.014	-	17044.775	
63.5	-	17044.505		17045.349	17045.357	-.008
64.5	17045.071	17045.084	-.013	-	17045.949	
65.5	-	17045.671		17046.494	17046.550	-.056**
66.5	17046.271	17046.268	.003	-	17047.160	
67.5	-	17046.873		17047.771	17047.779	-.008
68.5	17047.478	17047.488	-.010	-	17048.407	
69.5	-	17048.112		17049.034	17049.043	-.009
70.5	17048.730	17048.744	-.014	-	17049.689	
71.5	-	17049.386		17050.330	17050.344	-.014
72.5	17050.021	17050.036	-.015	-	17051.008	
73.5	-	17050.696		17051.703	17051.681	.022
74.5	17051.360	17051.364	-.004	-	17052.362	
75.5	-	17052.042		17053.032	17053.053	-.021
76.5	17052.710	17052.729	-.019	-	17053.753	
77.5	-	17053.424		17054.443	17054.462	-.019
78.5	17054.110	17054.129	-.019	-	17055.180	
79.5	-	17054.843		17055.903	17055.907	-.004
80.5	17055.561	17055.565	-.004	-	17056.643	
81.5	-	17056.297		17057.377	17057.388	-.011
82.5	17057.022	17057.038	-.016	-	17058.142	
83.5	-	17057.788		17058.911	17058.905	.006
84.5	17058.551	17058.547	.004	-	17059.678	

Appendix 2

YbS Line Positions

Rotational transitions in the $A0^{-}-X0^{-}$ and $B0^{-}-X0^{-}$ systems of ^{176}YbS, ^{174}YbS and ^{172}YbS. For each transition, the tables show the assigned rotational quantum number J, the measured line position in cm^{-1} and the residual between the observed and calculated values. Lines marked with * were excluded in the least-squares fit.

^{174}YbS 0 - 0 Band A-X System

	P Branch			R Branch		
J	Obs	Calc	Diff	Obs	Calc	Diff
0	-	.000		17541.611	17541.609	.002
1	17541.168	17541.167	.001	17541.824	17541.822	.002
2	17540.940	17540.937	.003	17542.029	17542.030	-.001
3	17540.705	17540.703	.002	17542.235	17542.232	.003
4	17540.463	17540.463	.000	17542.429	17542.429	.000
5	17540.218	17540.217	.001	17542.622	17542.620	.002
6	17539.965	17539.966	-.001	17542.810	17542.806	.004
7	17539.713	17539.709	.004	17542.985	17542.986	-.001
8	17539.446	17539.447	-.001	17543.162	17543.161	.001
9	17539.178	17539.180	-.002	17543.332	17543.330	.002
10	17538.908	17538.907	.001	17543.501	17543.494	.007*
11	17538.632	17538.629	.003	17543.659	17543.653	.006*
12	17538.344	17538.345	-.001	17543.817	17543.806	.011*
13	17538.056	17538.056	.000	17543.962	17543.953	.009*
14	17537.758	17537.761	-.003*	17544.101	17544.095	.006*
15	17537.461	17537.461	.000	17544.237	17544.232	.005*
16	17537.156	17537.156	.000	17544.366	17544.363	.003*
17	17536.845	17536.845	.000	17544.494	17544.489	.005*
18	17536.530	17536.529	.001	17544.615	17544.609	.006*
19	17536.204	17536.207	-.003*	17544.729	17544.724	.005*
20	17535.878	17535.880	-.002*	17544.840	17544.833	.007*
21	17535.546	17535.547	-.001*	17544.943	17544.937	.006*
22	17535.209	17535.209	.000*	17545.038	17545.035	.003*
23	17534.862	17534.865	-.003*	17545.134	17545.128	.006*
24	17534.513	17534.516	-.003*	17545.221	17545.215	.006*
25	17534.159	17534.162	-.003*	-	17545.297	
26	17533.795	17533.802	-.007*	-	17545.373	
27	17533.432	17533.437	-.005*	-	17545.443	
28	17533.061	17533.066	-.005*	-	17545.509	
29	17532.684	17532.689	-.005*	-	17545.568	
30	17532.303	17532.307	-.004*	-	17545.622	
31	17531.914	17531.920	-.006*	-	17545.671	
32	17531.521	17531.527	-.006*	-	17545.714	
33	17531.120	17531.129	-.009*	-	17545.751	
34	17530.715	17530.725	-.010*	-	17545.783	
35	17530.303	17530.316	-.013*	-	17545.809	
36	17529.901	17529.901	.000	-	17545.830	
37	17529.480	17529.481	-.001	-	17545.845	
38	17529.054	17529.055	-.001	-	17545.854	
39	17528.621	17528.624	-.003	-	17545.858	
40	17528.186	17528.187	-.001	-	17545.857	
41	17527.746	17527.745	.001	-	17545.849	
42	17527.296	17527.297	-.001	-	17545.836	
43	17526.848	17526.844	.004	-	17545.818	
44	17526.385	17526.385	.000	-	17545.794	
45	17525.921	17525.921	.000	-	17545.764	
46	17525.451	17525.451	.000	-	17545.728	
47	17524.976	17524.975	.001	-	17545.687	
48	17524.495	17524.494	.001	-	17545.640	
49	17524.005	17524.007	-.002	-	17545.588	

50	17523.517	17523.515	.002	-	17545.530	
51	17523.016	17523.017	-.001	-	17545.466	
52	17522.513	17522.514	-.001	-	17545.396	
53	17522.009	17522.005	.004	-	17545.321	
54	17521.491	17521.491	.000	-	17545.240	
55	17520.974	17520.970	.004	-	17545.153	
56	17520.445	17520.445	.000	-	17545.060	
57	17519.917	17519.913	.004	-	17544.962	
58	17519.375	17519.376	-.001	-	17544.858	
59	17518.835	17518.834	.001	-	17544.748	
60	17518.285	17518.285	.000	-	17544.633	
61	17517.731	17517.731	.000	-	17544.512	
62	17517.174	17517.172	.002	-	17544.384	
63	17516.608	17516.606	.002	-	17544.251	
64	17516.009	17516.035	-.026*	-	17544.113	
65	-	17515.459		-	17543.968	
66	-	17514.876		-	17543.818	
67	-	17514.288		-	17543.661	
68	-	17513.695		17543.501	17543.499	.002
69	-	17513.095		17543.332	17543.331	.001
70	-	17512.490		17543.162	17543.157	.005*
71	-	17511.879		17542.985	17542.977	.008*
72	-	17511.262		17542.798	17542.791	.007*
73	-	17510.640		17542.606	17542.600	.006*
74	-	17510.011		17542.407	17542.402	.005*
75	-	17509.377		17542.202	17542.198	.004*
76	-	17508.738		17541.993	17541.989	.004*
77	-	17508.092		17541.776	17541.773	.003
78	-	17507.441		17541.552	17541.552	.000
79	-	17506.783		17541.326	17541.324	.002
80	-	17506.120		17541.091	17541.091	.000
81	-	17505.451		17540.852	17540.851	.001
82	-	17504.777		17540.604	17540.605	-.001
83	-	17504.096		17540.349	17540.354	-.005
84	-	17503.409		17540.093	17540.096	-.003

0-1 Band

		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
0	-	.000		-	17177.227	
1	17176.786	17176.785	.001	-	17177.441	
2	17176.559	17176.558	.001	-	17177.650	
3	17176.324	17176.325	-.001	-	17177.854	
4	17176.089	17176.088	.001	-	17178.054	
5	17175.847	17175.847	.000	-	17178.250	
6	17175.600	17175.601	-.001	-	17178.440	
7	17175.351	17175.350	.001	-	17178.627	
8	17175.096	17175.094	.002	-	17178.808	
9	17174.835	17174.834	.001	-	17178.985	
10	17174.571	17174.570	.001	-	17179.157	
11	17174.300	17174.301	-.001	17179.325	17179.325	.000
12	17174.025	17174.027	-.002	17179.481	17179.487	-.006
13	17173.746	17173.748	-.002	17179.640	17179.646	-.006

14	17173.465	17173.465	.000	17179.793	17179.799	-.006
15	17173.177	17173.178	-.001	17179.944	17179.948	-.004
16	17172.885	17172.885	.000	17180.090	17180.093	-.003
17	17172.587	17172.588	-.001	17180.230	17180.232	-.002
18	17172.285	17172.287	-.002	17180.365	17180.367	-.002
19	17171.982	17171.981	.001	17180.493	17180.497	-.004
20	17171.670	17171.670	.000	17180.621	17180.623	-.002
21	17171.355	17171.354	.001	17180.741	17180.744	-.003
22	17171.033	17171.034	-.001	17180.861	17180.860	.001
23	17170.705	17170.710	-.005	17180.969	17180.972	-.003
24	17170.377	17170.380	-.003	17181.076	17181.079	-.003
25	17170.043	17170.046	-.003	17181.178	17181.181	-.003
26	17169.709	17169.708	.001	17181.282	17181.279	.003
27	17169.371	17169.365	.006	17181.378	17181.371	.007*
28	17169.025	17169.017	.008*	17181.459	17181.460	-.001
29	17168.665	17168.664	.001	17181.538	17181.543	-.005
30	17168.308	17168.307	.001	17181.622	17181.622	.000
31	17167.946	17167.945	.001	17181.682	17181.696	-.014*
32	17167.580	17167.578	.002	17181.767	17181.765	.002
33	17167.206	17167.207	-.001	17181.832	17181.829	.003
34	17166.832	17166.831	.001	17181.886	17181.889	-.003
35	17166.452	17166.451	.001	17181.940	17181.944	-.004
36	17166.067	17166.066	.001	17181.994	17181.994	.000
37	17165.679	17165.676	.003	17182.040	17182.040	.000
38	17165.281	17165.281	.000	17182.078	17182.080	-.002
39	17164.880	17164.882	-.002	17182.117	17182.116	.001
40	17164.478	17164.478	.000	17182.144	17182.147	-.003
41	17164.068	17164.069	-.001	-	17182.174	
42	17163.659	17163.656	.003	17182.197	17182.195	.002
43	17163.237	17163.238	-.001	-	17182.212	
44	17162.816	17162.815	.001	-	17182.224	
45	17162.387	17162.388	-.001	-	17182.231	
46	17161.953	17161.955	-.002	-	17182.233	
47	17161.517	17161.518	-.001	-	17182.230	
48	17161.076	17161.077	-.001	-	17182.223	
49	17160.630	17160.630	.000	-	17182.210	
50	17160.179	17160.179	.000	-	17182.193	
51	17159.723	17159.723	.000	-	17182.171	
52	17159.259	17159.262	-.003	-	17182.144	
53	17158.795	17158.797	-.002	17182.120	17182.112	.008*
54	17158.327	17158.326	.001	17182.071	17182.075	-.004
55	17157.852	17157.851	.001	17182.035	17182.034	.001
56	17157.369	17157.371	-.002	17181.988	17181.987	.001
57	17156.887	17156.887	.000	17181.933	17181.936	-.003
58	17156.397	17156.397	.000	17181.880	17181.879	.001
59	17155.902	17155.903	-.001	17181.827	17181.818	.009*
60	17155.405	17155.403	.002	17181.752	17181.751	.001
61	17154.900	17154.899	.001	17181.679	17181.680	-.001
62	17154.390	17154.391	-.001	17181.604	17181.603	.001
63	17153.876	17153.877	-.001	17181.520	17181.522	-.002
64	17153.357	17153.358	-.001	17181.439	17181.435	.004
65	17152.834	17152.835	-.001	17181.348	17181.344	.004
66	17152.304	17152.306	-.002	17181.248	17181.248	.000
67	17151.770	17151.773	-.003	17181.145	17181.146	-.001
68	17151.234	17151.235	-.001	17181.040	17181.039	.001
69	17150.689	17150.692	-.003	17180.930	17180.928	.002
70	17150.141	17150.144	-.003	17180.811	17180.811	.000

71	17149.590	17149.591	-.001	17180.683	17180.689	-.006
72	17149.033	17149.033	.000	17180.566	17180.562	.004
73	17148.471	17148.470	.001	17180.428	17180.430	-.002
74	17147.907	17147.903	.004	17180.295	17180.293	.002
75	17147.334	17147.330	.004	17180.152	17180.151	.001
76	17146.754	17146.752	.002	17180.002	17180.003	-.001
77	17146.169	17146.169	.000	17179.844	17179.851	-.007
78	17145.579	17145.582	-.003	17179.688	17179.693	-.005
79	-	17144.989		17179.531	17179.530	.001
80	-	17144.391		17179.366	17179.361	.005
81	-	17143.788		17179.194	17179.188	.006
82	-	17143.180		17179.009	17179.009	.000
83	-	17142.568		17178.825	17178.825	.000
84	-	17141.950		17178.637	17178.636	.001
85	-	17141.326		17178.443	17178.442	.001
86	-	17140.698		-	17178.242	
87	-	17140.065		-	17178.037	
88	-	17139.427		17177.826	17177.826	.000
89	-	17138.783		17177.611	17177.610	.001
90	-	17138.134		17177.387	17177.389	-.002
91	-	17137.480		17177.162	17177.163	-.001
92	-	17136.821		17176.928	17176.931	-.003
93	-	17136.157		17176.689	17176.693	-.004
94	-	17135.488		17176.453	17176.451	.002
95	-	17134.813		17176.206	17176.202	.004
96	-	17134.133		17175.951	17175.949	.002
97	-	17133.448		17175.690	17175.690	.000
98	-	17132.758		17175.427	17175.425	.002
99	-	17132.062		17175.156	17175.155	.001

1-1 Band

		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
0	-	.000		17501.861	17501.865	-.004
1	17501.424	17501.424	.000	17502.071	17502.078	-.007
2	17501.200	17501.196	.004	17502.281	17502.285	-.004
3	17500.959	17500.962	-.003	17502.481	17502.487	-.006
4	17500.722	17500.723	-.001	17502.684	17502.684	.000
5	17500.483	17500.480	.003	17502.878	17502.876	.002
6	17500.227	17500.231	-.004	17503.060	17503.063	-.003
7	17499.977	17499.976	.001	17503.244	17503.244	.000
8	17499.715	17499.717	-.002	17503.420	17503.420	.000
9	17499.450	17499.452	-.002	17503.592	17503.591	.001
10	17499.181	17499.182	-.001	17503.754	17503.757	-.003
11	17498.907	17498.907	.000	17503.916	17503.917	-.001
12	17498.627	17498.627	.000	17504.073	17504.073	.000
13	17498.340	17498.341	-.001	17504.223	17504.223	.000
14	17498.047	17498.051	-.004	17504.367	17504.368	-.001
15	17497.753	17497.755	-.002	17504.507	17504.507	.000
16	17497.452	17497.454	-.002	17504.639	17504.642	-.003
17	17497.144	17497.147	-.003	17504.767	17504.771	-.004
18	17496.836	17496.836	.000	17504.894	17504.895	-.001

19	17496.519	17496.519	.000	17505.009	17505.013	-.004
20	17496.195	17496.197	-.002	17505.126	17505.127	-.001
21	17495.869	17495.870	-.001	17505.231	17505.235	-.004
22	17495.536	17495.538	-.002	-	17505.338	
23	17495.200	17495.200	.000	17505.433	17505.435	-.002
24	17494.856	17494.858	-.002	17505.510	17505.528	-.018*
25	17494.510	17494.510	.000	17505.611	17505.615	-.004
26	17494.155	17494.157	-.002	17505.690	17505.697	-.007
27	17493.798	17493.798	.000	17505.766	17505.773	-.007
28	17493.433	17493.435	-.002	17505.838	17505.845	-.007
29	17493.065	17493.066	-.001	-	17505.911	
30	17492.691	17492.692	-.001	-	17505.971	
31	17492.309	17492.313	-.004	-	17506.027	
32	17491.926	17491.928	-.002	-	17506.077	
33	17491.538	17491.538	.000	-	17506.122	
34	17491.142	17491.144	-.002	-	17506.161	
35	17490.743	17490.744	-.001	-	17506.196	
36	17490.339	17490.338	.001	-	17506.225	
37	17489.928	17489.928	.000	-	17506.248	
38	17489.512	17489.512	.000	-	17506.267	
39	17489.095	17489.091	.004	-	17506.280	
40	17488.663	17488.664	-.001	-	17506.287	
41	17488.232	17488.233	-.001	-	17506.290	
42	17487.795	17487.796	-.001	-	17506.287	
43	17487.353	17487.354	-.001	-	17506.279	
44	17486.907	17486.907	.000	-	17506.265	
45	17486.456	17486.454	.002	-	17506.246	
46	17485.996	17485.997	-.001	-	17506.222	
47	17485.530	17485.534	-.004	-	17506.192	
48	17485.067	17485.065	.002	-	17506.157	
49	17484.592	17484.592	.000	-	17506.116	
50	17484.112	17484.113	-.001	-	17506.070	
51	17483.629	17483.629	.000	-	17506.019	
52	17483.137	17483.139	-.002	-	17505.963	
53	17482.642	17482.645	-.003	-	17505.901	
54	17482.145	17482.145	.000	-	17505.833	
55	17481.639	17481.639	.000	-	17505.760	
56	17481.130	17481.129	.001	-	17505.682	
57	17480.613	17480.613	.000	-	17505.598	
58	17480.094	17480.092	.002	-	17505.509	
59	17479.563	17479.565	-.002	-	17505.415	
60	17479.034	17479.034	.000	-	17505.315	
61	17478.495	17478.497	-.002	-	17505.209	
62	17477.953	17477.954	-.001	-	17505.098	
63	17477.404	17477.406	-.002	-	17504.982	
64	17476.854	17476.853	.001	-	17504.860	
65	17476.296	17476.295	.001	-	17504.733	
66	17475.731	17475.731	.000	-	17504.600	
67	17475.161	17475.162	-.001	17504.446	17504.462	-.016*
68	-	17474.588		17504.299	17504.318	-.019*
69	-	17474.008		17504.173	17504.169	.004
70	-	17473.423		17504.005	17504.014	-.009
71	-	17472.832		17503.853	17503.854	-.001
72	-	17472.236		17503.686	17503.688	-.002
73	-	17471.635		17503.519	17503.516	.003
74	-	17471.028		17503.339	17503.339	.000
75	-	17470.416		17503.156	17503.157	-.001

76	-	17469.798		17502.968	17502.969	-.001
77	-	17469.176		17502.776	17502.775	.001
78	-	17468.547		17502.576	17502.576	.000
79	-	17467.913		17502.373	17502.371	.002
80	-	17467.274		17502.159	17502.161	-.002
81	-	17466.630		17501.943	17501.944	-.001
82	-	17465.980		17501.724	17501.723	.001
83	-	17465.324		17501.497	17501.496	.001
84	-	17464.663		17501.264	17501.263	.001

1-2 Band

	P Branch			R Branch		
J	Obs	Calc	Diff	Obs	Calc	Diff
0	-	.000		17139.815	17139.814	.001
1	17139.373	17139.373	.000	17140.035	17140.027	.008
2	17139.153	17139.147	.006	17140.240	17140.236	.004
3	17138.920	17138.916	.004	17140.445	17140.441	.004
4	17138.681	17138.680	.001	17140.644	17140.641	.003
5	17138.444	17138.441	.003	17140.841	17140.837	.004
6	17138.200	17138.196	.004	-	17141.029	
7	17137.950	17137.948	.002	-	17141.216	
8	17137.691	17137.695	-.004	17141.403	17141.399	.004
9	17137.440	17137.438	.002	17141.578	17141.577	.001
10	17137.180	17137.176	.004	17141.750	17141.751	-.001
11	17136.912	17136.910	.002	17141.919	17141.920	-.001
12	17136.641	17136.640	.001	17142.090	17142.085	.005
13	17136.369	17136.365	.004	17142.249	17142.246	.003
14	17136.090	17136.086	.004	17142.406	17142.403	.003
15	17135.804	17135.802	.002	17142.560	17142.554	.006
16	17135.516	17135.514	.002	17142.704	17142.702	.002
17	17135.226	17135.222	.004	17142.851	17142.845	.006
18	17134.929	17134.925	.004	17142.984	17142.984	.000
19	17134.626	17134.624	.002	17143.119	17143.118	.001
20	17134.321	17134.318	.003	17143.253	17143.248	.005
21	17134.010	17134.009	.001	17143.378	17143.373	.005
22	17133.695	17133.694	.001	17143.494	17143.494	.000
23	17133.379	17133.376	.003	17143.612	17143.611	.001
24	17133.056	17133.053	.003	17143.721	17143.723	-.002
25	17132.727	17132.725	.002	17143.833	17143.831	.002
26	17132.396	17132.394	.002	-	17143.934	
27	17132.059	17132.058	.001	17144.029	17144.033	-.004
28	17131.721	17131.717	.004	17144.130	17144.127	.003
29	17131.373	17131.372	.001	17144.210	17144.217	-.007
30	17131.020	17131.023	-.003	17144.316	17144.302	.014*
31	17130.667	17130.669	-.002	17144.380	17144.383	-.003
32	17130.309	17130.311	-.002	-	17144.460	
33	17129.945	17129.948	-.003	17144.532	17144.532	.000
34	17129.580	17129.581	-.001	17144.607	17144.599	.008
35	17129.210	17129.210	.000	17144.666	17144.662	.004
36	17128.834	17128.834	.000	-	17144.721	
37	17128.460	17128.454	.006	17144.777	17144.775	.002
38	17128.075	17128.070	.005	17144.825	17144.825	.000
39	17127.682	17127.681	.001	17144.871	17144.870	.001

