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Fourier Transform and Diode Laser IR Spectra of Formaldehyde and its Application to Air Pollution Monitoring

Shachar Nadler

A Thesis

in

The Department

of

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ABSTRACT

Fourier Transform and Diode Laser IR Spectra of Formaldehyde and its Application to Air Pollution Monitoring.

Shachar Nadler, Ph.D.
Concordia University, 1986

High resolution FT-IR spectra have been recorded with a Bomem interferometer ($\Delta\nu$=~0.004 cm^{-1}) and covered the region from 890 to 1580 cm^{-1}. Over 3200 transitions in the ν_4, ν_6 and ν_3 bands of H_2CO have been assigned. Line positions have been analyzed using a least-squares-fit to a Watson reduced Hamiltonian. Since the 3 bands have been fitted simultaneously, the analysis included the extensive Coriolis coupling effects between the upper states. The fit yielded improved molecular constants including, for the first time, all the sixth order coefficients and a third order Coriolis coupling constant for the interaction between ν_6 and ν_3.

A tunable diode laser (TDL) has been used to determine absolute line strengths for 28 transitions in the ν_4 and ν_6 bands. These line strengths have been used to determine the dipole moment derivatives and consequently facilitated the prediction of the ν_4 and ν_6 band strengths.

The TDL system has also been used to study the effects of pressure broadening due to collision with foreign gases. Pressure broadening coefficients for air, H_2, O_2 and N_2 have been determined. These are very similar to theoretical literature values in the cases of air, N_2 and O_2. The H_2-H_2CO values are in good agreement with earlier experimental millimeter-wave results.

A method for the measurement of small amounts of H_2CO in air has been developed for use in domestic air pollution monitoring. Conventional reduced pressure techniques have been found unsuitable due to the adsorptive nature of formaldehyde. Our suggested technique employs the TDL spectrometer coupled with a multipass White cell (4-100 meter) and a cold trap (liq. N_2) installed between the sample cell and the analytical White cell. The cold trap allows the reduction of pressure within the White cell (to <10 torr) without loss of sample since the H_2CO is frozen out in the trap. The H_2CO sample is sublimated by heating and then analyzed. This method may employ relatively shorter absorption pathlengths since most of the original H_2CO sample (mass) is available for the analysis. Based on the mass of H_2CO present in 5 liter air samples in a 100 m optical pathlength this technique has demonstrated a limit of detection of 6×10^{-3} absorption units and a sensitivity of 4.4×10^{-5} m^{-1}. For the strongest line in $^{Q}Q_3$ of ν_1 (C-H stretch) this limits the detection to ~7 ppbv. The limit of

detection can be easily reduced to < 5 ppb by simply increasing the sample volume to 10 or 15 liters.

The standard 5 liter grab bags used for air sampling have been proven to be unsuitable for work with H_2CO. It has been demonstrated that due to adsorption and possibly polymerization these bags show a decreased H_2CO content with time. Consequently the construction of a mobile "super sniffer" has been suggested since samples of H_2CO could not be collected in the field and analyzed in the laboratory. The design and operational parameters of a super sniffer have been outlined. This unit may be easily modified (in the field) to allow for the analysis of other air pollutants.

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CHAPTER 1

INTRODUCTION

1.1 Introductory Remarks

Formaldehyde (H_2CO) is an important atmospheric pollutant both indoors and outdoors [1-3] and is also a molecule of considerable astrophysical interest [4-7]. Knowledge of line frequencies, absolute intensities and line shapes is necessary for quantitative analysis for both atmospheric and laboratory experiments since pressure and temperature changes can lead to frequency shifts and line shape variations.

The 3 μm C-H stretching vibration-rotation bands of H_2CO have been well studied at high resolution by several groups [8-11]. Recently the C=O stretching band has been studied using diode lasers [12]. The three low lying bands of H_2CO ν_3, ν_4 and ν_6 have been studied at low resolution ($\Delta\nu$~0.25 cm^{-1}) by Nakagawa and Morino [13] and at moderate resolution ($\Delta\nu$~0.05 cm^{-1}) by Allegrini at al. [14]. These three bands are the focal point of this experimental work.

1.2 Experimental Objectives

This project has four experimental objectives:

Part A: To obtain more accurate molecular constants for the ν_3, ν_4 and ν_6 bands.

Part B: To determine absolute line strengths for individual ro-vibrational lines.

Part C: To determine broadening parameters induced by collision with foreign gases.

Part D: To develop an analytical technique for the detection of H_2CO in ambient air at low ppb levels.

1.2.1 Part A: The Molecular Constants for the ν_3, ν_4 and ν_6 Bands of H_2CO.

High resolution FT-IR spectra have been recorded with a Bomem interferometer ($\Delta\nu$~0.004 cm^{-1}) covering the region from 890 to 1580 cm^{-1}. Using the ground-state-combination-difference technique IR transitions in the ν_3, ν_4 and ν_6 bands will be assigned. The assigned transitions will then be analyzed by means of least-squares to a sixth order Hamiltonian. The transitions for the three bands will be fit simultaneously. This will permit the analysis of the extensive Coriolis interaction between the bands. The fit will yield the rotational and Coriolis interaction constants from which all transitions in the region may be predicted.

1.2.2 Part B: Absolute Line Strength Determination for Individual Ro-Vibrational Lines in the ν_4 and ν_6 bands of H_2CO.

Using tunable diode lasers (TDLs) the absolute line strengths of several transitions will be determined. Since

the TDL spectrometer allows for Doppler limited resolution, the line strengths will be evaluated using the direct method [15]. This technique allows the determination of line strengths from the absorption profiles of individual transitions since for Doppler limited transitions, $\ln(I/I_o)$ is directly proportional to the line strength S. At present only band strengths are available in the literature [16,17].

The line strengths will be used to evaluate the dipole moment derivatives of their respective bands. These derivatives may in turn be used to predict the entire spectrum from the eigenvalues and eigenvectors of the Hamiltonian (obtained in Part A).

1.2.3 Part C: Foreign Gas Broadening Parameters

The TDL spectrometer will also be used for the evaluation of pressure broadening parameters induced by collision with foreign gases. The effects of air, H_2, O_2 and N_2 on several transitions in the ν_4 and ν_6 bands of H_2CO will be determined. The broadening parameters will be evaluated from plots of the absorption widths of individual transitions as a function of foreign gas pressure.

1.2.4 Part D: Trace Analysis of H_2CO in Ambient Air

In recent years TDLs have been used extensively to monitor trace gases. The literature covers a wide range of

analytical applications including the detection of NO_2 at <1 ppb levels, the measurment of pollutants (CO) at atmospheric pressures, and the detection of several gases simultaneously [18-25].

The aim of this work is to develope an analytical method for trace detection of H_2CO in ambient air. Hence, known analytical techniques will be modified to suit the detection of the "difficult to handle" H_2CO molecules [16]. These molecules adsorb easily to surfaces, have a tendency to polymerize, and are water soluble.

The experimental phase will evaluate and/or develop the following:

1. Transitions in the ν_4, ν_6 and ν_1 bands suitable for trace analysis. Transitions in the ν_1 band are several orders of magnitude stronger than those in ν_4 and ν_6 and therefore may be used with relatively shorter optical pathlengths or for detection of lower concentrations.
2. The detection of samples at reduced pressures in a long optical path cell technique.
3. The feasability of using 5 liter standard grab bags for field work (sample collection).
4. The lower limit of detection.
5. Preparation of calibration curves suitable for routine analysis
6. The design of mobile TDL system capable of on-site analysis.

CHAPTER 2

THEORY OF ASYMMETRIC TOP MOLECULAR SPECTRA

2.1 Introductory Remarks

The theoretical basis for both infrared (IR) and microwave (MW) spectroscopy is essentially the same. Using a Hamiltonian which represents the system under study and a proper set of wavefunctions one solves the Schrodinger equation $H\Psi = E\Psi$ for the eigenvalues and eigenvectors. These in turn yield, respectively, the energy levels and the intensities of the spectral lines.

The degree of difficulty in solving the Schrodinger equation, however, varies with the particular system and is a function of molecular size and symmetry. For asymmetric molecules the solution cannot be written in closed form, even in the rigid-rotor approximation. Rather, to obtain the energy levels, the Hamiltonian matrix is computed in some basis set and is then numerically diagonalized to yield the eigenvalues. It follows then that the accuracy of a predicted spectrum is governed by the quality of the equation of molecular motion used to generate the Hamiltonian operator.

The equation of motion is usually based on the rigid rotor-harmonic oscillator model. However, for meaningful results across a broad range of energy levels, it is

necessary to include terms accounting for non-rigid and anharmonic behaviour. Consideration must also be given to centrifugal distortion, and, when applicable, to Coriolis and Fermi interactions.

2.2 The Rigid Rotor - Harmonic Oscillator Hamiltonian

The quantum mechanical Hamiltonian operator for a polyatomic molecule can be expressed as

$$\hat{H} = T_E + T_N + V_{EN} + V_{NN} + V_{EE} \qquad (2\text{-}1)$$

where T_E and T_N represent, respectively, the kinetic energy of all the electrons and all the nuclei in terms of momentum. The potential energy terms V_{EN}, V_{NN} and V_{EE} arise from the electrostatic attraction and repulsion between electrons and nuclei. Consequently, the total energy of a molecule can be written as

$$E_{total} = E_{translation} + E_{rotation} + E_{vibration} + E_{electronic} + E_{trans-rot} + E_{trans-vib} + E_{rot-vib} \qquad (2\text{-}2)$$

The system can be greatly simplified by using the Born-Oppenheimer approximation [26]. This approximation assumes that the nuclei, owing to their much greater masses, move much more slowly than the electrons. Therefore, at any given time the motion of the electrons is the same as if the nuclei were fixed at their present instantaneous positions. This facilitates the separation of Schrodinger's equation

into an electronic part and a "mechanical" rotation vibration part. Each part may then be solved independently.

Further simplification may be achieved by describing the position of the nuclei in a molecule using a molecule-fixed coordinate system [27]. This axis system has its origin at the molecule's center of mass, and is rotating with the molecule. The orientation of the rotating system with respect to the space fixed axis may be described by a set of Euler angles. The molecule-fixed axis system eliminates the translation-coupled terms and allows the separation of the translational energy from the total energy equation. Hence, we are left with only the rotation-vibration energy

$$E_{rov} = E_{rot} + E_{vib} + E_{rot-vib} \qquad (2-3)$$

This is represented in the Hamiltonian in terms of kinetic and potential energies

$$H_{rov} = T_{rov} + V_{rov} \qquad (2-4)$$

The rotation-vibration Hamiltonian may now be solved, treating the molecule as a set of point masses representing the nuclei lying in some potential field. Here, the electronic energy as a function of nuclear positions, becomes the potential energy term.

The rotational kinetic energy is expressed in terms of angular momentum, while the vibrational energy may be stated

in harmonic oscillator form. Wilson and Howard [28] transformed the kinetic energy in the space-fixed frame to the molecule-fixed axis system. By doing so they obtained the following classical expression for the molecular kinetic energy

$$T = \sum_{\alpha\beta} 1/2 (J_\alpha - p_\alpha) \mu_{\alpha\beta} (J_\beta - p_\beta) + \sum_{i}^{3N-6} P_i^2 \qquad (2\text{-}5)$$

where the terms are defined in Table 2-1. Molecular vibrations are described relative to the molecular axes with the 3N-6 normal vibrational coordinates Q_i where N is the number of atoms. Hence, $P_i = \partial T/\partial Q_i$ is the vibrational momentum conjugate to the normal coordinates, Q_i. It is assumed here that the potential energy is a function only of the normal coordinates.

Starting with this classical expression (Equation 2-5) the quantum-mechanical Hamiltonian operator has been derived by Wilson and Howard [28], and later by Darling and Dennison [29]. More recently, Watson [30] has simplified the rather complicated original expressions to give a more general Hamiltonian for non-linear polyatomic molecules

$$\hat{H} = 1/2 \sum_{\alpha\beta} (\hat{J}_\alpha - \hat{p}_\alpha) \mu_{\alpha\beta} (\hat{J}_\beta - \hat{p}_\beta) + 1/2 \sum_i \hat{P}_i^2 + \hat{V}(Q_i) + U \qquad (2\text{-}6)$$

The last term, $U = -1/8h^2 \sum_\alpha \mu_{\alpha\beta}$ is a function only of the vibrational coordinates and therefore can be incorporated into the potential energy term. For practical purposes this Hamiltonian is usually simplified by expanding V and $\mu_{\alpha\beta}$

Table 2-1

Definition of Commonly Used Symbols

$\hat{}$ .....circumflex denotes operator

H .....Hamiltonian operator

J .....quantum number defining eigenvalues of the total angular momentum J

J_α ....component of total angular momentum, α = x,y, or z

p_α ....component of vibrational angular momentum, α = x,y,z

P_i ....linear momentum conjugate to the i^{th} normal coordinates

Q_i ....i^{th} normal coordinate

d_i degeneracy of Q_i

v_i .... quantum number of vibration of Q_i

I_α^v ....effective moment of inertia about α=x,y, or z in vibrational state v

$\mu_{\alpha\beta}$ ..inverse of moment of inertia matrix, or β=x,y,z

about equilibrium values as a Taylor series in the normal coordinates. This series, however, converges relatively slowly for light asymmetric molecules such as H_2O and H_2CO. A perturbation calculation can be made using a unitary transformation on the Hamiltonian making it diagonal in vibrational quantum numbers [31]. The Hamiltonian may then be rewritten as

$$\hat{H} = \hat{H}_{rot} + \hat{H}_{vib} \qquad (2\text{-}7)$$

where the rotational parameters are a function of the particular vibration under consideration. The zero order vibrational Hamiltonian is given by

$$\hat{H}_{vib} = 1/2 \sum_i (\hat{P}_i^2 + \hat{Q}_i^2) \qquad (2\text{-}8)$$

This gives rise to the harmonic oscillator vibrational energy levels defined by

$$E_{vib} = (v + d/2) \quad (cm^{-1}) \qquad (2\text{-}9)$$

Hence the total vibrational energy of a given molecule is

$$G(v_1, v_2, \ldots) = \sum_i \omega_i \, (v_i + d_i/2) \qquad (2\text{-}10)$$

where i runs over the 3N-6 normal vibrational modes. Providing that no resonances exist between the various vibrational states the rotational Hamiltonians may now be diagonalized to yield the rotational energies for the individual vibrational bands. The discussion will now focus

on the rotational Hamiltonian, specifically for the case of the asymmetric rotor which is characterized by three unequal moments of inertia.

If the molecular axes are fixed so that they coincide with the principal axes of inertia [32], then the lowest-order approximation for the rotational Hamiltonian may be stated in terms of the rigid rotor as

$$\hat{H}_{rot} = \hat{H}_{rigid} = B'_x \hat{J}_x^2 + B'_y \hat{J}_y^2 + B'_z \hat{J}_z^2 \qquad (2\text{-}11)$$

where the rotational constants $B'_\alpha = 1/2I_\alpha \text{ cm}^{-1}$ (α=x,y or z) and I_x, I_y, I_z are the principal moments of inertia of the molecule. The angular momentum components J_α are measured in units of $\hbar$, and obey commutation relations of the type

$$[\hat{J}_\alpha, \hat{J}_\beta] = \hat{J}_\alpha \hat{J}_\beta - \hat{J}_\beta \hat{J}_\alpha = -i\hat{J}_\gamma \qquad (2\text{-}12)$$

where the subscripts cyclically represent the molecule-fixed axes x,y and z.

By introducing centrifugal distortion, Wilson and Howard [28] derived the next higher order of approximation to H_{rot}, giving

$$\hat{H}_{rot} = \hat{H}_{rigid} + 1/4 \sum \tau_{\alpha\beta\gamma\delta} \hat{J}_\alpha \hat{J}_\beta \hat{J}_\gamma \hat{J}_\delta \qquad (2\text{-}13)$$

where the $\tau_{\alpha\beta\gamma\delta}$ coefficient in the quartic terms is given to a good approximation by [33]

$$\tau = -1/2 \sum_{ij} \mu^i_{\alpha\beta} (F^{-1}) \mu^j_{\alpha\beta} \qquad (2\text{-}14)$$

where i and j run over the 3N-6 internal displacement coordinates, which are used to evaluate both the inverse force field (F^{-1}) and the moment-of-inertia matrices. The general asymmetric rotor has 21 non-zero distortion coefficients, of which nine take on distinct values while the rest vanish due to symmetry. The nine distinct values are

$$\tau_{\alpha\alpha\alpha\alpha}, \tau_{\alpha\alpha\beta\beta} = \tau_{\beta\beta\alpha\alpha}$$

$$\tau_{\alpha\beta\alpha\beta} = \tau_{\alpha\beta\beta\alpha} = \tau_{\beta\alpha\alpha\beta} = \tau_{\beta\alpha\beta\alpha}$$

where α, β = x, y or z

By applying the commutation relations shown in equation (2-12) Kivelson and Wilson [9] have demonstrated that there are really only six independent distortion coefficients, and equation (2-13) can be written in a simpler form as

$$\hat{H}_{rot} = B_x \hat{J}_x^2 + B_y \hat{J}_y^2 + B_z \hat{J}_z^2 + 1/4 \, \tau'_{\alpha\beta\gamma\delta} \hat{J}_\alpha^2 \hat{J}_\beta^2 \qquad (2\text{-}15)$$

where
$$\tau'_{xxxx} = \tau_{xxxx}$$
$$\tau'_{yyyy} = \tau_{yyyy}$$
$$\tau'_{zzzz} = \tau_{zzzz}$$
$$\tau'_{xxyy} = \tau_{xxyy} + 2\tau_{xyxy}$$
$$\tau'_{yyzz} = \tau_{yyzz} + 2\tau_{yzyz}$$
$$\tau'_{xxzz} = \tau_{xxzz} + 2\tau_{xzxz}$$
$$B_x = B'_x + 1/4(3\tau_{xyxy} - 2\tau_{xzxz} - 2\tau_{yzyz})$$
$$B_y = B'_y + 1/4(3\tau_{yzyz} - 2\tau_{xyxy} - 2\tau_{xzxz})$$
$$B_z = B'_z + 1/4(3\tau_{xzxz} - 2\tau_{xyxy} - 2\tau_{yzyz})$$

Note, however, that the new rotational constants $B_{x,y,z}$ are now also corrected for distortion.

It was later shown by Dowling [35] that for planar asymmetric top molecules such as H_2CO, the six independent τ constants reduce to four independent coefficients. These H_{rot} models are however, only valid for a harmonic-oscillator approximation to the force field and for the equilibrium coefficients, not the vibrationally averaged ones that are observed in practice. If the energy levels of a molecule are known to high accuracy then this H_{rot} will yield a poor fit because of these two approximations. Watson [36] has demonstrated that the poor data fits obtained from the Kivelson and Wilson model are due to the fact that the matrix elements of the six $\tau_{\alpha\beta\gamma\delta}$ are linearly dependent on each other. Consequently, Watson developed a more general Hamiltonian which may be expanded to high orders in angular momentum operators that insures independence of the matrix elements of the effective operators. In this thesis, the rotational constants and distortion coefficients for formaldehyde were determined from a least-squares-fit to a sixth order Watson Hamiltonian. A detailed summary of the development of this Hamiltonian will now follow.

2.3 The Rotational Hamiltonian

The general rotational Hamiltonian for a particular vibrational band may be written as a power series in the angular momentum components $\hat{J}_x$, $\hat{J}_y$ and $\hat{J}_z$. By means of commutation relations this representation is reduced to the so-called standard form [36,37] given as

$$\hat{H}_{rot} = \sum_{pqr} h_{pqr} (\hat{J}_x^p \hat{J}_y^q \hat{J}_z^r + \hat{J}_z^r \hat{J}_y^q \hat{J}_x^p) \quad (2\text{-}16)$$

where the coefficients h_{pqr} can be either real or complex and p, q and r are integers. However, molecular model Hamiltonians must be invariant to both time reversal L [38] and to Hermitian conjugation denoted by the symbol * [32], so that

$$\hat{H}_{rot} = L\hat{H}_{rot}L^{-1} = \hat{H}_{rot}^* = (L\hat{H}_{rot}L^{-1})^* \quad (2\text{-}17)$$

Consequently, the standard expression is constrained by the fact that $\hat{H}_{rot}$ must be Hermitian, h_{pqr} has to be real and not complex, and the sum p+q+r is restricted to even integers. For orthorhombic molecules p,q and r are all even integers and some of the h_{pqr} coefficients can be shown to equal zero. By the use of unitary transformations the general non-orthorhombic asymmetric top Hamiltonian may be transformed to the orthorhombic form. The standard form Hamiltonian up to terms of sixth degree in J_α can be written [39] as

$$\hat{H}_{rot} = \hat{H}_2 + \hat{H}_4 + \hat{H}_6 \quad (2\text{-}18)$$

where

$$\hat{H}_2 = \sum_\alpha B_\alpha \hat{J}_\alpha^2$$

$$= B_x \hat{J}_x^2 + B_y \hat{J}_y^2 + B_z \hat{J}_z^2 \qquad (2\text{-}19)$$

$$\hat{H}_4 = \sum_{\alpha \neq \beta} T_{\alpha\beta} \hat{J}_\alpha^2 \hat{J}_\beta^2$$

$$= T_{xx} \hat{J}_x^4 + T_{yy} \hat{J}_y^4 + T_{zz} \hat{J}_z^4 + T_{xy} (\hat{J}_x^2 \hat{J}_y^2 + \hat{J}_y^2 \hat{J}_x^2)$$

$$+ T_{xz} (\hat{J}_x^2 \hat{J}_z^2 + \hat{J}_z^2 \hat{J}_x^2) + T_{yz} (\hat{J}_y^2 \hat{J}_z^2 + \hat{J}_z^2 \hat{J}_y^2) \qquad (2\text{-}20)$$

$$\hat{H}_6 = \sum_\alpha \phi_{\alpha\alpha\alpha} \hat{J}_\alpha^6 + \sum_{\alpha \neq \beta} \phi_{\alpha\alpha\beta} (\hat{J}_\alpha^4 \hat{J}_\beta^2 + \hat{J}_\beta^2 \hat{J}_\alpha^4)$$

$$+ \phi_{xyz} (\hat{J}_x^2 \hat{J}_y^2 \hat{J}_z^2 + \hat{J}_z^2 \hat{J}_y^2 \hat{J}_x^2)$$

$$= \phi_{xxx} \hat{J}_x^6 + \phi_{yyy} \hat{J}_y^6 + \phi_{zzz} \hat{J}_z^6 + \phi_{xxy} (\hat{J}_x^4 \hat{J}_y^2 + \hat{J}_y^2 \hat{J}_x^4)$$

$$+ \phi_{xxz} (\hat{J}_x^4 \hat{J}_z^2 + \hat{J}_z^2 \hat{J}_x^4) + \phi_{yyz} (\hat{J}_y^4 \hat{J}_z^2 + \hat{J}_z^2 \hat{J}_y^4)$$

$$+ \phi_{yyx} (\hat{J}_y^4 \hat{J}_x^2 + \hat{J}_x^2 \hat{J}_y^4) + \phi_{zzx} (\hat{J}_z^4 \hat{J}_x^2 + \hat{J}_x^2 \hat{J}_z^4)$$

$$+ \phi_{zzy} (\hat{J}_z^4 \hat{J}_y^2 + \hat{J}_y^2 \hat{J}_z^4) + \phi_{xyz} (\hat{J}_x^2 \hat{J}_y^2 \hat{J}_z^2 + \hat{J}_z^2 \hat{J}_y^2 \hat{J}_x^2) \qquad (2\text{-}21)$$

This Hamiltonian may be expanded to higher degrees in $\hat{J}_\alpha$. However, in general, for low quantum numbers the energy contributions from the various terms are such that $\hat{H}_2 >> \hat{H}_4 >> \hat{H}_6 \ldots\ldots$, so that the power series may be truncated according to the needs of the particular system. For highly flexible or light molecules, such a series may not converge at a satisfactory rate and an alternative treatment may be

preferable [40-42].

The coefficients $T_{\alpha\beta}$ are related to Kivelson and Wilson's parameters by $\mathcal{T}_{\alpha\alpha\beta\beta} = 4T_{\alpha\beta}$. At this point however, the Hamiltonian has 3 quadratic, 6 quartic and 10 sextic coefficients of which some are not determinable parameters. Unitary transformation of $\hat{H}_{rot}$ affects only the coefficients of the momentum operators while leaving the eigenvalues unchanged. Watson has made use of this fact and demonstrated that by a proper choice of unitary operators it is possible to eliminate many terms from the Hamiltonian so that it yields a set of determinable molecular constants from combinations of the indeterminable coefficients.

Watson constructed a unitary operator by means of the equation

$$\hat{U} = \exp(i\hat{S}) \tag{2-22}$$

where $\hat{S}$ is Hermitian. In order that $\hat{U}$ be invariant to time reversal, S must change sign under time reversal. Hence, $\hat{S}$ is given as an odd power series in the components of the angular momentum [37]

$$\hat{S} = \sum_{pqr} s_{pqr}(\hat{J}_x^p \hat{J}_y^q \hat{J}_z^r + \hat{J}_z^r \hat{J}_y^q \hat{J}_x^p) = \hat{S}_3 + \hat{S}_5 + \hat{S}_7 + \ldots \tag{2-23}$$

with p, q, and r all odd ,and real coefficients s_{pqr}. As in the case of the standard form $\hat{H}_{rot}$, this series may be truncated according to the particular case. This work utilizes the first two terms of this series, which are

$$\hat{S}_3 = s_{111}(\hat{J}_x\hat{J}_y\hat{J}_z + \hat{J}_z\hat{J}_y\hat{J}_x)$$

$$\hat{S}_5 = s_{311}(\hat{J}_x^3\hat{J}_y\hat{J}_z + \hat{J}_z\hat{J}_y\hat{J}_x^3) + s_{131}(\hat{J}_x\hat{J}_y^3\hat{J}_z + \hat{J}_z\hat{J}_y^3\hat{J}_x)$$
$$+ s_{113}(\hat{J}_x\hat{J}_y\hat{J}_z^3 + \hat{J}_z^3\hat{J}_y\hat{J}_x) \qquad (2\text{-}24)$$

The contact transformation of the rotational Hamiltonian may be written as

$$\tilde{H}_R = U^{-1}\hat{H}_{rot}U = \tilde{H}_2' + \tilde{H}_4' + \tilde{H}_6' + \ldots. \qquad (2\text{-}25)$$

where the terms of the transformed Hamiltonian are given by [37]

$$\tilde{H}_2' = \hat{H}_2$$

$$\tilde{H}_4' = \hat{H}_4 + i(\hat{H}_2,\hat{S}_3)$$

$$\tilde{H}_6' = \hat{H}_6 + i(\hat{H}_4,\hat{S}_3) - 1/4\{(\hat{H}_2,\hat{S}_3),\hat{S}_3\} + i(\hat{H}_2,\hat{S}_5) \qquad (2\text{-}26)$$

For each commutation of the type (A,B)=AB-BA the degree of a given term is reduced by one. The rearrangement of each $\tilde{H}_n'$ to the standard form produces terms of lower degree. The terms of the same degree are then collected to give

$$\tilde{H}_R = \tilde{H}_2 + \tilde{H}_4 + \tilde{H}_6 + \ldots. \qquad (2\text{-}27)$$

$\tilde{H}_R$ has now the same form as $\hat{H}_{rot}$. The new quadratic and quartic molecular constants are then related to the old ones by

$$\tilde{B}_x = B_x + 4(B_z - B_y)s_{111}$$

$$\tilde{B}_y = B_y + 4(B_x - B_z)s_{111}$$

$$\tilde{B}_z = B_z + 4(B_y - B_x)s_{111} \qquad (2\text{-}28)$$

$$\tilde{T}_{xx} = T_{xx} \,, \quad \tilde{T}_{yy} = T_{yy} \,, \quad \tilde{T}_{zz} = T_{zz}$$

$$\tilde{T}_{yz} = T_{yz} + 2(B_z - B_y)s_{111}$$

$$\tilde{T}_{xz} = T_{xz} + 2(B_x - B_z)s_{111}$$

$$\tilde{T}_{xy} = T_{xy} + 2(B_y - B_x)s_{111} \qquad (2\text{-}29)$$

The transformed sextic coefficients are listed in Watson's paper [37], while the higher order contributions for the quadratic and quartic terms are given by Typke [43].