40	17127.290	17127.287	.003	17144.908	17144.910	-.002
41	-	17126.890		17144.947	17144.947	.000
42	17126.489	17126.488	.001	-	17144.978	
43	17126.085	17126.081	.004	17145.003	17145.005	-.002
44	17125.673	17125.670	.003	-	17145.028	
45	17125.253	17125.254	-.001	-	17145.046	
46	17124.838	17124.835	.003	-	17145.059	
47	17124.410	17124.410	.000	-	17145.068	
48	17123.984	17123.982	.002	-	17145.073	
49	17123.548	17123.548	.000	-	17145.073	
50	17123.112	17123.111	.001	-	17145.068	
51	17122.670	17122.669	.001	-	17145.059	
52	17122.224	17122.222	.002	-	17145.045	
53	17121.771	17121.771	.000	-	17145.027	
54	17121.318	17121.316	.002	-	17145.004	
55	17120.856	17120.856	.000	17144.980	17144.977	.003
56	17120.392	17120.391	.001	-	17144.945	
57	-	17119.923		17144.905	17144.908	-.003
58	-	17119.449		17144.867	17144.867	.000
59	-	17118.972		17144.823	17144.821	.002
60	-	17118.489		17144.775	17144.770	.005
61	-	17118.003		17144.714	17144.715	-.001
62	-	17117.511		17144.655	17144.656	-.001
63	-	17117.016		17144.598	17144.591	.007
64	-	17116.515		17144.526	17144.522	.004
65	-	17116.011		17144.436	17144.449	-.013*
66	-	17115.501		17144.368	17144.370	-.002
67	-	17114.988		17144.285	17144.287	-.002
68	-	17114.469		17144.200	17144.200	.000
69	-	17113.947		17144.110	17144.108	.002
70	-	17113.419		17144.008	17144.011	-.003
71	-	17112.887		17143.907	17143.909	-.002
72	-	17112.351		17143.801	17143.803	-.002
73	-	17111.810		17143.690	17143.692	-.002
74	-	17111.265		17143.574	17143.576	-.002
75	-	17110.715		17143.460	17143.455	.005
76	-	17110.160		17143.330	17143.330	.000
77	-	17109.601		17143.198	17143.200	-.002
78	-	17109.037		17143.066	17143.066	.000
79	-	17108.469		17142.927	17142.926	.001
80	-	17107.896		17142.780	17142.782	-.002
81	-	17107.318		-	17142.633	
82	-	17106.736		17142.478	17142.479	-.001
83	-	17106.149		17142.325	17142.321	.004
84	-	17105.558		17142.154	17142.158	-.004
85	-	17104.962		17141.989	17141.989	.000
86	-	17104.362		17141.817	17141.817	.000
87	-	17103.756		17141.640	17141.639	.001
88	-	17103.147		-	17141.456	
89	-	17102.532		-	17141.269	
90	-	17101.913		17141.075	17141.077	-.002

2-2 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
1	-	17467.532		17468.176	17468.183	-.007**
2	17467.307	17467.304	.003	17468.384	17468.390	-.006**
3	17467.072	17467.072	.000	17468.584	17468.591	-.007**
4	17466.836	17466.834	.002	17468.792	17468.788	.004
5	17466.593	17466.591	.002	17468.978	17468.979	-.001
6	17466.345	17466.343	.002	17469.169	17469.165	.004
7	17466.091	17466.090	.001	17469.347	17469.346	.001
8	17465.837	17465.831	.006	17469.523	17469.522	.001
9	17465.570	17465.568	.002	17469.694	17469.692	.002
10	17465.298	17465.299	-.001	17469.858	17469.857	.001
11	17465.023	17465.025	-.002	17470.016	17470.018	-.002
12	17464.748	17464.746	.002	17470.173	17470.173	.000
13	17464.463	17464.462	.001	17470.321	17470.322	-.001
14	17464.173	17464.173	.000	17470.470	17470.467	.003
15	17463.879	17463.878	.001	17470.609	17470.606	.003
16	17463.583	17463.579	.004	17470.742	17470.741	.001
17	17463.274	17463.274	.000	17470.874	17470.870	.004
18	17462.962	17462.964	-.002	17470.997	17470.994	.003
19	17462.650	17462.649	.001	17471.115	17471.112	.003
20	17462.327	17462.328	-.001	17471.226	17471.226	.000
21	17462.003	17462.003	.000	17471.334	17471.334	.000
22	17461.676	17461.672	.004	17471.439	17471.437	.002
23	17461.342	17461.336	.006	17471.533	17471.535	-.002
24	17460.998	17460.995	.003	17471.629	17471.627	.002
25	17460.652	17460.649	.003	17471.713	17471.714	-.001
26	17460.300	17460.298	.002	17471.795	17471.796	-.001
27	17459.940	17459.941	-.001	17471.873	17471.873	.000
28	17459.580	17459.579	.001	17471.943	17471.944	-.001
29	17459.212	17459.212	.000	17472.009	17472.010	-.001
30	17458.840	17458.840	.000	17472.076	17472.070	.006
31	17458.464	17458.462	.002	17472.126	17472.125	.001
32	17458.080	17458.079	.001	-	17472.174	
33	17457.690	17457.690	.000	-	17472.216	
34	17457.297	17457.296	.001	-	17472.251	
35	17456.894	17456.895	-.001	-	17472.277	
36	17456.484	17456.487	-.003	-	17472.287	
37	17456.070	17456.069	.001	-	17472.252	
38	17455.637	17455.636	.001	-	17472.539	
39	17455.168	17455.158	.010	-	17472.472	
40	17455.006	17455.002	.004**	-	17472.457	
41	17454.501	17454.492	.009	-	17472.450	
42	17454.035	17454.034	.001	-	17472.443	
43	17453.584	17453.584	.000	-	17472.433	
44	17453.134	17453.134	.000	-	17472.419	
45	17452.685	17452.682	.003	-	17472.401	
46	17452.221	17452.226	-.005	-	17472.377	
47	17451.765	17451.765	.000	-	17472.350	
48	17451.300	17451.300	.000	-	17472.317	
49	17450.832	17450.829	.003	-	17472.279	
50	17450.355	17450.354	.001	-	17472.236	
51	17449.874	17449.875	-.001	-	17472.188	
52	17449.395	17449.390	.005	-	17472.134	
53	17448.896	17448.900	-.004	-	17472.076	

54	17448.405	17448.405	.000	-	17472.012	
55	17447.904	17447.905	-.001	-	17471.944	
56	17447.400	17447.400	.000	-	17471.870	

2-3 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
1	17107.812	17107.812	.000	-	17108.464	
2	-	17107.587		17108.673	17108.672	.001
3	17107.355	17107.357	-.002	17108.871	17108.876	-.005
4	17107.121	17107.122	-.001	17109.097	17109.076	.021**
5	17106.883	17106.883	.000	17109.281	17109.271	.010**
6	17106.638	17106.640	-.002	17109.466	17109.462	.004
7	17106.390	17106.393	-.003	17109.647	17109.649	-.002
8	17106.142	17106.141	.001	17109.825	17109.831	-.006
9	17105.884	17105.885	-.001	17110.001	17110.009	-.008
10	17105.625	17105.624	.001	17110.177	17110.183	-.006
11	17105.357	17105.359	-.002	17110.349	17110.352	-.003
12	17105.088	17105.090	-.002	17110.515	17110.517	-.002
13	17104.815	17104.817	-.002	17110.675	17110.677	-.002
14	17104.538	17104.539	-.001	17110.834	17110.833	.001
15	17104.257	17104.257	.000	17110.985	17110.985	.000
16	17103.972	17103.970	.002	17111.137	17111.132	.005
17	17103.677	17103.679	-.002	17111.271	17111.275	-.004
18	17103.382	17103.384	-.002	17111.412	17111.414	-.002
19	17103.083	17103.085	-.002	17111.549	17111.548	.001
20	17102.779	17102.781	-.002	17111.678	17111.678	.000
21	17102.474	17102.473	.001	17111.805	17111.804	.001
22	17102.158	17102.160	-.002	17111.926	17111.925	.001
23	17101.842	17101.843	-.001	17112.039	17112.041	-.002
24	17101.521	17101.522	-.001	17112.154	17112.154	.000
25	17101.196	17101.196	.000	17112.262	17112.261	.001
26	17100.866	17100.866	.000	17112.366	17112.365	.001
27	17100.532	17100.532	.000	17112.467	17112.464	.003
28	17100.193	17100.193	.000	17112.557	17112.558	-.001
29	17099.849	17099.850	-.001	17112.647	17112.648	-.001
30	17099.498	17099.502	-.004	17112.734	17112.733	.001
31	17099.147	17099.150	-.003	17112.813	17112.813	.000
32	17098.787	17098.793	-.006	17112.880	17112.888	-.008**
33	17098.427	17098.432	-.005	17112.963	17112.958	.005
34	17098.066	17098.065	.001	17113.020	17113.021	-.001
35	17097.692	17097.693	-.001	17113.081	17113.076	.005
36	17097.319	17097.315	.004	-	17113.115	
37	17096.929	17096.928	.001	17113.114	17113.111	.003
38	17096.525	17096.526	-.001	-	17113.429	
39	17096.080	17096.080	.000	17113.398	17113.394	.004
40	17095.961	17095.957	.004	-	17113.412	
41	17095.481	17095.481	.000	-	17113.438	
42	17095.060	17095.057	.003	17113.471	17113.466	.005
43	17094.639	17094.643	-.004	17113.499	17113.492	.007
44	17094.230	17094.230	.000	-	17113.514	
45	17093.809	17093.814	-.005	-	17113.533	
46	17093.393	17093.396	-.003	-	17113.548	

47	17092.974	17092.974	.000	-	17113.559	
48	17092.550	17092.548	.002	-	17113.565	
49	17092.120	17092.119	.001	-	17113.568	
50	17091.687	17091.685	.002	-	17113.566	
51	17091.248	17091.247	.001	-	17113.560	
52	17090.807	17090.805	.002	-	17113.550	
53	17090.361	17090.359	.002	-	17113.535	
54	17089.911	17089.909	.002	-	17113.516	
55	17089.454	17089.454	.000	-	17113.493	
56	17088.998	17088.996	.002	-	17113.466	
57	17088.532	17088.533	-.001	-	17113.434	
58	17088.067	17088.066	.001	-	17113.397	
59	17087.594	17087.594	.000	-	17113.357	
60	17087.118	17087.118	.000	-	17113.311	
61	17086.637	17086.639	-.002	-	17113.262	
62	17086.155	17086.154	.001	-	17113.208	
63	17085.666	17085.666	.000	-	17113.150	
64	17085.173	17085.173	.000	-	17113.087	

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0-0 Band *A-X* System

	P Branch			R Branch		
J	Obs	Calc	Diff	Obs	Calc	Diff
0	-	.000		17541.611	17541.610	.001
1	17541.168	17541.167	.001	17541.824	17541.824	.000
2	17540.940	17540.938	.002	17542.029	17542.032	-.003
3	17540.705	17540.702	.003	17542.235	17542.234	.001
4	17540.463	17540.462	.001	17542.429	17542.431	-.002
5	17540.218	17540.216	.002	17542.622	17542.623	-.001
6	17539.965	17539.964	.001	17542.810	17542.809	.001
7	17539.713	17539.707	.006	17542.985	17542.990	-.005
8	17539.446	17539.445	.001	17543.162	17543.165	-.003
9	17539.178	17539.177	.001	17543.332	17543.335	-.003
10	17538.908	17538.904	.004	17543.501	17543.499	.002
11	17538.632	17538.625	.007	17543.659	17543.658	.001
12	17538.344	17538.341	.003	17543.817	17543.811	.006
13	17538.056	17538.051	.005	17543.962	17543.959	.003
14	17537.758	17537.756	.002	17544.101	17544.102	-.001
15	17537.461	17537.455	.006*	17544.237	17544.239	-.002
16	17537.156	17537.149	.007*	17544.366	17544.370	-.004
17	17536.845	17536.838	.007*	17544.494	17544.496	-.002
18	17536.530	17536.521	.009*	17544.615	17544.616	-.001
19	17536.204	17536.199	.005*	17544.729	17544.731	-.002
20	17535.878	17535.871	.007*	17544.840	17544.841	-.001
21	17535.546	17535.538	.008*	17544.943	17544.945	-.002
22	17535.209	17535.199	.010*	17545.038	17545.043	-.005
23	17534.862	17534.855	.007*	17545.134	17545.136	-.002
24	17534.513	17534.505	.008*	17545.221	17545.224	-.003
25	17534.159	17534.150	.009*	-	17545.306	
26	17533.795	17533.790	.005*	-	17545.382	
27	17533.432	17533.424	.008*	-	17545.453	
28	17533.061	17533.052	.009*	-	17545.518	
29	17532.684	17532.675	.009*	-	17545.578	

30	17532.303	17532.293	.010*	-	17545.632	
31	17531.914	17531.905	.009*	-	17545.681	
32	17531.521	17531.511	.010*	-	17545.724	
33	17531.120	17531.112	.008*	-	17545.761	
34	17530.715	17530.708	.007*	-	17545.793	
35	17530.303	17530.298	.005*	-	17545.820	
36	17529.890	17529.882	.008*	-	17545.840	
37	17529.470	17529.462	.008*	-	17545.855	
38	17529.041	17529.035	.006*	-	17545.865	
39	17528.606	17528.603	.003*	-	17545.869	
40	17528.170	17528.166	.004*	-	17545.867	
41	17527.727	17527.723	.004*	-	17545.860	
42	17527.280	17527.274	.006*	-	17545.847	
43	17526.823	17526.820	.003*	-	17545.829	
44	17526.362	17526.360	.002	-	17545.804	
45	17525.897	17525.895	.002	-	17545.775	
46	17525.427	17525.424	.003	-	17545.739	
47	17524.951	17524.948	.003	-	17545.698	
48	17524.469	17524.466	.003	-	17545.651	
49	17523.978	17523.978	.000	-	17545.598	
50	17523.487	17523.485	.002	-	17545.540	
51	17522.987	17522.987	.000	-	17545.476	
52	17522.481	17522.482	-.001	-	17545.406	
53	17521.976	17521.973	.003	-	17545.331	
54	17521.457	17521.457	.000	-	17545.250	
55	17520.941	17520.936	.005	-	17545.163	
56	17520.410	17520.409	.001	-	17545.070	
57	17519.880	17519.877	.003	-	17544.972	
58	17519.340	17519.339	.001	-	17544.868	
59	17518.799	17518.795	.004	-	17544.758	
60	17518.245	17518.246	-.001	-	17544.642	
61	17517.689	17517.691	-.002	-	17544.520	
62	17517.131	17517.130	.001	-	17544.393	
63	17516.570	17516.564	.006	-	17544.260	
64	-	17515.992		-	17544.121	
65	-	17515.414		-	17543.976	
66	-	17514.831		-	17543.825	
67	-	17514.242		-	17543.668	
68	-	17513.647		17543.501	17543.506	-.005*
69	-	17513.046		17543.332	17543.337	-.005*
70	-	17512.440		17543.162	17543.163	-.001*
71	-	17511.828		17542.985	17542.983	.002*
72	-	17511.210		17542.798	17542.796	.002
73	-	17510.586		17542.606	17542.604	.002
74	-	17509.957		17542.407	17542.406	.001
75	-	17509.321		17542.202	17542.202	.000
76	-	17508.680		17541.993	17541.992	.001
77	-	17508.033		17541.776	17541.776	.000
78	-	17507.381		17541.552	17541.554	-.002
79	-	17506.722		17541.326	17541.326	.000
80	-	17506.058		17541.091	17541.091	.000
81	-	17505.387		17540.852	17540.851	.001
82	-	17504.711		17540.604	17540.605	-.001
83	-	17504.029		17540.349	17540.352	-.003
84	-	17503.341		17540.093	17540.094	-.001

0-1 Band

		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
1	-	17176.461		17177.119	17177.117	.002
2	17176.233	17176.233	.000	17177.329	17177.327	.002
3	17176.002	17176.000	.002	17177.528	17177.532	-.004
4	17175.762	17175.763	-.001	17177.730	17177.732	-.002
5	17175.520	17175.521	-.001	17177.926	17177.928	-.002
6	17175.274	17175.274	.000	17178.120	17178.119	.001
7	17175.024	17175.023	.001	17178.307	17178.306	.001
8	17174.767	17174.767	.000	17178.487	17178.487	.000
9	17174.508	17174.507	.001	17178.667	17178.665	.002
10	17174.244	17174.241	.003	17178.835	17178.837	-.002
11	17173.973	17173.972	.001	17179.002	17179.005	-.003
12	17173.693	17173.697	-.004	17179.163	17179.168	-.005
13	17173.419	17173.418	.001	17179.325	17179.327	-.002
14	17173.135	17173.135	.000	17179.476	17179.481	-.005
15	17172.846	17172.847	-.001	-	17179.630	
16	17172.553	17172.554	-.001	17179.773	17179.774	-.001
17	17172.255	17172.256	-.001	17179.912	17179.914	-.002
18	17171.953	17171.954	-.001	17180.050	17180.050	.000
19	17171.649	17171.648	.001	17180.179	17180.180	-.001
20	17171.355	17171.336	.019*	17180.305	17180.306	-.001
21	17171.033	17171.020	.013*	17180.426	17180.427	-.001
22	17170.705	17170.700	.005	17180.543	17180.544	-.001
23	17170.377	17170.374	.003	17180.656	17180.656	.000
24	17170.048	17170.044	.004	17180.745	17180.763	-.018*
25	17169.713	17169.710	.003	17180.862	17180.865	-.003
26	17169.376	17169.371	.005	17180.969	17180.963	.006*
27	17169.025	17169.027	-.002	17181.055	17181.056	-.001
28	17168.665	17168.678	-.013*	17181.145	17181.144	.001
29	17168.321	17168.325	-.004	17181.224	17181.228	-.004
30	17167.966	17167.967	-.001	17181.302	17181.307	-.005
31	17167.605	17167.605	.000	17181.378	17181.381	-.003
32	17167.236	17167.238	-.002	17181.458	17181.450	.008*
33	17166.867	17166.866	.001	17181.522	17181.515	.007*
34	17166.490	17166.489	.001	17181.571	17181.575	-.004
35	17166.109	17166.108	.001	17181.622	17181.630	-.008
36	17165.725	17165.722	.003	17181.682	17181.680	.002
37	17165.331	17165.332	-.001	-	17181.726	
38	17164.934	17164.936	-.002	-	17181.766	
39	17164.537	17164.536	.001	-	17181.802	
40	17164.132	17164.132	.000	-	17181.834	
41	17163.721	17163.722	-.001	-	17181.860	
42	17163.307	17163.308	-.001	-	17181.881	
43	17162.890	17162.889	.001	-	17181.898	
44	17162.466	17162.466	.000	-	17181.910	
45	17162.040	17162.038	.002	-	17181.917	
46	17161.604	17161.605	-.001	-	17181.920	
47	17161.167	17161.167	.000	-	17181.917	
48	17160.724	17160.724	.000	-	17181.909	
49	17160.277	17160.277	.000	-	17181.897	
50	17159.824	17159.825	-.001	-	17181.880	
51	17159.368	17159.368	.000	-	17181.858	

52	17158.907	17158.907	.000	-	17181.831	
53	17158.441	17158.440	.001	-	17181.799	
54	17157.971	17157.969	.002	-	17181.762	
55	17157.495	17157.493	.002	-	17181.720	
56	17157.014	17157.013	.001	-	17181.674	
57	17156.526	17156.527	-.001	-	17181.622	
58	17156.040	17156.037	.003	17181.562	17181.566	-.004
59	17155.542	17155.541	.001	-	17181.504	
60	17155.041	17155.041	.000	-	17181.437	
61	17154.537	17154.537	.000	-	17181.366	
62	17154.025	17154.027	-.002	17181.287	17181.289	-.002
63	17153.513	17153.512	.001	17181.209	17181.208	.001
64	17152.993	17152.993	.000	17181.126	17181.121	.005
65	17152.467	17152.468	-.001	17181.040	17181.030	.010*
66	17151.939	17151.939	.000	17180.930	17180.933	-.003
67	17151.407	17151.405	.002	17180.825	17180.832	-.007
68	17150.886	17150.866	.020*	17180.724	17180.725	-.001
69	17150.290	17150.322	-.032*	17180.613	17180.613	.000
70	-	17149.773		17180.496	17180.496	.000
71	-	17149.219		17180.371	17180.374	-.003
72	-	17148.660		17180.249	17180.247	.002
73	-	17148.097		17180.117	17180.115	.002
74	-	17147.528		-	17179.977	
75	-	17146.954		-	17179.835	
76	-	17146.375		17179.688	17179.687	.001
77	-	17145.792		17179.530	17179.534	-.004
78	-	17145.203		-	17179.376	
79	-	17144.609		17179.211	17179.213	-.002
80	-	17144.010		17179.045	17179.044	.001
81	-	17143.407		17178.869	17178.871	-.002
82	-	17142.798		17178.690	17178.692	-.002
83	-	17142.184		17178.507	17178.507	.000
84	-	17141.565		17178.314	17178.318	-.004
85	-	17140.940		17178.121	17178.123	-.002
86	-	17140.311		17177.923	17177.923	.000
87	-	17139.677		17177.713	17177.717	-.004
88	-	17139.037		17177.505	17177.506	-.001
89	-	17138.393		17177.290	17177.290	.000
90	-	17137.743		17177.068	17177.069	-.001
91	-	17137.088		17176.841	17176.842	-.001
92	-	17136.428		17176.610	17176.610	.000
93	-	17135.762		17176.373	17176.372	.001
94	-	17135.092		17176.130	17176.129	.001
95	-	17134.416		17175.879	17175.880	-.001
96	-	17133.735		17175.626	17175.626	.000
97	-	17133.049		17175.369	17175.367	.002
98	-	17132.357		17175.103	17175.102	.001

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		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
1	-	17501.396		17502.047	17502.051	-.004*
2	17501.169	17501.168	.001*	17502.263	17502.259	.004*
3	17500.932	17500.934	-.002*	17502.464	17502.462	.002*

4	17500.694	17500.695	-.001*	17502.665	17502.659	.006*
5	17500.454	17500.450	.004*	17502.855	17502.851	.004*
6	17500.202	17500.201	.001*	17503.043	17503.038	.005*
7	17499.947	17499.946	.001*	17503.223	17503.220	.003*
8	17499.691	17499.686	.005*	17503.400	17503.396	.004*
9	17499.422	17499.421	.001*	17503.572	17503.568	.004*
10	17499.153	17499.150	.003*	17503.736	17503.734	.002*
11	17498.873	17498.875	-.002*	17503.895	17503.894	.001
12	17498.593	17498.594	-.001*	17504.051	17504.050	.001
13	17498.306	17498.308	-.002	17504.202	17504.200	.002
14	17498.014	17498.017	-.003	17504.346	17504.345	.001
15	17497.715	17497.720	-.005	17504.487	17504.485	.002
16	17497.417	17497.419	-.002	17504.622	17504.620	.002
17	17497.110	17497.112	-.002	17504.750	17504.749	.001
18	17496.799	17496.800	-.001	17504.871	17504.873	-.002
19	17496.483	17496.482	.001	17504.994	17504.992	.002
20	17496.159	17496.160	-.001	17505.107	17505.106	.001
21	17495.831	17495.832	-.001	17505.214	17505.214	.000
22	17495.494	17495.499	-.005	17505.319	17505.317	.002
23	17495.160	17495.161	-.001	17505.417	17505.415	.002
24	17494.813	17494.818	-.005	17505.506	17505.508	-.002*
25	17494.470	17494.469	.001	17505.598	17505.595	.003*
26	17494.112	17494.116	-.004	17505.680	17505.677	.003*
27	17493.755	17493.757	-.002	17505.759	17505.754	.005*
28	17493.390	17493.392	-.002	17505.831	17505.825	.006*
29	17493.019	17493.023	-.004	17505.899	17505.891	.008*
30	17492.647	17492.648	-.001	-	17505.952	
31	17492.265	17492.268	-.003	17506.010	17506.008	.002*
32	17491.880	17491.883	-.003	-	17506.058	
33	17491.493	17491.493	.000	-	17506.103	
34	17491.096	17491.097	-.001	-	17506.143	
35	17490.695	17490.696	-.001	-	17506.177	
36	17490.285	17490.290	-.005	-	17506.206	
37	17489.877	17489.879	-.002	-	17506.230	
38	17489.462	17489.462	.000	-	17506.248	
39	17489.044	17489.041	.003	-	17506.261	
40	17488.613	17488.613	.000	-	17506.269	
41	17488.179	17488.181	-.002	-	17506.271	
42	17487.739	17487.744	-.005	-	17506.268	
43	17487.301	17487.301	.000	-	17506.260	
44	17486.851	17486.853	-.002	-	17506.246	
45	17486.398	17486.399	-.001	-	17506.227	
46	17485.939	17485.941	-.002	-	17506.203	
47	17485.475	17485.477	-.002	-	17506.173	
48	17485.012	17485.008	.004	-	17506.138	
49	17484.534	17484.533	.001	-	17506.097	
50	17484.050	17484.054	-.004	-	17506.052	
51	17483.569	17483.569	.000	-	17506.000	
52	17483.076	17483.078	-.002	-	17505.944	
53	17482.580	17482.583	-.003	-	17505.881	
54	17482.079	17482.082	-.003	-	17505.814	
55	17481.573	17481.576	-.003	-	17505.741	
56	17481.066	17481.064	.002	-	17505.663	
57	17480.548	17480.548	.000	-	17505.579	
58	17480.027	17480.026	.001	-	17505.490	
59	17479.496	17479.498	-.002	-	17505.395	
60	17478.968	17478.965	.003	-	17505.295	

61	17478.428	17478.427	.001	-	17505.189	
62	17477.883	17477.884	-.001	-	17505.078	
63	17477.336	17477.335	.001	-	17504.961	
64	17476.781	17476.781	.000	-	17504.839	
65	17476.217	17476.222	-.005	-	17504.712	
66	17475.653	17475.657	-.004	-	17504.579	
67	17475.085	17475.087	-.002	-	17504.440	
68	-	17474.512		-	17504.296	
69	-	17473.931		17504.149	17504.147	.002
70	-	17473.344		17503.995	17503.992	.003
71	-	17472.753		17503.833	17503.831	.002
72	-	17472.156		17503.670	17503.665	.005
73	-	17471.554		17503.496	17503.493	.003
74	-	17470.946		17503.317	17503.316	.001
75	-	17470.333		17503.133	17503.133	.000
76	-	17469.714		17502.946	17502.945	.001
77	-	17469.090		17502.754	17502.751	.003
78	-	17468.461		17502.553	17502.551	.002
79	-	17467.826		17502.345	17502.346	-.001
80	-	17467.186		17502.134	17502.135	-.001
81	-	17466.540		17501.915	17501.919	-.004
82	-	17465.889		17501.697	17501.697	.000
83	-	17465.232		17501.473	17501.469	.004
84	-	17464.570		17501.234	17501.236	-.002
85	-	17463.902		17500.994	17500.997	-.003
86	-	17463.229		17500.752	17500.752	.000

1-2 Band

	P Branch			R Branch		
J	Obs	Calc	Diff	Obs	Calc	Diff
1	-	17139.024		17139.678	17139.679	-.001
2	-	17138.797		-	17139.888	
3	17138.550	17138.566	-.016*	17140.096	17140.094	.002
4	17138.329	17138.330	-.001	-	17140.294	
5	17138.093	17138.090	.003	17140.493	17140.490	.003
6	17137.847	17137.845	.002	-	17140.682	
7	17137.598	17137.596	.002	17140.875	17140.870	.005
8	17137.345	17137.343	.002	17141.054	17141.053	.001
9	17137.086	17137.085	.001	17141.229	17141.232	-.003
10	17136.824	17136.823	.001	17141.403	17141.406	-.003
11	17136.554	17136.556	-.002	17141.578	17141.576	.002
12	17136.282	17136.285	-.003	17141.750	17141.741	.009
13	17136.012	17136.010	.002	-	17141.902	
14	17135.731	17135.730	.001	17142.068	17142.059	.009
15	17135.448	17135.446	.002	17142.210	17142.211	-.001
16	17135.195	17135.157	.038*	17142.365	17142.359	.006
17	17134.867	17134.865	.002	17142.503	17142.502	.001
18	17134.569	17134.567	.002	17142.641	17142.641	.000
19	17134.267	17134.266	.001	17142.779	17142.775	.004
20	17133.959	17133.960	-.001	17142.902	17142.905	-.003
21	17133.649	17133.649	.000	17143.036	17143.031	.005
22	17133.335	17133.334	.001	17143.155	17143.152	.003
23	17133.017	17133.015	.002	-	17143.269	

24	17132.692	17132.691	.001	17143.382	17143.381	.001
25	17132.365	17132.363	.002	17143.494	17143.489	.005
26	17132.031	17132.031	.000	17143.594	17143.592	.002
27	17131.697	17131.694	.003	17143.694	17143.691	.003
28	17131.352	17131.353	-.001	17143.788	17143.786	.002
29	-	17131.007		17143.872	17143.876	-.004
30	-	17130.657		-	17143.961	
31	17130.310	17130.303	.007*	-	17144.042	
32	17129.945	17129.944	.001*	17144.127	17144.119	.008
33	17129.580	17129.581	-.001*	17144.192	17144.191	.001
34	17129.210	17129.213	-.003*	17144.263	17144.259	.004
35	17128.834	17128.841	-.007*	17144.318	17144.322	-.004
36	17128.460	17128.465	-.005*	17144.380	17144.381	-.001
37	-	17128.084		17144.437	17144.435	.002
38	-	17127.699		17144.489	17144.484	.005
39	-	17127.309		17144.532	17144.530	.002
40	-	17126.915		-	17144.570	
41	17126.517	17126.516	.001	17144.607	17144.606	.001
42	17126.115	17126.113	.002	17144.641	17144.638	.003
43	17125.706	17125.706	.000	17144.666	17144.665	.001
44	17125.292	17125.294	-.002	-	17144.688	
45	17124.877	17124.878	-.001	-	17144.706	
46	17124.459	17124.457	.002	-	17144.719	
47	17124.030	17124.032	-.002	-	17144.728	
48	17123.601	17123.603	-.002	-	17144.733	
49	17123.170	17123.169	.001	-	17144.733	
50	17122.733	17122.730	.003	-	17144.728	
51	17122.290	17122.287	.003	-	17144.719	
52	17121.842	17121.840	.002	-	17144.705	
53	17121.390	17121.388	.002	-	17144.687	
54	17120.934	17120.932	.002	-	17144.664	
55	17120.473	17120.471	.002*	-	17144.636	
56	17120.009	17120.006	.003*	-	17144.604	
57	-	17119.536		-	17144.567	
58	-	17119.062		17144.526	17144.526	.000
59	-	17118.583		-	17144.480	
60	-	17118.100		17144.436	17144.430	.006
61	-	17117.613		-	17144.374	
62	-	17117.121		-	17144.315	
63	-	17116.624		17144.250	17144.250	.000
64	-	17116.123		-	17144.181	
65	-	17115.617		17144.110	17144.107	.003
66	-	17115.107		-	17144.029	
67	-	17114.593		17143.941	17143.946	-.005
68	-	17114.073		17143.859	17143.858	.001
69	-	17113.550		17143.770	17143.766	.004
70	-	17113.021		17143.673	17143.669	.004
71	-	17112.489		17143.574	17143.567	.007
72	-	17111.951		17143.460	17143.461	-.001
73	-	17111.410		17143.346	17143.349	-.003
74	-	17110.863		17143.235	17143.233	.002
75	-	17110.312		17143.115	17143.113	.002
76	-	17109.757		-	17142.988	
77	-	17109.197		17142.858	17142.857	.001
78	-	17108.632		17142.726	17142.723	.003
79	-	17108.063		17142.581	17142.583	-.002
80	-	17107.489		17142.442	17142.439	.003

81	-	17106.911		17142.289	17142.290	-.001
82	-	17106.328		17142.129	17142.136	-.007
83	-	17105.740		17141.978	17141.977	.001
84	-	17105.148		17141.815	17141.814	.001
85	-	17104.551		17141.640	17141.646	-.006
86	-	17103.950		17141.469	17141.472	-.003
87	-	17103.344		17141.293	17141.295	-.002
88	-	17102.733		17141.113	17141.112	.001

2-2 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
4	-	17466.787		17468.701	17468.745	-.044**
5	-	17466.544		17468.933	17468.936	-.003
6	-	17466.295		17469.096	17469.123	-.027**
7	-	17466.042		17469.304	17469.304	.000
8	17465.785	17465.783	.002	17469.475	17469.480	-.005
9	17465.522	17465.519	.003	17469.643	17469.651	-.008**
10	17465.251	17465.250	.001	17469.818	17469.817	.001
11	17464.978	17464.976	.002	17469.979	17469.978	.001
12	17464.697	17464.696	.001	17470.133	17470.133	.000
13	17464.413	17464.412	.001	17470.272	17470.283	-.011**
14	17464.123	17464.122	.001	17470.427	17470.428	-.001
15	17463.828	17463.827	.001	17470.571	17470.568	.003
16	17463.525	17463.527	-.002	17470.704	17470.703	.001
17	17463.226	17463.222	.004	17470.836	17470.832	.004
18	17462.914	17462.911	.003	17470.960	17470.956	.004
19	17462.598	17462.596	.002	17471.079	17471.076	.003
20	17462.274	17462.275	-.001	17471.189	17471.189	.000
21	17461.946	17461.949	-.003	17471.303	17471.298	.005
22	17461.620	17461.618	.002	17471.399	17471.402	-.003
23	17461.282	17461.282	.000	-	17471.500	
24	17460.940	17460.941	-.001	-	17471.593	
25	17460.592	17460.594	-.002	-	17471.681	
26	17460.245	17460.243	.002	-	17471.763	
27	17459.886	17459.886	.000	-	17471.841	
28	17459.526	17459.524	.002	-	17471.913	
29	17459.159	17459.157	.002	-	17471.980	
30	17458.784	17458.785	-.001	-	17472.042	
31	17458.407	17458.407	.000	-	17472.098	
32	17458.027	17458.025	.002	-	17472.150	
33	17457.639	17457.637	.002	-	17472.195	
34	17457.246	17457.244	.002	-	17472.236	
35	17456.844	17456.846	-.002	-	17472.272	
36	17456.445	17456.442	.003	-	17472.302	
37	17456.037	17456.033	.004	-	17472.326	
38	17455.637	17455.620	.017**	-	17472.346	
39	17455.202	17455.200	.002	-	17472.359	
40	17454.776	17454.776	.000	-	17472.367	
41	17454.342	17454.346	-.004	-	17472.370	
42	17453.913	17453.910	.003	-	17472.365	
43	17453.465	17453.469	-.004	-	17472.353	
44	17453.019	17453.021	-.002	-	17472.328	

45	17452.565	17452.565	.000	-	17472.271	
46	17452.095	17452.098	-.003	-	17472.450	
47	17451.598	17451.597	.001	-	17472.348	
48	17451.333	17451.333	.000	-	17472.296	
49	17450.788	17450.788	.000	-	17472.251	
50	17450.293	17450.294	-.001	-	17472.204	
51	17449.805	17449.805	.000	-	17472.153	
52	17449.312	17449.315	-.003	-	17472.098	
53	17448.822	17448.822	.000	-	17472.038	
54	-	17448.324		-	17471.973	
55	17447.824	17447.822	.002	-	17471.904	
56	17447.316	17447.315	.001	-	17471.829	

2-3 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
3	17106.989	17106.992	-.003	17108.513	17108.514	-.001
4	-	17106.757		17108.719	17108.714	.005
5	17106.516	17106.518	-.002	17108.909	17108.910	-.001
6	17106.274	17106.274	.000	17109.097	17109.101	-.004
7	17106.021	17106.026	-.005	17109.281	17109.288	-.007
8	17105.772	17105.774	-.002	17109.466	17109.471	-.005
9	17105.517	17105.517	.000	17109.647	17109.649	-.002
10	17105.255	17105.256	-.001	17109.825	17109.823	.002
11	17104.989	17104.991	-.002	17110.003	17109.993	.010**
12	17104.722	17104.722	.000	17110.159	17110.158	.001
13	17104.449	17104.448	.001	17110.316	17110.319	-.003
14	17104.168	17104.169	-.001	17110.474	17110.476	-.002
15	17103.885	17103.887	-.002	17110.622	17110.628	-.006
16	17103.599	17103.600	-.001	17110.773	17110.776	-.003
17	17103.308	17103.309	-.001	17110.917	17110.919	-.002
18	17103.012	17103.013	-.001	17111.064	17111.058	.006
19	17102.710	17102.713	-.003	17111.197	17111.193	.004
20	17102.407	17102.409	-.002	17111.321	17111.323	-.002
21	17102.102	17102.100	.002	17111.452	17111.449	.003
22	17101.789	17101.788	.001	17111.565	17111.571	-.006
23	17101.471	17101.470	.001	17111.683	17111.688	-.005
24	17101.149	17101.149	.000	17111.805	17111.801	.004
25	17100.821	17100.823	-.002	17111.926	17111.909	.017**
26	17100.493	17100.493	.000	17112.039	17112.014	.025**
27	17100.156	17100.158	-.002	17112.107	17112.113	-.006
28	17099.816	17099.819	-.003	17112.204	17112.208	-.004
29	17099.473	17099.476	-.003	17112.293	17112.299	-.006
30	17099.132	17099.129	.003	-	17112.386	
31	-	17098.777		17112.468	17112.468	.000
32	17098.428	17098.420	.008	-	17112.545	
33	17098.066	17098.060	.006	17112.619	17112.619	.000
34	17097.692	17097.695	-.003	17112.687	17112.687	.000
35	-	17097.326		-	17112.752	
36	17096.949	17096.952	-.003	17112.813	17112.812	.001
37	17096.576	17096.574	.002	-	17112.867	
38	17096.192	17096.192	.000	-	17112.917	
39	17095.807	17095.805	.002	-	17112.963	

40	17095.413	17095.413	.000	-	17113.005	
41	17095.016	17095.017	-.001	-	17113.041	
42	17094.614	17094.616	-.002	-	17113.071	
43	17094.230	17094.211	.019**	-	17113.094	
44	17093.809	17093.799	.010**	-	17113.106	
45	17093.393	17093.381	.012**	-	17113.086	
46	17092.959	17092.951	.008	-	17113.304	
47	17092.493	17092.489	.004	-	17113.240	
48	17092.267	17092.266	.001	-	17113.229	
49	17091.760	17091.761	-.001	-	17113.224	
50	17091.306	17091.308	-.002	-	17113.218	
51	17090.863	17090.862	.001	-	17113.210	
52	17090.418	17090.416	.002	-	17113.198	
53	17089.969	17089.966	.003	-	17113.182	
54	17089.515	17089.514	.001	-	17113.163	
55	17089.057	17089.057	.000	-	17113.139	
56	17088.598	17088.597	.001	-	17113.110	
57	17088.134	17088.133	.001	-	17113.078	
58	17087.666	17087.664	.002	-	17113.041	
59	17087.193	17087.191	.002	-	17113.000	
60	17086.716	17086.714	.002	-	17112.954	
61	17086.235	17086.233	.002	-	17112.904	
62	17085.749	17085.748	.001	-	17112.850	
63	17085.260	17085.258	.002	-	17112.791	

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0 - 0 Band *A*-*X* System

	P Branch			R Branch		
J	Obs	Calc	Diff	Obs	Calc	Diff
0	-	.000		17541.611	17541.620	-.009*
1	17541.168	17541.179	-.011*	17541.824	17541.833	-.009*
2	17540.940	17540.950	-.010*	17542.029	17542.040	-.011*
3	17540.705	17540.716	-.011*	17542.235	17542.242	-.007*
4	17540.463	17540.476	-.013*	17542.429	17542.438	-.009*
5	17540.218	17540.230	-.012*	17542.622	17542.629	-.007*
6	17539.965	17539.980	-.015*	17542.810	17542.815	-.005*
7	17539.713	17539.723	-.010*	17542.985	17542.995	-.010*
8	17539.446	17539.462	-.016*	17543.162	17543.169	-.007*
9	17539.178	17539.195	-.017*	17543.332	17543.338	-.006*
10	17538.908	17538.922	-.014*	17543.501	17543.502	-.001
11	17538.632	17538.644	-.012*	17543.659	17543.660	-.001
12	17538.344	17538.361	-.017*	17543.817	17543.812	.005
13	17538.056	17538.072	-.016*	17543.962	17543.959	.003
14	17537.758	17537.778	-.020*	17544.101	17544.101	.000
15	17537.461	17537.478	-.017*	17544.237	17544.237	.000
16	17537.156	17537.173	-.017*	17544.366	17544.368	-.002
17	17536.845	17536.863	-.018*	17544.494	17544.493	.001
18	17536.530	17536.547	-.017*	17544.615	17544.613	.002
19	17536.204	17536.225	-.021*	17544.729	17544.727	.002
20	17535.878	17535.898	-.020*	17544.840	17544.836	.004
21	17535.546	17535.566	-.020*	17544.943	17544.939	.004
22	17535.209	17535.228	-.019*	17545.038	17545.037	.001

23	17534.862	17534.885	-.023*	17545.134	17545.130	.004
24	17534.513	17534.536	-.023*	17545.221	17545.216	.005
25	17534.159	17534.182	-.023*	-	17545.298	
26	17533.795	17533.822	-.027*	-	17545.373	
27	17533.432	17533.457	-.025*	-	17545.444	
28	17533.061	17533.087	-.026*	-	17545.508	
29	17532.684	17532.711	-.027*	-	17545.568	
30	17532.303	17532.329	-.026*	-	17545.621	
31	17531.914	17531.942	-.028*	-	17545.669	
32	17531.521	17531.550	-.029*	-	17545.712	
33	17531.120	17531.152	-.032*	-	17545.749	
34	17530.715	17530.749	-.034*	-	17545.781	
35	17530.303	17530.340	-.037*	-	17545.806	
36	17529.901	17529.925	-.024*	-	17545.827	
37	17529.480	17529.506	-.026*	-	17545.842	
38	17529.054	17529.080	-.026*	-	17545.851	
39	17528.621	17528.650	-.029*	-	17545.854	
40	17528.186	17528.213	-.027*	-	17545.853	
41	17527.746	17527.771	-.025*	-	17545.845	
42	17527.296	17527.324	-.028*	-	17545.832	
43	17526.872	17526.871	.001	-	17545.813	
44	17526.412	17526.413	-.001	-	17545.789	
45	17525.949	17525.949	.000	-	17545.759	
46	17525.479	17525.480	-.001	-	17545.723	
47	17525.005	17525.005	.000	-	17545.682	
48	17524.525	17524.525	.000	-	17545.635	
49	17524.037	17524.039	-.002	-	17545.582	
50	17523.545	17523.547	-.002	-	17545.524	
51	-	17523.050		-	17545.460	
52	17522.547	17522.547	.000	-	17545.391	
53	17522.040	17522.039	.001	-	17545.316	
54	17521.525	17521.526	-.001	-	17545.235	
55	17521.008	17521.006	.002	-	17545.148	
56	17520.482	17520.481	.001	-	17545.056	
57	17519.950	17519.951	-.001	-	17544.958	
58	17519.413	17519.415	-.002	-	17544.854	
59	17518.870	17518.873	-.003	-	17544.745	
60	17518.324	17518.326	-.002	-	17544.630	
61	17517.772	17517.773	-.001	-	17544.509	
62	17517.215	17517.215	.000	-	17544.382	
63	17516.651	17516.651	.000	-	17544.250	
64	17516.034	17516.081	-.047*	-	17544.111	
65	-	17515.506		-	17543.967	
66	-	17514.925		-	17543.818	
67	-	17514.338		-	17543.662	
68	-	17513.746		17543.501	17543.501	.000
69	-	17513.148		17543.332	17543.334	-.002
70	-	17512.544		17543.162	17543.160	.002
71	-	17511.935		17542.985	17542.982	.003
72	-	17511.320		17542.798	17542.797	.001
73	-	17510.699		17542.606	17542.606	.000
74	-	17510.073		17542.407	17542.410	-.003*
75	-	17509.441		17542.202	17542.208	-.006*
76	-	17508.803		17541.993	17541.999	-.006*
77	-	17508.160		17541.776	17541.785	-.009*
78	-	17507.510		17541.552	17541.565	-.013*
79	-	17506.855		17541.326	17541.339	-.013*

80	-	17506.195		17541.091	17541.107	-.016*
81	-	17505.528		17540.852	17540.870	-.018*
82	-	17504.856		17540.604	17540.626	-.022*
83	-	17504.178		17540.349	17540.376	-.027*
84	-	17503.494		17540.093	17540.120	-.027*