Due to the fact that the determinable constants can only be a function of the energies, and cannot depend on the particular choice of unitary transformation, s_{pqr} must not appear in the expression for the determinable parameters. Hence, in equations (2-28) and (2-29) s_{111} should be eliminated by substitution. By doing so one also eliminates one molecular parameter. Consequently, a set of parameters which do not depend on the transformation is obtained:

$$\tilde{B}_x^{\cdot} = B_x - 2T_{yx}$$
$$\tilde{B}_y^{\cdot} = B_y - 2T_{xz}$$
$$\tilde{B}_z^{\cdot} = B_z - 2T_{xy}$$

$$T_{xx} \,, \quad T_{yy} \,, \quad T_{zz}$$
$$T_1 = T_{yz} + T_{xz} + T_{xy}$$
$$T_2 = B_x T_{yz} + B_y T_{xz} + B_z T_{xy} \qquad (2\text{-}30)$$

Similarly, the sextic part of the Hamiltonian may be reduced to seven determinable combinations of coefficients. The three rotational constants, the five quartic centrifugal distortion constants, and the seven sextic centrifugal distortion constants give a total of 15 determinable parameters from a sixth order asymmetric Hamiltonian. In general, a Hamiltonian of n^{th} degree has $n(n+4)/4$ determinable parameters (remembering that here n is an even integer).

Finally, in order to reduce the complexity of the matrix elements, the Hamiltonian is written in terms of the operators $\tilde{J}^2$, $\hat{J}_z$ and $\hat{J}_\pm$. Where, $\tilde{J}$ represents the total angular momentum, J_z is the component of $\tilde{J}$ along the z molecular principal axis, and $\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y$, in the symmetric top basis, acts as the lowering and raising operators of the quantum number K. This representation is given by [37]

$$\begin{aligned}\hat{H}_{rot} &= B_{200}\tilde{J}^2 + B_{020}\hat{J}_z^2 + B_{002}(\hat{J}_+^2 + \hat{J}_-^2) \\ &+ T_{400}\tilde{J}^4 + T_{220}\tilde{J}^2\hat{J}_z^2 + T_{040}\hat{J}_z^4 + T_{202}\tilde{J}^2(\hat{J}_+^2 + \hat{J}_-^2) \\ &+ 1/2T_{022}\{\hat{J}_z^2(\hat{J}_+^2 + \hat{J}_-^2) + (\hat{J}_+^2 + \hat{J}_-^2)\hat{J}_z^2\} \\ &+ T_{004}(\hat{J}_+^4 + \hat{J}_-^4) + \text{higher order terms} \qquad (2\text{-}31)\end{aligned}$$

where the subscripts of the coefficients refer to the powers of the operators $\tilde{J}$, $\hat{J}_z$ and $\hat{J}_\pm$. In the transformed

Hamiltonian the coefficients for the quadratic and quartic terms then become:

$$\tilde{B}_{200} = B_{200} + 4B_{002}s_{111}$$

$$\tilde{B}_{020} = B_{020} - 14B_{002}s_{111}$$

$$\tilde{B}_{002} = B_{002} + 2B_{002}s_{111}$$

$$\tilde{T}_{400} = T_{400} - 2B_{002}s_{111}$$

$$\tilde{T}_{202} = T_{202}$$

$$\tilde{T}_{220} = T_{220} + 12B_{002}s_{111}$$

$$\tilde{T}_{022} = T_{022} - 2B_{020}s_{111}$$

$$\tilde{T}_{040} = T_{040} - 10B_{002}s_{111}$$

$$\tilde{T}_{004} = T_{004} + B_{002}s_{111} \qquad (2\text{-}32)$$

2.4 The Reduced Hamiltonian

It was shown in the previous section that the rotational Hamiltonian may be reduced by a proper choice of s_{pqr}. This however, can be done in many ways [39,44]. To limit the possibilities it is convenient to consider only those reductions that eliminate specific cylindrical components from the Hamiltonian. The two most commonly used reductions, called AS (asymmetric) and NS (nearly symmetric) are obtained using two of Nielsen's molecular constants [45]

$$R_5 = (1/8)(-T_{xx} + T_{yy} + 2T_{xz} - 2T_{yz})$$

$$R_6 = (1/16)(T_{xx} + T_{yy} - 2T_{xy}) \qquad (2\text{-}33)$$

Under unitary transformation these become

$$\tilde{R}_5 = R_5 - (B_z - (1/2)(B_x - B_y))s_{111}$$

$$\tilde{R}_6 = R_6 + (1/4)(B_x - B_y)s_{111} \qquad (2\text{-}34)$$

The NS and AS forms may be obtained by setting respectively $\tilde{R}_5$ and $\tilde{R}_6$ to zero yielding

$$s_{111} = R_5/\{B_z - 1/2(B_x + B_y)\} = T_{022}/2B_{020} \qquad (2\text{-}35)$$

or

$$s_{111} = 4R_6/(B_x - B_y) = -T_{004}/B_{002} \qquad (2\text{-}36)$$

Observe that equation (2-35) may not be used for nearly spherical tops, where $B_x \simeq B_y \simeq B_z$ leads to an infinetly large s_{111}. Similarly equation (2-36) used in the AS case goes to infinity for nearly symmetric tops where $B_x \simeq B_y$. Hence, the choice of reduction form is governed by molecular symmetry. The Hamiltonian for formaldehyde was reduced using the AS form.

The choice for s_{111} using Equation (2-36) makes $\tilde{T}_{004} = 0$ so that the operator $(\hat{J}_+^4 + \hat{J}_-^4)$ is eliminated from Equation (2-31). Similarly, with proper choices of s_{113}, s_{131} and s_{311} one may drop three operators from the sextic term of $\tilde{H}_{rot}$. The reduced Hamiltonian may then be written as

$$\hat{H}^{AS} = \hat{H}_2^{AS} + \hat{H}_4^{AS} + \hat{H}_6^{AS} + \ldots \qquad (2\text{-}37)$$

where

$$\hat{H}_2^{AS} = 1/2(B_x^{AS} + B_y^{AS})\tilde{J}^2 + \{B_z^{AS} - 1/2(B_x^{AS} + B_y^{AS})\}\hat{J}_z^2 + 1/4(B_x^{AS} - B_y^{AS})(\hat{J}_+^2 - \hat{J}_-^2)$$

$$\hat{H}_4^{AS} = -\Delta_J\tilde{J}^4 - \Delta_{JK}\tilde{J}^2\hat{J}_z^2 - \Delta_K\hat{J}_z^4 - \delta_J\tilde{J}^2(\hat{J}_+^2 - \hat{J}_-^2) - 1/2\delta_K\{\hat{J}_z^2(\hat{J}_+^2 - \hat{J}_-^2) + (\hat{J}_+^2 - \hat{J}_-^2)\hat{J}_z^2\}$$

$$\hat{H}_6^{AS} = H_J\tilde{J}^6 + H_{JK}\tilde{J}^4\hat{J}_z^2 + H_{KJ}\tilde{J}^2\hat{J}_z^4 + H_K\hat{J}^6 + h_J\tilde{J}^4(\hat{J}_+^2 - \hat{J}_-^2) + 1/2h_{JK}\tilde{J}^2\{\hat{J}_z^2(\hat{J}_+^2 - \hat{J}_-^2) + (\hat{J}_+^2 - \hat{J}_-^2)\hat{J}_z^2\} + 1/2h_K\{\hat{J}_z^4(\hat{J}_+^2 - \hat{J}_-^2) + (\hat{J}_+^2 - \hat{J}_-^2)\hat{J}_z^4\}$$

The matrix of this Hamiltonian is in tri-diagonal form, which makes it relatively easy to solve. Therefore, the AS form is the one most commonly used.

2.5 Asymmetric Rotor Notation and Selection Rules

The rigid rotor Hamiltonian given in Equation (2-11) is usually rewritten as

$$\hat{H}_{rigid} = B_a\hat{J}_a^2 + B_b\hat{J}_b^2 + B_c\hat{J}_c^2 \qquad (2\text{-}38)$$

where the molecule fixed axes x,y, and z are now represented by some permutation of a, b and c. A further simplification introduces $A=B_a$ $B=B_b$ and $C=B_c$. According to convention A>B>C

since $I_a<I_b<I_c$. The original x,y, and z axes may be identified with the new labels in the six ways [46] shown in Table 2-2

Table 2-2

Axis Representation

	right hand permutations			left hand permutations		
	I^r	II^r	III^r	I^l	II^l	III^l
x	b	c	a	c	a	b
y	c	a	b	b	c	a
z	a	b	c	a	b	c

The rotational constants A, B and C may be used to define asymmetry parameters. These in turn indicate to what extent an asymmetric top approximates the limits of a symmetric top, i.e., when any two rotational constant are equal. The Wang asymmetry parameter b is given by

$$b = (B_y - B_x)/(2B_z - B_x - B_y) \qquad (2\text{-}39)$$

In the I^r axis permutation b becomes

$$b_p = (C - B)/(2A - B - C) \qquad (2\text{-}40)$$

The range of b_p is $-1 \leq b_p \leq 0$. Now, for a prolate symmetric

top where A>B=C, b_p=0. The other limit, b_p=-1 occurs for the oblate symmetric top where A=B>C. In the III^r representation b is defined as

$$b_o = (B - A)/(2C - A - B) \qquad (2\text{-}41)$$

The range here is $0 \leq b_o \leq 1$; where b_o is respectively 0 and I for oblate and prolate symmetric tops. The utilization of the remaining representations is not neccessary due to redundancy.

Another useful definition is given in terms of Ray's asymmetry parameter κ where

$$\kappa = (2B - A - C)/(A - C) \qquad (2\text{-}42)$$

Here the range is $-1 \leq \kappa \leq +1$, where κ is equal to -1 in the prolate limit and +1 in the oblate limit, κ=0 defines the most asymmetric case. The computed Ray parameter for H_2CO is κ=-0.961, hence formaldehyde is a near prolate asymmetric top. The limits of κ also suggest that an asymmetric top may be described in terms of its symmetric limits. A convenient method of representation consist of the symmetric wave-functions $\psi_{J,K,M}$ written as $|J,K,M\rangle$. The quantum numbers K and M represent respectively, the 2J+1 orientations of the total angular momentum in the molecule fixed axis system (J_z) and in the space fixed coordinate system (J_Z). In the absence of an external potential field, all M values are degenerate for a given K and they are not considered in the computation used in this thesis.

The matrices of the Hamiltonians discussed thus far are diagonal in J. Hence the only matrix elements required for the calculation of the energy levels are $\langle J,K'|\hat{H}|J,K\rangle$. Therefore the Hamiltonian may be diagonalized individually for each J value. In the rigid rotor representation, the only non-zero matrix elements are

$$\langle J,K|\hat{H}_{rigid}|J,K\rangle = (1/2)(B_x+B_y)J(J+1) + [B_z - (1/2)(B_x+B_y)]K^2$$

$$\langle J,K\pm2|\hat{H}_{rigid}|J,K\rangle = (1/4)(B_x-B_y)\{[J(J+1)-K(K\pm1)] \times [J(J+1)-(K\pm1)(K\pm2)]\}^{1/2} \qquad (2\text{-}43)$$

so that H_{rigid} is tri-diagonal. The calculation of the rotational energy level reduces to the diagonalization of this matrix for each value of J. Observe, however, that for a symmetric top ($B_x=B_y$) or a spherical top ($B_x=B_y=B_z$) the Hamiltonian is already diagonal.

The numerical diagonalization of asymmetric top Hamiltonian matrices is facilitated by the use of a new set of basis function $|J,K^+\rangle$ created by the Wang transformation [47]

$$|J,0^+\rangle = |J,0\rangle$$
$$|J,K^+\rangle = (1/2)\{|J,K\rangle + |J,-K\rangle\} \quad K>0$$
$$|J,K^-\rangle = (1/2)\{|J,K\rangle - |J,-K\rangle\} \quad K>0 \qquad (2\text{-}44)$$

Here one takes into account the symmetry properties of the asymmetric wavefunctions which belong to the group $V_{(a,b,c)}$

defined by an identity operator E and three two-fold rotational operators C_2^a, C_2^b, C_2^c, where a,b and c denote the molecular fixed axis. The character table for $V_{(a,b,c)}$ is given in Table 2-3 with +1 and -1 representing respectively, symmetric and antisymmetric wavefunctions for the given operator.

Table 2-3

Character Table for the Group $V_{(a,b,c)}$

operation				symmetry		Wang's sub-matrices	
E	C_2^a	C_2^b	C_2^c	K_a, K_c	type	J_{even}	J_{odd}
1	1	1	1	e,e	A_o	E^+	E^-
1	1	-1	-1	e,o	B_a	E^-	E^+
1	-1	1	-1	o,o	B_b	O^+	O^-
1	-1	-1	1	o,e	B_c	O^-	O^+

The rigid-rotor Hamiltonian is invariant to two-fold rotations C_2^α (α=x,y,z) which generate the point group $V_{(a,b,c)}$ (or D_2 group). Since the Wang functions are linear combinations of the symmetric top wavefunctions which trannsform with $V_{(a,b,c,)}$ operations, they may be used as a basis set yielding fully symmetrized sub- matrices. If $\hat{H}_{rot}$ is now set up in this basis, then the Hamiltonian matrix for each J (other then J=0 and J=1) can be partitioned into four independent tri-diagonal matrices. This can be done because the matrix elements connecting even and odd K's vanish along

with those connecting $|J,K^+\rangle$ and $|J,K^-\rangle$. Hence for a given J we may write

$$\hat{H}_R^J = E^+ + O^+ + E^- + O^- \qquad (2\text{-}45)$$

where + and - refer to matrices with only $|J,K^+\rangle$ or $|J,K^-\rangle$ elements. the E and O labels refer to whether K is even or odd. Upon computation, one obtains 2J+1 energy levels for each J, The advantage of using Wang's transformation lies in the fact that the original 2J+1 by 2J+1 matrix is reduced to four much smaller matrices. A general result for the asymmetric top Hamiltonian matrix of a given J is that for even J the E^+ block has dimension (J+2)/2 and the other three blocks have dimension J/2, whereas for odd J the E^- block has dimension (J-1)/2 and the other three blocks have dimension (J+1)/2. This results in significant computational efficiencies.

The asymmetric top rotational energy levels are designated ${}^{J}K_a,K_c$. This is obtained by considering a proccess in which the rotational constant B_α is varied smoothly from the prolate to the oblate symmetric conditions. Here K_a and K_c represent respectively the prolate and oblate limits of K. For intermediate values of B_α, the energy levels for a given J do not cross. Thus, ${}^{J}K_a,K_c$ specifies each energy level uniquely as can be seen in Figure 2-1. The symmetries of the wave functions with respect to C_2^a and C_2^c of $V_{(a,b,c)}$ are determined by K_a and K_c

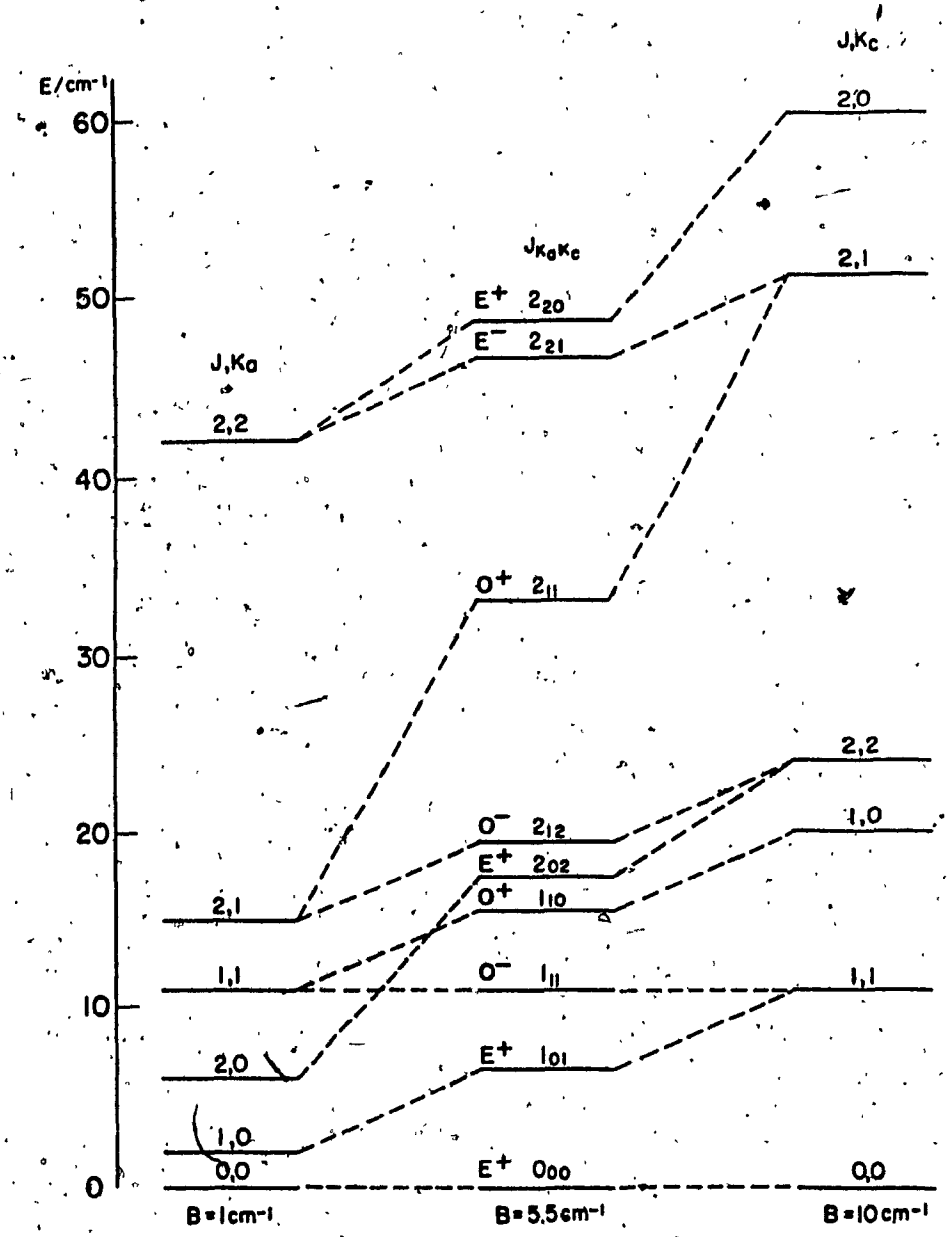


Figure 2-1: Correlation Diagram for the Asymmetric Rotor Energy Levels.

The correlation of J=0,1 and 2 energy levels of a rigid asymmetric top molecule having (A,B,C)=(10,5.5,1) cm^{-1} i.e., κ=0, with those for the prolate top having (A,B,C)=(10,1,1) cm^{-1} on the left, and with those for the oblate top having (A,B,C)=(10,10,1) cm^{-1} on the right.

according to the transformation $C_2^{\alpha}|J,K^+\rangle$, where α=a or c. The energy increases with increasing K_a and decreases with increasing K_c. Therefore the energy levels for a given J, in assending order, have the labels

$$(K_a,K_c) = (0,J)\ ,\ (1,J)\ ,\ (1,J-1)\ ,\ (2,J-1)\ ,\ (2,J-2)\ldots$$
$$\ldots(J-1,2)\ ,\ (J-1,1)\ ,\ (J,1)\ ,\ (J,0) \qquad (2\text{-}46)$$

Observe that for other then zero, each value of K_a or K_c occurs twice in succession, also that K_a+K_c must equal either J or J+1.

In the case of the I^r representation, sixth order AS form Hamiltonian, the only non-zero matrix elements are

$$\begin{aligned}\langle J,K|\hat{H}_R^{AS}|J,K\rangle &= 1/2[B+C]J(J+1) + \{A-1/2[B+C]\}K^2 \\ &\quad - \Delta_J J^2(J+1)^2 - \Delta_{JK}J(J+1)K^2 - \Delta_K K^4 \\ &\quad + H_J J^3(J+1)^3 + H_{JK}J^2(J+1)^2K^2 \\ &\quad + H_{KJ}J(J+1)K^4 + H_K K^6\end{aligned}$$

$$\begin{aligned}\langle J,K\pm2|\hat{H}_R^{AS}|J,K\rangle &= \{1/4[B-C] - \delta_J J(J+1) \\ &\quad - 1/2\delta_K[(K\pm2)^2+K^2] + h_J J^2(J+1)^2 \\ &\quad + 1/2h_{JK}J(J+1)[(K\pm2)+K^2] \\ &\quad + 1/2h_K[(K\pm2)^4+K^4]\} \\ &\quad \times \{[J(J+1)-K(K\pm1)][J(J+1)-(K\pm1)(K\pm2)]\}^{1/2}\end{aligned} \qquad (2\text{-}47)$$

Hence, the form of the energy matrix is identical to that for the rigid rotor.

Transitions between energy levels are designated using $J'K_a'K_c'$ for an upper state energy, and $J''K_a''K_c''$ for a lower state. In an asymmetric top the type and nature of a given transition is governed by two selection rules. The first rule states that only transitions with $\Delta J=J'-J''=0,\pm1$ are allowed. The second selection rule is a function of the orientation of the dipole moment ($\vec{\mu}$) along the molecular axes a, b and c. Combinations of odd and even K_a and K_c transitions are classified as type a, b and c (Table 2-4). For the case of H_2CO the three vibrational bands ν_3, ν_4 and ν_6 investigated here are type a, type c and type b respectively and are illustrated in Figure 2-2.

The permanent dipole moment for H_2CO is along the a axis (I^r representation). This gives rise to the pure rotational spectrum of this molecule. For vibrational-rotational transitions one must be concerned with the instantaneous dipole moment induced by the vibration. In this case, the selection rules for changes in K_a and K_c are a function of the transformation of the components of the dipole moment for a given vibration and can be determined from Table 2-3. For the direction cosine matrix (described in the next section) to be non-zero as required for rotational transitions, the product of the characters of the initial and final rotational wave function as well as that

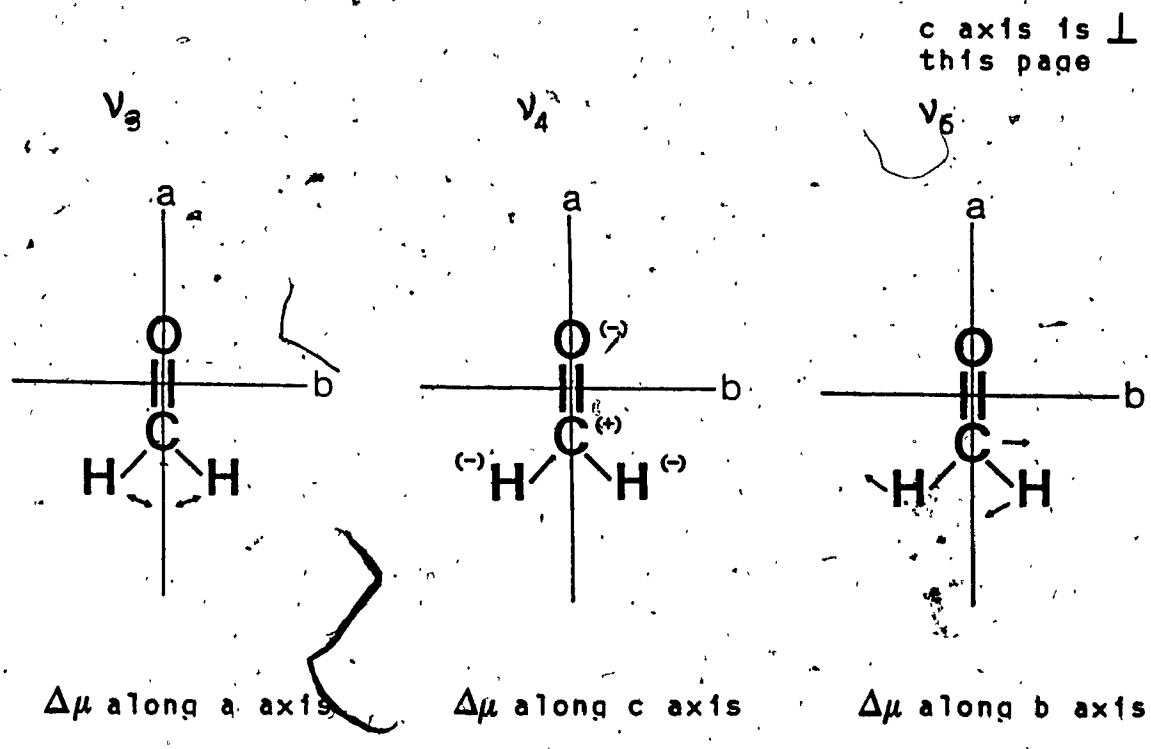
Table 2-4

Asymmetric Top Selection Rules

	ΔK_a	ΔK_c	classification
μ_a	even	odd	type a
μ_b	odd	odd	type b
μ_c	odd	even	type c

Figure 2-2

The ν_3, ν_4 and ν_6 Vibrations and Their Relation to μ.



of the dipole moment change must be +1. This can be seen clearly if Table 2-3 is rewritten as a multiplication table in terms of the transformation of the permanent dipole moment along the a,b,c molecule-fixed axes [46,49] as shown in Table 2-5.

Table 2-5

Direction of the Dipole Moment Permitting Transitions Between Rotational States

	K_aK_c	A ee	B_a eo	B_b oo	B_c oe
A	ee	-	a	b	c
B_a	eo	a	-	c	b
B_b	oo	b	c	-	a
B_c	oe	c	b	a	-

For the ν_3 vibration belonging to the B_a symmetry species the instantaneous dipole moment transforms according to B_a, so the selection rules for K_a and K_c are

$$oe \leftrightarrow oo \text{ and } eo \leftrightarrow ee.$$

Similarly, ν_4 with B_c symmetry yields

$$eo \leftrightarrow oo\ ,\ ee \leftrightarrow oe$$

and ν_6 with B_b symmetry has

$$ee \leftrightarrow oo\ ,\ eo \leftrightarrow oe$$

For a given vibration $\Delta J=0,+1,-1$ coresponds to the Q, R and P-branches, respectively. However, due to the nature of the asymmetric top, each branch splits into a series of sub-branches as a function of K. In the case of the near prolate top, the sub-branches are governed by K_a, where, for a given K_a one finds a cluster of transitions due to J and K_c. For example, the notation $^{Q}P_5(7)$ in ν_3 represent two possible transitions for $K_a=5$ where Q means that $\Delta K_a=0$; P and 7 stand for $\Delta J=-1$ and $J''=7$, respectively. Hence, the notation represent the transitions $(6_{5,1} \leftarrow 7_{5,2})$ and $(6_{5,2} \leftarrow 7_{5,3})$ in the ν_3 band.

2.6 Line Intensities

According to the Beer-Lambert law, the transmission of radiation through a homogeneous gas sample is described by the relation:

$$I = I_0 e^{-k(\nu)X} \qquad (2\text{-}48)$$

where $k(\nu)$ is the absorption coefficient, $\ln(I/I_0)$ is the absorption ratio and, X is the optical density. The absorption coefficient is a function of both line strength and line shape. The line strength or intensity, S, is defined to be the integral of the absorption coefficient

over the line profile:

$$S = \int_{-\infty}^{\infty} k(\nu)\,d\nu \qquad (2\text{-}49)$$

Hence, S is the area under the curve. In terms of fundamental molecular quantities, the strength of a spectral line arising from the transition from state A to state B is given by [46,48]:

$$S_A^B = [8\pi^3/(3hc)](n/G)\nu_{AB}\mathrm{Exp}(-hcE_A/kT) * [1-\mathrm{Exp}(-hc\,\nu_{AB}/kT)]\,|\langle A|\mu|B\rangle|^2 \qquad (2\text{-}50)$$

where n is the total number of absorbing molecules per cm^3 per atmosphere, G is the total partition function and $|\langle A|\mu|B\rangle|^2$ is the square of the transition dipole moment matrix element. The rotation-vibration partition function is given by

$$G = \sum_J g_j e^{(-E_J''/kT)} \qquad (2\text{-}51)$$

where g_i is the statistical weight or degeneracy of the energy state E_j'' of the vibrating-rotating molecule.

The square of the dipole moment matrix element is given by:

$$|\langle A|\mu|B\rangle|^2 = \sum_{f=X,Y,Z} |\langle i|\,\mu_f|f\rangle|^2 \qquad (2\text{-}52)$$

where i and f are the initial and final state of all the sublevels in the transition A to B and, μ_f is the component of the dipole moment along the X,Y,Z space fixed axes. In the absence of an external field the X,Y,Z components of the

dipole moment are equal so that only one component has to be evaluated. The chosen component can then be related to the dipole moment relative to the molecule-fixed axis with the direction cosines, ϕ_{Fg}. For example, working with the Z component yields

$$|\langle A|\mu|B\rangle|^2 = 3|\langle i|\mu_Z|f\rangle|^2 \qquad (2\text{-}53)$$

with

$$\mu_Z = \sum_g z_g \mu_g$$

where g is summed over the 3 molecule-fixed axes a,b,c.