0-1 Band

		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
4	-	17176.409		17178.368	17178.371	-.003
5	-	17176.168		17178.559	17178.566	-.007
6	-	17175.922		17178.755	17178.757	-.002
7	-	17175.671		17178.939	17178.942	-.003
8	-	17175.416		17179.123	17179.124	-.001
9	17175.158	17175.157	.001	-	17179.300	
10	17174.892	17174.893	-.001	-	17179.472	
11	17174.616	17174.624	-.008	-	17179.639	
12	17174.347	17174.350	-.003	17179.800	17179.802	-.002
13	17174.077	17174.072	.005	-	17179.960	
14	17173.791	17173.790	.001	-	17180.113	
15	17173.501	17173.503	-.002	17180.268	17180.262	.006*
16	17173.208	17173.211	-.003	-	17180.406	
17	17172.911	17172.914	-.003	17180.543	17180.545	-.002
18	-	17172.613		-	17180.680	
19	17172.285	17172.307	-.022*	17180.809	17180.810	-.001
20	17171.982	17171.997	-.015*	17180.929	17180.935	-.006
21	17171.670	17171.682	-.012*	17181.056	17181.056	.000
22	17171.355	17171.363	-.008*	-	17181.172	
23	17171.033	17171.038	-.005*	17181.282	17181.283	-.001
24	17170.705	17170.710	-.005*	17181.383	17181.390	-.007
25	17170.377	17170.376	.001	17181.491	17181.492	-.001
26	17170.043	17170.038	.005	17181.586	17181.589	-.003
27	17169.709	17169.695	.014*	17181.682	17181.682	.000
28	17169.371	17169.348	.023*	17181.767	17181.770	-.003
29	17169.025	17168.996	.029*	-	17181.853	
30	17168.665	17168.639	.026*	-	17181.931	
31	17168.280	17168.278	.002	-	17182.005	
32	17167.912	17167.912	.000	-	17182.074	
33	17167.542	17167.541	.001	-	17182.138	
34	17167.164	17167.166	-.002	17182.197	17182.198	-.001
35	17166.787	17166.786	.001	17182.248	17182.253	-.005
36	17166.403	17166.401	.002	17182.300	17182.303	-.003
37	17166.012	17166.012	.000	17182.345	17182.348	-.003
38	17165.617	17165.618	-.001	17182.388	17182.389	-.001
39	17165.220	17165.219	.001	17182.425	17182.424	.001
40	17164.816	17164.816	.000	17182.455	17182.455	.000
41	17164.409	17164.408	.001	17182.482	17182.481	.001
42	17163.997	17163.995	.002	17182.507	17182.503	.004
43	17163.580	17163.578	.002	-	17182.519	
44	17163.154	17163.156	-.002	-	17182.531	
45	17162.727	17162.729	-.002	-	17182.538	
46	17162.296	17162.297	-.001	-	17182.540	
47	17161.862	17161.861	.001	-	17182.538	

48	17161.423	17161.420	.003	-	17182.530	
49	17160.980	17160.974	.006	-	17182.518	
50	17160.524	17160.523	.001	-	17182.501	
51	17160.069	17160.068	.001	-	17182.478	
52	17159.609	17159.608	.001	-	17182.451	
53	17159.146	17159.143	.003	-	17182.420	
54	17158.678	17158.674	.004	-	17182.383	
55	17158.201	17158.199	.002	17182.340	17182.341	-.001
56	17157.724	17157.720	.004	17182.296	17182.295	.001
57	17157.238	17157.236	.002	17182.242	17182.243	-.001
58	17156.748	17156.747	.001	17182.187	17182.187	.000
59	17156.255	17156.254	.001	17182.120	17182.125	-.005
60	17155.758	17155.755	.003	-	17182.059	
61	17155.252	17155.252	.000	17181.988	17181.988	.000
62	17154.743	17154.744	-.001	17181.916	17181.912	.004
63	17154.229	17154.231	-.002	17181.827	17181.830	-.003
64	17153.710	17153.714	-.004	-	17181.744	
65	17153.187	17153.191	-.004	-	17181.653	

1-1 Band

	P Branch			R Branch		
J	Obs	Calc	Diff	Obs	Calc	Diff
4	-	17500.755		17502.710	17502.712	-.002
5	17500.502	17500.512	-.010*	17502.905	17502.904	.001
6	17500.259	17500.263	-.004	-	17503.090	
7	17500.010	17500.009	.001	-	17503.271	
8	17499.748	17499.750	-.002	-	17503.447	
9	17499.481	17499.486	-.005	-	17503.618	
10	17499.212	17499.216	-.004	-	17503.783	
11	17498.941	17498.942	-.001	-	17503.943	
12	17498.661	17498.662	-.001	-	17504.098	
13	17498.378	17498.377	.001	-	17504.248	
14	17498.084	17498.087	-.003	-	17504.393	
15	17497.789	17497.791	-.002	-	17504.532	
16	17497.490	17497.491	-.001	-	17504.666	
17	17497.183	17497.185	-.002	-	17504.795	
18	17496.873	17496.874	-.001	-	17504.919	
19	17496.558	17496.558	.000	-	17505.037	
20	17496.236	17496.236	.000	-	17505.150	
21	17495.908	17495.910	-.002	-	17505.258	
22	17495.576	17495.578	-.002	-	17505.361	
23	17495.242	17495.241	.001	-	17505.459	
24	17494.897	17494.899	-.002	-	17505.551	
25	17494.552	17494.551	.001	-	17505.638	
26	17494.197	17494.199	-.002	-	17505.719	
27	17493.841	17493.841	.000	-	17505.796	
28	17493.478	17493.478	.000	-	17505.867	
29	17493.108	17493.110	-.002	-	17505.933	
30	17492.735	17492.736	-.001	-	17505.993	
31	17492.356	17492.358	-.002	-	17506.049	
32	17491.972	17491.974	-.002	-	17506.099	
33	17491.583	17491.585	-.002	-	17506.144	
34	17491.189	17491.191	-.002	-	17506.183	

35	17490.790	17490.791	-.001	-	17506.217	
36	17490.386	17490.387	-.001	-	17506.246	
37	17489.975	17489.977	-.002	-	17506.270	
38	17489.560	17489.562	-.002	-	17506.288	
39	17489.143	17489.141	.002	-	17506.301	
40	17488.716	17488.716	.000	-	17506.309	
41	17488.285	17488.285	.000	-	17506.311	
42	17487.848	17487.849	-.001	-	17506.308	
43	17487.406	17487.407	-.001	-	17506.300	
44	17486.959	17486.961	-.002	-	17506.286	
45	17486.512	17486.509	.003	-	17506.267	
46	17486.050	17486.052	-.002	-	17506.243	
47	17485.590	17485.590	.000	-	17506.213	
48	17485.122	17485.122	.000	-	17506.178	
49	17484.651	17484.649	.002	-	17506.138	
50	17484.169	17484.171	-.002	-	17506.092	
51	17483.687	17483.688	-.001	-	17506.041	
52	17483.196	17483.199	-.003	-	17505.984	
53	17482.704	17482.705	-.001	-	17505.922	
54	17482.205	17482.206	-.001	-	17505.855	
55	17481.704	17481.702	.002	-	17505.782	
56	17481.196	17481.192	.004	-	17505.704	
57	17480.677	17480.677	.000	-	17505.620	
58	17480.158	17480.157	.001	-	17505.531	
59	17479.631	17479.631	.000	-	17505.437	
60	17479.097	17479.100	-.003	-	17505.337	
61	17478.565	17478.564	.001	-	17505.232	
62	17478.023	17478.022	.001	-	17505.121	
63	17477.476	17477.476	.000	-	17505.005	
64	17476.927	17476.923	.004	-	17504.883	
65	17476.365	17476.366	-.001	-	17504.756	
66	17475.801	17475.803	-.002	-	17504.624	
67	17475.238	17475.235	.003	-	17504.486	
75	-	17470.497		17503.187	17503.183	.004
76	-	17469.880		-	17502.995	
77	-	17469.258		17502.802	17502.802	.000
78	-	17468.631		17502.602	17502.603	-.001
79	-	17467.998		17502.394	17502.399	-.005
80	-	17467.360		17502.189	17502.189	.000
81	-	17466.717		17501.975	17501.973	.002
82	-	17466.068		17501.751	17501.752	-.001
83	-	17465.413		17501.529	17501.525	.004
84	-	17464.753		17501.292	17501.292	.000
85	-	17464.088		17501.053	17501.054	-.001
86	-	17463.417		-	17500.810	
87	-	17462.741		17500.561	17500.561	.000

1-2 Band

		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
10	17137.527	17137.520	.007	-	17142.087	
11	17137.263	17137.254	.009	-	17142.256	

12	17136.998	17136.984	.014	-	17142.421	
13	17136.729	17136.710	.019*	-	17142.582	
14	17136.438	17136.432	.006	-	17142.738	
15	17136.157	17136.149	.008	-	17142.890	
16	17135.866	17135.861	.005	-	17143.037	
17	17135.573	17135.570	.003	-	17143.180	
18	17135.275	17135.274	.001	-	17143.319	
19	17134.982	17134.973	.009	-	17143.453	
20	17134.675	17134.668	.007	-	17143.583	
21	17134.362	17134.359	.003	-	17143.708	
22	17134.048	17134.046	.002	-	17143.829	
23	17133.731	17133.728	.003	-	17143.945	
24	17133.411	17133.405	.006	-	17144.057	
25	17133.081	17133.079	.002	-	17144.165	
26	-	17132.748		-	17144.268	
27	-	17132.412		-	17144.367	
28	-	17132.072		17144.464	17144.461	.003
29	-	17131.728		-	17144.551	
30	17131.373	17131.380	-.007*	17144.641	17144.637	.004
31	17131.020	17131.027	-.007*	17144.721	17144.718	.003
32	17130.667	17130.669	-.002	17144.794	17144.794	.000
33	17130.309	17130.308	.001	17144.869	17144.866	.003
34	17129.945	17129.942	.003	-	17144.934	
35	-	17129.571		-	17144.997	
36	-	17129.196		17145.052	17145.056	-.004
37	-	17128.817		17145.109	17145.110	-.001
38	-	17128.433		17145.158	17145.159	-.001
39	17128.044	17128.045	-.001	17145.201	17145.205	-.004
40	17127.655	17127.652	.003	17145.245	17145.245	.000
41	17127.258	17127.255	.003	17145.281	17145.281	.000
42	-	17126.854		17145.310	17145.313	-.003
43	17126.448	17126.448	.000	17145.340	17145.340	.000
44	17126.043	17126.037	.006	17145.370	17145.363	.007*
45	17125.622	17125.623	-.001	17145.396	17145.381	.015*
46	17125.201	17125.204	-.003	-	17145.394	
47	17124.781	17124.780	.001	-	17145.403	
48	17124.349	17124.352	-.003	-	17145.408	
49	17123.926	17123.919	.007	-	17145.408	
50	17123.485	17123.482	.003	-	17145.403	
51	17123.046	17123.041	.005	-	17145.394	
52	17122.597	17122.595	.002	-	17145.380	
53	17122.149	17122.145	.004	-	17145.361	
54	17121.689	17121.690	-.001	17145.336	17145.338	-.002
55	17121.234	17121.230	.004	17145.309	17145.311	-.002
56	17120.765	17120.767	-.002	17145.281	17145.279	.002
57	17120.294	17120.298	-.004	17145.241	17145.242	-.001
58	-	17119.826		17145.199	17145.200	-.001
59	-	17119.348		17145.152	17145.154	-.002
60	-	17118.866		17145.099	17145.103	-.004

2-2 Band

J	P Branch OBS	CALC	DIFF	R Branch OBS	CALC	DIFF
2	17467.356	17467.344	.012**	-	17468.427	
3	17467.111	17467.111	.000	17468.635	17468.628	.007**
4	17466.875	17466.874	.001	17468.828	17468.824	.004**
5	-	17466.631		-	17469.015	
6	17466.390	17466.383	.007**	-	17469.200	
7	-	17466.130		17469.388	17469.380	.008**
8	17465.886	17465.872	.014**	17469.559	17469.555	.004**
9	17465.610	17465.609	.001	17469.723	17469.725	-.002
10	-	17465.340		17469.887	17469.889	-.002
11	17465.067	17465.066	.001	17470.048	17470.048	.000
12	17464.788	17464.787	.001	17470.200	17470.202	-.002
13	17464.504	17464.502	.002	17470.346	17470.350	-.004
14	17464.213	17464.212	.001	-	17470.493	
15	17463.916	17463.917	-.001	-	17470.630	
16	17463.616	17463.616	.000	-	17470.761	
17	17463.316	17463.310	.006**	-	17470.887	
18	17462.994	17462.998	-.004	-	17471.006	
19	17462.676	17462.680	-.004	-	17471.118	
20	17462.357	17462.356	.001	-	17471.221	
27	17460.147	17460.141	.006	-	17471.981	
28	17459.739	17459.732	.007	-	17472.040	
29	17459.348	17459.343	.005	-	17472.098	
30	17458.966	17458.958	.008	-	17472.154	
31	17458.576	17458.574	.002	-	17472.206	
32	17458.193	17458.187	.006	-	17472.254	
33	17457.799	17457.796	.003	-	17472.298	
34	17457.403	17457.402	.001	-	17472.336	
35	17457.005	17457.003	.002	-	17472.370	
36	17456.599	17456.599	.000	-	17472.400	
37	17456.193	17456.191	.002	-	17472.424	
38	17455.780	17455.777	.003	-	17472.443	
39	17455.360	17455.359	.001	-	17472.457	
40	17454.939	17454.936	.003	-	17472.466	
41	17454.501	17454.508	-.007**	-	17472.470	
42	17454.078	17454.075	.003	-	17472.469	
43	17453.643	17453.637	.006	-	17472.462	
44	17453.184	17453.194	-.010**	-	17472.451	
45	17452.743	17452.746	-.003	-	17472.434	
46	17452.295	17452.293	.002	-	17472.412	
47	17451.840	17451.834	.006	-	17472.385	
48	17451.367	17451.371	-.004	-	17472.353	
49	17450.905	17450.903	.002	-	17472.316	
50	17450.427	17450.429	-.002	-	17472.273	
51	17449.945	17449.950	-.005	-	17472.226	
52	17449.475	17449.467	.008**	-	17472.173	
53	17448.976	17448.978	-.002	-	17472.115	
54	17448.484	17448.484	.000	-	17472.051	
55	17447.984	17447.985	-.001	-	17471.983	
56	17447.478	17447.481	-.003	-	17471.909	

2-3 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
4	-	17107.473		17109.423	17109.423	.000
12	-	17105.442		17110.856	17110.857	-.001
13	-	17105.168		17111.014	17111.016	-.002
14	-	17104.890		-	17111.170	
15	17104.611	17104.607	.004	17111.321	17111.320	.001
16	17104.318	17104.320	-.002	-	17111.465	
17	17104.019	17104.027	-.008**	-	17111.604	
18	17103.731	17103.730	.001	17111.742	17111.738	.004
19	-	17103.428		-	17111.866	
20	17103.121	17103.120	.001	-	17111.986	
21	17102.805	17102.807	-.002	-	17112.096	
22	-	17102.485		-	17112.188	
23	17102.159	17102.153	.006	-	17112.240	
24	17101.814	17101.804	.010	-	17112.760	
25	-	17101.414		-	17112.753	
26	-	17101.493		-	17112.809	
27	17101.052	17101.045	.007	-	17112.885	
28	17100.667	17100.659	.008	-	17112.967	
29	17100.299	17100.294	.005	-	17113.049	
30	17099.934	17099.934	.000	-	17113.130	
31	17099.574	17099.575	-.001	-	17113.208	
32	17099.214	17099.215	-.001	-	17113.282	
33	17098.848	17098.852	-.004	-	17113.353	
34	17098.484	17098.485	-.001	-	17113.420	
35	17098.117	17098.115	.002	-	17113.483	
36	17097.739	17097.741	-.002	-	17113.542	
37	17097.358	17097.363	-.005	-	17113.596	
38	17096.976	17096.981	-.005	17113.649	17113.647	.002
39	-	17096.595		17113.694	17113.693	.001
40	-	17096.205		-	17113.735	
41	-	17095.811		-	17113.773	
42	-	17095.413		17113.805	17113.806	-.001
43	-	17095.010		17113.837	17113.835	.002
44	-	17094.603		-	17113.860	
45	-	17094.192		17113.881	17113.880	.001
46	17093.772	17093.777	-.005	-	17113.896	
47	17093.354	17093.357	-.003	-	17113.908	
48	-	17092.933		-	17113.915	
49	-	17092.505		-	17113.918	
50	17092.072	17092.072	.000	-	17113.917	
51	17091.634	17091.636	-.002	-	17113.911	
52	17091.195	17091.195	.000	-	17113.900	
53	17090.751	17090.749	.002	-	17113.886	
54	17090.300	17090.300	.000	-	17113.867	
55	17089.845	17089.846	-.001	-	17113.843	
56	17089.386	17089.388	-.002	-	17113.815	
57	17088.926	17088.925	.001	-	17113.783	
58	17088.459	17088.458	.001	-	17113.746	
59	17087.987	17087.987	.000	-	17113.705	
60	17087.514	17087.512	.002	-	17113.660	

61	17087.032	17087.032	.000	-	17113.610	
62	17086.548	17086.548	.000	-	17113.555	
63	17086.062	17086.060	.002	-	17113.496	
64	17085.564	17085.567	-.003	-	17113.433	
65	17085.074	17085.070	.004	-	17113.365	

^{174}YbS 0 - 0 Band *B*-*X* System

		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
1	-	21095.843		21096.528	21096.523	.005
2	-	21095.622		21096.758	21096.754	.004
3	21095.408	21095.403	.005	21096.990	21096.988	.002
4	21095.185	21095.187	-.002	21097.226	21097.224	.002
5	21094.971	21094.973	-.002	21097.464	21097.463	.001
6	21094.760	21094.761	-.001	21097.704	21097.703	.001
7	21094.553	21094.552	.001	21097.947	21097.946	.001
8	21094.341	21094.344	-.003	21098.182	21098.191	-.009
9	21094.136	21094.139	-.003	21098.439	21098.437	.002
10	21093.934	21093.936	-.002	21098.684	21098.686	-.002
11	21093.733	21093.735	-.002	21098.937	21098.936	.001
12	21093.533	21093.536	-.003	21099.187	21099.187	.000
13	21093.336	21093.338	-.002	21099.438	21099.439	-.001
14	21093.141	21093.141	.000	21099.692	21099.693	-.001
15	21092.946	21092.946	.000	21099.947	21099.947	.000
16	21092.752	21092.752	.000	21100.201	21100.201	.000
17	21092.560	21092.558	.002	21100.456	21100.456	.000
18	21092.366	21092.365	.001	21100.709	21100.711	-.002
19	21092.174	21092.173	.001	21100.963	21100.965	-.002
20	21091.981	21091.980	.001	21101.208	21101.219	-.011*
21	21091.788	21091.787	.001	21101.471	21101.471	.000
22	21091.592	21091.593	-.001	21101.723	21101.722	.001
23	21091.393	21091.398	-.005	21101.972	21101.970	.002
24	21091.205	21091.201	.004	21102.219	21102.216	.003
25	21091.003	21091.002	.001	21102.458	21102.459	-.001
26	21090.804	21090.801	.003	21102.694	21102.697	-.003
27	21090.599	21090.596	.003	21102.934	21102.931	.003
28	21090.387	21090.388	-.001	21103.165	21103.159	.006
29	21090.176	21090.174	.002	21103.379	21103.380	-.001
30	21089.954	21089.955	-.001	21103.592	21103.593	-.001
31	21089.732	21089.729	.003	21103.793	21103.797	-.004
32	21089.495	21089.496	-.001	21103.990	21103.991	-.001
33	21089.254	21089.253	.001	21104.173	21104.171	.002
34	21088.995	21088.999	-.004	21104.337	21104.338	-.001
35	21088.730	21088.733	-.003	21104.483	21104.488	-.005
36	21088.446	21088.453	-.007	21104.622	21104.618	.004
37	21088.154	21088.156	-.002	21104.726	21104.727	-.001
38	21087.842	21087.840	.002	21104.813	21104.811	.002
39	21087.503	21087.502	.001	-	21104.866	
40	21087.140	21087.139	.001	-	21104.889	
41	21086.750	21086.748	.002	-	21104.874	
42	21086.328	21086.325	.003	-	21104.818	
43	21085.872	21085.864	.008	21104.726	21104.714	.012*

44	21085.352	21085.361	-.009	21104.563	21104.556	.007*
45	21084.826	21084.811	.015*	21104.337	21104.337	.000*
46	21084.215	21084.207	.008*	-	21104.050	
47	21083.553	21083.543	.010*	21103.793	21103.685	.108*
48	21082.845	21082.810	.035*	-	21103.234	
49	21082.101	21081.999	.102*	21103.592	21102.686	.906*
50	21081.404	21081.103	.301*	-	21102.029	
51	21081.015	21080.109	.906*	-	21101.251	

^{174}YbS 0-1 Band

	P Branch			R Branch		
J	Obs	Calc	Diff	Obs	Calc	Diff
2	20731.241	20731.245	-.004	20732.378	20732.377	.001
3	20731.025	20731.028	-.003	20732.617	20732.613	.004
4	20730.812	20730.815	-.003	20732.854	20732.852	.002
5	20730.603	20730.605	-.002	20733.096	20733.094	.002
6	20730.396	20730.398	-.002	20733.342	20733.340	.002
7	20730.196	20730.194	.002	20733.588	20733.588	.000
8	20729.997	20729.993	.004	20733.834	20733.839	-.005
9	20729.800	20729.796	.004	20734.091	20734.093	-.002
10	20729.604	20729.601	.003	20734.347	20734.349	-.002
11	20729.409	20729.408	.001	20734.607	20734.608	-.001
12	20729.217	20729.218	-.001	20734.867	20734.869	-.002
13	20729.032	20729.031	.001	20735.130	20735.131	-.001
14	20728.846	20728.846	.000	20735.396	20735.396	.000
15	20728.661	20728.662	-.001	20735.662	20735.662	.000
16	20728.483	20728.481	.002	20735.928	20735.929	-.001
17	20728.303	20728.301	.002	20736.196	20736.198	-.002
18	20728.124	20728.123	.001	20736.468	20736.467	.001
19	20727.944	20727.945	-.001	20736.732	20736.736	-.004
20	20727.767	20727.769	-.002	20737.000	20737.006	-.006
21	20727.593	20727.593	.000	20737.278	20737.275	.003
22	20727.404	20727.417	-.013*	20737.544	20737.544	.000
23	20727.243	20727.240	.003	20737.813	20737.811	.002
24	20727.066	20727.063	.003	20738.079	20738.077	.002
25	20726.882	20726.885	-.003	20738.341	20738.340	.001
26	20726.701	20726.705	-.004	20738.601	20738.599	.002
27	20726.523	20726.523	.000	20738.859	20738.855	.004
28	20726.335	20726.337	-.002	20739.108	20739.106	.002
29	20726.150	20726.148	.002	20739.353	20739.351	.002
30	20725.954	20725.954	.000	20739.591	20739.589	.002
31	20725.758	20725.754	.004	20739.819	20739.819	.000
32	20725.546	20725.547	-.001	20740.038	20740.039	-.001
33	20725.328	20725.332	-.004	20740.246	20740.247	-.001
34	20725.103	20725.106	-.003	20740.441	20740.441	.000
35	20724.871	20724.870	.001	20740.618	20740.620	-.002
36	20724.619	20724.619	.000	20740.779	20740.780	-.001
37	20724.352	20724.353	-.001	20740.920	20740.919	.001
38	20724.068	20724.069	-.001	20741.030	20741.034	-.004
39	20723.761	20723.764	-.003	20741.126	20741.120	.006
40	20723.435	20723.434	.001	-	20741.175	
41	20723.076	20723.077	-.001	20741.206	20741.194	.012*

42	20722.691	20722.688	.003	20741.167	20741.170	-.003
43	20722.271	20722.262	.009	-	20741.100	
44	20721.790	20721.795	-.005	20740.992	20740.976	.016*
45	20721.303	20721.281	.022*	-	20740.791	
46	20720.722	20720.713	.009*	20740.587	20740.538	.049*
47	20720.101	20720.085	.016*	20740.314	20740.207	.107*
48	20719.426	20719.388	.038*	20740.104	20739.790	.314*
49	20718.719	20718.614	.105*	20740.208	20739.275	.933*
50	20718.065	20717.754	.311*	-	20738.651	
51	20717.722	20716.796	.926*	-	20737.904	

^{172}YbS 0-0 Band *B-X* System

	P Branch			R Branch		
J	Obs	Calc	Diff	Obs	Calc	Diff
3	-	21095.596		21097.178	21097.184	-.006
4	21095.379	21095.379	.000	21097.423	21097.420	.003
5	21095.165	21095.165	.000	21097.657	21097.659	-.002
6	21094.974	21094.953	.021*	21097.900	21097.901	-.001
7	21094.749	21094.744	.005	21098.142	21098.144	-.002
8	21094.553	21094.536	.017*	21098.389	21098.389	.000
9	21094.341	21094.331	.010*	21098.636	21098.637	-.001
10	21094.136	21094.128	.008*	21098.884	21098.886	-.002
11	21093.934	21093.927	.007*	21099.136	21099.137	-.001
12	21093.733	21093.727	.006	21099.387	21099.389	-.002
13	21093.533	21093.530	.003	21099.642	21099.643	-.001
14	21093.335	21093.333	.002	21099.898	21099.897	.001
15	21093.141	21093.138	.003	21100.153	21100.153	.000
16	21092.946	21092.945	.001	21100.408	21100.409	-.001
17	21092.752	21092.752	.000	21100.665	21100.665	.000
18	21092.560	21092.560	.000	21100.921	21100.922	-.001
19	21092.366	21092.368	-.002	21101.180	21101.178	.002
20	21092.174	21092.176	-.002	21101.436	21101.434	.002
21	21091.981	21091.984	-.003	21101.691	21101.689	.002
22	21091.788	21091.792	-.004	21101.948	21101.943	.005
23	21091.591	21091.599	-.008*	21102.219	21102.194	.025*
24	21091.398	21091.404	-.006*	21102.458	21102.443	.015*
25	21091.205	21091.207	-.002	21102.694	21102.689	.005
26	21091.007	21091.008	-.001	21102.934	21102.932	.002
27	21090.804	21090.807	-.003	21103.165	21103.170	-.005
28	21090.599	21090.601	-.002	21103.398	21103.403	-.005
29	21090.387	21090.391	-.004	21103.631	21103.629	.002
30	21090.176	21090.176	.000	21103.849	21103.848	.001
31	21089.954	21089.954	.000	21104.057	21104.058	-.001
32	21089.732	21089.726	.006	21104.262	21104.258	.004
33	21089.494	21089.488	.006	21104.448	21104.447	.001
34	21089.254	21089.241	.013*	21104.622	21104.622	.000
35	21088.996	21088.982	.014*	21104.772	21104.782	-.010
36	21088.710	21088.709	.001	21104.919	21104.924	-.005
37	21088.422	21088.421	.001	21105.051	21105.045	.006
38	21088.115	21088.116	-.001	21105.143	21105.143	.000
39	21087.791	21087.790	.001	21105.218	21105.215	.003
40	21087.439	21087.441	-.002	-	21105.257	

41	21087.065	21087.066	-.001	21105.256	21105.265	-.009*
42	21086.655	21086.661	-.006*	21105.218	21105.235	-.017*
43	21086.212	21086.222	-.010*	21105.143	21105.161	-.018*
44	21085.733	21085.744	-.011*	21105.051	21105.037	.014*
45	21085.205	21085.223	-.018*	-	21104.859	
46	21084.669	21084.653	.016*	-	21104.618	
47	21083.997	21084.027	-.030*	21104.313	21104.308	.005*
48	21083.378	21083.340	.038*	21104.057	21103.919	.138*
49	21082.601	21082.583	.018*	21103.962	21103.443	.519*
50	21081.880	21081.748	.132*	-	21102.869	
51	21081.349	21080.825	.524*	-	21102.187	

^{172}YbS 0-1 Band

		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
3	20730.892	20730.891	.001	20732.482	20732.479	.003
4	20730.679	20730.678	.001	20732.720	20732.719	.001
5	20730.466	20730.468	-.002	20732.963	20732.962	.001
6	20730.259	20730.261	-.002	20733.213	20733.208	.005
7	20730.054	20730.057	-.003	20733.460	20733.458	.002
8	20729.859	20729.856	.003	20733.710	20733.710	.000
9	20729.659	20729.658	.001	20733.964	20733.964	.000
10	20729.467	20729.463	.004	20734.219	20734.222	-.003
11	20729.270	20729.271	-.001	20734.475	20734.482	-.007
12	20729.082	20729.082	.000	20734.736	20734.744	-.008
13	20728.894	20728.895	-.001	20734.998	20735.008	-.010*
14	20728.708	20728.710	-.002	20735.271	20735.274	-.003
15	20728.530	20728.527	.003	20735.538	20735.542	-.004
16	20728.344	20728.347	-.003	20735.813	20735.811	.002
17	20728.170	20728.168	.002	20736.081	20736.081	.000
18	20727.988	20727.990	-.002	20736.351	20736.353	-.002
19	20727.812	20727.814	-.002	20736.626	20736.625	.001
20	20727.643	20727.639	.004	20736.899	20736.897	.002
21	20727.464	20727.464	.000	20737.169	20737.169	.000
22	20727.294	20727.290	.004	20737.442	20737.441	.001
23	20727.117	20727.115	.002	20737.712	20737.711	.001
24	20726.940	20726.941	-.001	20737.983	20737.980	.003
25	20726.765	20726.765	.000	20738.245	20738.247	-.002
26	20726.591	20726.587	.004	20738.515	20738.511	.004
27	20726.406	20726.408	-.002	20738.774	20738.772	.002
28	20726.229	20726.226	.003	20739.027	20739.028	-.001
29	20726.042	20726.041	.001	20739.280	20739.279	.001
30	20725.851	20725.851	.000	20739.525	20739.523	.002
31	20725.648	20725.655	-.007	20739.759	20739.760	-.001
32	20725.451	20725.454	-.003	20740.000	20739.987	.013*
33	20725.238	20725.244	-.006	20740.207	20740.204	.003
34	20725.022	20725.025	-.003	20740.410	20740.407	.003
35	20724.797	20724.796	.001	20740.589	20740.596	-.007
36	20724.554	20724.554	.000	20740.771	20740.767	.004
37	-	20724.297		20740.915	20740.919	-.004
38	20724.022	20724.023	-.001	20741.030	20741.047	-.017*
39	20723.733	20723.729	.004	-	20741.149	

40	20723.435	20723.412	.023*	-	20741.221	
41	20723.076	20723.069	.007	-	20741.258	
42	20722.691	20722.695	-.004	20741.257	20741.255	.002
43	20722.277	20722.287	-.010*	20741.206	20741.208	-.002
44	20721.839	20721.839	.000	-	20741.109	
45	20721.358	20721.346	.012*	-	20740.953	
46	20720.824	20720.803	.021*	20740.831	20740.731	.100*
47	20720.215	20720.201	.014*	20740.543	20740.435	.108*
48	20719.633	20719.535	.098*	20740.298	20740.056	.242*
49	20718.901	20718.794	.107*	-	20739.584	
50	20718.216	20717.971	.245*	-	20739.007	
51	20717.722	20717.055	.667*	-	20738.313	

Appendix 3

YbOH Line Positions

Rotational transitions in the $\tilde{A}^2\Pi - \tilde{X}^2\Sigma^-$ system of ^{174}YbOH and ^{172}YbOH. For each transition, the tables show the assigned rotational quantum number J, the measured line position in cm^{-1} and the residual between the observed and calculated values. Lines marked with ** were excluded in the least-squares fit.

^{174}YbOH (000)–(000) Band

	$Q_{11}(ef)$			$R_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
30.5	-	17331.989		17332.538	17332.542	-.004
31.5	17332.509	17332.511	-.002	17333.076	17333.081	-.005
32.5	17333.044	17333.050	-.006	17333.635	17333.636	-.001
33.5	17333.604	17333.604	.000	17334.208	17334.207	.001
34.5	17334.174	17334.174	.000	17334.792	17334.793	-.001
35.5	17334.757	17334.759	-.002	17335.393	17335.396	-.003
36.5	17335.358	17335.361	-.003	17336.014	17336.014	.000
37.5	17335.976	17335.978	-.002	17336.647	17336.647	.000
38.5	17336.606	17336.610	-.004	17337.297	17337.297	.000
39.5	17337.258	17337.259	-.001	17337.962	17337.962	.000
40.5	17337.920	17337.923	-.003	17338.642	17338.643	-.001
41.5	17338.597	17338.603	-.006	17339.345	17339.339	.006
42.5	17339.289	17339.298	-.009	17340.054	17340.051	.003
43.5	17340.008	17340.009	-.001	17340.781	17340.779	.002
44.5	17340.734	17340.736	-.002	17341.519	17341.522	-.003
45.5	17341.477	17341.479	-.002	17342.286	17342.281	.005
46.5	17342.237	17342.237	.000	17343.063	17343.056	.007
47.5	17343.007	17343.010	-.003	17343.849	17343.847	.002
48.5	17343.800	17343.800	.000	17344.655	17344.653	.002
49.5	17344.603	17344.605	-.002	-	17345.474	
50.5	-	17345.425		17346.315	17346.311	.004
51.5	17346.263	17346.262	.001	17347.168	17347.164	.004
52.5	17347.112	17347.113	-.001	17348.039	17348.032	.007
53.5	17347.982	17347.981	.001	17348.917	17348.916	.001
54.5	17348.864	17348.864	.000	17349.817	17349.816	.001
55.5	17349.763	17349.762	.001	17350.737	17350.731	.006
56.5	17350.674	17350.676	-.002	17351.664	17351.661	.003
57.5	17351.603	17351.606	-.003	17352.613	17352.607	.006
58.5	17352.551	17352.551	.000	-	17353.569	
59.5	-	17353.511		-	17354.546	
60.5	-	17354.487		17355.542	17355.538	.004
61.5	17355.483	17355.479	.004	-	17356.546	
62.5	-	17356.486		17357.561	17357.569	-.008
63.5	17357.515	17357.508	.007	17358.613	17358.608	.005
64.5	17358.551	17358.546	.005	17359.663	17359.662	.001
65.5	17359.600	17359.599	.001	17360.734	17360.732	.002
66.5	17360.670	17360.668	.002	17361.812	17361.817	-.005
67.5	17361.748	17361.752	-.004	17362.915	17362.917	-.002
68.5	17362.854	17362.851	.003	17364.030	17364.032	-.002
69.5	17363.966	17363.965	.001	17365.164	17365.163	.001
70.5	17365.096	17365.095	.001	17366.307	17366.310	-.003
71.5	17366.238	17366.241	-.003	17367.461	17367.471	-.010
72.5	17367.410	17367.401	.009	17368.642	17368.648	-.006
73.5	17368.576	17368.577	-.001	17369.838	17369.840	-.002
74.5	17369.773	17369.768	.005	17371.047	17371.047	.000
75.5	17370.974	17370.974	.000	-	17372.270	
76.5	-	17372.196		17373.498	17373.507	-.009
77.5	17373.432	17373.433	-.001	17374.762	17374.760	.002
78.5	17374.685	17374.684	.001	-	17376.028	

	$R_{11}(ee)$			$P_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
1.5	-	17326.063		17322.185	17322.178	.007
2.5	-	17327.073		17321.248	17321.247	.001
3.5	-	17328.099		17320.337	17320.331	.006
4.5	-	17329.141		17319.441	17319.431	.010
5.5	-	17330.198		17318.552	17318.547	.005
6.5	17331.270	17331.271	-.001	17317.677	17317.678	-.001
7.5	-	17332.360		17316.825	17316.826	-.001
8.5	17333.464	17333.464	.000	17315.995	17315.989	.006
9.5	17334.582	17334.584	-.002	17315.165	17315.168	-.003
10.5	17335.718	17335.719	-.001	17314.364	17314.363	.001
11.5	17336.873	17336.870	.003	17313.569	17313.574	-.005
12.5	17338.035	17338.037	-.002	17312.799	17312.801	-.002
13.5	17339.216	17339.219	-.003	17312.041	17312.044	-.003
14.5	17340.419	17340.416	.003	-	17311.303	
15.5	17341.632	17341.629	.003	17310.575	17310.578	-.003
16.5	17342.861	17342.857	.004	17309.866	17309.868	-.002
17.5	17344.104	17344.101	.003	17309.172	17309.175	-.003
18.5	17345.377	17345.360	.017**	17308.496	17308.498	-.002
19.5	17346.638	17346.635	.003	17307.831	17307.836	-.005
20.5	17347.926	17347.925	.001	17307.187	17307.191	-.004
21.5	17349.231	17349.230	.001	17306.558	17306.561	-.003
22.5	17350.555	17350.551	.004	17305.949	17305.948	.001
23.5	17351.889	17351.887	.002	17305.347	17305.350	-.003
24.5	17353.240	17353.238	.002	17304.766	17304.769	-.003
25.5	17354.606	17354.604	.002	17304.203	17304.204	-.001
26.5	17355.985	17355.986	-.001	17303.656	17303.655	.001
27.5	17357.385	17357.383	.002	17303.119	17303.121	-.002
28.5	17358.799	17358.795	.004	17302.604	17302.604	.000
29.5	17360.223	17360.222	.001	17302.101	17302.103	-.002
30.5	17361.669	17361.664	.005	17301.617	17301.618	-.001
31.5	17363.125	17363.122	.003	17301.150	17301.149	.001
32.5	17364.596	17364.594	.002	17300.696	17300.696	.000
33.5	17366.083	17366.082	.001	17300.259	17300.260	-.001
34.5	17367.583	17367.584	-.001	17299.841	17299.839	.002
35.5	17369.097	17369.102	-.005	17299.435	17299.435	.000
36.5	17370.636	17370.634	.002	17299.047	17299.046	.001
37.5	17372.182	17372.182	.000	17298.675	17298.674	.001
38.5	17373.739	17373.744	-.005	17298.319	17298.318	.001
39.5	17375.321	17375.321	.000	17297.980	17297.977	.003
40.5	17376.897	17376.913	-.016**	17297.653	17297.653	.000
41.5	17378.518	17378.520	-.002	17297.347	17297.346	.001
42.5	17380.145	17380.142	.003	17297.056	17297.054	.002
43.5	17381.773	17381.778	-.005	17296.780	17296.778	.002
44.5	17383.421	17383.429	-.008	17296.518	17296.519	-.001
45.5	17385.095	17385.095	.000	17296.283	17296.276	.007
46.5	17386.774	17386.776	-.002	17296.050	17296.048	.002
47.5	17388.466	17388.471	-.005	17295.839	17295.837	.002
48.5	17390.177	17390.181	-.004	-	17295.642	
49.5	-	17391.905		17295.461	17295.464	-.003
50.5	17393.639	17393.644	-.005	17295.289	17295.301	-.012**
51.5	17395.400	17395.397	.003	17295.156	17295.154	.002
52.5	17397.165	17397.165	.000	17295.025	17295.024	.001

53.5	17398.946	17398.948	-.002	17294.908	17294.910	-.002
54.5	-	17400.744		17294.808	17294.812	-.004
55.5	17402.548	17402.555	-.007	17294.727	17294.730	-.003
56.5	-	17404.381		17294.664	17294.664	.000
57.5	-	17406.221		-	17294.614	
58.5	17408.069	17408.075	-.006	-	17294.580	
59.5	17409.937	17409.943	-.006	-	17294.563	
60.5	17411.826	17411.826	.000	-	17294.562	
61.5	17413.726	17413.722	.004	-	17294.576	
62.5	17415.634	17415.633	.001	-	17294.607	
63.5	17417.559	17417.558	.001	-	17294.654	
64.5	17419.497	17419.497	.000	-	17294.717	
65.5	17421.454	17421.450	.004	-	17294.796	
66.5	17423.425	17423.418	.007	-	17294.892	
67.5	17425.405	17425.399	.006	-	17295.003	
68.5	-	17427.393		-	17295.130	
69.5	17429.415	17429.402	.013**	-	17295.274	

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(000)–(100) Band

	$R_{11}(ee)$			$P_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
4.5	-	16799.832		16790.129	16790.131	-.002
5.5	-	16800.904		16789.276	16789.264	.012**
6.5	-	16801.995		16788.415	16788.415	.000
7.5	-	16803.105		16787.600	16787.585	.015**
8.5	-	16804.233		16786.772	16786.774	-.002
9.5	-	16805.380		16785.979	16785.982	-.003
10.5	-	16806.545		16785.210	16785.209	.001
11.5	-	16807.728		16784.455	16784.454	.001
12.5	-	16808.930		16783.720	16783.718	.002
13.5	-	16810.151		16782.995	16783.001	-.006
14.5	-	16811.389		16782.305	16782.303	.002
15.5	-	16812.647		16781.626	16781.624	.002
16.5	-	16813.922		16780.965	16780.963	.002
17.5	-	16815.216		16780.319	16780.322	-.003
18.5	-	16816.528		16779.697	16779.699	-.002
19.5	-	16817.859		16779.098	16779.095	.003
20.5	16819.211	16819.207	.004	16778.510	16778.511	-.001
21.5	16820.589	16820.574	.015**	16777.942	16777.945	-.003
22.5	16821.967	16821.959	.008	16777.401	16777.397	.004
23.5	16823.364	16823.363	.001	16776.872	16776.869	.003
24.5	16824.791	16824.784	.007	16776.362	16776.360	.002
25.5	16826.225	16826.224	.001	16775.870	16775.870	.000
26.5	16827.677	16827.682	-.005	16775.399	16775.399	.000
27.5	16829.153	16829.158	-.005	16774.948	16774.946	.002
28.5	16830.651	16830.652	-.001	16774.512	16774.513	-.001
29.5	16832.163	16832.164	-.001	16774.093	16774.098	-.005
30.5	16833.692	16833.694	-.002	16773.703	16773.703	.000
31.5	16835.245	16835.242	.003	16773.326	16773.326	.000
32.5	16836.802	16836.808	-.006	16772.963	16772.969	-.006
33.5	-	16838.392		16772.630	16772.630	.000
34.5	-	16839.994		16772.318	16772.311	.007

35.5	-	16841.613		16772.010	16772.010	.000
36.5	-	16843.251		16771.742	16771.729	.013**
37.5	-	16844.906		16771.463	16771.466	-.003
38.5	-	16846.580		16771.222	16771.223	-.001
39.5	-	16848.271		16770.986	16770.998	-.012**
40.5	-	16849.979		16770.800	16770.793	.007
41.5	-	16851.706		16770.621	16770.606	.015**
42.5	-	16853.450		16770.436	16770.438	-.002
43.5	-	16855.211		16770.290	16770.290	.000