In the case of H_2CO, if we assume that there is no mixing among the states ν_3, ν_4 and ν_6 then ν_3 has no change in μ_b and μ_c, so only μ_a needs to be considered in Equation (2-53). Similarly, for ν_4 and ν_6 if it is assumed that there is no mixing then only μ_c and μ_b respectively need to be considered (Figure 2-1). In the case for ν_3 Equation (2-53) then becomes:

$$|\langle A|\mu|B\rangle|^2 = 3|\langle i|\phi_{Za}\mu_a|f\rangle|^2 \qquad (2\text{-}54)$$

If it is assumed that there is no interaction between rotation and vibration, ie., where μ_g does not depend on the rotational coordinates, then Equation (2-54) for ν_3 may be written as

$$|\langle A|\mu|B\rangle|^2 = 3|\langle R_i|\phi_{Za}|R_f\rangle|^2 \, |\langle v_i|\mu_a|v_f\rangle|^2 \times \beta \qquad (2\text{-}55)$$

where

$$|R_i\rangle|v_i\rangle = |i\rangle \quad \text{and} \quad |R_f\rangle|v_f\rangle = |f\rangle$$

and β is the nuclear spin degeneracy and is 3 for transitions where K_a is odd and is 1 for transitions where K_a is even in the lower state.

Recalling that we are dealing with the case where there is no mixing between vibrational states we find

$$v_i = \text{ground state}, \quad v_f = v_3 \text{ or } v_4 \text{ or } v_6$$

$$R_i^j = \sum_n T_{jn}^T |J,K\rangle_n$$

$$R_f^m = \sum_l S_{ml}^T |J,K\rangle_l \tag{2-56}$$

where S is the eigenvector transformation matrix that diagonalizes the upper state Hamiltonian (superscript T represents transpose of...), T is the eigenvector matrix that diagonalizes the lower state Hamiltonian, and $|J,K\rangle_n$ represents the n^{th} symmetric top basis set. Thus Equation (2-55) may be written in more compact form as [13,53]

$$|\langle A|\mu|B\rangle|^2 = \{\langle v_i|\mu|v_f\rangle[\sum_n T_{fn}^T \sum_l S_{ml}^T \langle J'',K''|\mu|J',K'\rangle]\}^2$$

$$= (\partial\mu/\partial Q)^2 \langle v_i|Q|v_f\rangle^2 [T^T U_a S]_{jm}^2 \tag{2-57}$$

where $[U_a]$ is the dipole moment matrix along the a axis, Q is the normal coordinate matrix, and $(\partial\mu/\partial Q)$ is the dipole moment derivative.

In the actual case presented in this thesis there is mixing between the vibrational states v_3, v_4 and v_6 so that Equation (2-55) no longer holds, in the sense that we must consider transition components along more than one axis.

However, the principle is the same and we may still write the intensity in the form of Equation (2-57). But unlike the case of Equation (2-57) the vibrational terms do not simply factor out and the correct expression becomes

$$|\langle i|\mu|f\rangle|^2 = \sum_n T_{in}^T \sum_1 U_{n1}^2 S_{if} \qquad (2\text{-}58)$$

where the full matrix U now has μ_a type term for rotational basis sets in the v_3=1 manifold, μ_b terms for the v_6=1 manifold and μ_c type terms for the v_4=1 manifold. A given transition will be now governed by the expression

$$|\langle i|\mu|f\rangle|^2 = \{(\partial\mu/\partial Q_3)z_3 + (\partial\mu/\partial Q_4)z_4 + (\partial\mu/\partial Q_6)z_6\}^2 \qquad (2\text{-}59)$$

where z_3 depends only upon the rotational quantum numbers in the v_3=1 manifold and the ground state, z_4 depends only upon the rotational quantum numbers in the v_4=1 manifold and the ground state, etc. For example, z_3 is represented as

$$z_3 = \sum_i a_i \sum_j b_j \langle v_3=0|\delta Q|v_3=1\rangle\langle J'',K''|F\phi_{zg}|J',K'\rangle \qquad (2\text{-}60)$$

where a and b are the basis set coefficients ($\int X\hat{O}p.Y d\tau = \int\sum a_i\phi_i\ \hat{O}p.\ \sum b_j\phi_j\ d\tau$). The Z terms are easily calculated from matrix elements given in reference [53].

Equation (2-59) may be used to determine the dipole moment derivatives from measured line strengths for several transitions. This is accomplished by a least-squares fit of the measured strengths to Equation (2-59). Note that not only the magnitude of the derivatives but their relative

signs are important. The results of this type of analysis for 27 lines will be presented at the end of Chapter 5. Once the dipole moment derivatives are determined the entire spectrum may be calculated from the eigenvalues and eigenvectors of the Hamiltonian.

2.7 Coriolis Perturbations

Perturbations between close lying energy levels are common phenomena in molecular spectroscopy. These perturbations may be caused by either Fermi or Coriolis interactions. Fermi resonance is due to mixing of states by terms in the potential energy while Coriolis interaction is due to mixing of states caused by terms in the kinetic energy. Coriolis interactions can occur between vibrational levels of different species while for Fermi resonance only states of the same vibrational and rotational species may interact. Since the effects of Fermi resonance were not observed in the 10 μm bands of H_2CO, it will not be described any further in this section.

When a polyatomic molecule rotates and vibrates simultaneously, two apparent forces can be observed. One is the centrifugal force; the second is the Coriolis force. The magnitude of these forces is given by

$$F_{centrifugal} = mr\omega^2 \qquad (2\text{-}56)$$

$$F_{Coriolis} = 2mv_a\omega\sin\varphi \qquad (2\text{-}57)$$

where m is the mass of the particle, v_a its apparent velocity with respect to the moving coordinate system, r its distance from the axis of rotation, ω the angular velocity of the coordinate system with respect to a fixed coordinate system, and φ the angle between the axis of rotation and the direction of v_a. The Coriolis force, unlike the centrifugal force, occurs only for a particle moving with respect to the rotating axis ($v_a \neq 0$) and is directed at right angles to both the direction of motion and the axis of rotation. The coupling which has been observed between rotation and vibration has been related to this Coriolis force. Coriolis interaction can be classified as either a rotational or vibrational perturbation [58]. It is a rotational perturbation when the interaction between two vibrational levels of different species results in a specific change in the rotational constant B. In a vibrational perturbation one finds either a change in the rotational constant accompanied by a shift in the vibrational level or a systematic change in the rotational constant alone. A shift of only the vibrational level is always due to Fermi resonance [50]. With ν_3 at 1500.17 cm^{-1}, ν_4 at 1167.26 cm^{-1}, and ν_6 at 1249.09 cm^{-1}, H_2CO is the classic example of rotational perturbations [45,50-52]. These are induced by the proximity of

the bands. The P-branch of ν_6 overlaps the R-branch of ν_4, and its R-branch overlaps the P-branch of ν_3. The band overlaps cause two strong Coriolis interactions observed previously. These are between the $K_a'=2$ level in ν_6 and the $K_a'=4$ level in ν_4, and between the $K_a'=6$ level of ν_6 and the $K_a'=3$ level in ν_3. The rovibrational model for H_2CO must include the relevent Coriolis terms to account for these perturbations. The following quantum mechanical description of Coriolis interaction is based on derivations by Nielsen [45], Allen and Cross [46], Mills et al. [53,54] and Nakagawa et al. [13,52].

Coriolis interaction is caused by the coupling of the total angular momentum components P_α and the vibrational angular momentum p_α. The main term of interaction for each band is included in its first order Hamiltonian as

$$H_{21(Cor.)} = -\sum_\alpha 2B_\alpha^e p_\alpha P_\alpha \qquad (2\text{-}58)$$

$$= -2\sum_\alpha B_\alpha^e P_\alpha \sum_{ss'} \zeta_{ss'}^\alpha (\omega_{s'}/\omega_s)^{1/2} q_s p_{s'}, \qquad (2\text{-}59)$$

where B_α^e stands for the equilibrium rotational constant around the α axis and $\zeta_{ss'}^\alpha$ for the Coriolis coupling constants derived from the vibration-rotation interaction constants α_s^α. The normal coordinate q_s, the conjugate momenta p_s and the angular momentum operators P_α are all dimensionless. According to Jahn's rule [31], if the product of the symmetry species of two vibrational modes contain the species of rotation, $\Gamma(q_{s'}) \otimes \Gamma(q_s) \in \Gamma(J_\alpha)$,

Coriolis interaction may take place between the modes ω_s and $\omega_{s'}$, or between the states $(v_s, v_{s'})$ and $(v_s+1, v_{s'}-1)$.

The first order Hamiltonian component H_{21} is usually isolated by a perturbation method [45], and contains the $\zeta_{ss'}$ terms which represent the extent of interaction between the states in question. The transformed Hamiltonian may now be written as the sum of two terms

$$H_{21(s,s')} = \tilde{H}_{21} + H_{21}^{*} \tag{2-60}$$

in which $\tilde{H}_{21}$ is the resonance term with nonvanishing matrix elements only between the resonating states, and H_{21}^{*} is a term with no such matrix elements. The contact transformation with a proper S_{21}^{*} function [56] eliminates H_{21}^{*} from the first order Hamiltonian and transforms H_{21} into

$$\tilde{H}_{21} = -[(\omega_s+\omega_{s'})/(\omega_s\omega_{s'})^{1/2}] \times (q_s p_{s'} - q_{s'} p_s) \sum_{\alpha} B_\alpha \zeta_{ss',p_\alpha}^{\alpha} \tag{2-61}$$

The transformation yields a somewhat modified vibration-rotation ineteraction constant, α_s^{α}. The unperturbed α_s^{α} may be obtained [56] by replacing $\zeta_{ss'}^{\alpha}$, by

$$-(\zeta_{ss'}^{\alpha})^2 (B_\alpha/\omega_s)(\omega_s-\omega_{s'})^2[\omega_s(\omega_s+\omega_{s'})]^{-1} \tag{2-62}$$

The term $\tilde{H}_{21}$ can then be evaluated by solving a secular equation obtained from a matrix with off-diagonal elements

$$\langle v_s, v_{s'} | \tilde{H}_{21} | v_s+1, v_{s'}-1 \rangle = i\, \xi_{vv',p_\alpha} \tag{2-63}$$

where

$$\xi_{vv'} = 2B_\alpha \zeta^\alpha_{ss'}[(\omega_{s'}/\omega_s)^{1/2} + (\omega_s/\omega_{s'})^{1/2}] \times [(v_s+1)v_{s'}/4]^{1/2} \quad (2\text{-}64)$$

In cases of strong Coriolis resonance as for ν_4 with ν_6 of H_2CO, a second order correction constant, η, may be extracted from the term $\tilde{H}_{22}$. Using a derivation similar to that of $\xi_{vv'}$, $\eta_{vv'}$ may be obtained from the $\tilde{H}_{22}$ term by solving a secular matrix with off-diagonal elements

$$\langle v_s, v_{s'} | \tilde{H}_{22} | v_s+1, v_{s'}-1 \rangle = \eta_{vv'}(P_\alpha P_\beta + P_\beta P_\alpha) \quad (2\text{-}65)$$

The type of Coriolis interactions in H_2CO are governed as usual by symmetry. Formaldehyde belongs to the C_{2v} point group (Table 2-6). For the I^r representation the axes are labeled as z=a, x=b, and y=c. Therefore, since ν_4 belongs to the B_1 representation, ν_6 to the B_2 representation, and ν_3 to the A_1 representation one obtains

a type Coriolis interaction for ν_4/ν_6 since

$$B_1 \otimes B_2 = 1 \quad 1 \quad -1 \quad -1 = A_2 \ (P_a)$$

b type Coriolis interaction for ν_3/ν_4 since

$$A_2 \otimes B_1 = 1 \quad -1 \quad -1 \quad 1 = B_2 \ (P_b)$$

and c type Coriolis interaction for ν_6/ν_3 since

$$B_2 \otimes A_2 = 1 \quad -1 \quad 1 \quad -1 = B_1 \ (P_c)$$

Symmetry also restricts the interaction between the rotational species in each set of bands to be as shown below.

Band	Symmetry Type	Angular Momentum comp.	C_{2v} Point group			
			E	$C_2(a)$	$\sigma_v(ba)$	$\sigma_v'(ca)$
ν_3	A_1	A	1	1	1	1
ν_4	B_1	P_b	1	-1	-1	1
ν_6	B_2	P_c	1	-1	1	-1
	A_2	P_a	1	1	-1	-1

Table 2-6: The C_{2v} Point Group Table in The I^r Representation.

ν_6/ν_4, a type Coriolis	ν_3/ν_4, b type Coriolis	ν_3/ν_6, c type Coriolis
$E^+ \; P_a \; E^-$	$E^+ \; P_b \; O^+$	$E^+ \; P_c \; O^-$
$E^- \; P_a \; E^+$	$E^- \; P_b \; O^-$	$E^- \; P_c \; O^+$
$O^+ \; P_a \; O^-$	$O^+ \; P_b \; E^+$	$O^+ \; P_c \; E^-$
$O^- \; P_a \; O^+$	$O^- \; P_b \; E^-$	$O^- \; P_c \; E^+$

The matrix elements for rotation in the symmetric top basis are

$$\langle J,K|P_a|J,K\rangle = \hbar K \tag{2-66}$$

$$\langle J,K|P_b|J,K\pm1\rangle = 1/2(\hbar)[J(J+1)-K(K\pm1)]^{1/2} \tag{2-67}$$

$$\langle J,K|P_c|J,K\pm1\rangle = \pm i/2(\hbar)[J(J+1)-K(K\pm1)]^{1/2} \tag{2-68}$$

and the second order in the same basis may be stated as

$$\langle J,K|(P_bP_c+P_cP_b)|J,K\pm2\rangle = \pm\hbar^2/2[J(+1)-K(K\pm1)]^{1/2} \times[J(J+1)-K(K\pm1)(K\pm2)]^{1/2} \tag{2-69}$$

The Coriolis interaction is one of vibration-rotation. Hence vibrational angular momentum must be taken into consideration. It has been shown [13] that by doing so one obtains

$$\begin{aligned}
\langle v,J,K|\hat{H}|v',J,K\rangle &= i\xi^a_{vv'}K \\
\langle v,J,K|\hat{H}|v',J,K\pm1\rangle &= i/2\xi^b_{vv'}[J(J+1)-K(K\pm1)]^{1/2} \\
\langle v,J,K|\hat{H}|v',J,K\pm1\rangle &= \mp1/2\xi^c_{vv'}[J(J+1)-K(K\pm1)]^{1/2}
\end{aligned} \tag{2-70}$$

$$\langle v,J,K|\hat{H}|v',J,K\pm2\rangle = \mp i/2\eta^{bc}_{vv'}[J(J+1)-K(K\pm1)]^{1/2} \times[J(J+1)-(K\pm1)(K\pm2)]^{1/2} \tag{2-71}$$

The matrix elements shown above are imaginary, but they can be made real by the proper choice of phase factors. The phase factors may be chosen corresponding to symmetry species of the vibrational states [13,45]; for example, 1 for A_1, -i for A_2, i for B_1, and -1 for B_2. Introducing these factors into the vibrational-rotational products and labeling the interacting modes observed in H_2CO yields the final matrix elements used by Johns [14] in an earlier analysis of the Coriolis interactions in formaldehyde.

$$\langle v_4,J,K|\hat{H}|v_6,J,K\rangle = \xi^a_{64}K \qquad (2\text{-}72)$$

$$\langle v_4,J,K|\hat{H}|v_6,J,K\pm2\rangle = \eta^{bc}_{64}[J(J+1)-K(K\pm1)]^{1/2} \times[J(J+1)-(K\pm1)(K\pm2)]^{1/2} \qquad (2\text{-}73)$$

$$\langle v_4,J,K|\hat{H}|v_3,J,K\pm1\rangle = -1/2\xi^b_{34}[J(J+1)-K(K\pm1)]^{1/2} \qquad (2\text{-}73)$$

$$\langle v_6,J,K|\hat{H}|v_3,J,K\pm1\rangle = \mp1/2\xi^c_{36}[J(J+1)-K(K\pm1)]^{1/2} \qquad (2\text{-}74)$$

The first and second order Coriolis interaction constants, ξ and η, are obtained from the least squares fit to the observed transitions.

The quintic third order Hamiltonian term, $\tilde{H}_{23}$, can be used to characterize the accidental Coriolis interaction between $K'_a=3$ of ν_3 and $K'_a=6$ of ν_6. For asymmetric tops $\tilde{H}_{23}$ is purely off-diagonal in v_s, and is calculated from a series of other Hamiltonian terms including H_{21} and H_{22} discussed above. Hence, $\tilde{H}_{23}$ is a mixed Coriolis Hamiltonian term which allows for $\Delta K=\pm3$ interactions needed to treat

this particular local resonance. The expression for $\tilde{H}_{23}$ is given by Aliev and Watson [57] as

$$\tilde{H}_{23} = \sum_{\alpha\beta\gamma} \sum_{s,s'} Y_{ss'} q_s p_{s'} P_\alpha P_\beta P_\gamma \qquad (2\text{-}75)$$

where Y is the third order Coriolis coupling constant. The derivation of $\tilde{H}_{23}$ and its contact transformation, as well as the evaluation of Y are described in detail in the literature [31,56,57].

The molecular symmetry and the particular Coriolis interaction govern the choice of axis assignment in equation (2-75) i.e. α, β, and γ for $p_\alpha P_\alpha P_\beta P_\gamma$. As in the case for the first order Coriolis between ν_3 and ν_6 the vibrational angular momentum p becomes p_c (along the c axis). To get $\Delta K=\pm 3$ coupling one must have the condition that the axes $\beta,\gamma \neq a$ since P_a is diagonal in K (Equation (2-72)). The possible products are:

$$P_c P_c P_c^2,\ P_c P_c P_b^2,\ P_c P_c P_b P_c,\ P_c P_c P_c P_b, \ldots \text{ etc.}$$

Since the entire term should be symmetric and so terms such as $P_c P_c P_b P_c$ must drop out yielding only $P_c P_c P_c^2 = P_c P_c^3$ and $P_c P_c P_b^2$. Both these products give the same J and K dependence. For pure rotational transitions using P_c^3 one obtains

$$\langle J,K|P_c^3|J,K\pm 3\rangle = \langle J,K|P_c|J,K\pm 1\rangle\langle J,K\pm 1|P_c|J,K\pm 2\rangle \times \langle J,K\pm 2|P_c|J,K\pm 3\rangle$$

$$= -i\hbar/8\ [J(J+1)-K(K\pm1)]^{1/2}$$
$$\times\ [J(J+1)-(K\pm1)(K\pm2)]^{1/2}$$
$$\times\ [J(J+1)-(K\pm2)(K\pm3)]^{1/2} \qquad (2\text{-}76)$$

Introducing Y, p_c, and q, from Equation (2-75), i.e. the interacting vibrational modes, the final off-diagonal term of the Hamiltonian takes the form

$$\langle v_6,J,K|\hat{H}|v_3,J,K\pm3\rangle = z_{36}\ [J(J+1)-K(K\pm1)]^{1/2}$$
$$\times\ [J(J+1)-(K\pm1)(K\pm2)]^{1/2}$$
$$\times\ [J(J+1)-(K\pm2)(K\pm3)]^{1/2}$$
$$= z_{36}\,\hbar(J,K) \qquad (2\text{-}77)$$

where z_{36} is a third order Coriolis coupling constant for the interaction between ν_3 and ν_6 and may be obtained from the least squares fit of the observed transitions.

CHAPTER 3

INSTRUMENTATION AND DATA ACQUISITION

3.1 Introduction

The qualitative and quantitative analysis of H_2CO has been carried out using two very high resolution techniques: Fourier transform infrared (FT-IR), and Doppler limited, tunable diode laser (TDL) spectroscopies. The FT-IR has been used for wide range survey spectroscopy, while the diode laser spectrometer has been used for the determination of individual line strengths, pressure broadened widths, and analytical trace analysis.

This chapter begins with a brief description of the FT-IR spectra. The laser spectrometer as well as the procedures used to obtain a spectrum are described in the next section. Several examples of TDL spectra are then shown and discussed to illustrate the capabilities of this technique and to show typical characteristics of the spectrum of H_2CO.

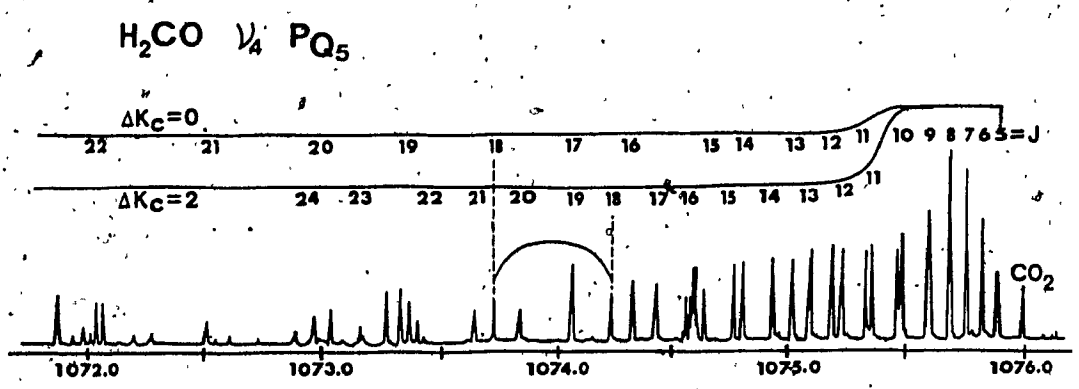
3.1 FT-IR Survey Spectra

High resolution FT-IR spectra of H_2CO from 890 to 1580 cm^{-1} have been recorded with a Bomem interferometer at the Herzberg Institute of Astrophysics in Ottawa. This

instrument has an unapodized resolution of ~0.0024 cm^{-1}. The spectrum reported was apodized with a Happ-Genzel function yielding an observed width of ~0.004 cm^{-1}. The spectrum contained nearly 4000 transitions arising from the ν_3, ν_4, and ν_6 bands. A peak finder program running on the PDP-11 computer of the Bomem interferometer provided a measured wavenumber listing for these transitions. A trace of CO_2 gas introduced into the sample cell provided for absolute calibration [59]. A typical FT-IR spectrum of H_2CO is shown in Figure 3-1.

3.3 TDL Experimental Apparatus

The Pb-salt tunable semiconductor diode lasers (TDL's) used in this work were fabricated by Spectra Physics/Laser Analytics division. Lasing in these semiconductors results from stimulated emission across the energy gap between the conduction and valence bands. A population inversion is achieved by applying a forward-bias current to the diode and thereby injecting charge carriers across the p-n junction. The recombination of these charge carriers facilitate the gain mechanism for laser action. The end faces of the laser crystals made by cleaving along natural crystal planes form the laser resonator. The TDL crystals are typically 400 μm long with a cross-section of 200 X 200 μm. The lasing frequencies of TDLs is governed by the specific composition of the crystal. $Pb_{1-x}Sn_xSe$ lasers can be made to operate



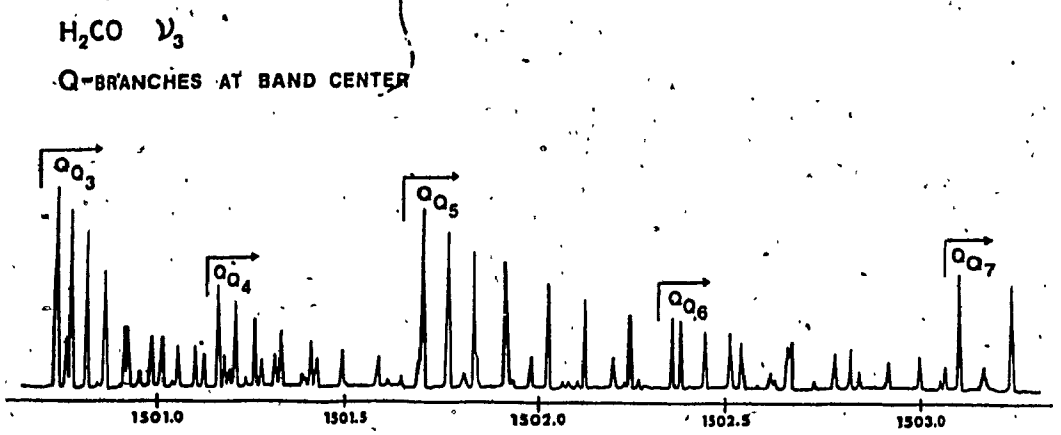


Figure 3-1: Two Typical Examples of FT-IR Spectra.

from about 300 to 1200 cm^{-1} and $PbS_{1-x}Se_x$ from 1200 to 2500 cm^{-1} by selective variation of x during fabrication. Both types of TDL's were used in this experimental work.

The output of any one TDL can be tuned across a range of 20-200 cm^{-1} by varying the crystal temperature from 10K to 100K, which in turn changes the band gap energy in the semiconductor and to some extent its index of refraction. Most diode lasers oscillate in several modes simultaneously, separated in wavelength by the cavity mode spacing of several wavenumbers. In most cases, however, single modes may be isolated by a grating monochromator. Several reviews of Pb-salt TDL's detailing their fabrication and operation have been published [23,60].

Line parameter measurements for H_2CO were made using a modified Laser analytics Model LS-3 spectrometer and the following procedure. One of the four tunable diode lasers mounted in a closed-cycle cryogenic refrigerator is temperature tuned to the desired wavelength within the tuning range of the laser emission. At this set wavelength, fine tuning of up to 1 cm^{-1} is accomplished with small temperature variations (I^2R heating) induced by the laser current control module (LCM). The laser current is sawtooth modulated at ~50 Hz and is synchronized to both a sectored blade chopper and a signal averager in a manner similar to that described by Jennings [15]. The output from the grating spectrometer is detected with a liquid nitrogen cooled

HgCdTe (or InSb) detector and is amplified by an EG&G Model 113 pre-amplifier. The signal is then sent to an EG&G Model 4203 signal averager and transmitted either to an X-Y recorder or via an RS-232 interface to an IBM PC computer. The relative calibration of the wavenumber scale was provided by a 3" solid germanium etalon with a fringe spacing in the region studied of ~0.016 cm^{-1}. The precise transition wavenumbers of H_2CO and etalon fringe spacings were obtained by reference to well known N_2O lines [63].

A Laser Analytics Model LO-3 multiple traversal absorption cell was used as the sample cell. This cell has White's optical configuration [61,62], and is adjustable for optimal pathlengths of 4.17 to 100.17 meters. Formaldehyde vapour was generated by heating analytical grade paraformaldehyde and introduced into the White cell through a liquid nitrogen trap. In order to prevent both sample polymerization and insure absorption lines having Doppler widths, the pressure of all H_2CO samples was maintained at <0.1 Torr. The optical path of the White cell was adjusted so as to allow 15-20% transmission for all transitions being measured. Pressure measurements were made with a Datamatrics Model 572A capacitance manometer which was frequently calibrated with reference to a Kontes McLeod gauge (0.001-1.000 mm Hg). A block diagram of the spectrometer and support equipment is shown in Figure 3-2.

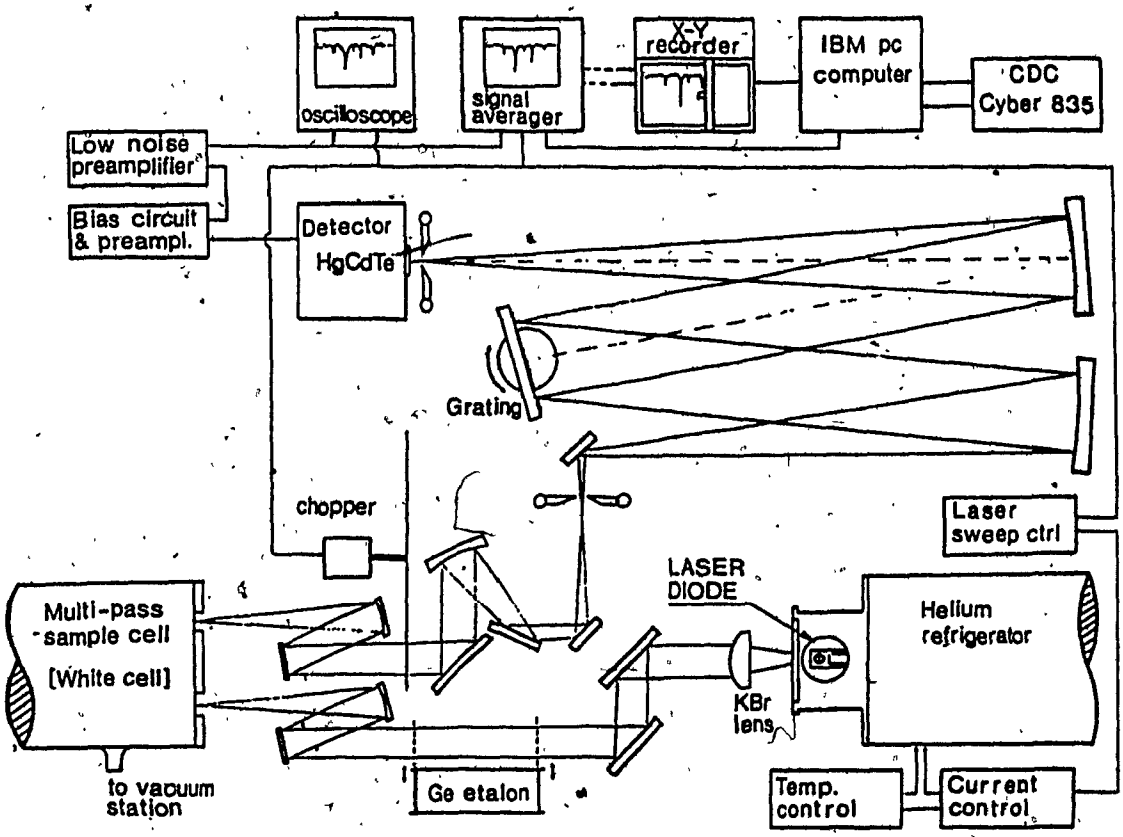


Figure 3-2: Schematic Diagram of the TDL Spectrometer.