^{172}YbOH (000)–(000) Band

	$Q_{11}(\mathit{ef})$			$R_{12}(\mathit{ff})$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
41.5	17338.696	17338.694	.002	17339.426	17339.434	-.008
42.5	17339.393	17339.392	.001	-	17340.148	
43.5	17340.107	17340.105	.002	17340.874	17340.878	-.004
44.5	17340.834	17340.834	.000	17341.617	17341.623	-.006
45.5	17341.581	17341.578	.003	17342.393	17342.384	.009
46.5	17342.340	17342.338	.002	17343.155	17343.161	-.006
47.5	17343.113	17343.113	.000	17343.950	17343.953	-.003
48.5	17343.904	17343.904	.000	17344.760	17344.761	-.001
49.5	17344.719	17344.711	.008	-	17345.584	
50.5	-	17345.533		17346.420	17346.423	-.003
51.5	17346.380	17346.371	.009	17347.276	17347.277	-.001
52.5	17347.225	17347.225	.000	17348.140	17348.147	-.007
53.5	17348.093	17348.093	.000	-	17349.032	
54.5	17348.977	17348.978	-.001	17349.931	17349.933	-.002
55.5	17349.880	17349.878	.002	17350.845	17350.850	-.005
56.5	17350.795	17350.793	.002	17351.779	17351.782	-.003
57.5	17351.727	17351.724	.003	17352.730	17352.729	.001
58.5	17352.669	17352.670	-.001	-	17353.692	
59.5	-	17353.632		-	17354.670	
60.5	-	17354.609		17355.663	17355.663	.000
61.5	17355.606	17355.602	.004	-	17356.672	
62.5	-	17356.610		17357.695	17357.696	-.001
63.5	17357.638	17357.633	.005	17358.739	17358.736	.003
64.5	17358.676	17358.672	.004	17359.793	17359.791	.002
65.5	17359.725	17359.726	-.001	17360.861	17360.861	.000
66.5	17360.795	17360.795	.000	17361.941	17361.947	-.006
67.5	17361.873	17361.879	-.006	17363.050	17363.048	.002
68.5	17362.979	17362.979	.000	17364.169	17364.164	.005
69.5	17364.094	17364.094	.000	17365.302	17365.295	.007
70.5	17365.224	17365.225	-.001	17366.445	17366.442	.003
71.5	17366.365	17366.370	-.005	17367.606	17367.604	.002
72.5	17367.526	17367.531	-.005	17368.777	17368.781	-.004
73.5	17368.703	17368.707	-.004	17369.979	17369.973	.006
74.5	17369.893	17369.898	-.005	17371.179	17371.180	-.001
75.5	17371.103	17371.104	-.001	-	17372.402	
76.5	-	17372.326		17373.649	17373.640	.009
77.5	17373.556	17373.562	-.006	17374.891	17374.892	-.001
78.5	17374.814	17374.813	.001	-	17376.160	

	$R_{11}(ee)$			$P_{12}(ff)$		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
1.5	-	17326.077		17322.185	17322.189	-.004
2.5	-	17327.088		17321.248	17321.256	-.008
3.5	-	17328.115		17320.337	17320.340	-.003
4.5	-	17329.158		17319.441	17319.439	.002
5.5	-	17330.217		17318.552	17318.554	-.002
6.5	-	17331.291		17317.677	17317.684	-.007
7.5	-	17332.381		17316.825	17316.831	-.006
8.5	-	17333.486		17315.995	17315.994	.001
9.5	-	17334.608		17315.165	17315.172	-.007
10.5	-	17335.744		17314.364	17314.367	-.003
11.5	-	17336.897		17313.569	17313.577	-.008
12.5	-	17338.065		17312.799	17312.804	-.005
13.5	-	17339.248		17312.041	17312.046	-.005
14.5	17340.454	17340.447	.007	-	17311.304	
15.5	17341.660	17341.661	-.001	17310.575	17310.578	-.003
16.5	17342.899	17342.891	.008	17309.866	17309.869	-.003
17.5	17344.142	17344.137	.005	17309.172	17309.175	-.003
18.5	17345.414	17345.398	.016**	17308.496	17308.497	-.001
19.5	17346.668	17346.674	-.006	17307.831	17307.835	-.004
20.5	17347.971	17347.965	.006	17307.187	17307.190	-.003
21.5	17349.274	17349.272	.002	17306.558	17306.560	-.002
22.5	17350.601	17350.595	.006	17305.949	17305.946	.003
23.5	17351.936	17351.932	.004	17305.347	17305.349	-.002
24.5	17353.290	17353.285	.005	17304.766	17304.767	-.001
25.5	17354.656	17354.654	.002	17304.203	17304.202	.001
26.5	17356.045	17356.037	.008	17303.656	17303.652	.004
27.5	17357.441	17357.436	.005	17303.119	17303.119	.000
28.5	17358.857	17358.850	.007	17302.604	17302.602	.002
29.5	17360.288	17360.279	.009	17302.101	17302.101	.000
30.5	17361.732	17361.723	.009	17301.617	17301.616	.001
31.5	17363.188	17363.182	.006	17301.150	17301.147	.003
32.5	17364.661	17364.657	.004	17300.696	17300.694	.002
33.5	17366.150	17366.146	.004	17300.259	17300.257	.002
34.5	17367.649	17367.651	-.002	17299.841	17299.837	.004
35.5	17369.166	17369.170	-.004	17299.435	17299.432	.003
36.5	17370.710	17370.705	.005	17299.047	17299.044	.003
37.5	17372.256	17372.254	.002	17298.675	17298.672	.003
38.5	17373.812	17373.818	-.006	17298.319	17298.316	.003
39.5	17375.395	17375.398	-.003	17297.980	17297.976	.004
40.5	17376.993	17376.992	.001	17297.653	17297.652	.001
41.5	17378.591	17378.601	-.010	17297.347	17297.344	.003
42.5	17380.223	17380.224	-.001	17297.056	17297.053	.003
43.5	17381.856	17381.863	-.007	17296.780	17296.777	.003
44.5	17383.511	17383.516	-.005	17296.518	17296.518	.000
45.5	17385.176	17385.184	-.008	17296.283	17296.275	.008
46.5	17386.863	17386.867	-.004	17296.050	17296.048	.002
47.5	17388.559	17388.564	-.005	17295.839	17295.837	.002
48.5	17390.271	17390.276	-.005	-	17295.643	
49.5	-	17392.002		17295.461	17295.464	-.003
50.5	17393.738	17393.743	-.005	17295.289	17295.302	-.013**
51.5	17395.492	17395.499	-.007	17295.156	17295.156	.000
52.5	17397.266	17397.269	-.003	17295.025	17295.026	-.001

53.5	17399.059	17399.053	.006	17294.908	17294.912	-.004
54.5	-	17400.852		17294.808	17294.814	-.006
55.5	17402.660	17402.665	-.005	17294.727	17294.732	-.005
56.5	-	17404.493		17294.664	17294.667	-.003
57.5	-	17406.335		-	17294.617	
58.5	17408.184	17408.191	-.007	-	17294.584	
59.5	17410.054	17410.061	-.007	-	17294.567	
60.5	17411.948	17411.946	.002	-	17294.566	
61.5	17413.846	17413.845	.001	-	17294.581	
62.5	17415.754	17415.757	-.003	-	17294.612	
63.5	17417.691	17417.684	.007	-	17294.659	
64.5	17419.629	17419.625	.004	-	17294.722	
65.5	17421.579	17421.580	-.001	-	17294.801	
66.5	17423.560	17423.549	.011	-	17294.897	
67.5	17425.538	17425.532	.006	-	17295.008	

Appendix 4

CaS Line Positions

Rotational transitions in the $A^1\Sigma^+$ – $X^1\Sigma^+$ system of CaS. For each transition, the tables show the assigned rotational quantum number J, the measured line position in cm^{-1} and the residual between the observed and calculated values. Lines marked with * were excluded in the least-squares fit.

CaS 0-0 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
0	-	.000		15194.759	15194.760	-.001
1	15194.073	15194.074	-.001	15195.069	15195.073	-.004
2	15193.702	15193.702	.000	15195.366	15195.366	.000
3	15193.308	15193.310	-.002	15195.636	15195.639	-.003
4	15192.898	15192.898	.000	15195.890	15195.893	-.003
5	15192.467	15192.467	.000	15196.128	15196.127	.001
6	15192.011	15192.015	-.004	15196.338	15196.341	-.003
7	15191.544	15191.544	.000	15196.528	15196.535	-.007
8	15191.052	15191.054	-.002	15196.705	15196.710	-.005
9	15190.539	15190.543	-.004	15196.823	15196.864	-.041*
10	15190.015	15190.013	.002	15196.987	15196.999	-.012*
11	15189.465	15189.463	.002	15197.101	15197.114	-.013*
12	15188.892	15188.893	-.001	15197.197	15197.210	-.013*
13	15188.306	15188.303	.003	15197.276	15197.285	-.009
14	15187.697	15187.694	.003	-	15197.341	
15	15187.068	15187.065	.003	-	15197.377	
16	15186.419	15186.416	.003	-	15197.393	
17	15185.749	15185.748	.001	-	15197.389	
18	15185.062	15185.060	.002	-	15197.365	
19	15184.352	15184.351	.001	-	15197.322	
20	15183.625	15183.624	.001	-	15197.258	
21	15182.878	15182.876	.002	-	15197.175	
22	15182.111	15182.109	.002	-	15197.072	
23	15181.323	15181.322	.001	15196.948	15196.949	-.001
24	15180.520	15180.515	.005	15196.806	15196.806	.000
25	15179.692	15179.689	.003	15196.641	15196.643	-.002
26	15178.851	15178.842	.009	15196.459	15196.461	-.002
27	15177.979	15177.976	.003	15196.259	15196.258	.001
28	15177.092	15177.091	.001	15196.034	15196.036	-.002
29	15176.187	15176.185	.002	15195.792	15195.794	-.002
30	15175.264	15175.260	.004	15195.528	15195.531	-.003
31	15174.319	15174.315	.004	15195.250	15195.249	.001
32	15173.354	15173.350	.004	15194.946	15194.947	-.001
33	15172.369	15172.365	.004	15194.622	15194.625	-.003
34	15171.366	15171.361	.005	15194.284	15194.283	.001
35	15170.339	15170.337	.002	15193.918	15193.921	-.003
36	15169.297	15169.293	.004	15193.537	15193.539	-.002
37	15168.229	15168.229	.000	15193.137	15193.138	-.001
38	15167.147	15167.146	.001	15192.712	15192.716	-.004
39	15166.047	15166.043	.004	15192.272	15192.274	-.002
40	15164.923	15164.920	.003	15191.811	15191.812	-.001
41	15163.781	15163.777	.004	15191.327	15191.330	-.003
42	15162.620	15162.614	.006	15190.817	15190.828	-.011
43	15161.435	15161.432	.003	15190.305	15190.307	-.002
44	15160.234	15160.230	.004	15189.757	15189.765	-.008
45	15159.012	15159.008	.004	15189.198	15189.203	-.005
46	15157.771	15157.766	.005	15188.619	15188.621	-.002
47	15156.518	15156.504	.014	15188.016	15188.019	-.003
48	15155.231	15155.223	.008	15187.389	15187.397	-.008

49	-	15153.922		15186.749	15186.754	-.005
50	-	15152.600		15186.087	15186.092	-.005
51	-	15151.259		15185.408	15185.410	-.002
52	-	15149.899		15184.704	15184.707	-.003
53	-	15148.518		15183.980	15183.984	-.004
54	-	15147.117		15183.237	15183.242	-.005
55	-	15145.697		15182.475	15182.479	-.004
56	-	15144.257		15181.691	15181.695	-.004
57	15142.803	15142.797	.006	15180.890	15180.892	-.002
58	-	15141.317		15180.053	15180.069	-.016*
59	-	15139.817		15179.220	15179.225	-.005
60	-	15138.297		15178.357	15178.361	-.004
61	15136.769	15136.757	.012	15177.468	15177.477	-.009
62	15135.210	15135.198	.012	15176.565	15176.572	-.007
63	15133.627	15133.618	.009	15175.644	15175.648	-.004
64	15132.029	15132.019	.010	15174.701	15174.703	-.002
65	15130.406	15130.399	.007	15173.736	15173.738	-.002
66	-	15128.760		15172.746	15172.752	-.006
67	15127.105	15127.101	.004	15171.742	15171.747	-.005
68	15125.430	15125.422	.008	15170.710	15170.721	-.011
69	15123.724	15123.723	.001	15169.670	15169.674	-.004
70	15122.003	15122.003	.000	15168.600	15168.607	-.007
71	15120.268	15120.264	.004	15167.520	15167.520	.000
72	15118.509	15118.505	.004	15166.408	15166.413	-.005
73	-	15116.726		15165.280	15165.285	-.005
74	15114.932	15114.927	.005	15164.130	15164.137	-.007
75	15113.115	15113.108	.007	15162.961	15162.968	-.007
76	15111.276	15111.269	.007	15161.773	15161.779	-.006
77	15109.421	15109.410	.011	15160.564	15160.569	-.005
78	15107.530	15107.530	.000	15159.331	15159.339	-.008
79	15105.621	15105.631	-.010*	15158.088	15158.089	-.001
80	15103.727	15103.712	.015*	15156.814	15156.818	-.004
81	15101.783	15101.772	.011	15155.526	15155.527	-.001
82	15099.816	15099.813	.003	-	15154.215	
83	15097.836	15097.833	.003	-	15152.882	
84	15095.838	15095.833	.005	-	15151.529	
85	-	15093.814		-	15150.155	
86	15091.773	15091.774	-.001	-	15148.761	

1-0 Band

		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
0	-	.000		15602.202	15602.202	.000
1	15601.514	15601.518	-.004	15602.511	15602.512	-.001
2	15601.144	15601.144	.000	15602.797	15602.802	-.005
3	15600.754	15600.750	.004	15603.068	15603.071	-.003
4	15600.329	15600.335	-.006	15603.299	15603.318	-.019*
5	15599.904	15599.898	.006	15603.540	15603.545	-.005
6	15599.443	15599.441	.002	15603.743	15603.750	-.007
7	15598.969	15598.962	.007	15603.925	15603.935	-.010*
8	15598.466	15598.463	.003	15604.091	15604.098	-.007
9	15597.946	15597.943	.003	-	15604.241	
10	15597.405	15597.401	.004	-	15604.362	

11	15596.840	15596.839	.001	-	15604.463	
12	15596.260	15596.256	.004	-	15604.542	
13	15595.658	15595.652	.006	-	15604.601	
14	15595.033	15595.027	.006	-	15604.638	
15	15594.383	15594.381	.002	-	15604.654	
16	15593.717	15593.714	.003	-	15604.650	
17	15593.036	15593.026	.010*	-	15604.624	
18	15592.322	15592.317	.005	-	15604.577	
19	15591.591	15591.587	.004	-	15604.509	
20	15590.840	15590.836	.004	15604.418	15604.420	-.002
21	15590.067	15590.064	.003	15604.295	15604.310	-.015*
22	15589.273	15589.271	.002	15604.177	15604.179	-.002
23	-	15588.457		15604.025	15604.027	-.002
24	15587.622	15587.622	.000	15603.848	15603.854	-.006
25	15586.766	15586.767	-.001	15603.657	15603.659	-.002
26	15585.888	15585.890	-.002	15603.443	15603.444	-.001
27	15584.994	15584.992	.002	15603.204	15603.207	-.003
28	15584.073	15584.074	-.001	15602.949	15602.949	.000
29	15583.133	15583.134	-.001	15602.669	15602.671	-.002
30	15582.175	15582.173	.002	15602.366	15602.371	-.005
31	15581.192	15581.192	.000	15602.047	15602.049	-.002
32	15580.192	15580.189	.003	15601.704	15601.707	-.003
33	15579.167	15579.166	.001	15601.342	15601.344	-.002
34	15578.121	15578.121	.000	15600.957	15600.959	-.002
35	15577.055	15577.056	-.001	15600.552	15600.553	-.001
36	15575.968	15575.969	-.001	15600.127	15600.126	.001
37	15574.859	15574.862	-.003	15599.671	15599.678	-.007
38	-	15573.733		15599.212	15599.209	.003
39	15572.584	15572.583	.001	15598.719	15598.718	.001
40	15571.413	15571.413	.000	15598.208	15598.207	.001
41	15570.220	15570.221	-.001	15597.670	15597.674	-.004
42	15569.006	15569.009	-.003	15597.122	15597.120	.002
43	15567.770	15567.775	-.005	15596.546	15596.544	.002
44	15566.516	15566.521	-.005	15595.948	15595.947	.001
45	15565.241	15565.245	-.004	15595.331	15595.329	.002
46	15563.946	15563.949	-.003	15594.688	15594.690	-.002
47	15562.629	15562.631	-.002	15594.037	15594.030	.007
48	15561.292	15561.292	.000	15593.349	15593.348	.001
49	-	15559.932		15592.649	15592.645	.004
50	-	15558.552		15591.926	15591.920	.006
51	-	15557.150		15591.180	15591.175	.005
52	-	15555.727		15590.411	15590.408	.003
53	-	15554.283		15589.626	15589.619	.007
54	15552.824	15552.818	.006	15588.783	15588.809	-.026*
55	-	15551.332		15587.982	15587.978	.004
56	15549.820	15549.825	-.005	15587.134	15587.126	.008
57	15548.295	15548.296	-.001	15586.259	15586.252	.007
58	15546.747	15546.747	.000	15585.356	15585.357	-.001
59	-	15545.177		15584.449	15584.440	.009
60	-	15543.585		15583.507	15583.502	.005
61	-	15541.972		15582.549	15582.542	.007
62	15540.334	15540.338	-.004	15581.568	15581.561	.007
63	15538.676	15538.684	-.008	15580.567	15580.559	.008
64	15536.997	15537.007	-.010	15579.516	15579.535	-.019*
65	15535.306	15535.310	-.004	15578.492	15578.489	.003
66	15533.585	15533.592	-.007	15577.427	15577.422	.005
67	15531.843	15531.852	-.009	15576.336	15576.334	.002

68	15530.084	15530.092	-.008	15575.231	15575.224	.007
69	15528.306	15528.310	-.004	-	15574.092	
70	15526.502	15526.507	-.005	15572.937	15572.939	-.002
71	15524.680	15524.682	-.002	15571.771	15571.765	.006
72	15522.831	15522.837	-.006	15570.573	15570.568	.005
73	15520.963	15520.970	-.007	15569.348	15569.351	-.003
74	15519.077	15519.082	-.005	15568.112	15568.111	.001
75	15517.167	15517.173	-.006	15566.848	15566.850	-.002
76	15515.237	15515.243	-.006	15565.573	15565.567	.006
77	15513.283	15513.291	-.008	15564.263	15564.263	.000
78	-	15511.319		15562.947	15562.937	.010
79	15509.324	15509.325	-.001	15561.596	15561.589	.007
80	15507.308	15507.309	-.001	15560.224	15560.220	.004
81	15505.271	15505.272	-.001	-	15558.829	
82	15503.201	15503.215	-.014	-	15557.416	
83	15501.129	15501.135	-.006	-	15555.981	
84	15499.030	15499.035	-.005	-	15554.525	
85	-	15496.913		15553.060	15553.047	.013

1-1 Band

	P Branch			R Branch		
J	Obs	Calc	Diff	Obs	Calc	Diff
5	15141.255	15141.255	.000	-	15144.901	
6	15140.807	15140.807	.000	-	15145.117	
7	15140.344	15140.341	.003	-	15145.313	
8	15139.851	15139.855	-.004	-	15145.490	
9	15139.349	15139.349	.000	-	15145.647	
10	15138.838	15138.825	.013*	-	15145.786	
11	15138.298	15138.281	.017*	-	15145.905	
12	15137.724	15137.718	.006	-	15146.004	
13	15137.142	15137.136	.006	-	15146.084	
14	15136.540	15136.534	.006	-	15146.145	
15	15135.919	15135.913	.006	-	15146.187	
16	15135.277	15135.273	.004	-	15146.209	
17	15134.616	15134.613	.003	-	15146.212	
18	15133.936	15133.934	.002	-	15146.195	
19	15133.242	15133.236	.006	-	15146.159	
20	15132.523	15132.519	.004	15146.099	15146.103	-.004
21	15131.782	15131.782	.000	15146.023	15146.029	-.006
22	15131.024	15131.026	-.002	15145.928	15145.934	-.006
23	15130.246	15130.251	-.005	15145.817	15145.821	-.004
24	15129.454	15129.456	-.002	15145.693	15145.687	.006
25	15128.640	15128.642	-.002	15145.537	15145.535	.002
26	15127.807	15127.809	-.002	15145.364	15145.363	.001
27	15126.956	15126.957	-.001	15145.167	15145.171	-.004
28	15126.081	15126.085	-.004	15144.962	15144.961	.001
29	15125.191	15125.194	-.003	15144.726	15144.730	-.004
30	15124.280	15124.283	-.003	15144.479	15144.480	-.001
31	15123.349	15123.353	-.004	15144.210	15144.211	-.001
32	15122.403	15122.404	-.001	15143.918	15143.922	-.004
33	15121.439	15121.436	.003	15143.612	15143.614	-.002
34	15120.453	15120.448	.005	15143.286	15143.286	.000
35	15119.442	15119.441	.001	15142.934	15142.939	-.005

36	15118.418	15118.415	.003	15142.570	15142.572	-.002
37	15117.368	15117.369	-.001	15142.183	15142.186	-.003
38	15116.313	15116.304	.009*	15141.777	15141.780	-.003
39	15115.216	15115.219	-.003	15141.348	15141.354	-.006
40	15114.110	15114.116	-.006	15140.906	15140.909	-.003
41	15112.989	15112.992	-.003	15140.442	15140.445	-.003
42	15111.844	15111.850	-.006	15139.961	15139.961	.000
43	15110.688	15110.688	.000	15139.456	15139.457	-.001
44	15109.516	15109.507	.009*	15138.934	15138.933	.001
45	15108.305	15108.306	-.001	15138.398	15138.390	.008
46	15107.085	15107.086	-.001	15137.825	15137.828	-.003
47	15105.850	15105.847	.003	15137.246	15137.245	.001
48	15104.584	15104.588	-.004	15136.654	15136.644	.010*
49	15103.313	15103.310	.003	15136.023	15136.022	.001
50	15102.009	15102.012	-.003	15135.381	15135.381	.000
51	15100.698	15100.695	.003	15134.721	15134.720	.001
52	15099.356	15099.358	-.002	15134.042	15134.039	.003
53	15098.004	15098.003	.001	15133.341	15133.339	.002
54	15096.633	15096.627	.006	15132.624	15132.619	.005
55	15095.237	15095.232	.005	15131.878	15131.879	-.001
56	15093.821	15093.818	.003	15131.121	15131.119	.002
57	15092.387	15092.384	.003	15130.337	15130.340	-.003
58	15090.938	15090.931	.007	15129.541	15129.541	.000
59	-	15089.459		15128.754	15128.722	.032*
60	-	15087.966		15127.878	15127.883	-.005
61	-	15086.455		15127.033	15127.024	.009
62	-	15084.923		15126.142	15126.146	-.004
63	-	15083.373		15125.232	15125.248	-.016*
64	-	15081.803		15124.335	15124.330	.005