3.4 Data Acquisition

Experimental data were obtained from six sets of spectra, taken in duplicate on three different occasions. This allowed analysis of variance within and between runs. A typical spectrum is shown in Figure 3-3. Maximum energy (I_o) was recorded through the evacuated White cell at the beginning and end of each set of spectra and compared with the I_o obtained for the individual traces. Pressure broadening effects were evaluated using an average of only the initial and final I_o values since the 100% transmission (background) at elevated pressures became indeterminable. A saturation absorption scan was made in order to verify whether the shutter zero was equivalent to the 100% absorption level. It has been found that the two agreed well, and so the shutter zero was used as the I=0 level. The full width at half height (FWHM) at $(1/2)\ln(I_o/I)$ (i.e. FWHM at $I' = \sqrt{I_o I}$) was measured by direct comparison with the Ge etalon transmission peaks (fringes) nearest each spectral feature. Etalon fringes were generally used for both the conversion of the tuning current axis (X-axis) to wavenumbers and the linearization of this axis. The need for linearization arises from the fact that the lasers do not tune linearly with current. The spacings between the fringes were calibrated using well known N_2O lines taken from Guelachvili [63]. The separation of the interference fringes of the Ge etalon vary as a function of both wave

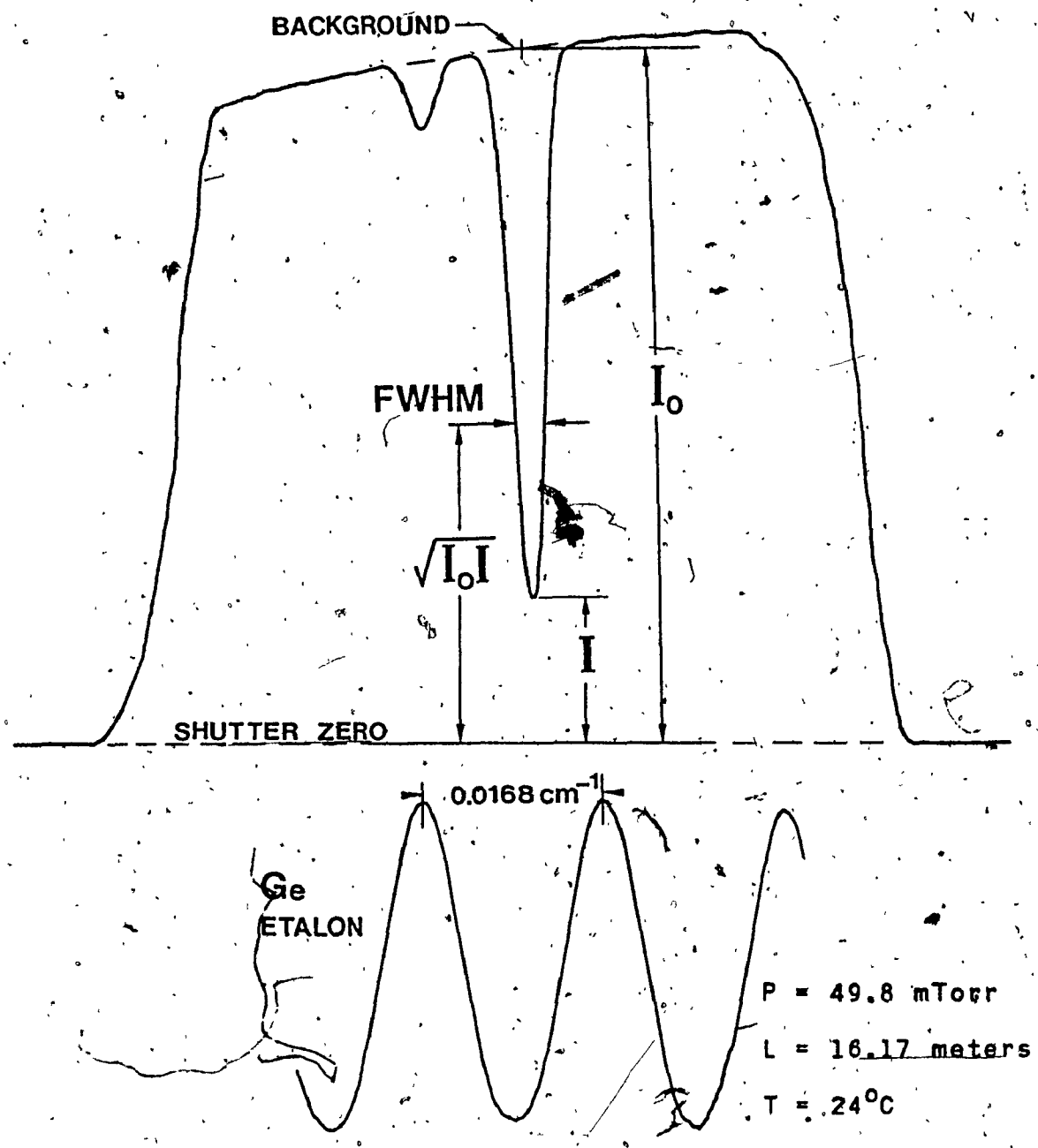


Figure 3-3: Measureable Parameters From TDL Spectra.

Absorption spectrum of the $18_{2,17} \leftarrow 18_{1,17}$ transition in the ν_4 band of H_2CO at 1172.38603 cm^{-1}. Interference fringes from Ge 7.62 cm etalon are used to provide relative calibration of the wavelength scale.

length and temperature and therefore needed frequent calibration. The above procedure for data collection was repeated at several different pressures: 0 to 70 mTorr H_2CO for line intensity studies; and 0 to 25 Torr for foreign gas broadening measurements. Each series of data points collected formed the basis for a Beer's law plot and statistical evaluation of the results.

The identification of individual transition lines prior to analysis was obtained by comparing survey (~0.5 cm^{-1}) TDL scans with the FT-IR data. Single isolated lines were identified using N_2O lines and etalon fringes. Typical TDL survey spectra are shown in Figures 3-4 and 3-5.

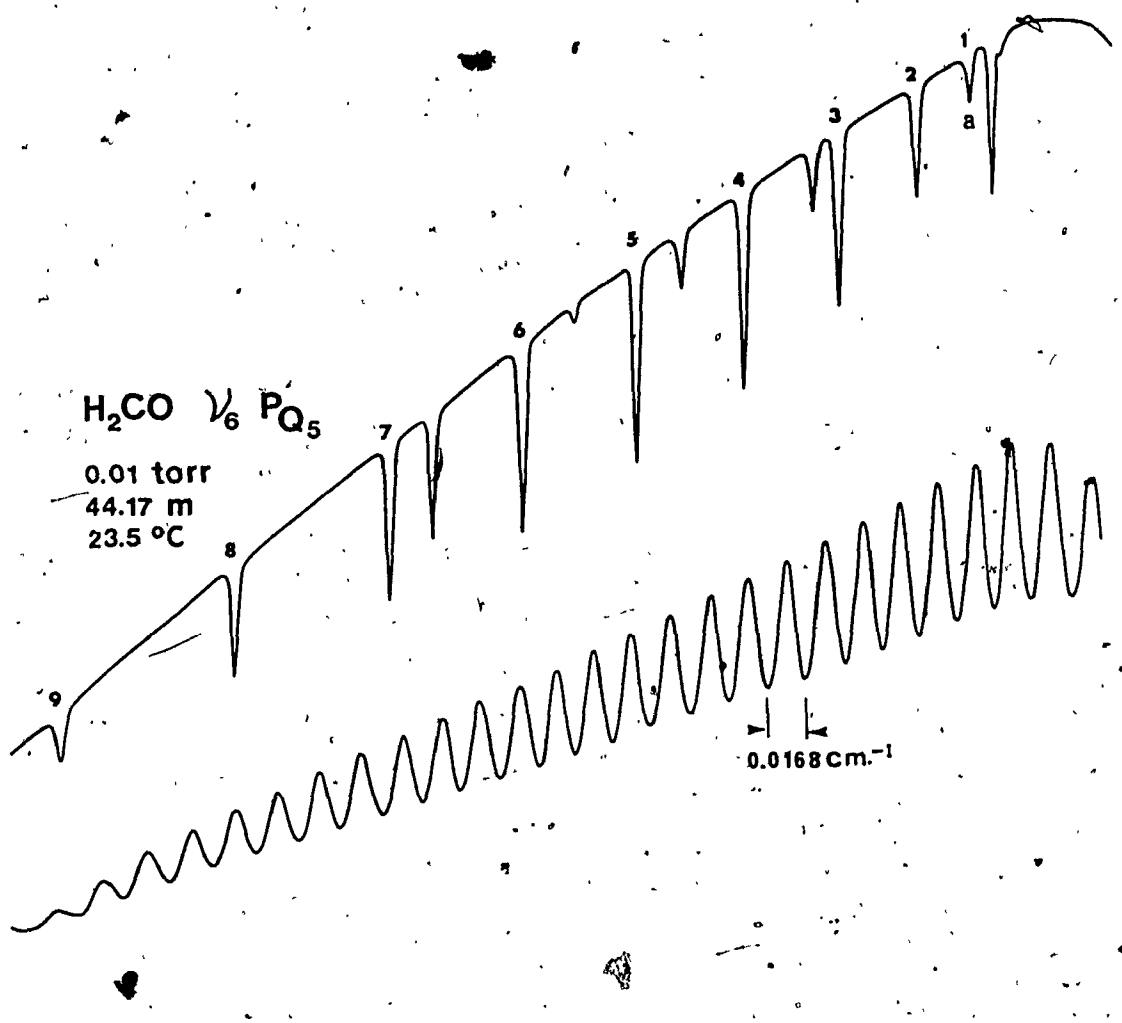


Figure 3-4: Survey Spectra of a Selected Region in the ν_6 band of H_2CO Recorded with a TDL.

a. The numbers 1-9 are used only as identifiers of the $^PQ_5$ series, i.e. 1 represents the transitions $5_{4,1}^{\circ} \leftarrow 5_{5,0}$ and $5_{4,2} \leftarrow 5_{5,1}$ at 1192.84237 cm^{-1}

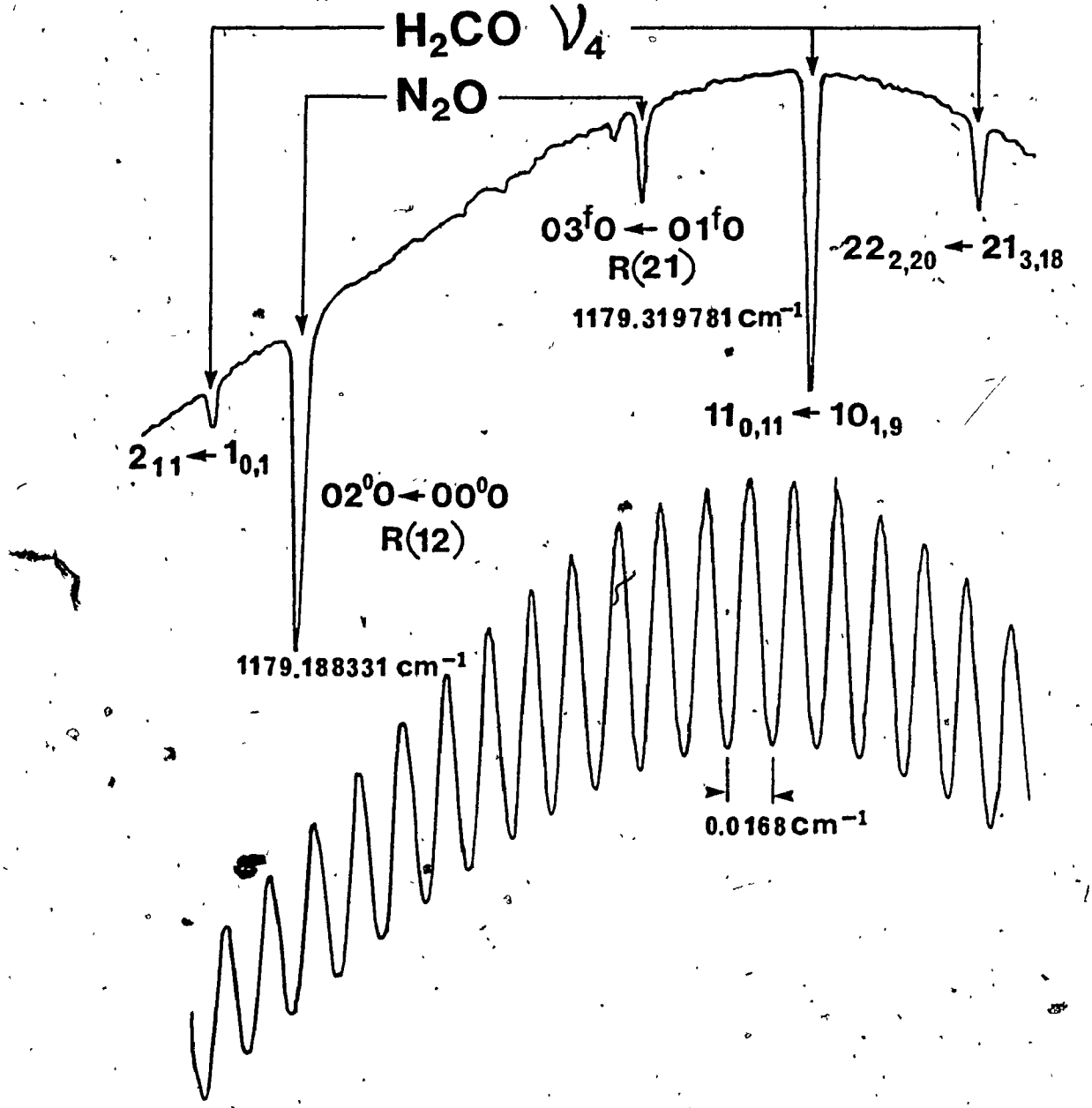


Figure 3-5: TDL Survey Spectra: Identification of Transitions in υ_4 of H_2CO Using Ge Etalon Fringes for Relative Calibration and N_2O for Absolute Calibration.

CHAPTER 4

EXPERIMENTAL RESULTS - H_2CO LINE ASSIGNMENTS, AND DETERMINATION OF LINE STRENGTHS AND BROADENING COEFFICIENTS

4.1 Introduction

In this chapter, a description of the method used for the assignment of the H_2CO transitions will be presented. These quantum number assignments were used in the simultaneous analysis of the ν_3, ν_4 and ν_6 vibration-rotation bands discussed in Chapter 5. The techniques used for evaluation of line strengths and foreign-gas pressure broadening parameters, and the final results will also be presented.

4.2 Frequency Assignments

The observed transitions obtained from the FT-IR spectrum were assigned using the ground-state-combination-difference (GSCD) technique. This method determines the upper state energy levels by combination of observed infrared transition wavenumbers and the appropriate calculated ground state energy values obtained from microwave spectra. Governed by the selection rules, an upper energy state may be reached by several different paths. Hence, the known

parts of a combination may be used to predict the frequencies of the unknown parts. An example of this powerful technique is shown in Figure 4-1 where, using the selection rules for ν_4, a transition diagram was constructed for $K''_a=1$. The six energy levels for the lower states were calculated from molecular constants derived from recent microwave data [64]. The two $^RQ_1$ infrared transition energies were selected using an educated guess. Using these values, the energies X_1, X_2, X_3, and X_4 were computed. These agreed within several milliwavenumbers with the existing FT-IR data, indicating that the transition model and the original guess for $^RQ_1$ were correct. Hence, the transitions shown in Figure 4-1 were assigned to these six IR wavenumbers

The ground state energy levels were generated from the ground state rotational constants reported by Cornet and Winnewisser [64], using a computer program written by Maki [65]. The energy levels generated consisted of all values up to $J''=30$ and $K''_a=10$.

Over 1000 assigned IR transitions given by Allegrini et al. [14], for $J<15$ in ν_3, ν_4, and ν_6 of H_2CO, took much of the guess work out of the initial utilization of the ground state combination difference. Using the GSCD technique, 3400 transitions were assigned of which over 3000 were used in the determination of the rotational constants for the three H_2CO bands. The observed wavevenumbers and their respective assignments are listed in Appendix A.

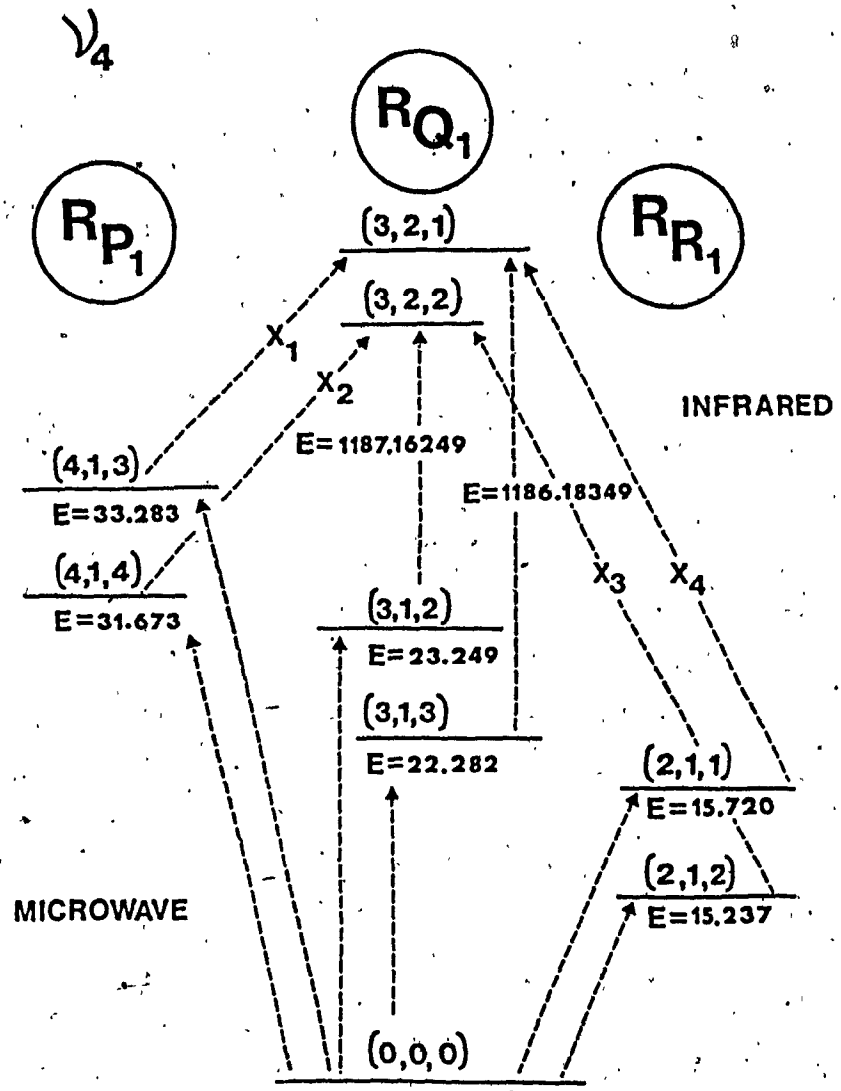


Figure 4-1: A Schematic Diagram of the Ground-State-Combination-Difference Technique.

4.3 Line Strength Determinations

The measurement of line strength is simplified considerably when performed with a laser spectrometer, since the instrument function defined by the laser profile is usually much narrower in bandwidth than typical observed linewidths. Hence, rather than using the somewhat cumbersome equivalent width technique [66-68], the strength of a line can be determined by the direct method from the line center absorption [15,69]. A brief decription of the direct method follows.

The intensity $I(\nu)$, of a single absorption line is given by Beer's law as

$$I(\nu) = I_o(\nu)\ \mathrm{Exp}[-k(\nu)\ X] \qquad (4\text{-}1)$$

where I_o is the intensity if there is no absorption, $k(\nu)$ is the absorption coeficient, and X is the optical density i.e. the pressure-pathlength product (PL). For a Doppler line shape the absorption coeficient has the form

$$k(\nu) = (S/\gamma_D)(\ln 2/\pi)^{1/2}\mathrm{EXP}[-\ln 2((\nu-\nu_o)/\gamma_D)^2] \qquad (4\text{-}2)$$

where γ_D is the Doppler half width and is equal to HWHM of the $k(\nu)$ profile, ν_o is the frequency at line center, and S is the line strength. The Doppler half width is given by

$$\gamma_D = \nu_o[(2kT\ln 2)/(mc^2)] \qquad (4\text{-}3)$$

where k is the Boltzmann constant, T is the temperature, m

is the molecular mass, and c is the speed of light. From the line center transmission, $\tau_o = I(\nu_o)/I_o(\nu_o)$ one can solve for the line strength S as

$$S = - (\gamma_D \ln \tau_o)/[PL(\ln 2/\pi)^{1/2}] \quad (4\text{-}4)$$

In terms of line center wavenumbers one finds [15]

$$S = - (2\pi kT/mc^2)^{1/2} (\nu_o/PL) \ln \tau_o \quad (4\text{-}5)$$

$$= - (0.5794)(\nu_o/PL)(T/M)^{1/2} \ln \tau_o \quad (4\text{-}6)$$

where ν_o is in cm^{-1}, P is the pressure in milliTorr, L is the absorption pathlength in cm, and M is the molar mass in grams.

The line strength for the 28 transitions measured were determined using Equation (4-6). Each transition was evaluated at several pressures (minimum 5) yielding a Beer's Law plot of $\ln(1/\tau_o)$ versus optical density (PL). Since the pathlength used was fixed, corrections to the pressure reading could be calculated from the X-intercept of the plot. The pressure correction to the capacitance manometer (-6 to -15 millitorr) obtained from the plots were in good agreement with spot calibrations using a McLeod Gauge. All pressure readings were corrected prior to use in the line intensity calculations. A typical Beer's Law plot is shown in Figure 4-2 for the for the transition $18_{2,17} \leftarrow 18_{1,17}$ of ν_4.

The resulting line strengths are listed in Table 4-1.

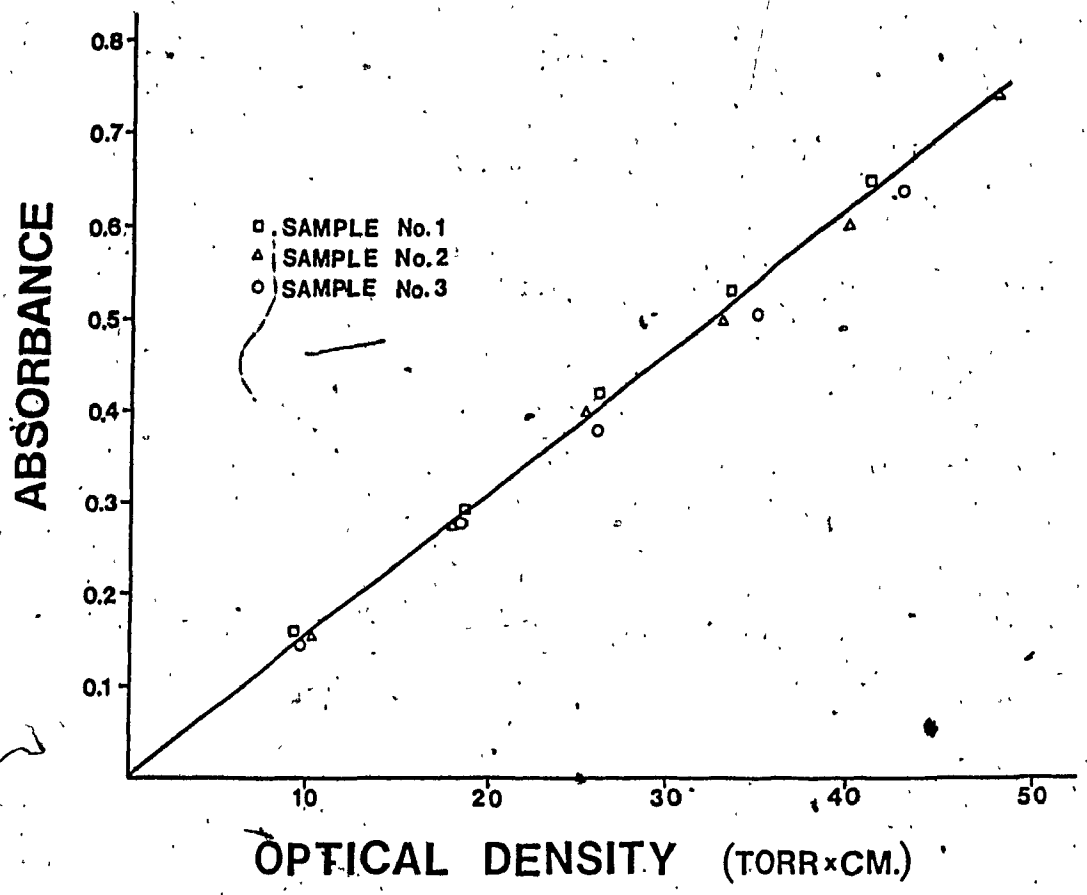


Figure 4-2: Beer's Law Plot of Absorbance vs. Optical Density for the $^{18}_{2,17} \leftarrow {}^{18}_{1,17}$ Transition at 1172.38603 cm^{-1} in the ν_4 band of H_2CO.

Table 4-1: Observed Line Strengths in the ν_4 and ν_6 Bands of H_2CO at 24±1°C.

FREQUENCY cm^{-1}	BAND	TRANSITION UPPER (J',K'_a,K'_c)	TRANSITION LOWER (J'',K''_a,K''_c)	AVERAGE INTENSITY $cm^{-2}atm^{-1}$
1148.33511	ν_6	(17, 4,14)	(18, 5,13)	$(3.225\pm0.126)\times10^{-3}$
1148.34523	ν_4	(11, 2, 9)	(10, 3, 7)	$(2.113\pm0.050)\times10^{-2}$
1148.36004	ν_6	(17, 4,13)	(18, 5,14)	$(3.395\pm0.151)\times10^{-3}$
1148.47042	ν_4	(3, 0, 3)	(4, 1, 3)	$(4.737\pm0.195)\times10^{-2}$
1148.50854	ν_4	(16, 1,15)	(16, 2,15)	$(1.866\pm0.075)\times10^{-2}$
1159.13578	ν_4	(1, 0, 1)	(1, 1, 1)	$(2.953\pm0.170)\times10^{-2}$
1159.27164	ν_4	(2, 0, 2)	(2, 1, 2)	$(4.846\pm0.304)\times10^{-2}$
1159.29738	ν_4	(28, 2,27)	(28, 1,27)	$(5.936\pm0.405)\times10^{-3}$
1159.39157	ν_4	(15, 2,13)	(14, 3,11)	$(1.883\pm0.064)\times10^{-2}$
1159.41214	ν_6	(6, 6, 1) (6, 6, 0)	(7, 7, 0) (7, 7, 1)	$(1.488\pm0.056)\times10^{-2}$
1159.43953	ν_4	(9, 1, 9)	(8, 2, 7)	$(7.429\pm0.327)\times10^{-3}$
1159.47176	ν_4	(3, 0, 3)	(3, 1, 3)	$(6.663\pm0.463)\times10^{-2}$
1172.38603	ν_4	(18, 2,17)	(18, 1,17)	$(3.208\pm0.062)\times10^{-2}$
1172.52555	ν_4	(6, 1, 6)	(6, 0, 6)	$(2.843\pm0.148)\times10^{-2}$
1180.64464	ν_6	(12, 2,11)	(13, 3,10)	$(1.898\pm0.100)\times10^{-2}$
1180.73250	ν_6	(4, 4, 1) (4, 4, 0)	(5, 5, 0) (5, 5, 1)	$(3.841\pm0.235)\times10^{-2}$
1180.80804	ν_4	(24, 0,24)	(23, 1,22)	$(2.613\pm0.074)\times10^{-3}$
1180.83214	ν_4	(11, 2,10)	(11, 1,10)	$(3.400\pm0.208)\times10^{-2}$
1180.88324	ν_6	(13, 2,11)	(14, 3,12)	$(1.651\pm0.116)\times10^{-2}$

continued.....

Table 4-1 (cont'd)

FREQUENCY cm^{-1}	BAND	TRANSITION UPPER (J', K_a', K_c')	TRANSITION LOWER (J'', K_a'', K_c'')	AVERAGE INTENSITY $cm^{-2}atm^{-1}$
1192.60831	V_6	(10, 4, 7)	(10, 5, 6)	$(2.800\pm0.091)\times10^{-2}$
		(10, 4, 6)	(10, 5, 5)	
1192.62677	V_6	(3, 3, 1)	(4, 4, 0)	$(2.000\pm0.092)\times10^{-2}$
		(3, 3, 0)	(4, 4, 1)	
1192.66566	V_6	(9, 4, 6)	(9, 5, 5)	$(2.800\pm0.096)\times10^{-2}$
		(9, 4, 5)	(9, 5, 4)	
1192.71773	V_6	(8, 4, 5)	(8, 5, 4)	$(2.492\pm0.123)\times10^{-2}$
		(8, 4, 4)	(8, 5, 3)	
1192.73689	V_6	(18, 1,17)	(19, 2,18)	$(6.010\pm0.228)\times10^{-3}$
1192.76481	V_6	(7, 4, 4)	(7, 5, 3)	$(2.165\pm0.075)\times10^{-2}$
		(7, 4, 3)	(7, 5, 2)	
1192.79547	V_6	(10, 1,10)	(11, 2, 9)	$(5.890\pm0.173)\times10^{-3}$
1192.80640	V_6	(6, 4, 3)	(6, 5, 2)	$(1.648\pm0.060)\times10^{-2}$
		(6, 4, 2)	(6, 5, 1)	
1192.84237	V_6	(5, 4, 2)	(5, 5, 1)	$(9.772\pm0.202)\times10^{-3}$
		(5, 4, 1)	(5, 5, 0)	

The absorptivity coefficient obtained from the slope (least squares fit) of the Beer's law function for a given data set routinely yielded a relative standard deviation of less than 3% and a linear correlation of >0.998. However, when absorption coefficients for a given transition obtained in several experiments (days apart) were averaged, the error increased to between 3 and 8% of the mean value. This is clearly demonstrated in the scatter obtained from 3 different H_2CO samples shown in figure 4-2. The error in reproducibility may be attributed to vibrations caused by the helium refrigerator and possibly to shifts in lasing modes [15,70,71].

The overall reliability of the TDL system and technique used was initialy evaluated on transitions in the N_2O calibrating gas [72]. The results obtained for five transitions in the $2\nu_2$ band were in excellent agreement with literature values obtained by other techniques [73,74].

4.4 Pressure Broadenning by Foreign Gases

Foreign-gas collision broadening parameters were evaluated by recording the absorption lineshapes of a fixed amount of H_2CO at a number of different pressures of the broadening gas. Pressure induced widths were then determined from a plot of line width versus the partial pressure of the foreign-gas. The H_2CO pressure was again maintained sufficiently low (<100 milliTorr) to insure an initial

Doppler lineshape. The low sample pressure limited the amount of foreign gas used to < 30 Torr, since the absorption lines became weaker as they get wider. This effect is illustrated in Figure 4-3.

The lineshape of a pressure broadened line is governed by the perturbation of exterior systems upon the absorber molecule. A smearing of the energy levels results from these disturbances which produces a probability distribution of the energy level shifts. For a collision broadened line, the lineshape function takes the form

$$k(\nu) = (1/\pi)\{\gamma_L/[(\nu-\nu_o)^2+\gamma_L^2]\} \qquad (4-7)$$

where γ_L, the half width at half height, is the reciprocal of the relaxation time and is proportional to the pressure. This function is known as the Lorentz lineshape. The observed spectra of of a broadened line however, is generally a convolution of Doppler and Lorentzian functions called a Voigt profile. At elevated pressures the lineshape is governed by the Lorentzian function yielding a linear relationship between the HWHM and the applied pressure (Figure 4-4). However, since the pressure range used here was limited to <30 Torr, the contribution of the Doppler function is still significant. The Lorentzian widths were obtained from the empirical relationship [80]

$$\gamma_L = \gamma_V\{7.7254-6.7254[1+0.3195(\gamma_D/\gamma_V)^2]^{1/2}\} \qquad (4-8)$$

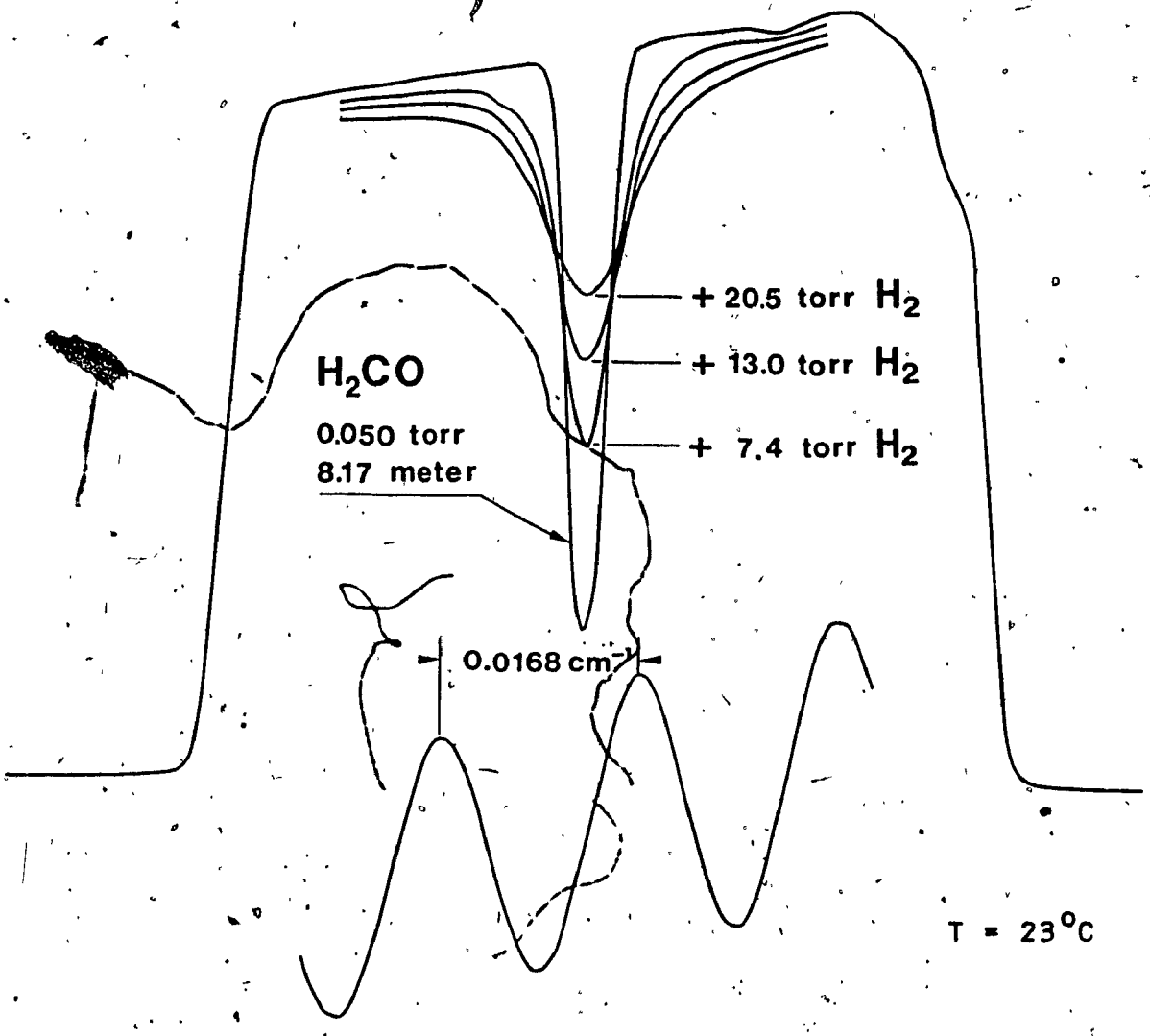


Figure 4-3: TDL Spectra for Hydrogen Pressure Broadening Experiments on the $3_{0,3} \leftarrow 3_{1,3}$ transition at 1159.47176 cm^{-1} of the ν_4 band of H_2CO.

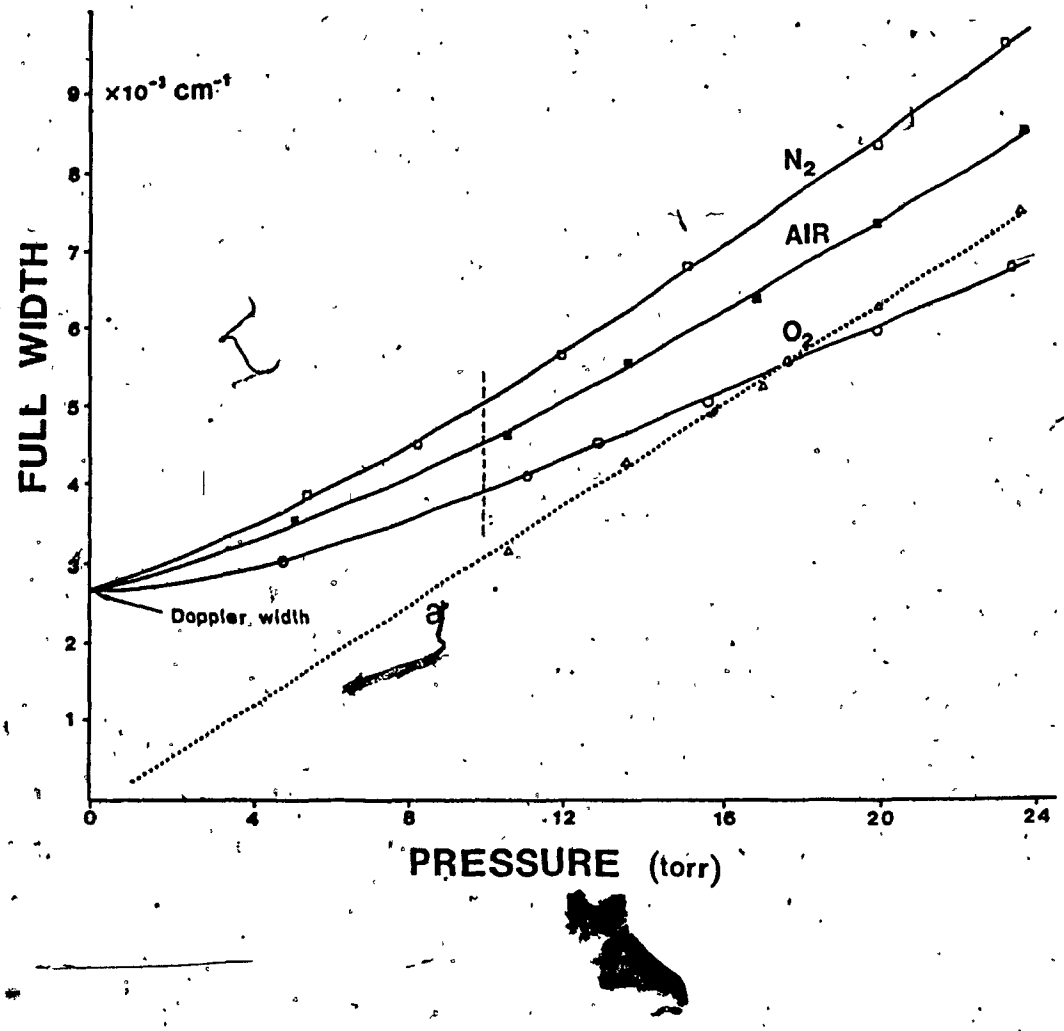


Figure 4-4: Plots of Foreign Gas Broadening Collision Widths (FWHM) of X-H_2CO (X=air, N_2 or O_2) as a Function of Pressure.

a. Dotted line represents the Lorentzian full-width as a function of pressure for air broadening derived from Voigt profile calculations.

where γ_V is the half-width of the observed Voigt profile. The Lorentzian results obtained here were then verified by use of a numerical convolution simulation similar to that described by Blass and Halsey [79]. Plotting the Lorentzian widths as a function of applied pressure yielded a linear relationship with an intercept close to zero (10^{-4} to 10^{-6} cm^{-1}). From the slopes of these plots all pressure broadening coefficients were evaluated. A typical plot (line marked a) is shown in Figure 4-4 for air broadening. It should be noted here that the kinetic theory of gases does not account for all observed phenomenon concerning halfwidth measurements. It is necessary to treat the problem at a higher level [75], where interactions such as the dependence of the halfwidth on J, the rotational quantum number are also considered [76].

The results for pressure broadening due to collision with air, H_2, O_2, and N_2 at room temperature (24 1°C) are listed in Table 4-2. The effect of air broadening may also be evaluated from the broadening contributions of O_2 and N_2 by the use of the relation

$$\gamma_{air} = P_{O_2} \gamma_{O_2} + P_{N_2} \gamma_{N_2} \qquad (4\text{-}9)$$

where the P_i are the partial atmospheric pressures of O_2 and N_2 (0.20946 and 0.78084 atm., respectively) and γ_i are the respective HWHM. Using this relationship yielded a computed air broadening coefficient of 0.128 cm^{-1}/atm. for the

transition $3_{0,3} \leftarrow 3_{1,3}$ of ν_4. This agrees quite well with the observed value of 0.126(10) cm^{-1}/atm.

The results obtained for air, O_2, and N_2 are in reasonable agreement with theoretical values obtained by Tejwani et al. [77]. The theoretical values listed in Table 4-2 represent average, intensity weighted broadening coefficients. The broadening coefficients for H_2 are also in reasonable agreement with the results of the experimental millimeter work reported by Nerfe [78].

Table 4-2: Foreign Gas Pressure Broadening Coefficients for H_2CO.[a]

WAVENUMBER (cm^{-1})	TRANSITION	BROADENING GAS			
		air	H_2	O_2	N_2
1159.47176	ν_4: $3_{0,3} \leftarrow 3_{1,3}$	0.126(10)	0.139(9)	0.090(8)	0.140(9)
1192.76481	ν_6: $7_{4,4} \leftarrow 7_{5,3}$ $7_{4,3} \leftarrow 7_{5,2}$	0.119(10)	0.158(18)		
1192.71773	ν_6: $8_{4,5} \leftarrow 8_{5,4}$ $8_{4,4} \leftarrow 8_{5,3}$	0.117(7)	0.166(18)		
1105.93457	ν_4: $14_{1,13} \leftarrow 15_{2,13}$	0.115(8)			
Millimeter broadening (avg.)			0.139[b]		
Theoretical Broadening (avg.)		0.107[c]		0.062[c]	0.120[c]

a. These values are half width at half height and for a temp. of 24±1°C.
b. From Nerfe [78]
c. From Tejwani et al. [77]

CHAPTER 5

ROTATIONAL ANALYSIS OF ν_3, ν_4 AND ν_6 BANDS OF FORMALDEHYDE

5.1 Introduction

In this Chapter, the least-squares analysis of the observed transitions of the ν_3, ν_4, and ν_6 bands of H_2CO will be presented. The aim of this analysis is to find a set of molecular constants that can most accurately reproduce the measured wavenumbers for a given Hamiltonian model. Generally, if sets of data for a molecule exist for both ultraviolet and microwave transitions or both infrared and microwave transitions, then the data sets can be combined to determine more accurate molecular constants for the common vibrational level(s); subsequent predictions and identifications of previously unassigned transitions are then aided. In this study the molecular constants were evaluated using a combination of vibrational (IR) and pure rotational (microwave) data.

The analysis technique involves an iterative process in which the RMS (root-mean-square) differences between the observed and calculated wavenumbers are minimized using the least-squares technique. The RMS minimization is obtained by iterative adjustment of the parameters of the Hamiltonian. A block diagram of the process is shown in Figure 5-1. To predict the transitions (calculated values)

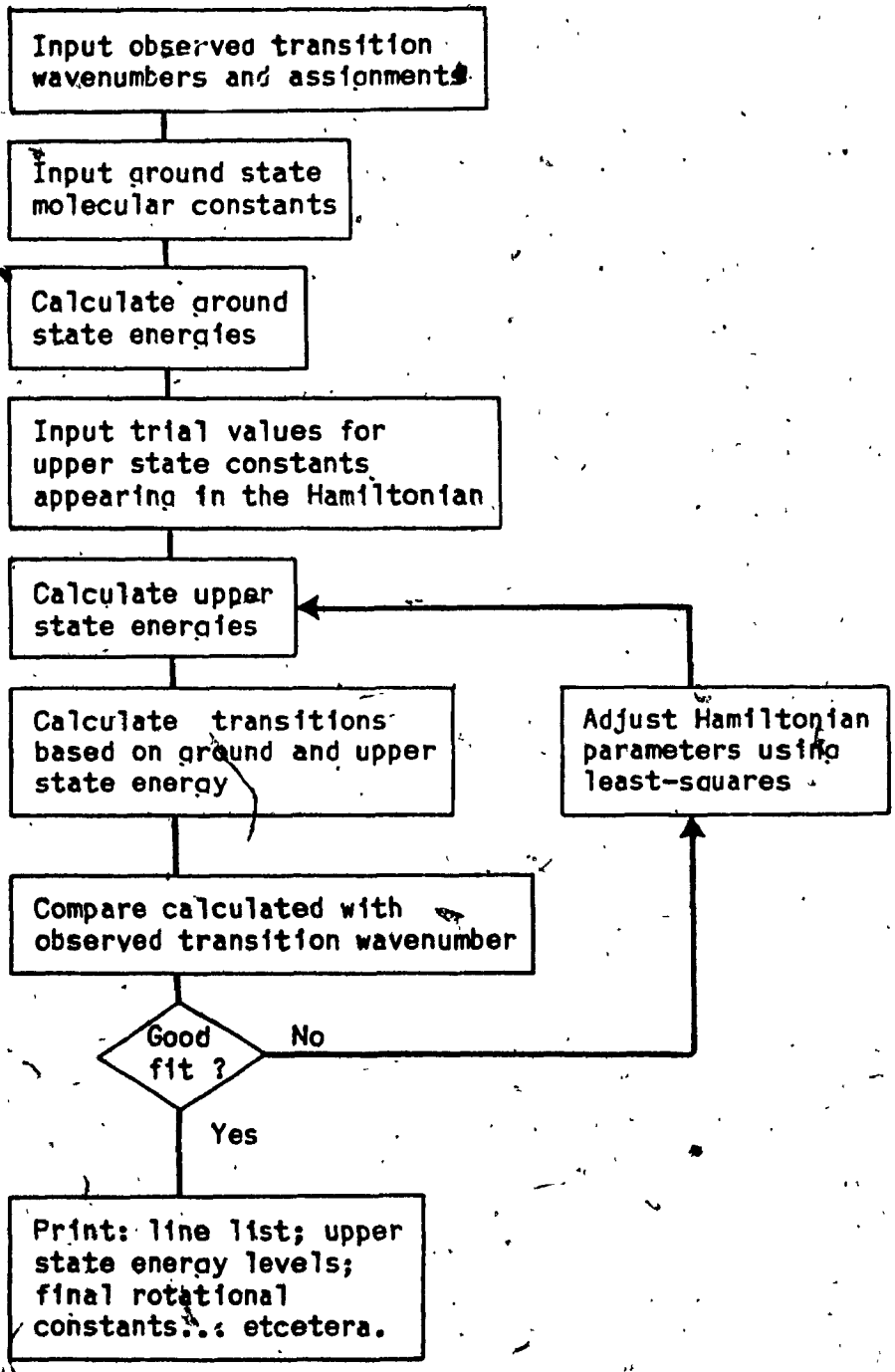


Figure 5-1: Block diagram of computer program used for the determination of asymmetric top molecular constants by least-squares fitting.

one needs both the ground and upper vibrational state molecular constants. The upper state set of constants are the quantities being adjusted and optimized in the fit.

The least-squares fitting technique was also applied to the observed line strengths. This fit computed the dipole moments for the three bands under study and facilitated the prediction of their spectra.

5.2 Least-Square Fitting to the Model Hamiltonian

Least-squares fitting to the rotational Hamiltonian of the transition wavenumbers was performed simultaneously for the ν_3, ν_4 and ν_6 bands using a computer program written and discribed by Johns [14] and modified by Reuter [81]. Hence only a summary will be presented here, stressing those points important for the interpretation of the results.

The aim of the program is to find a set of statistically significant molecular constants, C_i, that can most accurately predict the measured wavenumbers from the Hamiltonian

$$\tilde{H}_R = \sum_i C_i \Omega_i \qquad (5\text{-}1)$$

where Ω_i is a quantum mechanical operator. An iterative approach is used in the least-squares fitting routine since the calculated wavenumbers, ν_i^{cal}, are not a linear function

of the C_i. This is done by making an initial "guess" for the C_i and then finding the set of corrections, δC_i, that best solve the linear equations

$$\nu_i^{obs} - \nu_i^{cal} = \sum_k X_{ik}\, \delta C_k \qquad (5\text{-}2)$$

where ν_i^{obs} is the observed frequency, i runs over N transitions, k runs over M coefficients, and X_{ik} is the wavenumber derivative of transition i with respect to coefficient k ($\partial\nu_i^{cal}/\partial C_k$). The best set of corrections, δC_k, in a least-squares sense are those that minimize the goodness of fit (RMS) relationship

$$(RMS)^2 = \chi^2 = \sum_{i=1}^{N} w_i (\nu_i^{obs} - \nu_i^{cal})^2 \qquad (5\text{-}3)$$

where $w_i = 1/\sigma_i^2$ is the weight of the i^{th} transition, and σ_i is the error assigned to that transition. The weighting is particularly important when the fitting involves mixed data sources. e.g. microwave and IR; where the σ in the microwave data is usually several orders of magnitude smaller than that for IR data. Upon minimization of χ^2 a new set of constants are generated, $C_i(new) = C_i(old) + \delta C_i$, which in turn are used to generate a new set of ν_i^{cal}. The iteration procedure is repeated to convergence, when the changes δC_i are smaller than some desired measure of precision. In this analysis δC_i had to satisfy the relationship $|\delta C_i| < \sigma(C_i)$, where $\sigma(C_i)$ is the least-squares estimate of the standard deviation of the C_i constants.

In order to minimize the RMS given by Equation (5-3)

the fitting program has to compute ν_i^{cal}, δC_i, and $\partial\nu_i/\partial C_k$. The fitting program uses a full Wang factorization described in Chapter 2, and using the Hellman-Feynmann theorem [82] calculates the required Jacobian matrix of partial derivatives of wavenumbers with respect to molecular parameters ($\partial\nu/\partial C$) by the eigenvector transformation method. The wavenumber derivatives are differences between the energy derivatives $\partial E_i/\partial C_i$. Since the energy levels are eigenvalues of $\tilde{H}_R$ which is a linear function of the C_i parameters, the frequency derivatives may be given as follows. Starting with the reduced Hamiltonian given by Equation (5-1) $\tilde{H}_R = \sum_k C_k \Omega_k$, where C_k is the k^{th} molecular constant and Ω_k is the k^{th} quantum mechanical operator, the i^{th} eigenvalue, E_i, is then

$$E_i = \sum_k C_k \langle i|\Omega_k|i\rangle \qquad (5\text{-}4)$$

where i is the i^{th} upper state eigenfunction. The derivative of E_i with respect to the k^{th} molecular constant is

$$\partial E_i/\partial C_k = \langle i|\Omega_k|i\rangle \qquad (5\text{-}5)$$

Now, for pure rotational transitions, the i^{th} frequency is

$$\nu_{ij}^{cal} = E_i - E_j$$

therefore

$$\partial\nu_{ij}^{cal}/\partial C_k = \partial E_i/\partial C_k - \partial E_j/\partial C_k$$

$$= \langle i|\Omega_k|i\rangle - \langle j|\Omega_k|j\rangle \qquad (5\text{-}6)$$

where j is the j^{th} upper state wavefunction. For vibrational transitions the i^{th} frequency is given by

$$\nu_{ij} = \nu_{o,n} + E'_i - E''_j \qquad (5\text{-}7)$$

The band center is represented by $\nu_{o,n}$ and is the separation between the J'=0 and J"=0 levels. The rotational eigenvalues E'_i and E''_j are measured relative to the J'=0 and J"=0 levels, respectively. In addition, the derivatives of the lower state energy are a function of the ground state molecular parameters which are kept fixed in the fit. Thus, the derivative with respect to molecular parameter k becomes simply

$$\partial\nu_{ij}/\partial C_k = \partial E'_i/\partial C_k = \langle i|\Omega_k|i\rangle \qquad (5\text{-}8)$$

In summary, the diagonalization process yields both the eigenvalues and the eigenvectors. The latter quantities are used for the construction of the Jacobian matrix having the elements described by Equations (5-6) and (5-8).

To find the set of C_i that minimizes χ^2 one generates the needed normal equations from the conditions $(\partial\chi^2/\partial C_j)=0$. The normal equations are [83,84]

$$Y = A\delta C \qquad (5\text{-}9)$$

where

$$Y_k = \sum_j w_j y_j x_{jk}$$

$$A_{ki} = \sum_j w_j x_{jk} x_{ji}$$

The corrections δC_i may be found by inverting the normal matrix A to give

$$\underset{\sim}{\delta C} = A^{-1}\underset{\sim}{Y} \qquad (5\text{-}10)$$

The inverse of A can be determined rapidly by matrix inversion techniques designed for the computer. However, if the determinant of A is very small, numerical errors may creep into the calculation of the inverse. This can be due to near linear dependence in the independent variables [85] or from a lack of sufficient experimental data to determine some of the C_i independent of the others. This analysis used matrix inversion to solve Equation (5-9) although other techniques are available, e.g. the Graham-Schmidt orthonormalization procedure [84,86,87]. Problems which could have arised from matrix inversion were eliminated by inserting a numerical ridge, i.e. the diagonal elements of A were not allowed to drop below a certain value.

Quantities determined for each fit were: the best fit values for the Hamiltonian coefficients, C_i; the estimated standard deviation of each coefficient, $\sigma(C_i)$; the correlation coefficient matrix, ρ_{ik}; the calculated wavenumber, ν_i^{cal}; the residuals, $\nu_i^{obs}-\nu_i^{cal}$; the standard deviation of the fit, σ_R; and the weighted standard deviation of the fit, σ_F. The standard deviation of the fit is given as

$$\sigma_R = \{(N-M)^{-1}\sum_{i=1}^{N}(\nu_i^{obs}-\nu_i^{cal})^2\}^{1/2} \qquad (5\text{-}11a)$$

the weighted standard deviation of the fit is given by

$$\sigma_F = \{(N-M)^{-1} \sum_{i=1}^{N} w_i (\nu_i^{obs} - \nu_i^{cal})^2\}^{1/2} \qquad (5\text{-}11b)$$

A reasonable fit for a set of accurately weighted observations will yeild a value near unity for σ_F.

5.3 Input To The Fitting Program

The input data consisted of the following.

1. Ground state molecular constants.
2. Initial values for the upper state molecular constants.
3. The observed FT-IR transition wavenumbers, their assigned quantum numbers, and their respective weights, and
4. Some observed excited state microwave transitions for the v_3=1, v_4=1, and v_6=1 states.

The rotational constants for the ground state of H_2CO were taken from Cornet and Winnewisser [64]. The constants included all the sextic coefficients. The initial upper states constants for the three bands were taken from Allegrini at al. [14]. These included quartic terms and 1st and 2nd order Coriolis coefficients. Both ground and upper state constants are listed in Table 5-1. A total of 3214 observed IR transitions in the ν_3, ν_4, and ν_6 bands were used in the fit. Although the FT-IR spectra contained several hundred additional absorptions, we decided to limit

Table 5-1: Ground State, and Initial Upper States Rotational Constants.