2-1 Band

		P Branch			R Branch	
J	Obs	Calc	Diff	Obs	Calc	Diff
19	-	15538.797		15551.667	15551.672	-.005
20	-	15538.056		15551.588	15551.591	-.003
21	-	15537.295		15551.489	15551.489	.000
22	-	15536.514		-	15551.367	
23	15535.717	15535.711	.006	15551.220	15551.224	-.004
24	15534.898	15534.889	.009	15551.058	15551.060	-.002
25	15534.048	15534.046	.002	15550.876	15550.876	.000
26	15533.174	15533.182	-.008	15550.674	15550.671	.003
27	-	15532.298		15550.449	15550.446	.003
28	15531.389	15531.393	-.004	15550.201	15550.200	.001
29	15530.459	15530.468	-.009*	15549.935	15549.933	.002
30	15529.516	15529.523	-.007	15549.646	15549.646	.000
31	15528.555	15528.556	-.001	15549.340	15549.338	.002
32	15527.572	15527.570	.002	15549.010	15549.009	.001
33	15526.561	15526.562	-.001	15548.664	15548.659	.005
34	15525.536	15525.535	.001	15548.295	15548.289	.006
35	15524.487	15524.486	.001	15547.899	15547.898	.001
36	15523.412	15523.418	-.006	15547.490	15547.487	.003
37	15522.333	15522.328	.005	15547.058	15547.054	.004
38	15521.219	15521.219	.000	15546.602	15546.601	.001

39	15520.086	15520.088	-.002	-	15546.128	
40	15518.934	15518.937	-.003	15545.632	15545.633	-.001
41	15517.765	15517.766	-.001	15545.123	15545.118	.005
42	15516.572	15516.574	-.002	15544.577	15544.582	-.005
43	15515.360	15515.361	-.001	15544.023	15544.025	-.002
44	15514.130	15514.128	.002	15543.446	15543.448	-.002
45	15512.869	15512.875	-.006	15542.839	15542.849	-.010*
46	-	15511.600		15542.225	15542.230	-.005
47	15510.302	15510.306	-.004	-	15541.590	
48	15508.992	15508.990	.002	-	15540.930	
49	-	15507.654		15540.235	15540.248	-.013*
50	15506.286	15506.298	-.012*	15539.532	15539.546	-.014*
51	-	15504.921		-	15538.822	
52	15503.516	15503.523	-.007	-	15538.078	
53	-	15502.105		-	15537.313	
54	-	15500.666		-	15536.528	
55	15499.214	15499.207	.007	-	15535.721	
56	15497.733	15497.727	.006	-	15534.893	
57	15496.232	15496.227	.005	-	15534.045	
58	15494.707	15494.705	.002	-	15533.176	
59	15493.165	15493.164	.001	-	15532.285	
60	15491.603	15491.601	.002	-	15531.374	
61	15490.028	15490.018	.010*	-	15530.442	
62	15488.410	15488.414	-.004	-	15529.489	
63	15486.793	15486.790	.003	-	15528.515	
64	-	15485.145		-	15527.520	
65	15483.477	15483.480	-.003	15526.504	15526.504	.000
66	15481.794	15481.793	.001	15525.464	15525.467	-.003
67	15480.090	15480.086	.004	15524.410	15524.408	.002
68	15478.357	15478.359	-.002	15523.331	15523.329	.002
69	15476.611	15476.611	.000	15522.228	15522.229	-.001
70	-	15474.842		15521.105	15521.108	-.003
71	15473.051	15473.052	-.001	15519.954	15519.966	-.012*
72	15471.239	15471.242	-.003	15518.797	15518.803	-.006
73	15469.409	15469.411	-.002	15517.614	15517.618	-.004
74	15467.561	15467.559	.002	15516.411	15516.413	-.002
75	15465.692	15465.686	.006	-	15515.186	
76	15463.797	15463.793	.004	15513.935	15513.939	-.004
77	15461.879	15461.879	.000	15512.658	15512.670	-.012*
78	-	15459.945		-	15511.380	
79	15457.988	15457.989	-.001	15510.067	15510.069	-.002
80	15456.019	15456.013	.006	15508.738	15508.736	.002
81	15454.017	15454.016	.001	15507.383	15507.383	.000
82	15452.000	15451.998	.002	15506.010	15506.008	.002
83	-	15449.960		15504.615	15504.612	.003
84	15447.901	15447.901	.000	15503.201	15503.195	.006
85	-	15445.820		15501.753	15501.757	-.004
86	-	15443.720		15500.293	15500.297	-.004
87	-	15441.598		15498.827	15498.816	.011*
88	15439.451	15439.455	-.004*	-	15497.314	
89	15437.304	15437.292	.012*	-	15495.791	
90	15435.127	15435.108	.019*	-	15494.246	

3-1 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
4	15951.590	15951.585	.005	-	15954.546	
5	15951.141	15951.147	-.006	-	15954.767	
6	15950.695	15950.687	.008	-	15954.965	
7	15950.212	15950.206	.006	-	15955.142	
8	15949.711	15949.703	.008	-	15955.297	
9	15949.185	15949.178	.007	-	15955.430	
10	15948.638	15948.632	.006	-	15955.541	
11	-	15948.064		-	15955.631	
12	15947.477	15947.474	.003	-	15955.699	
13	15946.862	15946.862	.000	-	15955.745	
14	15946.235	15946.229	.006	-	15955.769	
15	15945.569	15945.574	-.005	-	15955.772	
16	15944.893	15944.897	-.004	-	15955.752	
17	15944.195	15944.198	-.003	-	15955.711	
18	15943.476	15943.478	-.002	15955.649	15955.648	.001
19	15942.735	15942.736	-.001	15955.563	15955.563	.000
20	15941.972	15941.972	.000	15955.456	15955.457	-.001
21	15941.185	15941.187	-.002	15955.317	15955.328	-.011**
22	15940.372	15940.380	-.008	15955.176	15955.178	-.002
23	15939.550	15939.551	-.001	15955.007	15955.006	.001
24	15938.698	15938.700	-.002	15954.810	15954.812	-.002
25	15937.833	15937.828	.005	15954.595	15954.596	-.001
26	15936.930	15936.934	-.004	15954.359	15954.358	.001
27	15936.017	15936.018	-.001	15954.101	15954.099	.002
28	15935.074	15935.080	-.006	15953.811	15953.817	-.006
29	15934.117	15934.121	-.004	15953.513	15953.514	-.001
30	15933.131	15933.140	-.009	15953.189	15953.189	.000
31	15932.131	15932.137	-.006	15952.847	15952.842	.005
32	15931.112	15931.113	-.001	15952.475	15952.473	.002
33	15930.064	15930.067	-.003	15952.084	15952.082	.002
34	15928.998	15928.999	-.001	15951.671	15951.669	.002
35	15927.907	15927.909	-.002	15951.235	15951.235	.000
36	15926.792	15926.798	-.006	15950.784	15950.778	.006
37	15925.659	15925.665	-.006	15950.304	15950.300	.004
38	15924.507	15924.510	-.003	15949.804	15949.799	.005
39	15923.329	15923.333	-.004	15949.282	15949.277	.005
40	15922.136	15922.135	.001	15948.739	15948.732	.007
41	15920.918	15920.915	.003	15948.178	15948.166	.012**
42	15919.674	15919.673	.001	15947.582	15947.578	.004
43	15918.412	15918.410	.002	15946.970	15946.968	.002
44	15917.125	15917.124	.001	15946.341	15946.336	.005
45	15915.824	15915.817	.007**	15945.686	15945.681	.005
46	15914.492	15914.488	.004	15945.003	15945.005	-.002
47	15913.136	15913.138	-.002	15944.306	15944.307	-.001
48	15911.766	15911.765	.001	15943.585	15943.587	-.002
49	15910.369	15910.371	-.002	15942.834	15942.845	-.011**
50	15908.953	15908.955	-.002	15942.082	15942.080	.002
51	15907.518	15907.518	.000	15941.296	15941.294	.002
52	15906.053	15906.058	-.005	15940.498	15940.486	.012**
53	15904.573	15904.577	-.004	15939.656	15939.656	.000
54	15903.073	15903.074	-.001	15938.803	15938.803	.000

55	15901.546	15901.549	-.003	15937.933	15937.929	.004
56	15900.000	15900.003	-.003	-	15937.032	
57	15898.433	15898.434	-.001	15936.116	15936.113	.003
58	-	15896.844		15935.178	15935.172	.006
59	15895.235	15895.232	.003	15934.208	15934.209	-.001
60	15893.593	15893.598	-.005	15933.217	15933.224	-.007**
61	15891.942	15891.942	.000	15932.217	15932.216	.001
62	15890.274	15890.264	.010**	15931.185	15931.186	-.001
63	15888.566	15888.564	.002	15930.131	15930.133	-.002
64	15886.843	15886.842	.001	15929.060	15929.057	.003
65	15885.098	15885.098	.000	-	15927.953	
66	15883.329	15883.330	-.001	15926.792	15926.769	.023**
67	15881.534	15881.536	-.002	15925.739	15925.742	-.003
68	15879.661	15879.661	.000	-	15924.563	
69	15877.941	15877.944	-.003	-	15923.374	
70	15876.073	15876.076	-.003	-	15922.166	
71	15874.195	15874.197	-.002	-	15920.935	
72	15872.300	15872.299	.001	-	15919.683	
73	15870.383	15870.380	.003	-	15918.409	
74	15868.438	15868.439	-.001	-	15917.112	
75	15866.483	15866.477	.006	-	15915.790	
76	15864.494	15864.492	.002	-	15914.418	
77	15862.487	15862.483	.004	-	15913.108	
78	15860.442	15860.424	.018**	-	15911.716	
79	15858.424	15858.427	-.003	-	15910.307	
80	15856.363	15856.349	.014**	-	15908.877	
81	15854.252	15854.254	-.002	-	15907.425	
82	15852.134	15852.139	-.005	-	15905.950	
83	15849.998	15850.001	-.003	-	15904.454	
84	15847.840	15847.842	-.002	-	15902.935	
85	15845.661	15845.662	-.001	-	15901.394	
86	15843.462	15843.459	.003	-	15899.830	
87	15841.237	15841.234	.003	-	15898.244	
88	15838.988	15838.988	.000	-	15896.636	

3-2 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
3	15496.912	15496.911	.001	-	15499.214	
4	-	15496.501		-	15499.463	
5	15496.080	15496.072	.008	-	15499.692	
6	15495.626	15495.622	.004	-	15499.900	
7	15495.153	15495.153	.000	-	15500.089	
8	-	15494.663		-	15500.257	
9	15494.155	15494.153	.002	-	15500.405	
10	15493.625	15493.624	.001	-	15500.533	
11	15493.074	15493.074	.000	-	15500.641	
12	15492.504	15492.504	.000	-	15500.729	
13	-	15491.914		-	15500.797	
14	15491.307	15491.304	.003	-	15500.844	
15	-	15490.674		-	15500.872	
16	15490.028	15490.024	.004	-	15500.879	
17	15489.350	15489.353	-.003	-	15500.866	

18	15488.662	15488.663	-.001	-	15500.833	
19	15487.951	15487.953	-.002	-	15500.780	
20	15487.228	15487.223	.005	-	15500.707	
21	15486.471	15486.472	-.001	-	15500.614	
22	15485.705	15485.702	.003	15500.508	15500.500	.008
23	15484.906	15484.911	-.005	15500.370	15500.366	.004
24	15484.094	15484.101	-.007	15500.214	15500.212	.002
25	15483.263	15483.270	-.007	15500.038	15500.038	.000
26	15482.416	15482.419	-.003	15499.845	15499.844	.001
27	15481.543	15481.549	-.006	15499.630	15499.630	.000
28	15480.656	15480.658	-.002	15499.398	15499.395	.003
29	15479.741	15479.747	-.006	15499.141	15499.140	.001
30	15478.816	15478.816	.000	15498.861	15498.865	-.004
31	15477.865	15477.865	.000	15498.574	15498.570	.004
32	15476.885	15476.894	-.009	15498.257	15498.254	.003
33	15475.896	15475.903	-.007	15497.923	15497.919	.004
34	15474.888	15474.892	-.004	15497.563	15497.563	.000
35	15473.860	15473.861	-.001	15497.188	15497.187	.001
36	15472.808	15472.810	-.002	15496.792	15496.790	.002
37	15471.739	15471.739	.000	15496.379	15496.374	.005
38	15470.646	15470.648	-.002	15495.936	15495.937	-.001
39	15469.533	15469.536	-.003	15495.483	15495.480	.003
40	15468.401	15468.405	-.004	-	15495.002	
41	15467.250	15467.254	-.004	15494.505	15494.505	.000
42	15466.082	15466.082	.000	15493.989	15493.987	.002
43	15464.885	15464.890	-.005	15493.448	15493.449	-.001
44	15463.674	15463.679	-.005	15492.895	15492.890	.005
45	15462.443	15462.447	-.004	15492.317	15492.311	.006
46	15461.192	15461.195	-.003	15491.711	15491.712	-.001
47	15459.929	15459.924	.005	15491.093	15491.093	.000
48	15458.628	15458.632	-.004	15490.449	15490.453	-.004
49	15457.319	15457.320	-.001	15489.795	15489.793	.002
50	15455.987	15455.988	-.001	15489.115	15489.113	.002
51	15454.632	15454.636	-.004	15488.410	15488.412	-.002
52	15453.257	15453.263	-.006	15487.698	15487.691	.007
53	-	15451.871		15486.953	15486.950	.003
54	-	15450.459		15486.192	15486.188	.004
55	-	15449.026		15485.406	15485.405	.001
56	15447.572	15447.574	-.002	-	15484.603	
57	15446.106	15446.101	.005	15483.784	15483.780	.004
58	15444.605	15444.608	-.003	15482.936	15482.936	.000
59	15443.118	15443.095	.023**	15482.079	15482.072	.007
60	15441.572	15441.562	.010**	15481.190	15481.188	.002
61	15440.008	15440.009	-.001	15480.281	15480.283	-.002
62	15438.435	15438.435	.000	15479.359	15479.357	.002
63	-	15436.841		15478.408	15478.410	-.002
64	-	15435.227		15477.441	15477.441	.000
65	-	15433.592		15476.449	15476.447	.002
66	15431.928	15431.935	-.007	15475.379	15475.374	.005
67	-	15430.254		15474.463	15474.460	.003
68	15428.488	15428.494	-.006	15473.399	15473.396	.003
69	15426.892	15426.893	-.001	15472.324	15472.323	.001
70	-	15425.142		15471.237	15471.232	.005
71	15423.379	15423.383	-.004	15470.125	15470.122	.003
72	15421.599	15421.607	-.008**	15468.991	15468.991	.000
73	-	15419.811		15467.842	15467.840	.002
74	-	15417.995		15466.661	15466.667	-.006**

75	15416.157	15416.159	-.002	15465.487	15465.472	.015**
76	15414.301	15414.303	-.002	15464.240	15464.229	.011**
77	15412.421	15412.424	-.003	15463.053	15463.049	.004
78	15410.497	15410.497	.000	-	15461.788	
79	15408.636	15408.633	.003	15460.513	15460.513	.000
80	15406.689	15406.690	-.001	-	15459.218	
81	15404.730	15404.732	-.002	-	15457.903	
82	15402.755	15402.755	.000	-	15456.567	
83	15400.770	15400.759	.011**	-	15455.211	
84	15398.749	15398.742	.007	-	15453.834	
85	15396.707	15396.705	.002	-	15452.437	
86	15394.644	15394.648	-.004	-	15451.019	
87	15392.573	15392.571	.002	-	15449.581	

4-2 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
4	15898.962	15898.961	.001	-	15901.912	
5	15898.525	15898.527	-.002	-	15902.133	
6	-	15898.072		-	15902.334	
7	-	15897.595		-	15902.512	
8	15897.096	15897.097	-.001	-	15902.670	
9	15896.574	15896.577	-.003	-	15902.806	
10	15896.033	15896.036	-.003	-	15902.921	
11	15895.476	15895.474	.002	-	15903.014	
12	15894.893	15894.891	.002	-	15903.086	
13	15894.287	15894.287	.000	-	15903.137	
14	15893.660	15893.661	-.001	-	15903.166	
15	15893.008	15893.014	-.006	-	15903.174	
16	15892.344	15892.345	-.001	-	15903.161	
17	15891.656	15891.656	.000	-	15903.126	
18	15890.944	15890.945	-.001	-	15903.070	
19	15890.210	15890.213	-.003	15902.997	15902.992	.005
20	15889.455	15889.459	-.004	15902.899	15902.893	.006
21	15888.681	15888.684	-.003	15902.781	15902.773	.008
22	15887.888	15887.888	.000	15902.634	15902.631	.003
23	15887.071	15887.071	.000	15902.468	15902.468	.000
24	15886.234	15886.232	.002	15902.287	15902.283	.004
25	15885.378	15885.372	.006	15902.078	15902.077	.001
26	15884.488	15884.490	-.002	15901.847	15901.849	-.002
27	15883.585	15883.587	-.002	15901.599	15901.599	.000
28	15882.653	15882.663	-.010**	15901.330	15901.328	.002
29	15881.716	15881.717	-.001	15901.041	15901.035	.006
30	15880.748	15880.749	-.001	15900.717	15900.719	-.002
31	15879.762	15879.760	.002	15900.387	15900.381	.006
32	15878.746	15878.749	-.003	15900.015	15900.020	-.005
33	15877.709	15877.715	-.006	15899.635	15899.633	.002
34	15876.653	15876.658	-.005	15899.221	15899.217	.004
35	15875.576	15875.576	.000	15898.750	15898.752	-.002
36	15874.463	15874.464	-.001	-	15898.094	
37	15873.306	15873.305	.001	15898.119	15898.125	-.006
38	15871.952	15871.952	.000	15897.551	15897.549	.002
39	15871.290	15871.288	.002	15897.017	15897.016	.001

40	15870.035	15870.017	.018**	15896.477	15896.475	.002
41	15868.790	15868.789	.001	15895.918	15895.918	.000
42	15867.554	15867.554	.000	15895.346	15895.342	.004
43	15866.305	15866.304	.001	15894.742	15894.746	-.004
44	15865.036	15865.034	.002	15894.127	15894.129	-.002
45	15863.743	15863.745	-.002	15893.490	15893.490	.000
46	15862.434	15862.434	.000	15892.821	15892.828	-.007
47	15861.101	15861.102	-.001	15892.144	15892.142	.002
48	15859.753	15859.748	.005	15891.421	15891.424	-.003
49	15858.372	15858.369	.003	15890.629	15890.634	-.005
50	15856.956	15856.959	-.003	15890.210	15890.192	.018
51	15855.478	15855.477	.001	15889.289	15889.301	-.012**
52	15854.339	15854.342	-.003**	15888.494	15888.493	.001
53	15852.759	15852.760	-.001	15887.678	15887.676	.002
54	15851.262	15851.260	.002	15886.841	15886.842	-.001
55	15849.755	15849.753	.002	15885.991	15885.989	.002
56	15848.227	15848.228	-.001	15885.100	15885.116	-.016**
57	15846.694	15846.685	.009**	15884.220	15884.221	-.001
58	15845.119	15845.121	-.002	15883.323	15883.305	.018**
59	15843.533	15843.536	-.003	15882.375	15882.368	.007
60	15841.930	15841.931	-.001	15881.410	15881.410	.000
61	15840.306	15840.305	.001	15880.432	15880.430	.002
62	15838.655	15838.657	-.002	15879.429	15879.429	.000
63	15836.988	15836.989	-.001	15878.403	15878.406	-.003
64	15835.297	15835.299	-.002	15877.366	15877.361	.005
65	15833.587	15833.588	-.001	15876.292	15876.295	-.003
66	15831.853	15831.855	-.002	15875.206	15875.207	-.001
67	15830.099	15830.102	-.003	15874.098	15874.098	.000
68	15828.322	15828.327	-.005	15872.966	15872.967	-.001
69	15826.526	15826.531	-.005	15871.814	15871.814	.000
70	15824.708	15824.713	-.005	15870.644	15870.640	.004
71	15822.869	15822.875	-.006	15869.448	15869.444	.004
72	15821.017	15821.014	.003	15868.225	15868.226	-.001
73	15819.136	15819.133	.003	15866.986	15866.986	.000
74	15817.235	15817.230	.005	15865.720	15865.725	-.005
75	15815.311	15815.306	.005	15864.487	15864.442	.045**
76	15813.349	15813.360	-.011**	15863.150	15863.137	.013**
77	-	15811.393		-	15861.811	
78	15809.416	15809.405	.011**	15860.450	15860.463	-.013**
79	15807.400	15807.396	.004	15859.102	15859.093	.009**
80	15805.358	15805.364	-.006	-	15857.701	
81	-	15803.312		-	15856.287	
82	-	15801.238		15854.860	15854.851	.009
83	-	15799.143		15853.398	15853.394	.004
84	-	15797.026		15851.908	15851.915	-.007
85	-	15794.888		15850.417	15850.414	.003
86	-	15792.729		15848.886	15848.891	-.005

4-3 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
1	-	15448.612		15449.595	15449.596	-.001
2	-	15448.245		15449.883	15449.885	-.002