	Ground State[a] in MHz	Upper States[b] in cm^{-1} $v_4 = 1$	$v_6 = 1$	$v_3 = 1$	
ν_o		1167.258	1249.091	1500.176	
A	281970.5723	9.2890	9.4881	9.46697	
B	38836.04557	1.287243	1.298244	1.300078	
C	34002.20344	1.135716	1.129886	1.129318	
Δ_K	19.42374	2.346	11.861	7.586	$X10^{-4}$
Δ_{JK}	1.29050	2.413	8.025	2.421	$X10^{-5}$
Δ_J	0.0752953	2.412	2.539	2.825	$X10^{-6}$
δ_K	1.0260307	2.33	4.64	5.00	$X10^{-5}$
δ_J	0.0104567	2.71	3.53	5.11	$X10^{-7}$
H_K	$4.499X10^{-3}$				
H_{KJ}	$-1.1218X10^{-4}$				
H_{JK}	$2.9019X10^{-5}$				
H_J	$3.1435X10^{-8}$				
h_K	$1.3721X10^{-3}$				
h_{JK}	$1.5666X10^{-5}$				
h_J	$4.2399X10^{-8}$				

ξ^a_{64}	10.0728
η^{bc}_{64}	0.002498
ξ^b_{34}	1.28841
ξ^c_{36}	0.75368

a) From Reference 64. b) From Reference 14.

the fit to transitions with $J \leq 29$. These transitions were the most accurately measured and were sufficient to yield an accurate and reliable set of molecular constants which in turn could be used to predict all the transitions in their respective bands. The observations used (ν_i^{obs}) along with their respective quantum numbers and weights are listed in Table A-1 of Appendix A.

The observed microwave transitions for the $v_3=1$, $v_4=1$, and $v_6=1$ excited vibrational states were taken from Oka et al [88], Chardon et al [89], and Dangoisse et al [90]. The observations included 14 transitions in ν_3, 31 transitions in ν_4, and 29 transitions in ν_6. These transitions along with their respective quantum numbers and weights are listed at the end of Table A-1 of Appendix A. The microwave data which were given in MHz were converted to wavenumbers using a value for the speed of light of $c=2.99792458 \times 10^{10}$ cm/sec.

5.4 Wavenumbers Fit; Results and Discussion

In this section the results of two separate fits are discussed. These fits are hereafter called fit A and fit B.

Fit A was obtained using the input described in the previous section and included in the fit all transitions up to 10 standard deviations from the fit. The results obtained from this fit are listed in Table A-1 of Appendix A. Out of the 3214 IR transitions fitted, 187 lines had residuals >

0.002 cm^{-1} and only 45 lines had residuals > 0.005 cm^{-1}. Most of these transition were blended lines or transitions with high J and K_a values. Overall this fit yielded excellent results with a RMS standard deviation of

$$\sigma_R = 0.00093 \text{ cm}^{-1}$$

and a weighted standard deviation of σ_F=1.13.

The rotational parameters obtained from this simultaneous analysis of the ν_3, ν_4, and ν_6 bands (fit A) are listed in Table 5-2. The correlation matrix for fit A shown in Table 5-3 reveals, however, that some of the 53 fitted constants are dependent on each other. There are 26 dependencies (underscored in the Table) with correlations > 0.800. Allegrini [14] also noted these dependencies and reported very high correlations between rotational parameters of ν_4 and ν_6 and their Coriolis coupling constants ξ_{64} and η_{64}. The relevence of high correlations between the independent variables in least squares fits is discussed in detail by Albritton et al. [83] and will not be dealt with here. From the point of view of our Hamiltonian model, however, it means that different sets of coefficients (rotational constants) might yield equivalent fits. This prompted a series of additional least squares fits culminating in fit B.

Fit B differs from fit A only in its initial upper state constants. The initial parameters for fit B were obtained from the results of a fit A modified to fit only transitions up to J'=15 and K'_a=5. The resulting rotational

Table 5-2: Molecular Constants for the ν_4, ν_6 and ν_3 Bands of H_2CO.

*Results of fit A and Fit B.

The constants are given in cm^{-1}. The uncertainties in parentheses are 1 from the least-squares fits, right-adjusted to the last digit of the parameter.

** These parameters were fixed to the ground state values.

	Fit A $V_4 = 1$	Fit B $V_4 = 1$	
ν_o	1167.25657 (6)	1167.25652 (6)	
A	9.287915 (27)	9.274998 (27)	
B	1.288481 (4)	1.288090 (2)	
C	1.1356828 (7)	1.1356943 (7)	
Δ_K	1.0116 (61)	0.7293 (61)	$X10^{-4}$
Δ_{JK}	3.5932 (70)	3.4893 (69)	$X10^{-5}$
Δ_J	2.3851 (15)	2.3772 (15)	$X10^{-6}$
δ_K	1.963 (20)	1.750 (20)	$X10^{-5}$
δ_J	2.7902 (52)	2.7559 (52)	$X10^{-7}$
H_K	-7.818 (78)	-9.224 (76)	$X10^{-7}$
H_{KJ}	-4.65 (17)	-3.92 (18)	$X10^{-8}$
H_{JK}	-2.34 (35)	-4.12 (35)	$X10^{-9}$
H_J	**	**	$X10^{-12}$
h_J	**	**	$X10^{-12}$
h_{JK}	2.20 (42)	2.06 (42)	$X10^{-9}$
h_K	1.07 (23)	2.13 (23)	$X10^{-7}$

continues.....

Table 5-2: Continued

	Fit A $V_6 = 1$	Fit B $V_6 = 1$	
ν_o	1249.09454 (6)	1249.09465 (6)	
A	9.473186 (27)	9.501472 (26)	
B	1.2981327 (8)	1.2981322 (8)	
C	1.1314955 (9)	1.1316572 (9)	
Δ_K	1.2098 (6)	1.2368 (6)	$\times 10^{-3}$
Δ_{JK}	5.2081 (58)	5.3599 (57)	$\times 10^{-5}$
Δ_J	2.5598 (13)	2.5589 (13)	$\times 10^{-6}$
δ_K	4.156 (26)	4.166 (26)	$\times 10^{-5}$
δ_J	3.6950 (66)	3.675 (66)	$\times 10^{-7}$
H_K	1.097 (71)	1.236 (71)	$\times 10^{-6}$
H_{KJ}	7.28 (15)	5.90 (14)	$\times 10^{-8}$
H_{JK}	3.48 (36)	4.50 (36)	$\times 10^{-9}$
H_J	**	**	$\times 10^{-11}$
h_J	**	**	$\times 10^{-11}$
h_{JK}	-0.235 (29)	-1.6534 (70)	$\times 10^{-10}$
h_K	5.75 (48)	7.38 (10)	$\times 10^{-8}$

continues.....

Table 5-2: Continued

	Fit A $V_3 = 1$	Fit B $V_3 = 1$	
ν_o	1500.17474 (7)	1500.17456 (7)	
A	9.467042 (11)	9.467124 (11)	
B	1.298742 (4)	1.299127 (4)	
C	1.127668 (1)	1.127517 (1)	
Δ_K	6.8277 (37)	6.8755 (37)	$\times 10^{-4}$
Δ_{JK}	4.2596 (70)	4.2387 (65)	$\times 10^{-5}$
Δ_J	2.7660 (14)	2.7665 (14)	$\times 10^{-6}$
δ_K	5.628 (42)	5.510 (44)	$\times 10^{-5}$
δ_J	4.7232 (75)	4.746 (75)	$\times 10^{-7}$
H_K	1.966 (37)	2.083 (45)	$\times 10^{-7}$
H_{KJ}	-1.121 (19)	-0.753 (22)	$\times 10^{-7}$
H_{JK}	1.422 (72)	1.073 (76)	$\times 10^{-8}$
H_J	**	**	$\times 10^{-12}$
h_J	**	**	$\times 10^{-12}$
h_{JK}	2.36 (36)	2.90 (36)	$\times 10^{-9}$
h_K	9.98 (44)	7.90 (47)	$\times 10^{-7}$
	Coriolis Constants		
ξ^a_{64}	10.069126 (98)	10.016327 (98)	
ξ^b_{34}	-1.43933 (45)	-1.39372 (45)	
ξ^c_{36}	0.978624 (38)	0.999699 (39)	
η^{bc}_{64}	-0.0032417(29)	-0.0033324(29)	
z_{36}	-4.02 (16) $\times 10^{-6}$	-5.82 (16) $\times 10^{-6}$	

	1	2	3	4	5	6	7	8	9	10	11	12	15	16	17
1	1.0000														
2	0.2785	1.0000													
3	-0.1121	-0.0483	1.0000												
4	0.4282	-0.0803	-0.0109	1.0000											
5	0.2276	0.1501	0.2453	-0.2026	1.0000										
6	-0.0755	0.0587	0.5576	-0.0923	0.0164	1.0000									
7	-0.0181	-0.1849	0.6795	0.1130	-0.0384	0.1632	1.0000								
8	0.1111	-0.0747	-0.2348	0.0280	0.1203	-0.4021	0.0261	1.0000							
9	0.3014	-0.0039	-0.0777	0.9186	-0.2827	-0.0892	-0.0066	0.0259	1.0000						
10	0.0883	-0.3714	0.3402	-0.0098	0.2735	0.0367	0.5780	0.1802	-0.3072	1.0000					
11	-0.0224	0.3463	-0.2795	-0.0856	0.1807	0.0174	-0.7288	-0.2668	0.0994	-0.8187	1.0000				
12	-0.3071	0.0498	-0.3916	-0.3973	-0.2959	-0.0930	-0.0695	-0.0191	-0.2654	-0.1441	-0.0033	1.0000			
15	0.1047	-0.0718	-0.4717	-0.0089	0.2022	-0.7849	-0.3245	0.6614	0.0127	0.0191	-0.0133	-0.0357	1.0000		
16	-0.0555	0.3548	-0.3542	-0.0316	-0.0483	-0.0287	-0.7460	-0.3500	0.1340	-0.8381	0.9533	0.0422	-0.0711	1.0000	
17	-0.8417	-0.2817	0.1756	-0.1705	-0.1050	0.0316	0.0645	-0.0769	-0.1109	-0.0247	0.0104	0.0359	-0.0637	0.0255	1.0000
18	0.0503	-0.2574	-0.2088	0.0105	-0.1299	0.0341	-0.2812	-0.1082	0.0357	-0.1778	0.2075	0.0233	-0.0485	0.2483	-0.0683
19	-0.0398	0.3804	0.2051	-0.0097	0.0428	0.0523	0.2677	0.0086	-0.0142	0.0671	-0.1322	0.0310	-0.1000	-0.1415	0.1092
20	-0.1469	0.1160	0.0089	-0.3263	0.0582	0.0107	-0.0359	-0.0122	-0.3048	-0.0522	0.0567	0.0739	0.0016	0.0459	0.4208
21	-0.1956	-0.3681	0.0273	0.0352	-0.3540	-0.0282	0.1797	0.0366	0.0127	0.1652	-0.3066	0.0417	-0.0111	-0.2372	0.2773
22	0.0622	-0.3162	-0.0004	0.0546	-0.1697	0.3149	-0.0703	-0.2259	0.0314	-0.0102	0.0357	-0.0030	-0.3408	0.0720	-0.0904
23	0.0216	-0.1627	0.2899	0.0204	0.0581	0.0813	0.5128	0.1782	-0.0986	0.5639	-0.5982	-0.0346	-0.0148	-0.6496	0.0392
24	0.0395	-0.0890	-0.0282	-0.0555	0.0445	-0.0960	0.1171	0.1600	-0.1164	0.2828	-0.2804	0.0191	0.1495	-0.2918	-0.0368
25	-0.1200	0.1201	-0.0153	-0.3099	0.0702	0.0150	-0.1047	-0.0834	-0.3282	-0.0751	0.1450	0.0545	-0.0351	0.1519	0.3415
26	0.1007	-0.1120	0.1803	-0.0583	-0.0013	0.0476	0.4809	0.2933	-0.1241	0.5208	-0.6620	0.0353	0.0735	-0.7191	-0.0588
27	-0.0817	0.3644	-0.2328	0.0523	-0.1219	-0.0978	-0.5110	-0.2747	0.2058	-0.7494	0.7436	0.0240	-0.0561	0.8262	0.0821
28	0.0350	-0.0295	0.0334	0.0716	0.0431	0.0182	-0.0033	-0.0233	0.0608	0.0025	-0.0292	-0.0719	-0.0168	0.0209	-0.2872
31	-0.0044	0.0750	-0.1608	-0.0757	0.1180	-0.4456	0.0042	0.2813	-0.0858	0.1272	-0.1389	-0.0222	0.4679	-0.1575	-0.0049
32	-0.0642	0.3809	-0.2697	0.0268	-0.0489	-0.1046	-0.5915	-0.2592	0.1983	-0.8073	0.8393	0.0194	-0.0157	0.8933	0.0524
33	-0.1613	-0.2327	-0.0390	-0.0114	-0.0401	0.0118	-0.1146	-0.0674	0.0018	-0.0497	0.1041	-0.0117	-0.0109	0.1056	0.1325
34	-0.2526	-0.9433	0.0294	0.0540	-0.1054	0.0256	0.0349	0.0202	-0.0071	0.2804	-0.2016	-0.0979	0.0423	-0.2178	0.2522
35	-0.1066	-0.2827	0.1150	0.0092	-0.0054	0.0145	0.2046	0.0926	-0.0360	0.2487	-0.2613	-0.0245	0.0183	-0.2773	0.1141
36	-0.1470	-0.3367	-0.0259	-0.0086	-0.0360	0.0089	-0.0759	-0.0345	-0.0122	0.0245	0.0358	-0.0227	0.0100	0.0298	0.1172
37	-0.0642	0.0199	-0.0991	-0.0101	-0.0392	0.0184	-0.2112	-0.1299	0.0298	-0.1980	0.2408	0.0135	-0.0487	0.2565	0.0281
38	-0.0405	-0.0855	0.0096	-0.0151	-0.0151	0.0663	-0.0040	-0.0476	-0.0272	0.0462	-0.0219	0.0013	-0.0592	-0.0259	0.0355
39	0.0151	0.0219	0.1874	0.0073	0.0604	-0.0378	0.3486	0.1951	-0.0358	0.2663	-0.3496	-0.0105	0.0659	-0.3684	0.0055
40	0.0209	-0.0239	0.0703	0.0145	-0.0045	0.0088	0.1316	0.0525	-0.0066	0.1075	-0.1435	-0.0054	-0.0023	-0.1432	-0.0182
41	-0.0786	-0.1560	-0.1097	-0.0244	-0.0289	0.0222	-0.2243	-0.1129	-0.0038	-0.1271	0.2158	-0.0006	-0.0229	0.2169	0.0465
42	-0.0879	-0.3200	0.2483	0.0290	0.0199	-0.0366	0.4569	0.2476	-0.0435	0.4312	-0.5231	-0.0436	0.0913	-0.5467	0.0960
43	-0.0317	-0.0094	-0.2368	-0.0106	-0.0659	0.0401	-0.4483	-0.2478	0.0490	-0.3526	0.4622	0.0136	-0.0786	0.4845	0.0035
44	0.1938	0.1476	-0.8157	0.0148	0.0266	-0.0181	0.0390	0.0469	0.0017	0.0258	-0.0532	0.0072	0.0236	-0.0545	-0.1844
47	0.0021	0.0377	-0.0330	0.0153	-0.0257	-0.0135	-0.0670	-0.0334	0.0351	-0.0996	0.0940	0.0015	-0.0065	0.1078	-0.0069
48	-0.0280	-0.0065	-0.2419	-0.0104	-0.0648	0.0366	-0.4553	-0.2474	0.0503	-0.3588	0.4692	0.0134	-0.0748	0.4913	0.0012
49	0.8814	0.3616	-0.2095	0.0776	0.0664	-0.0453	-0.0709	0.0956	0.0292	0.0052	-0.0282	0.0138	0.0800	-0.0342	-0.8948
50	-0.2493	-0.9886	0.0651	0.0612	-0.0962	0.0121	0.1075	0.0680	-0.0129	0.3511	-0.2859	-0.1066	0.0668	-0.3072	0.2541
51	0.1069	0.5898	-0.0135	-0.0199	0.0910	-0.0762	-0.1069	-0.0248	0.0585	-0.3352	0.2893	0.0212	0.0271	0.3018	-0.1056
52	-0.8587	-0.4818	0.2052	-0.0629	-0.0786	0.0456	0.0829	-0.0800	-0.0290	0.0480	-0.0169	-0.0279	-0.0669	-0.0141	0.8726
53	0.0615	-0.1926	0.0675	-0.0510	-0.0178	0.2457	0.1353	-0.0564	-0.1411	0.3492	-0.2974	-0.0154	-0.1872	-0.3165	-0.0702

Table 5-3: Correlation Matrix from Least-Squares-Fit: Results From Fit A.

a. The numbers 1-48 represent cyclically the rotational constants for ν_4, ν_6 and ν_3. 49-53 represent the Coriolis constants.

	18	19	20	21	22	23	24	25	26	27	28	31	32	33	34
18	1.0000														
19	-0.4341	1.0000													
20	-0.1431	0.1073	1.0000												
21	0.3475	0.0214	-0.1273	1.0000											
22	0.6599	-0.0173	-0.1061	0.2073	1.0000										
23	-0.6376	0.5685	0.0840	0.0607	-0.1582	1.0000									
24	0.1538	-0.2931	0.0129	0.1249	-0.1903	0.0360	1.0000								
25	-0.0704	0.0341	0.9309	-0.2234	-0.0332	-0.0303	0.0249	1.0000							
26	-0.2948	0.2792	-0.0108	0.3992	-0.1968	0.6548	0.1832	-0.2621	1.0000						
27	0.3794	-0.1524	0.0192	-0.1231	0.1443	-0.7980	-0.2821	0.1464	-0.8139	1.0000					
28	-0.2604	-0.3294	-0.4129	-0.3032	-0.1806	-0.0789	-0.0090	-0.2980	-0.1388	-0.0065	1.0000				
31	0.0649	-0.2845	-0.0497	0.1332	-0.5098	-0.2360	0.5871	-0.0406	0.1181	-0.0946	0.0388	1.0000			
32	0.3155	-0.1746	0.0377	-0.2634	0.0796	-0.7885	-0.3361	0.1456	-0.8034	0.9711	0.0295	-0.1368	1.0000		
33	0.0848	-0.1187	-0.0751	0.0833	0.0849	-0.0300	-0.0071	-0.0618	-0.0736	0.0047	0.0320	-0.0365	0.0196	1.0000	
34	0.2772	-0.4015	-0.1139	0.3337	0.3467	0.1247	0.0744	-0.1068	0.0588	-0.3175	0.0348	-0.1178	-0.3158	0.3086	1.0000
35	0.0399	-0.0957	-0.0191	0.1007	0.0665	0.1019	0.0310	-0.0396	0.1146	-0.1849	-0.0026	-0.0086	-0.2006	0.0855	0.1448
36	0.1214	-0.1650	-0.0960	0.1267	0.1230	-0.0057	0.0036	-0.0893	-0.0289	-0.0594	0.0346	-0.0423	-0.0455	0.7927	0.3379
37	0.0285	-0.0387	-0.0630	-0.0165	0.0320	-0.0732	-0.0129	-0.0392	-0.1273	0.1099	0.0302	-0.0311	0.1312	0.5127	0.1624
38	-0.0368	0.0107	-0.0002	0.0400	0.0213	0.1154	0.0356	-0.0140	0.0988	-0.1397	-0.0029	-0.0337	-0.1223	0.1193	0.2309
39	-0.0548	0.0788	0.0244	-0.0231	-0.0903	0.0417	-0.0117	-0.0038	0.1105	-0.0735	-0.0083	0.0719	-0.1152	-0.1834	-0.2771
40	-0.0226	0.0454	-0.0147	0.0273	0.0020	0.0538	-0.0130	-0.0177	0.0443	-0.0452	0.0016	-0.0062	-0.0736	0.0033	0.0927
41	0.0822	-0.1101	-0.0673	0.0643	0.0809	-0.0360	-0.0091	-0.0540	-0.0663	0.0134	0.0246	-0.0465	0.0501	0.5851	0.2069
42	0.0435	-0.0550	-0.0593	0.1148	0.0340	0.0930	0.0173	-0.0901	0.1534	-0.1953	0.0168	0.0411	-0.2576	0.0387	0.1381
43	0.0678	-0.1026	-0.0306	0.0005	0.0986	-0.0774	0.0078	0.0061	-0.1639	0.1179	0.0145	-0.0809	0.1751	0.2534	0.2347
44	-0.0232	0.0408	0.0213	-0.0532	-0.0291	0.0119	0.0202	0.0169	0.0568	-0.0173	-0.0137	0.0280	-0.0230	-0.6797	-0.2385
47	0.0332	-0.0050	-0.0176	-0.0056	0.0228	-0.0794	-0.0433	0.0056	-0.1171	0.1306	0.0088	-0.0256	0.1170	0.0408	0.0643
48	0.0719	-0.1058	-0.0276	0.0001	0.1007	-0.0831	0.0070	0.0091	-0.1671	0.1237	0.0131	-0.0814	0.1817	0.2227	0.2240
49	0.0768	-0.0344	-0.0559	-0.1573	0.0758	0.0001	0.0597	-0.0457	0.1552	-0.0835	-0.0093	0.0062	-0.0693	-0.1836	-0.3322
50	0.2873	-0.4134	-0.1151	0.3447	0.3478	0.1331	0.0780	-0.1127	0.0827	-0.3466	0.0347	-0.1044	-0.3537	0.2439	0.9601
51	-0.1430	0.3291	0.0701	-0.2968	-0.2757	-0.2729	-0.1358	0.0945	-0.2603	0.4437	0.0276	0.0868	0.4424	-0.1795	-0.6111
52	-0.0208	-0.0418	0.0339	0.2057	-0.0090	0.0207	-0.0460	0.0249	-0.1322	0.0272	0.0056	-0.0250	0.0116	0.2089	0.4506
53	-0.1268	0.0430	-0.0013	0.1753	0.1192	0.4788	0.2266	-0.0629	0.5055	-0.6156	-0.0315	-0.0671	-0.5911	0.0985	0.2805

	35	36	37	38	39	40	41	42	43	44	47	48	49	50	51
35	1.0000														
36	0.0817	1.0000													
37	-0.0276	0.0058	1.0000												
38	0.3239	0.0058	0.2891	1.0000											
39	0.6810	-0.0661	-0.4345	-0.1581	1.0000										
40	-0.5399	-0.0447	0.0124	-0.2422	-0.2146	1.0000									
41	-0.0608	0.8782	-0.0572	0.0732	-0.2473	-0.0881	1.0000								
42	0.4149	0.0137	-0.1569	-0.1899	0.6974	0.1804	-0.3738	1.0000							
43	-0.3252	0.1209	0.5381	0.2887	-0.8392	-0.1746	0.3462	-0.8433	1.0000						
44	-0.3250	-0.4157	-0.3905	-0.3283	0.0359	0.0554	-0.2637	-0.0737	-0.1200	1.0000					
47	-0.6905	-0.0663	0.1748	-0.4775	-0.4883	0.7357	-0.0660	-0.0246	0.0776	0.0707	1.0000				
48	-0.3475	0.1326	0.4632	0.2479	-0.8413	-0.1940	0.3634	-0.8613	0.9942	-0.0918	0.0710	1.0000			
49	-0.1365	-0.1724	-0.0618	-0.0403	0.0045	0.0191	-0.0810	-0.1288	-0.0210	0.2205	0.0018	-0.0171	1.0000		
50	0.2703	0.3485	-0.0044	0.0910	-0.0537	0.0141	0.1786	0.2850	0.0488	-0.1489	-0.0348	0.0464	-0.3346	1.0000	
51	-0.2326	0.2392	-0.0684	-0.1282	0.2030	0.0638	-0.1819	0.0013	-0.2360	0.0932	0.0643	-0.2372	0.1345	-0.5971	1.0000
52	0.1814	0.2144	0.0572	0.0511	-0.0125	-0.0157	0.1031	0.1638	0.0272	-0.2289	-0.0067	0.0232	-0.9817	0.4581	-0.2769
53	-0.0281	0.1007	0.1673	0.1927	-0.4106	-0.1694	0.1929	-0.3854	0.4942	-0.0224	-0.1106	0.5002	0.0945	0.2067	-0.5312

	52	53
52	1.0000	
53	-0.0568	1.0000

WEIGHTED STANDARD DEVIATION = 0.113E+01

UNWEIGHTED STANDARD DEVIATION = 0.933E-03

LEAST SQUARES ITERATIVE PROCEDURE COMPLETE.

constants from fit B are also listed in Table 5-2. These are significantly different from the results obtained from fit A. Yet, the standard deviation of fit B is nearly identical to that of fit A (σ_R=0.00091 cm^{-1}) and both sets of constants predict the same calculated frequencies. Hence, the high correlation between the parameters does allow for similar results from different sets of molecular constants.

Both A and B fittings were also tried where only transitions within four standard deviations of the fit were included. The resulting rotational constants in these cases were again significantly different but had an improved standard deviation of σ_R<0.0006 cm^{-1}. These attempts turned out not to be very useful since too many transitions were excluded from the fitting process.

The continuing discussion refers to the parameters obtained from fit A as the final results, although at this point either one of the two sets may be presented as such. Using the sextic Hamiltonian terms significantly improved the overall fit reducing the σ_R of the fit by a factor of 5. The improvements were noticed for transition series with high J and K_a values. Without the sextic terms these series showed an incremental divergence in the residuals as a function of J for J>15. However, preliminary fittings indicated that not all the sextic coefficients could be used in the fit. Two of these coefficients, namely, H_J and h_J converged in the fit to yield values of the order of 10^{-12}

cm^{-1}. From the matrix elements shown in Equation (2-47) one can see that H_J and h_J are the coefficients of $J^3(J+1)^3$ and $J^2(J+1)^2$ respectively. As such, even for the highest J used (J=29), the products yielded contributions on the order of 10^{-4} and 10^{-7} cm^{-1}. These values are of no significance since they are smaller than the resolution of the FT-IR spectrometer used (~0.004 cm^{-1}). Consequently, these two coefficients were fixed during the fit to the more accurate ground state values as indicated in Table 5-2.

The 3rd order Coriolis constant, z_{36}, had a suprisingly small effect on the local resonance between ν_3 and ν_6. It improved the calculated values for many transitions having J>15 by an average of 0.4 milliwavenumbers. Basically it is difficult at this point to estimate the real contribution of z_{36}.

The high correlations between the coefficients of the Hamiltonian are due in large part to the symmetry of the formaldehyde molecule. The near symmetric top (κ=-0.961) character of H_2CO coupled with the strong Coriolis interactions between the bands is the main cause for the observed correlations. These in turn, allow for some of the fitted Hamiltonian constants to compensate for or contribute to other constants. This being manifested in multiple sets of rotational constants (e.g. fits A and B) and the apparent small contribution of some of the coefficients.

Presently we are searching among the unassigned

transitions of the FT-IR spectra for series having high J and K_a (K_a>8). Fitting such series might cause a convergence to only one set of molecular constants. However, even without these extra transitions the best set of constants may be determined graphically from a predicted spectra, i.e. when both the eigenvalues and eigenvectors obtained from a given fit are used simultaneously.

5.5 Intensity Fitting

The 27 observed line strengths for ν_4 and ν_6 discussed and listed in chapter 4 along with eleven ratio estimated line strengths for ν_3 were used to determine the dipole moment derivatives $\partial\mu/\partial Q_x$ (x=3, 4 or 6). These derivatives may in turn be used to predict the entire spectrum from the eigenvalues and eigenvectors of the Hamiltonian.

The derivatives $\partial\mu/\partial Q_3$, $\partial\mu/\partial Q_4$, and $\partial\mu/\partial Q_6$ were evaluated using a least-squares fitting program. The fitting involved an iterative process similar to that used for the transition wavenumbers fit. The weighted RMS differences to be minimized is given by

$$(RMS)^2 = \chi^2 = \sum_i^N w_i (S_i^{obs} - S_i^{cal})^2 \quad (5\text{-}13)$$

where $w_i = 1/\sigma_i^2$ is the weight of the i^{th} line strength, and

σ_i is the error assigned to that observation. S_i^{cal} is obtained from Equation (2-59). The iterative process involves generating estimates of $\partial\mu/\partial Q_x$ such that

$$\partial\mu/\partial Q_x(\text{new}) = \partial\mu/\partial Q_x(\text{old}) + \delta(\partial\mu/\partial Q_x).$$

These in turn are used to generate a new set of S_i^{cal}. The iterative process continues until $\delta(\partial\mu/\partial Q_x) < \sigma(\partial\mu/\partial Q_x)$ where $\sigma(\partial\mu/\partial Q_x)$ is the estimated standard deviation of the dipole moment derivative. The correction factor $\delta(\partial\mu/\partial Q_x)$ is evaluated as follows. From Equation (2-59) one obtains

$$\begin{aligned} S_i^{cal} = {} & (\partial\mu/\partial Q_4)^2 z_4^2 + (\partial\mu/\partial Q_6)^2 z_6^2 + (\partial\mu/\partial Q_3)^2 z_3^2 \\ & + 2(\partial\mu/\partial Q_4)(\partial\mu/\partial Q_6) z_4 z_6 + 2(\partial\mu/\partial Q_4)(\partial\mu/\partial Q_3) z_4 z_3 \\ & + 2(\partial\mu/\partial Q_6)(\partial\mu/\partial Q_3) z_6 z_3 \end{aligned} \qquad (5\text{-}14)$$

Hence, the normal equations may be written as

$$wD^T\Delta S = D^T wD\delta P \qquad (5\text{-}15)$$

where $\Delta S_i = S_i^{cal} - S_i^{obs}$, $\delta P_x = (\partial\mu/\partial Q_x)$ and D, the Jacobian matrix is given by $D_{ix} = \partial S_i^{cal}/\partial(\partial\mu/\partial Q_x)$ and is evaluated from Equation (5-14) where i runs over the number of observations and x=3,4 or 6, i.e. the three contributing dipole moment derivatives. For example, the i^{th} row of this matrix contains the following 3 elements

$$\begin{aligned} \partial S_i^{cal}/\partial(\partial\mu/\partial Q_4) = {} & 2(\partial\mu/\partial Q_4) z_4^2 + 2(\partial\mu/\partial Q_6) z_4 z_6 \\ & + 2(\partial\mu/\partial Q_3) z_4 z_3 \end{aligned}$$

$$\partial s_i^{cal}/\partial(\partial\mu/\partial Q_6) = 2(\partial\mu/\partial Q_6)z_6^2 + 2(\partial\mu/\partial Q_4)z_4z_6 + 2(\partial\mu/\partial Q_3)z_6z_3$$

$$\partial s_i^{cal}/\partial(\partial\mu/\partial Q_3) = 2(\partial\mu/\partial Q_3)z_3^2 + 2(\partial\mu/\partial Q_4)z_4z_3 + 2(\partial\mu/\partial Q_6)z_6z_3$$

It should be noticed here that in the absence of interactions between the bands the 2nd and 3rd terms of all the elements drop out.

5.6 Intensity fitting; Results and Discussion

The results of the least-squares fitting of the line strengths are listed in Table 5-4. This fit which was based on the eigenvectors obtained from fit A (described above) yielded a standard deviation of σ_R=0.00404 $cm^{-2}atm^{-1}$. This is a good fit with an RMS proportional to the experimental error. The σ_R is somewhat smaller when the 11 estimated line strengths for ν_3 are not used. However, these were needed for the evaluation of the dipole moment of ν_3 which in turn was used in the evaluation of the magnitude of energy mixing between the bands.

The values for the effective dipole moments obtained from this fit are:

$$(\partial\mu/\partial Q_4) = 2.408(44)\times10^{-3}\ cm^{-1}atm^{-1/2}$$

$$(\partial\mu/\partial Q_6) = -3.092(40)\times10^{-3}\ cm^{-1}atm^{-1/2}$$

$$(\partial\mu/\partial Q_3) = 1.69(18)\times10^{-3}\ cm^{-1}atm^{-1/2}$$

JU	KAU	KCU	VU[a]	JL	KAL	KCL	OBS INT	OBS-CAL	FREQ	WT
17	4	14	2	18	5	13	0.3225E-02	-0.8798E-03	1148.3347	4.7383
11	2	9	1	10	3	7	0.2113E-01	0.2987E-03	1148.3452	0.3009
17	4	13	2	18	5	14	0.3395E-02	-0.7146E-03	1148.3602	3.2992
3	0	3	1	4	1	3	0.4737E-01	0.6102E-02	1148.4702	0.0198
16	1	15	1	16	2	15	0.1866E-01	0.2189E-02	1148.5083	0.1337
1	0	1	1	1	1	1	0.2953E-01	0.6159E-03	1159.1356	0.0260
2	0	2	1	2	1	2	0.4846E-01	0.9827E-03	1159.2716	0.0081
28	2	27	1	28	1	27	0.5936E-02	0.6334E-03	1159.2876	0.4586
15	2	13	1	14	3	11	0.1883E-01	-0.6959E-03	1159.3920	0.1837
9	1	9	1	8	2	7	0.7429E-02	0.1965E-03	1159.4396	0.7035
3	0	3	1	3	1	3	0.6663E-01	0.1642E-02	1159.4715	0.0035
18	2	17	1	18	1	17	0.3208E-01	0.3744E-02	1172.3859	0.1957
6	1	6	1	6	0	6	0.2843E-01	0.4681E-03	1172.5255	0.0343
12	2	11	2	13	3	10	0.1898E-01	-0.1705E-02	1180.6443	0.0752
4	4	1	2	5	5	0	0.1921E-01	-0.2606E-03	1180.7330	0.0540
24	0	24	1	23	1	22	0.2613E-02	-0.7444E-03	1180.8080	13.7373
11	2	10	1	11	1	10	0.3400E-01	-0.1982E-02	1180.8324	0.0174
13	2	11	2	14	3	12	0.1651E-01	-0.3688E-02	1180.8831	0.0559
10	4	7	2	10	5	6	0.1400E-01	0.1407E-02	1192.6082	0.3555
3	3	1	2	4	4	0	0.1000E-01	0.4628E-03	1192.6270	0.3555
9	4	6	2	9	5	5	0.1400E-01	0.1930E-02	1192.6657	0.3265
8	4	5	2	8	5	4	0.1246E-01	0.1405E-02	1192.7181	0.1957
18	1	17	2	19	2	18	0.6010E-02	-0.1123E-02	1192.7374	1.4471
7	4	4	2	7	5	3	0.1083E-01	0.1358E-02	1192.7652	0.5209
10	1	10	2	11	2	9	0.5890E-02	-0.4981E-03	1192.7954	2.5135
6	4	3	2	6	5	2	0.8240E-02	0.1029E-02	1192.8068	0.8358
5	4	2	2	5	5	1	0.4886E-02	0.7429E-03	1192.8428	7.3743
16	3	14	3	17	3	15	0.3260E-01	0.4423E-02	1460.5795	0.0018
10	1	10	3	11	1	11	0.6260E-01	-0.9457E-02	1474.5636	0.0005
7	1	6	3	8	1	7	0.7070E-01	0.2707E-02	1480.5772	0.0004
6	0	6	3	7	0	7	0.3010E-01	0.6901E-02	1483.4343	0.0021
3	3	1	3	3	3	0	0.3250E-01	-0.1104E-01	1500.7334	0.0018
9	5	5	3	9	5	4	0.1840E-01	0.2022E-02	1502.0204	0.0058
7	7	1	3	7	7	0	0.2010E-01	0.2710E-02	1503.1104	0.0047
9	1	8	3	8	1	7	0.5524E-01	-0.6834E-02	1523.3220	0.0006
13	0	13	3	12	0	12	0.2450E-01	0.6134E-02	1531.2509	0.0031
14	2	13	3	13	2	12	0.2047E-01	0.6708E-02	1534.9392	0.0047
20	3	17	3	19	3	16	0.1981E-01	0.6861E-02	1552.1402	0.0047

NUMBER OF LINES FIT = 38

ROTATIONAL PARTITION FUNCTION = 0.282383D+04

Table 5-4: Results From Least-squares Fitting of Line Strengths.

a. The numbers 1,2 and 3 represent respectively ν_4, ν_6 and ν_3

The ratio of $(\partial\mu/\partial Q_4)/(\partial\mu/\partial Q_6)=-0.779(12)$ representing the magnitude of perturbation [54] between the two bands, compares well with the value of -0.8(1) obtained by Nakagawa and Morino [13]. The effective dipole moments were converted to conventional units (Debye/amu$^{1/2}$Å). These compare favorably (within ±15%) with literature values (Table 5-4).

The least-squares fit also computed the rotational partition function yielding G=2823.83. This value is in good agreement with G_r=2832.91 obtained from the empirical relationship [91]

$$G_r \cong 1/\sigma[(\pi/ABC)\cdot(kT/h)^3]^{1/2} \qquad (5\text{-}16)$$

where A, B, and C are the ground state rotational constants (MHz), T is the temperature (K), and σ is a measure of symmetry and is equal to 2 for the C_{2v} group.

The band strengths were computed by summations using

$$B_x = \sum_i k(\nu)_{xi} \qquad (5\text{-}17)$$

where i runs over all calculated line strengths within a given band, x (x=3,4, or 6). These summations yielded the following band strengths

B_4 = 16.013 cm^{-2}atm^{-1}

B_6 = 35.424 cm^{-2}atm^{-1}

B_3 = 11.632 cm^{-2}atm^{-1}

These values were converted to conventional units of km/mole using the ideal gas law (cm^{-2}atm^{-1}=Tx8.2056x10^{-4}km/atm [48]) and are compared to literature values [16,17] in Table 5-5.

Table 5-5. Calculated Dipole Moment Derivatives and Band Strengths.

Dipole Moment derivatives

(Debye/amu$^{1/2}$Å)

derivative	This work	Nakanaga et al [16]
$(\partial\mu/\partial Q_4)$	0.332(6)[a]	0.39
$(\partial\mu/\partial Q_6)$	0.442(6)	0.47
$(\partial\mu/\partial Q_3)$	0.264(28)	

Band Strength

(km/mole)

	This work	Nakagana et al [16] cal.	Nakagana et al [16] obs.	Histasune and Eggers [17]
ν_4, ν_6	12.53(84)	16.83	16.41(65)	9.9(5)
ν_4	3.90(37)	7.53	6.49(64)	
ν_6	8.63(82)	9.30	9.94(97)	
ν_3	2.83(27)	12.01	11.1(1.0)	

a. The uncertainties in parentheses are 1 standard deviation, right adjusted to the last digit.

It should be noted here that none of the literature values for either the dipole moments or band strengths were obtained from direct line strength measurments. For example, the values quoted from Nakanaga et al [16] were obtained from low resolution (0.25 cm^{-1}) FT-IR band measurements and band simulation.

Since in this work the line strengths were not measured directly for transitions in ν_3, we have little confidence in the values of $(\partial\mu/\partial Q_3)$ and B_3. However, when in several calulations this dipole moment was varied in magnitude from 1/10 to x10 its current value, little change has been noticed in the band strengths of ν_4 and ν_6. This indicates that ν_3 has a relatively weak interaction with the other bands. It is estimated that B_3 should be about 3 times the reported value. This will increase $(\partial\mu/\partial Q_3)$ by a factor of $\sqrt{3}$ which in turn will cause only 1.8% change in B_4 and <1% change in B_6. Based on this reasoning we have high confidence in the values presented here for ν_4 and ν_6.

The goodness of the fit was checked by comparing the wavenumbers and relative line strengths of the predicted transitions to those of the observed (FT-IR). A stick diagram of such a comparison is presented in Figure 5-2.

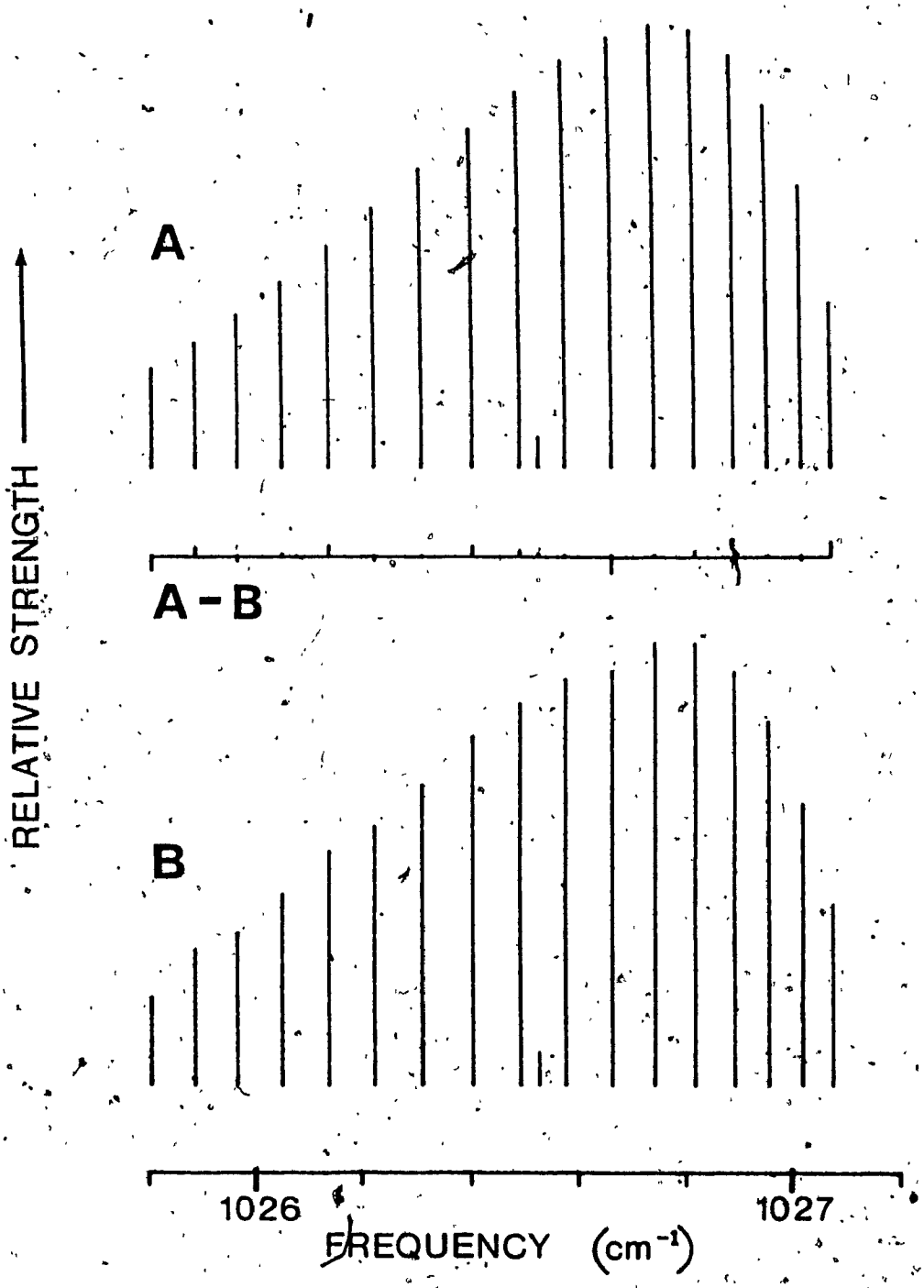


Figure 5-2: Stick Diagram Comparing Observed and Calculated Wavenumbers and Line Strengths for P_{Q_7} of ν_4.

A. Calculated
B. Observed (FT-IR)

CHAPTER 6

TRACE ANALYSIS OF FORMALDEHYDE IN AMBIENT AIR

6.1 Introduction

In this Chapter, the potential application of the TDL spectrometer to trace analysis of H_2CO in ambient air will be discussed. The aim here is to develop a rapid analysis technique capable of measuring air samples containing H_2CO concentrations at the low ppb level.

In the past decade, TDL systems have been used in a wide range of analytical applications, from trace analysis of gases at the <1 ppb level to fully automated on-line monitoring of gases and liquids [18-25,92,93]. Since the techniques and methodology are covered in the literature, the task here is rather heavily oriented to sample collection and handling prior to and during analysis. The ease with which H_2CO polymerizes and adsorbs to surfaces complicates its routine analysis. In addition, due to pressure broadening effect the spectroscopic technique requires reduced sample pressures. These three factors reduce the analyte concentration by several orders of magnitude. Analyte loss may be compensated by increasing the optical path length. This, however, is limited by hardware cost and size.

The results obtained from the TDL determinations were always compared with results obtained from the Laser Thermal

Lens (LTL) [94-98] technique, and to those obtained from the well established NIOSH colorimetric technique [99]. The LTL technique is currently also evaluated and developed at Concordia University by Dr. Langford's group for air pollution monitoring [100-102].

6.2 Preliminary Analysis

The initial attempts at determining H_2CO in air were carried out using a conventional spectroscopic technique. Samples of 10 ppm H_2CO in air prepared in a one liter glass bulb by passing dry air over a pellet of reagent grade paraformaldehyde [101] were introduced into the White cell. The cell pressure was then reduced to <10 Torr and the path length adjusted to 100.17 meters. The result from monitoring several strong transitions in the 10 μm region (ν_4 and ν_6 bands) were always negative, i.e. no absorption was observed.

The next step was to install the cold trap (liquid N_2) shown in Figure 6-1 between the sample cell and the White cell. This allowed for the reduction of pressure without loss of sample since the H_2CO was frozen out in the cold trap. This yielded detections as low as 1 ppm (Figure 6-2). It was observed, however, that identical samples yielded a variety of absorption values. We attributed this to the following potential causes: polymerization, surface adsorption and/or poor trapping mechanism of sample. The steps

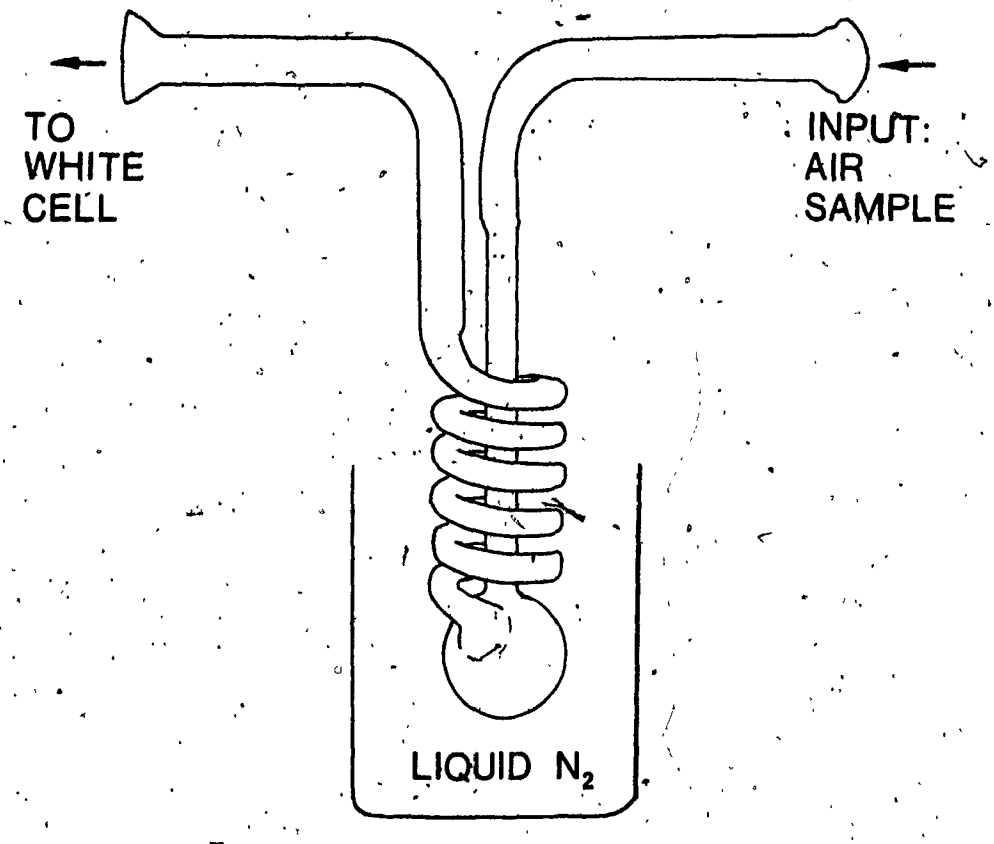


Figure 6-1: Formaldehyde Sampling Apparatus for Trapping H_2CO from a Fixed Volume of Air.

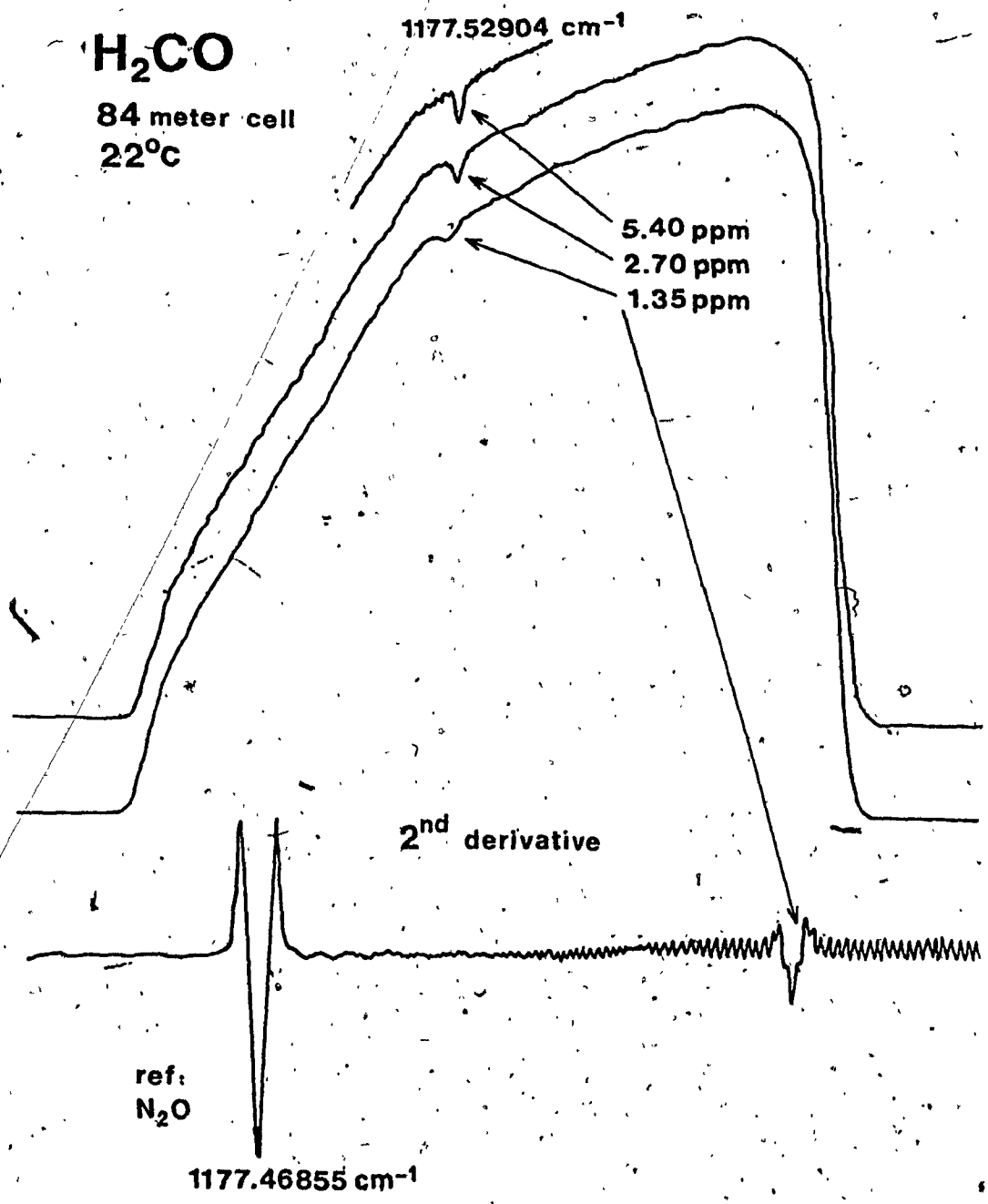


Figure 6-2: First Efforts at Determining H_2CO in Air Concentrations Using the Cold Trap.

taken to eliminate or reduce these problems as well as the measures taken to improve the lower limit of detection are described in the following section.

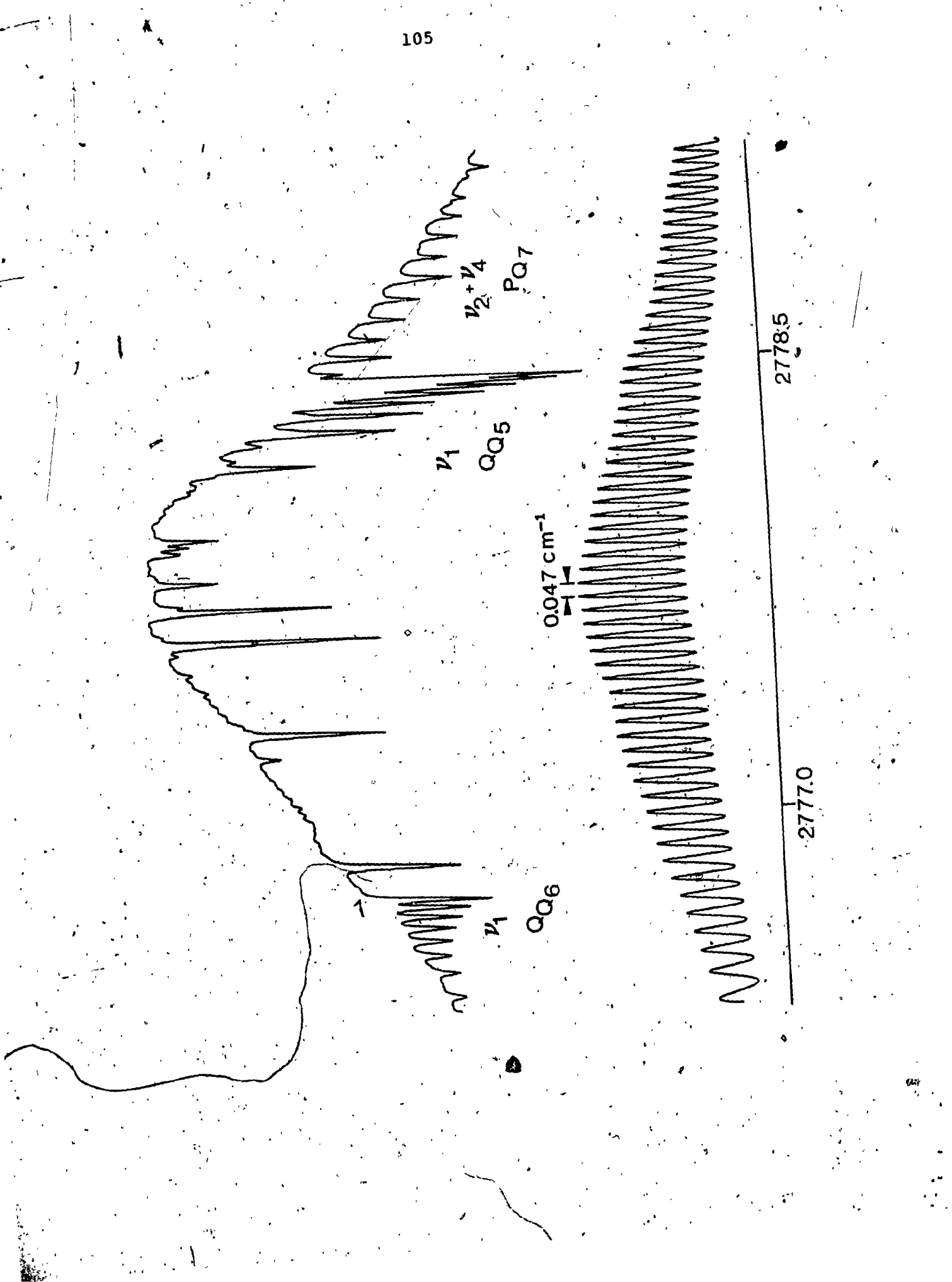
6.3 Experimental

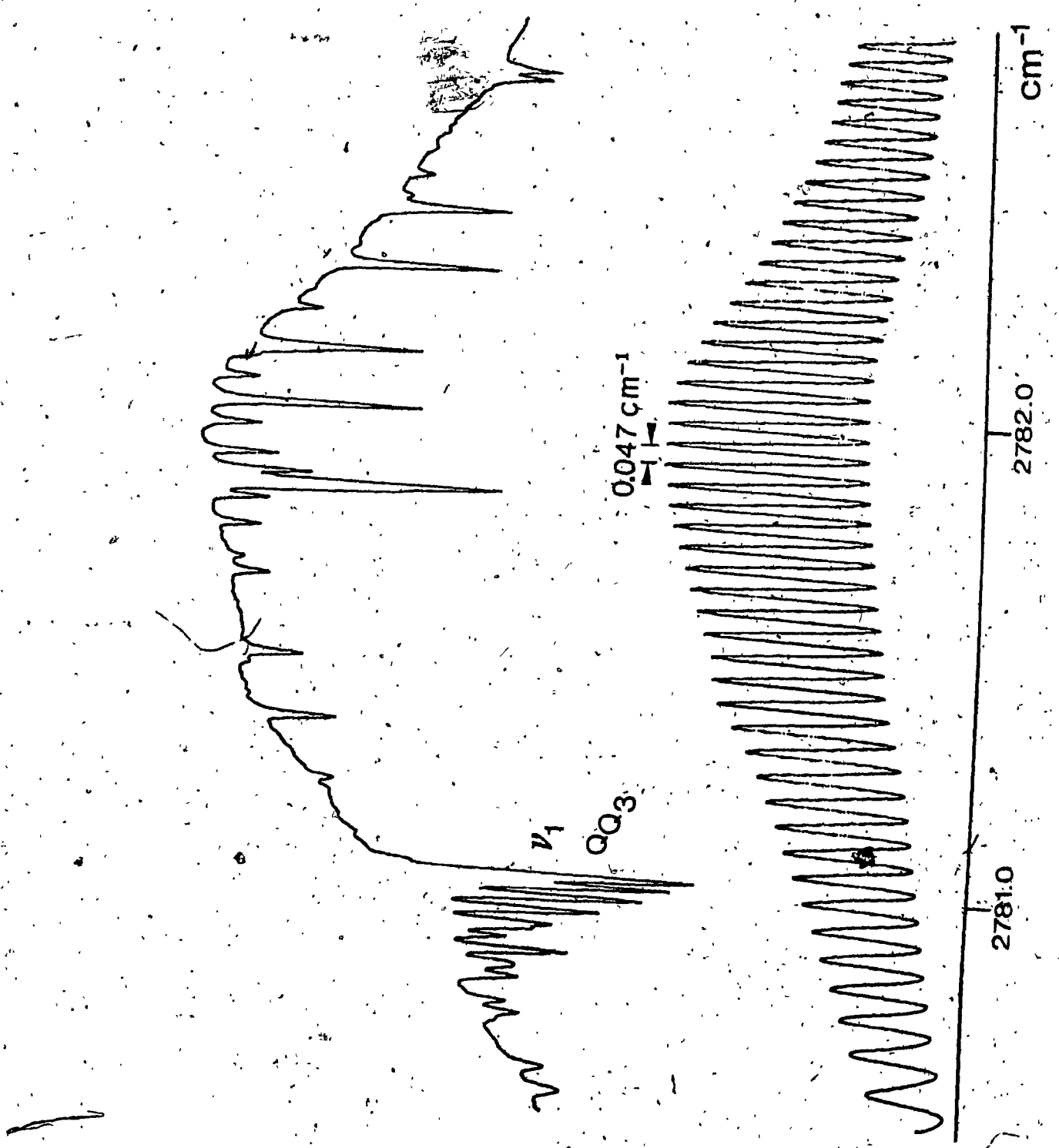
Two steps were taken to improve the lower limit of detection. The first was to switch to the 3 μm spectral region. Transitions in the ν_1 (C-H stretch) band are much stronger than those of the ν_4 and ν_6 bands [103]. The second step was to use standard 5 liter grab bags. Since the cold trap allows the analysis to be mass based rather than volume based, this increased 5 fold the the number of molecules introduced into the White cell for analysis. The reusable multilayer (polyethylene inner layer) gas sampling bags were obtained from Applied Research Products Ltd, Quebec. Samples were obtained routinely from environmental chambers at Technitrol Canada Ltd, from the McGill University Laboratory for Occupational Hygiene, and from several sites at Concordia University.