3	-	15447.859		15450.153	15450.154	-.001
4	15447.444	15447.452	-.008**	15450.405	15450.403	.002
5	15447.024	15447.026	-.002	15450.633	15450.633	.000
6	15446.581	15446.581	.000	15450.843	15450.843	.000
7	15446.106	15446.116	-.010**	15451.028	15451.033	-.005
8	15445.631	15445.631	.000	15451.204	15451.204	.000
9	15445.129	15445.127	.002	15451.340	15451.355	-.015**
10	15444.605	15444.603	.002	-	15451.487	
11	15444.058	15444.059	-.001	-	15451.599	
12	15443.500	15443.496	.004	-	15451.691	
13	15442.913	15442.914	-.001	-	15451.764	
14	15442.310	15442.311	-.001	-	15451.817	
15	15441.687	15441.689	-.002	-	15451.850	
16	15441.048	15441.048	.000	-	15451.863	
17	15440.386	15440.387	-.001	-	15451.857	
18	15439.706	15439.706	.000	-	15451.831	
19	15439.008	15439.006	.002	-	15451.786	
20	15438.288	15438.286	.002	-	15451.720	
21	15437.544	15437.547	-.003	-	15451.635	
22	15436.787	15436.787	.000	15451.526	15451.531	-.005
23	15436.011	15436.009	.002	15451.404	15451.406	-.002
24	15435.211	15435.210	.001	15451.260	15451.262	-.002
25	15434.389	15434.392	-.003	15451.097	15451.097	.000
26	15433.556	15433.554	.002	15450.914	15450.913	.001
27	15432.697	15432.697	.000	15450.710	15450.709	.001
28	15431.818	15431.820	-.002	15450.475	15450.485	-.010**
29	15430.923	15430.922	.001	15450.241	15450.240	.001
30	15430.008	15430.005	.003	15449.973	15449.976	-.003
31	15429.070	15429.068	.002	15449.691	15449.690	.001
32	15428.118	15428.111	.007	15449.383	15449.382	.001
33	15427.134	15427.133	.001	15449.046	15449.051	-.005
34	15426.148	15426.133	.015**	15448.693	15448.692	.001
35	15425.116	15425.110	.006	15448.290	15448.286	.004
36	15424.058	15424.059	-.001	15447.689	15447.689	.000
37	15422.961	15422.962	-.001	15447.785	15447.782	.003
38	15421.674	15421.673	.001	15447.274	15447.271	.003
39	15421.073	15421.075	-.002	15446.804	15446.802	.002
40	15419.870	15419.872	-.002	15446.328	15446.329	-.001
41	15418.713	15418.713	.000	15445.835	15445.842	-.007**
42	15417.548	15417.549	-.001	15445.340	15445.337	.003
43	15416.369	15416.371	-.002	15444.820	15444.813	.007
44	15415.171	15415.175	-.004	15444.271	15444.270	.001
45	15413.962	15413.962	.000	15443.709	15443.707	.002
46	15412.730	15412.729	.001	15443.118	15443.123	-.005
47	15411.477	15411.476	.001	15442.516	15442.516	.000
48	15410.206	15410.203	.003	15441.880	15441.880	.000
49	15408.908	15408.907	.001	15441.168	15441.172	-.004
50	15407.584	15407.581	.003	15440.810	15440.814	-.004
51	15406.186	15406.185	.001	15440.008	15440.010	-.002
52	15405.132	15405.139	-.007	15439.285	15439.289	-.004
53	15403.639	15403.647	-.008	15438.561	15438.562	-.001
54	15402.238	15402.238	.000	15437.817	15437.820	-.003
55	15400.823	15400.823	.000	15437.057	15437.060	-.003
56	15399.371	15399.394	-.023**	15436.280	15436.281	-.001
57	15397.946	15397.947	-.001	15435.481	15435.483	-.002
58	15396.480	15396.481	-.001	15434.656	15434.666	-.010**
59	15395.003	15394.996	.007	15433.826	15433.828	-.002

60	15393.497	15393.493	.004	15432.968	15432.972	-.004
61	15391.973	15391.970	.003	15432.089	15432.095	-.006
62	15390.434	15390.427	.007	15431.196	15431.199	-.003
63	15388.867	15388.866	.001	15430.272	15430.283	-.011**
64	15387.284	15387.284	.000	15429.341	15429.347	-.006
65	15385.683	15385.683	.000	15428.401	15428.391	.010**
66	15384.065	15384.063	.002	15427.417	15427.415	.002
67	15382.427	15382.423	.004	15426.424	15426.419	.005
68	15380.768	15380.764	.004	15425.401	15425.404	-.003
69	15379.084	15379.085	-.001	-	15424.368	
70	15377.384	15377.386	-.002	-	15423.313	
71	15375.675	15375.668	.007	-	15422.238	

5-3 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
2	15849.154	15849.123	.031**	-	15850.756	
3	-	15848.734		-	15851.020	
4	15848.347	15848.324	.023**	-	15851.264	
5	15847.920	15847.893	.027**	-	15851.486	
6	15847.469	15847.441	.028**	-	15851.688	
7	15846.998	15846.969	.029**	-	15851.869	
8	15846.501	15846.476	.025**	-	15852.029	
9	15845.985	15845.962	.023**	-	15852.168	
10	15845.456	15845.427	.029**	-	15852.286	
11	15844.893	15844.872	.021**	-	15852.383	
12	15844.320	15844.295	.025**	-	15852.460	
13	15843.712	15843.698	.014**	-	15852.516	
14	15843.104	15843.080	.024**	-	15852.550	
15	15842.461	15842.441	.020**	-	15852.564	
16	15841.802	15841.782	.020**	-	15852.558	
17	15841.122	15841.102	.020**	-	15852.530	
18	15840.414	15840.400	.014**	-	15852.481	
19	-	15839.679		15852.419	15852.412	.007**
20	15838.952	15838.936	.016**	15852.326	15852.321	.005**
21	15838.186	15838.172	.014**	15852.216	15852.210	.006**
22	15837.399	15837.388	.011**	15852.082	15852.078	.004**
23	15836.593	15836.583	.010**	15851.931	15851.924	.007**
24	15835.767	15835.757	.010**	15851.754	15851.750	.004**
25	15834.918	15834.911	.007**	15851.562	15851.556	.006**
26	15834.051	15834.043	.008**	15851.341	15851.340	.001
27	15833.162	15833.155	.007**	15851.108	15851.103	.005
28	15832.252	15832.246	.006**	15850.851	15850.845	.006
29	15831.321	15831.316	.005**	15850.573	15850.567	.006
30	15830.367	15830.366	.001	15850.272	15850.267	.005
31	15829.396	15829.394	.002	15849.951	15849.947	.004
32	15828.395	15828.402	-.007	15849.606	15849.605	.001
33	15827.384	15827.389	-.005	15849.245	15849.243	.002
34	15826.360	15826.356	.004	15848.864	15848.859	.005
35	15825.298	15825.301	-.003	15848.451	15848.455	-.004
36	15824.222	15824.226	-.004	15848.037	15848.030	.007
37	15823.130	15823.130	.000	15847.583	15847.583	.000
38	15822.022	15822.013	.009**	15847.114	15847.116	-.002

39	15820.874	15820.876	-.002	15846.631	15846.628	.003
40	15819.712	15819.717	-.005	15846.117	15846.119	-.002
41	15818.531	15818.538	-.007	15845.589	15845.588	.001
42	15817.331	15817.338	-.007	15845.037	15845.037	.000
43	15816.109	15816.118	-.009	15844.462	15844.465	-.003
44	15814.871	15814.876	-.005	15843.864	15843.872	-.008**
45	15813.610	15813.614	-.004	15843.237	15843.257	-.020**
46	15812.330	15812.330	.000	15842.629	15842.622	.007
47	15811.015	15811.027	-.012**	15841.964	15841.966	-.002
48	15809.707	15809.702	.005	15841.288	15841.288	.000
49	15808.359	15808.356	.003	15840.592	15840.589	.003
50	15806.984	15806.990	-.006	15839.912	15839.870	.042**
51	15805.598	15805.602	-.004	15839.166	15839.129	.037**
52	15804.193	15804.194	-.001	15838.370	15838.367	.003
53	15802.767	15802.765	.002	15837.585	15837.584	.001
54	15801.302	15801.316	-.014**	15836.781	15836.780	.001
55	15799.844	15799.845	-.001	15835.958	15835.954	.004
56	15798.351	15798.353	-.002	15835.109	15835.107	.002
57	-	15796.841		15834.240	15834.239	.001
58	15795.306	15795.307	-.001	15833.363	15833.350	.013**
59	-	15793.752		15832.439	15832.438	.001
60	15792.180	15792.177	.003	15831.506	15831.506	.000
61	15790.570	15790.580	-.010	15830.541	15830.551	-.010**
62	15788.958	15788.961	-.003	15829.577	15829.574	.003
63	15787.312	15787.322	-.010	-	15828.575	
64	15785.674	15785.660	.014**	15827.546	15827.551	-.005
65	15783.977	15783.975	.002	15826.509	15826.501	.008
66	15782.282	15782.267	.015**	15825.425	15825.419	.006
67	15780.531	15780.533	-.002	15824.279	15824.285	-.006
68	-	15778.767		15822.985	15822.983	.002
69	15776.958	15776.950	.008**	15822.747	15822.737	.010
70	15774.957	15774.966	-.009	15821.254	15821.255	-.001
71	15774.031	15774.037	-.006	15820.028	15820.019	.009
72	15771.871	15771.872	-.001	15818.805	15818.805	.000
73	15769.950	15769.955	-.005	15817.583	15817.583	.000
74	15768.060	15768.059	.001	15816.352	15816.347	.005
75	-	15766.156		15815.097	15815.092	.005
76	15764.240	15764.239	.001	15813.820	15813.819	.001
77	15762.298	15762.304	-.006	15812.527	15812.525	.002
78	15760.310	15760.351	-.041**	15811.219	15811.212	.007
79	-	15758.378		15809.881	15809.877	.004
80	15756.383	15756.384	-.001	15808.520	15808.522	-.002
81	15754.367	15754.371	-.004	15807.147	15807.146	.001
82	15752.347	15752.337	.010**	15805.755	15805.748	.007
83	15750.319	15750.283	.036**	-	15804.330	
84	15748.203	15748.208	-.005	-	15802.891	
85	-	15746.113		-	15801.430	
86	15743.997	15743.997	.000	-	15799.949	
87	15741.856	15741.860	-.004	-	15798.446	
88	-	15739.702		-	15796.922	
89	15737.518	15737.524	-.006	-	15795.376	
90	15735.324	15735.325	-.001	-	15793.810	

5-4 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
20	-	15391.360		15404.748	15404.745	.003
21	-	15390.632		15404.671	15404.669	.002
22	-	15389.884		15404.571	15404.574	-.003
23	-	15389.118		15404.462	15404.459	.003
24	-	15388.332		15404.327	15404.325	.002
25	-	15387.527		15404.172	15404.172	.000
26	-	15386.703		15404.002	15404.000	.002
27	-	15385.860		15403.805	15403.808	-.003
28	15384.993	15384.998	-.005	15403.599	15403.598	.001
29	15384.113	15384.117	-.004	-	15403.368	
30	15383.221	15383.217	.004	15403.121	15403.118	.003
31	15382.294	15382.298	-.004	15402.851	15402.850	.001
32	15381.358	15381.359	-.001	15402.564	15402.562	.002
33	15380.407	15380.402	.005	15402.250	15402.255	-.005
34	15379.425	15379.425	.000	15401.927	15401.929	-.002
35	15378.432	15378.430	.002	15401.585	15401.583	.002
36	15377.411	15377.415	-.004	15401.226	15401.219	.007
37	15376.389	15376.381	.008**	15400.833	15400.835	-.002
38	15375.326	15375.329	-.003	15400.432	15400.432	.000
39	15374.252	15374.257	-.005	-	15400.009	
40	15373.162	15373.166	-.004	15399.572	15399.567	.005
41	15372.047	15372.056	-.009	15399.101	15399.106	-.005
42	15370.924	15370.927	-.003	15398.623	15398.626	-.003
43	15369.778	15369.779	-.001	15398.127	15398.126	.001
44	15368.603	15368.611	-.008	15397.607	15397.607	.000
45	15367.421	15367.425	-.004	15397.059	15397.069	-.010**
46	15366.224	15366.220	.004	15396.515	15396.511	.004
47	15364.971	15364.995	-.024**	15395.938	15395.934	.004
48	15363.759	15363.752	.007	15395.347	15395.338	.009
49	15362.493	15362.489	.004	-	15394.722	
50	15361.218	15361.208	.010**	-	15394.087	
51	15359.907	15359.907	.000	-	15393.433	
52	15358.585	15358.587	-.002	-	15392.760	
53	15357.248	15357.248	.000	-	15392.066	
54	15355.891	15355.890	.001	-	15391.354	
55	15354.509	15354.513	-.004	-	15390.622	
56	15353.116	15353.116	.000	-	15389.870	
57	15351.707	15351.701	.006	-	15389.099	
58	15350.258	15350.266	-.008	-	15388.309	
59	15348.813	15348.812	.001	-	15387.498	
60	15347.338	15347.339	-.001	-	15386.668	
61	-	15345.846		-	15385.818	
62	15344.335	15344.334	.001	-	15384.947	
63	15342.792	15342.802	-.010	15384.060	15384.055	.005
64	15341.244	15341.250	-.006	15383.140	15383.141	-.001
65	15339.682	15339.677	.005	15382.190	15382.202	-.012**
66	15338.090	15338.082	.008**	15381.236	15381.233	.003
67	-	15336.463		15380.217	15380.214	.003
68	15334.817	15334.814	.003	15379.032	15379.030	.002
69	15333.122	15333.116	.006	15378.900	15378.902	-.002
70	15331.241	15331.251	-.010	15377.523	15377.540	-.017

71	15330.418	15330.445	-.027	-	15376.427	

6-4 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
2	15800.313	15800.315	-.002	-	15801.942	
3	-	15799.928		-	15802.206	
4	15799.520	15799.521	-.001	-	15802.450	
5	15799.094	15799.094	.000	-	15802.673	
6	15798.645	15798.646	-.001	-	15802.876	
7	15798.173	15798.178	-.005	-	15803.059	
8	15797.692	15797.689	.003	-	15803.221	
9	15797.181	15797.180	.001	-	15803.362	
10	-	15796.651		-	15803.483	
11	-	15796.101		-	15803.584	
12	15795.531	15795.531	.000	-	15803.664	
13	15794.935	15794.940	-.005	-	15803.724	
14	-	15794.329		-	15803.763	
15	15793.694	15793.698	-.004	-	15803.781	
16	15793.040	15793.046	-.006	-	15803.779	
17	15792.369	15792.373	-.004	-	15803.757	
18	15791.681	15791.681	.000	-	15803.714	
19	15790.964	15790.967	-.003	15803.655	15803.650	.005
20	-	15790.233		15803.573	15803.565	.008
21	15789.481	15789.479	.002	15803.470	15803.460	.010
22	15788.707	15788.704	.003	15803.334	15803.334	.000
23	15787.913	15787.909	.004	15803.195	15803.187	.008
24	15787.093	15787.092	.001	15803.027	15803.020	.007
25	15786.258	15786.256	.002	15802.837	15802.831	.006
26	15785.404	15785.398	.006	15802.620	15802.621	-.001
27	15784.520	15784.519	.001	15802.391	15802.390	.001
28	15783.620	15783.620	.000	15802.137	15802.138	-.001
29	15782.696	15782.699	-.003	15801.860	15801.863	-.003
30	15781.757	15781.757	.000	15801.564	15801.567	-.003
31	15780.791	15780.793	-.002	15801.246	15801.247	-.001
32	-	15779.808		15800.907	15800.905	.002
33	15778.793	15778.800	-.007	15800.535	15800.537	-.002
34	15777.763	15777.768	-.005	15800.141	15800.142	-.001
35	15776.707	15776.711	-.004	15799.716	15799.717	-.001
36	15775.628	15775.628	.000	15799.254	15799.253	.001
37	15774.513	15774.515	-.002	15798.741	15798.737	.004
38	15773.358	15773.363	-.005	15798.142	15798.130	.012**
39	15772.158	15772.159	-.001	15797.306	15797.304	.002
40	15770.867	15770.864	.003	-	15795.785	
41	15769.350	15769.351	-.001	15798.202	15798.212	-.010
42	15767.144	15767.144	.000	15797.241	15797.239	.002
43	15768.891	15768.885	.006	15796.498	15796.502	-.004
44	15767.222	15767.225	-.003	15795.830	15795.831	-.001
45	15765.802	15765.801	.001	15795.181	15795.178	.003
46	15764.441	15764.444	-.003	15794.539	15794.524	.015**
47	15763.104	15763.104	.000	15793.860	15793.860	.000
48	15761.766	15761.764	.002	15793.185	15793.184	.001
49	15760.404	15760.415	-.011**	15792.490	15792.491	-.001

50	15759.052	15759.053	-.001	15791.780	15791.782	-.002
51	15757.665	15757.676	-.011**	15791.094	15791.054	.040**
52	15756.280	15756.281	-.001	-	15790.307	
53	15754.907	15754.869	.038**	-	15789.542	
54	15753.444	15753.438	.006	-	15788.756	
55	15751.971	15751.988	-.017**	-	15787.951	
56	15750.516	15750.519	-.003	-	15787.127	
57	15749.028	15749.030	-.002	-	15786.282	
58	-	15747.522		-	15785.416	
59	15745.990	15745.994	-.004	-	15784.531	
60	15744.445	15744.447	-.002	-	15783.625	
61	15742.876	15742.879	-.003	-	15782.699	
62	15741.291	15741.291	.000	-	15781.752	
63	15739.684	15739.683	.001	-	15780.784	
64	15738.054	15738.055	-.001	-	15779.796	
65	15736.404	15736.406	-.002	-	15778.787	
66	15734.742	15734.737	.005	-	15777.756	
67	15733.052	15733.048	.004	-	15776.704	
68	15731.341	15731.337	.004	-	15775.629	
69	15729.609	15729.605	.004	-	15774.531	
70	15727.850	15727.851	-.001	-	15773.404	
71	15726.074	15726.073	.001	-	15772.233	
72	15724.269	15724.268	.001	-	15770.870	
73	15722.423	15722.419	.004	-	15770.234	
74	15720.377	15720.378	-.001	-	15768.896	
75	15719.064	15719.064	.000	-	15767.639	
76	15717.054	15717.049	.005	-	15766.336	
77	15715.128	15715.116	.012**	-	15765.210	
78	15713.136	15713.136	.000	-	15763.895	
79	15711.337	15711.334	.003	-	15762.587	
80	15709.342	15709.344	-.002	-	15761.265	
81	15707.355	15707.361	-.006**	-	15759.924	
82	15705.349	15705.364	-.015**	-	15758.563	
83	-	15703.349		-	15757.183	
84	15701.280	15701.315	-.035**	-	15755.782	
85	15699.186	15699.261	-.075**	-	15754.361	
86	15697.014	15697.187	-.173**	-	15752.919	

Extra Lines included in Fit for Perturber 7

40	-	15779.546		15800.013	15800.012	.001
41	15775.176	15775.176	.000	15792.816	15792.818	-.002
42	15771.378	15771.370	.008**	-	15788.894	
43	15763.491	15763.490	.001	-	15784.604	

6-5 Band

	P Branch			R Branch		
J	OBS	CALC	DIFF	OBS	CALC	DIFF
2	-	15355.976		15357.606	15357.603	.003
3	-	15355.595		15357.867	15357.872	-.005
4	-	15355.194		15358.125	15358.123	.002
5	15354.775	15354.776	-.001	15358.361	15358.355	.006
6	-	15354.338		-	15358.568	

7	15353.880	15353.882	-.002	15358.759	15358.762	-.003
8	15353.406	15353.407	-.001	-	15358.938	
9	15352.915	15352.913	.002	-	15359.095	
10	15352.399	15352.401	-.002	-	15359.233	
11	15351.873	15351.870	.003	-	15359.352	
12	15351.322	15351.320	.002	-	15359.453	
13	15350.755	15350.752	.003	-	15359.535	
14	15350.166	15350.164	.002	-	15359.598	
15	15349.556	15349.559	-.003	-	15359.642	
16	15348.928	15348.934	-.006	-	15359.667	
17	15348.301	15348.291	.010**	-	15359.674	
18	15347.632	15347.628	.004	-	15359.661	
19	15346.945	15346.947	-.002	-	15359.630	
20	15346.242	15346.248	-.006	-	15359.580	
21	15345.508	15345.529	-.021**	-	15359.510	
22	15344.792	15344.792	.000	-	15359.422	
23	15344.031	15344.035	-.004	-	15359.314	
24	15343.261	15343.260	.001	-	15359.188	
25	15342.465	15342.466	-.001	-	15359.042	
26	15341.654	15341.653	.001	-	15358.876	
27	15340.820	15340.820	.000	15358.692	15358.691	.001
28	15339.972	15339.968	.004	15358.487	15358.486	.001
29	15339.098	15339.097	.001	15358.260	15358.261	-.001
30	15338.210	15338.206	.004	15358.015	15358.016	-.001
31	-	15337.295		15357.750	15357.749	.001
32	15336.363	15336.364	-.001	15357.458	15357.461	-.003
33	15335.415	15335.412	.003	15357.149	15357.150	-.001
34	15334.436	15334.439	-.003	15356.811	15356.813	-.002
35	15333.449	15333.442	.007	15356.450	15356.447	.003
36	15332.422	15332.420	.002	15356.046	15356.045	.001
37	15331.375	15331.369	.006	15355.592	15355.592	.000
38	15330.286	15330.283	.003	15355.049	15355.049	.000
39	15329.140	15329.145	-.005	15354.287	15354.290	-.003
40	15327.914	15327.918	-.004	15352.837	15352.839	-.002
41	15326.471	15326.475	-.004	15355.335	15355.336	-.001
42	15324.341	15324.340	.001	15354.436	15354.435	.001
43	15326.154	15326.153	.001	15353.775	15353.770	.005
44	15324.566	15324.568	-.002	15353.169	15353.174	-.005
45	15323.221	15323.221	.000	15352.599	15352.598	.001
46	15321.942	15321.942	.000	15352.028	15352.022	.006
47	15320.681	15320.683	-.002	15351.443	15351.439	.004
48	15319.419	15319.424	-.005	15350.840	15350.844	-.004
49	15318.156	15318.159	-.003	-	15350.235	
50	15316.887	15316.882	.005	15349.606	15349.610	-.004
51	15315.579	15315.591	-.012**	-	15348.969	
52	15314.289	15314.285	.004	-	15348.311	
53	15313.007	15312.962	.045**	-	15347.635	
54	15311.630	15311.623	.007**	-	15346.942	

Extra Lines included in Fit for Perturber 7

40	-	15336.588		15357.065	15357.064	.001
41	-	15332.294		-	15349.942	
42	15328.580	15328.565	.015**	-	15346.095	

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