Several survey spectra were taken in the ν_1 band (Figure 6-3). The strong transitions in the $^{Q}Q_3$ sub-branch were selected for monitoring. Analytical measurements were taken only from the transition $^3{}_{3,1} \leftarrow {}^3{}_{3,0}$ (the strongest line in the branch). It should be noted here that the selection of monitoring lines in the ν_1 band is also

Figure 6-3: Survey Scans of Portions of the ν_1 Band of H_2CO in the 3 μm Region. The Strong $^QQ_3$ Branch Lines were Selected for Monitoring.

Conditions: 5 Torr H_2CO in 10 cm. cell at 24°C.


$\nu_2+\nu_4$
PQ_7
ν_1
QQ_5
0.047 cm^{-1}
ν_1
QQ_6
2778.5
2777.0


0.047 cm⁻¹
ν_1 QQ_3
2782.0
2781.0
cm⁻¹

governed by their distance from interfering H_2O lines. Hence, the $^QQ_3$ sub-branch has been chosen not only for its strong transitions but also because the nearest H_2O line is 0.4 cm^{-1} away [104]. Working with these transitions allowed determinations of < 1 ppm. The results obtained from identical sample bags however, demonstrated very poor reproducibility. Grab bags containing 1 ppm H_2CO have yielded 0.170 ppm on LTL analysis and ~0.03 ppm on TDL determinations. More importantly, the TDL results never agreed with the NIOSH determinations and it was impossible to construct calibration curves. Poor results were still obtained even after the White cell and access ports were heated (80°C) to reduce adsorption.

Since the cold trap yielded the mass of H_2CO from a given volume of air, it was decided to prepare liquid standards containing equivalent masses (1 ppb in 5 liter = 6.131×10^{-9} grams). The standard solutions were prepared by dissolving paraformaldehyde in water at 120°C (in an autoclave [105]). The concentrations were such that 1 liter contained the equivalent mass of 10 or 20 ppb in 5 liters of air. These standards produced excellent calibration curves (Figures 6-4 and 6-5) with linear correlation coefficients of R = 0.999. From the spectra observed detection limits of 6×10^{-3} absorbance units (twice the signal to noise ratio) were determined. The sensitivity determined from the slope of the Beer's plots for a 100 meter optical path length is

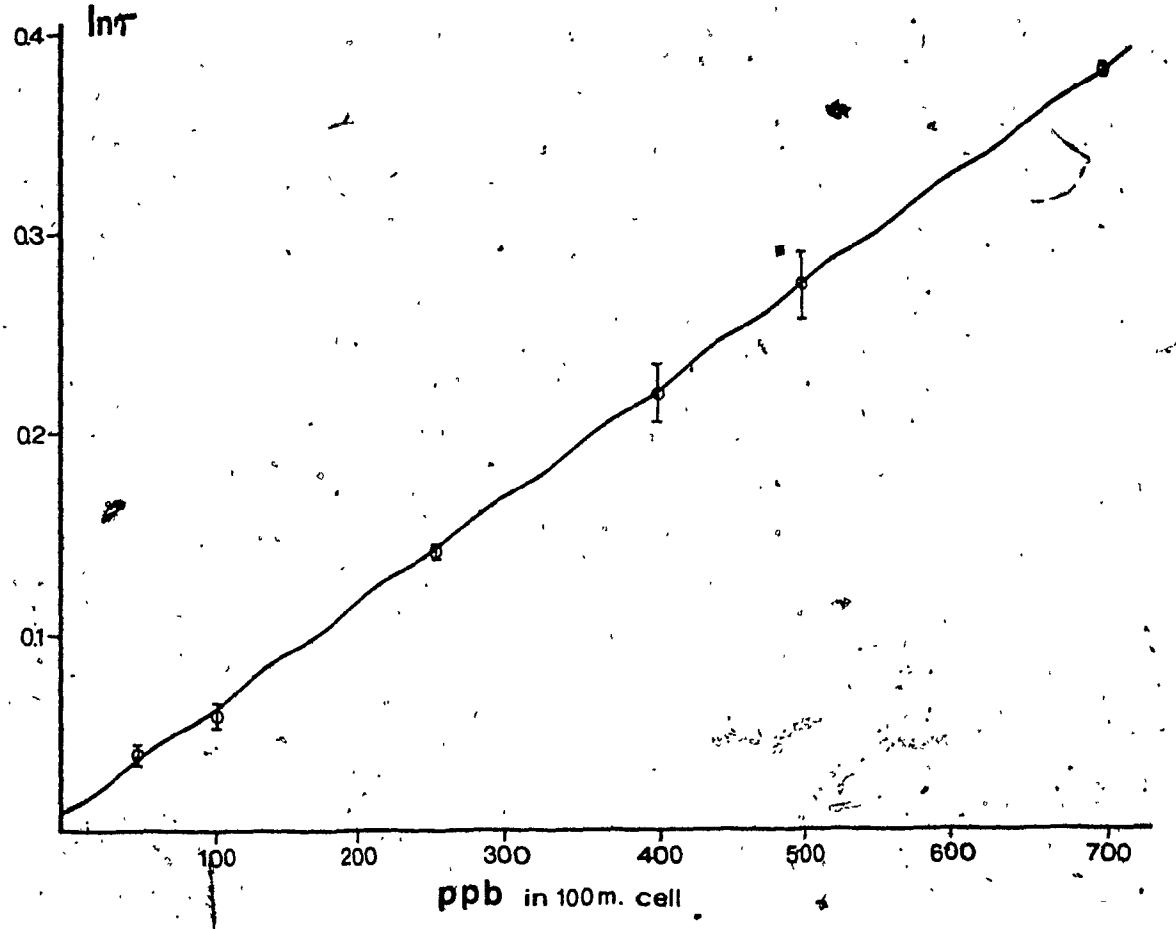


Figure 6-4: Analytical Detection Curve (Beer's plot) for the Transition $3_{3,1} \leftarrow 3_{3,0}$ of ν_1 Using Standard Solutions. The plot was constructed from the following data.

Conc. (ppb)	$\ln(I_o/I)$
50	0.039 (5)
100	0.060 (6)
250	0.142 (3)
400	0.218 (15)
500	0.273 (18)
700	0.381 (3)

* Error bars represent 1 standard deviation.

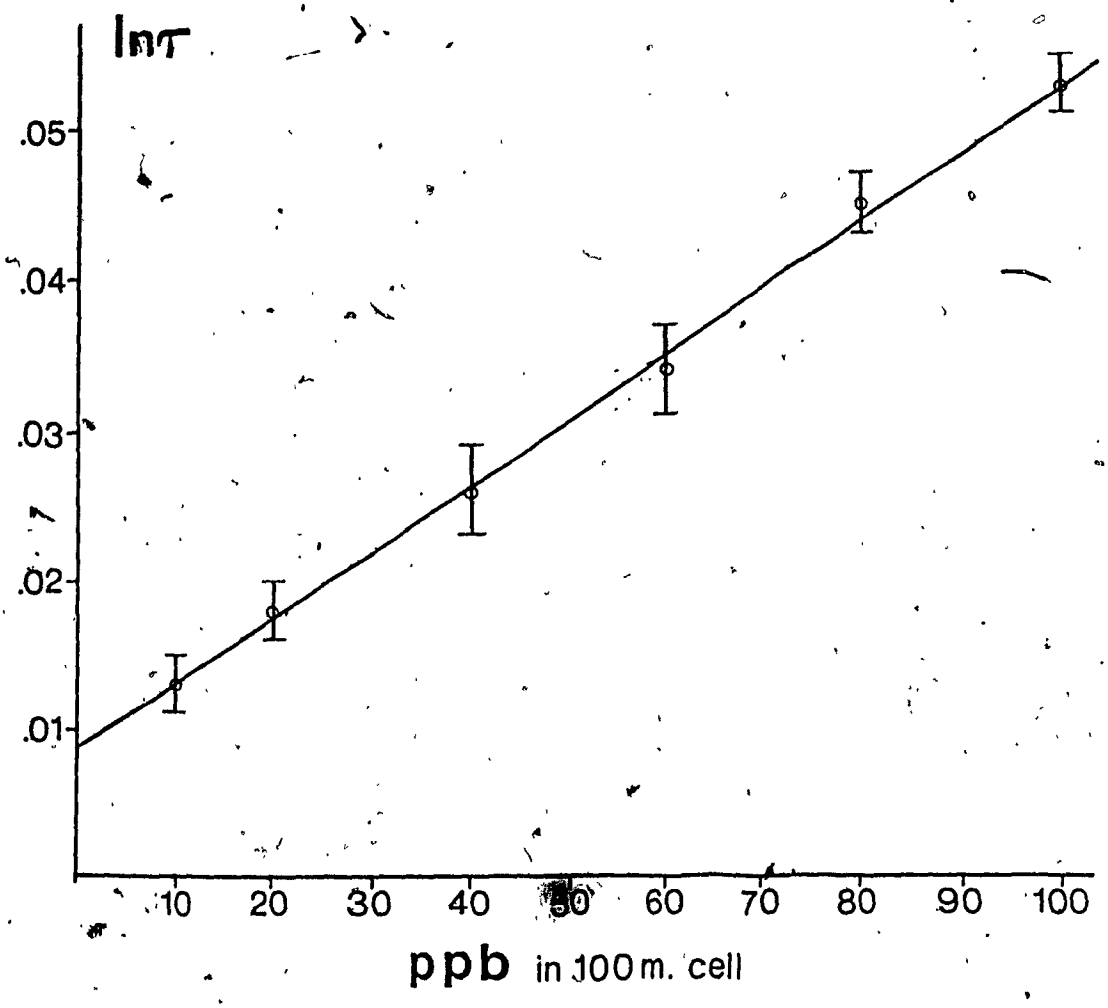


Figure 6-5: Same as Figure 6-4 but For Lower Concentration of 10-100 ppb.

The plot was constructed from the following data:

Conc. (ppb)	$\ln(I_o/I)$
10	0.013(2)
20	0.018(2)
40	0.026(3)
60	0.034(3)
80	0.045(2)
100	0.053(2)

4.4×10^{-5} m^{-1}. For the strongest line in Q_{Q_3} of ν_1 this limits the detection to ~7 ppb/v. This lower limit of detection is based on 5 liter samples. With the use of larger trap designs and by sampling larger volumes such as 10 liters or more the detection limit would come down to 5 ppb. Note, however, that the choice of sample volume is governed by the design of the cold trap, since ice (moisture from air) must be prevented from clogging the trap.

The attention was then focused on the grab bags. Using the same standard solution, an equivalent amount of 100 (and 200) ppb was evaporated into several bags. These were analyzed as a function of time spent within each bag. The 100 ppb bags were evaluated about 1/2 hour after the fill yielding an absorption of about 20 ppb. The 200 ppb bags were evaluated as shown below:

STARTING WITH 200 ppb

TIME (hrs)	YIELD
0.5	~75 ppb
3.0	~80 ppb
6.0	~60 ppb
24.0	~12 ppb

It becomes evident from this behaviour that the main cause for sample loss is due to adsorption and/or polymerization. This opinion was reinforced by proving that the cold trap is quite efficient in both trapping and delivering H_2CO molecules. The combined volume of the White cell and connecting hoses is about 16.5 liters. This volume was

evacuated and laboratory air (room air) was introduced through the cold trap to a final room pressure. Upon analysis (figure 6-6) the trapped sample yielded an absorption of $\ln(I_o/I) = 0.045(5)$. From the calibration curve (Figure 6-5) this is equivalent to 80(9) ppb. Converting this result to the equivalent mass in 5 liters yields 24±3 ppb. This was in good agreement with both the NIOSH analysis (22 ppb) and the LTL (20 ppb) results.

The formaldehyde adsorbs so readily to most surfaces that remote sampling using bulbs, grab bags, etc. seems very suspect (see trace c of Figure 6-6). If the samples are immediately processed on the site by being put into solution as in both the LTL and NIOSH techniques or via a trap in the TDL method they will be acceptable. However, storage and subsequent transportation for even a few hours will give misleading low results as demonstrated above. Eventually all results appear to show 10-20 ppb which is unfortunately close to ambient room air levels and would be interpreted as acceptable.

This problem of sampling means that a mobile system would be the optimum setup for TDL air sampling, especially for H_2CO. A layout for a proposed "Super Sniffer" system is given in the following section

6.4 The Mobile TDL "Super Sniffer" System

The proposed mobile TDL spectrometer is illustrated in

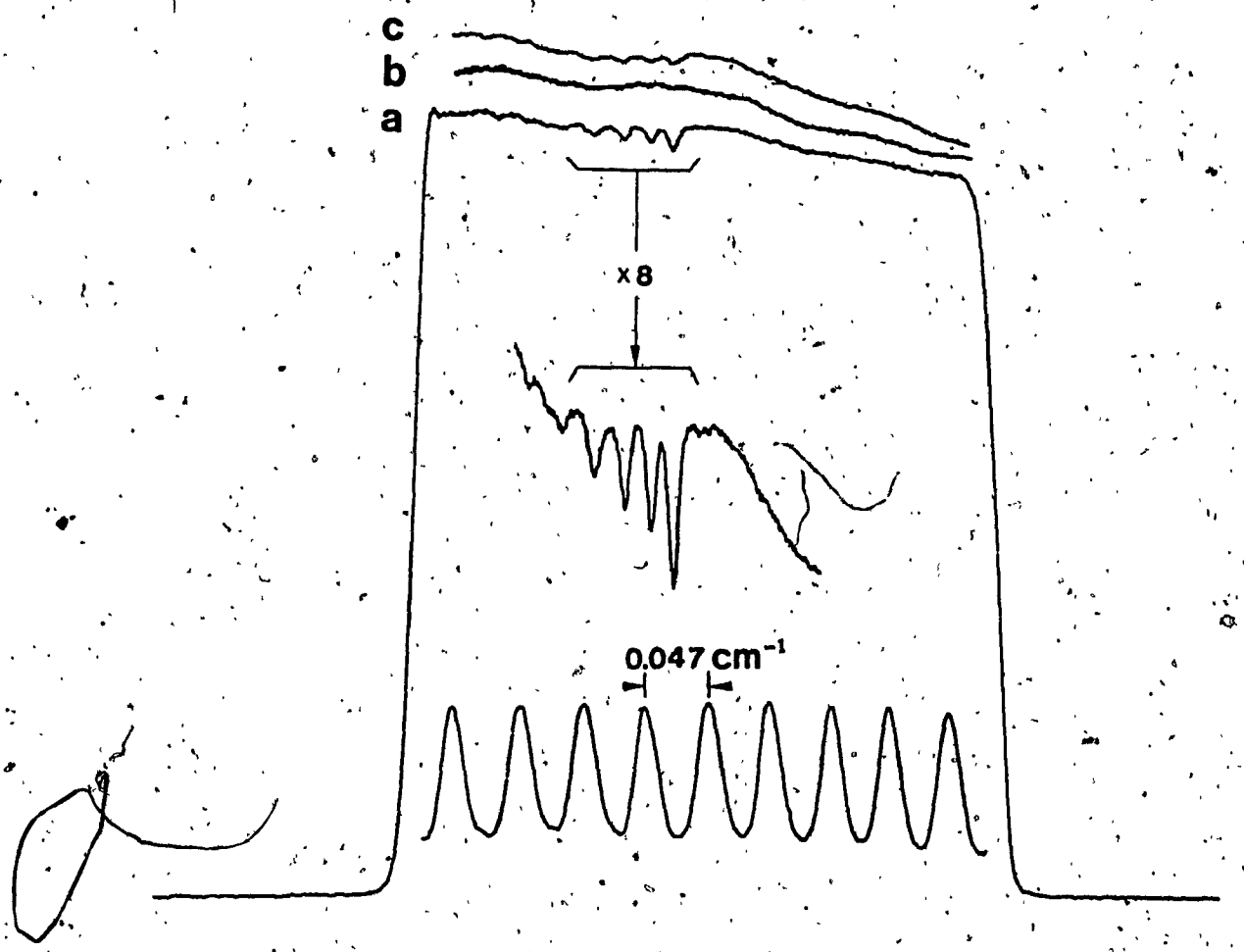


Figure 6-6: Detection of H_2CO in Laboratory air by the TDL System Using the Cold Trap and 100.17 meter Optical Path Length.

Trace a: the H_2CO absoption peaks due to $^{Q}Q_3$ transitions. Measurements were taken only for the transition $3_{3,1} \leftarrow 3_{3,0}$ (strongest line). Trace b: the background. Trace c: the desorption spectra after 3 hrs of heating the White cell under vacuum.

Figures 6-7,8,9. This Super Sniffer is a double beam, frequency locked system and completely self contained. It is flexible enough to allow flowing air methods such as have been proposed by other workers for NO_x and SO_x problems [18,19,24] as well as for a trapping system. The frequency locking allows a simpler setup than in our laboratory system. The system is double beam so that the diode lasers can be locked to a monitoring frequency from the reference cell to prevent drifting. If one wishes to apply this system to other gases besides H_2CO this is easily done. The proposed system would even allow use as a laboratory system by the installation of a small 0.25 meter monochromator if needed for selecting new monitoring frequencies. Once the proper frequencies have been chosen it could be removed for the remote field work. Systems of this type have been demonstrated already by other groups for mobile astronomical and tropospheric monitors [15,106].

An integral alignment system containing a HeNe laser and pellical beam splitter is also included. This facilitates quick alignment and peaking up the system (mobile units are in need of frequent alignment). The alignment system will also permit rapid switching of monitoring lasers. Four lasers can be mounted in the refrigerator cold head allowing the monitoring of up to four gases. The White cell can be either 0.5 or 1.0 meter in base length depending on how small a cart one wishes to construct. The analytical

pressures would be monitored by several capacitance manometers, covering the desired working range.

The electronic system (Figure 6-9) provides for feedback stabilization of the diode wavelength and if one wishes to incorporate a microcomputer then it would be possible to automate the switching between diodes to monitor more than one gas automatically. The system would use HgCdTe detectors for work in the 5-16 μm range and InSb detectors in the 3-5 μm region.

In summary, the proposed mobile Super Sniffer would be a multi-purpose state-of-the-art analytical spectrometer. The system could be easily upgraded and/or modified to meet specific needs. The size of the unit would be governed mainly by the choice of White cell. e.g. using a 1 meter cell the dimensions would be l=1.5 m, h=1.0 m, and w=0.85 m. The system has been designed to be self contained except for plugging in to the electrical outlet where it is used. Requirements are for 110V for everything except the helium compressor which requires 220V. The design is more elaborate than that used by other groups with the intention that it can double as the laboratory system.

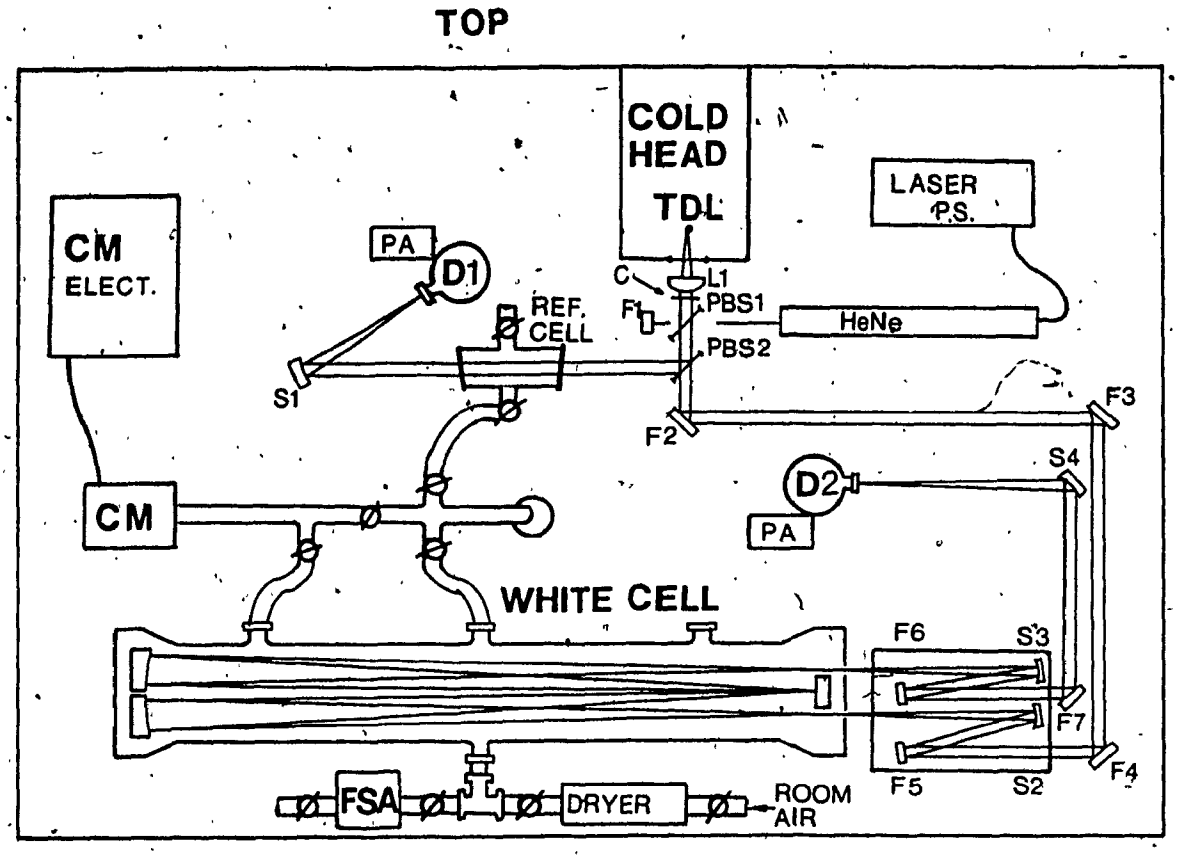


Figure 6-7: Top View of the Proposed Mobile TDL System; The "Super Sniffer".

The labels are interpreted as: detectors (D1, D2), diode lasers (TDL), capacitance manometer (CM), formaldehyde sampling apparatus (FSA), flat mirrors (F1-F7), spherical mirrors (S1-S4), pellical beam splitter (PBS1), ZnSe beam splitter (PBS2), chopper (C), KBr lens (L1), and preamplifiers (PA). The scale is mainly determined by the base length of the White cell (0.5 m or 1.0 m).

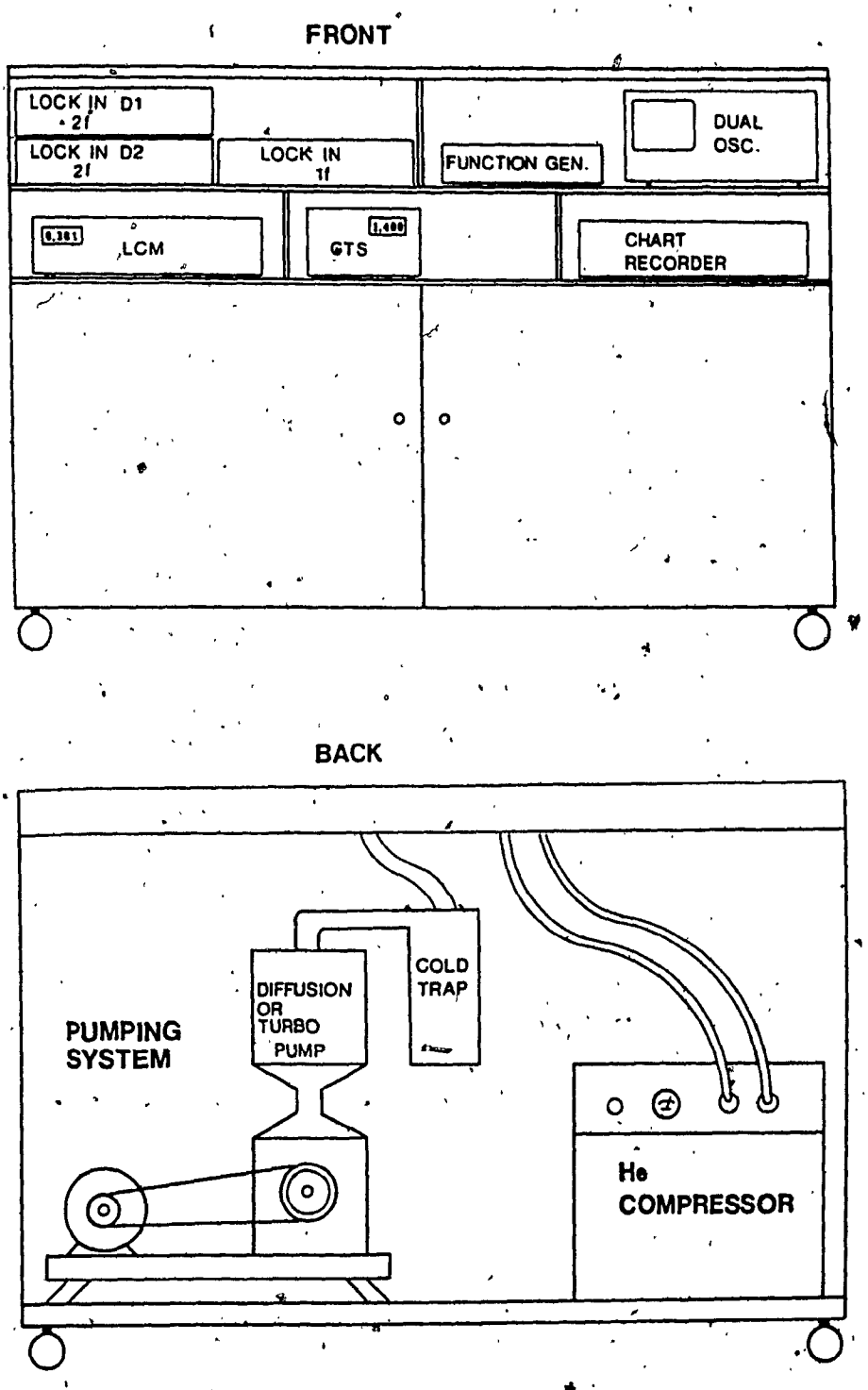


Figure 6-8: Side Views of the Mobile TDL System.

The CTS is the laser temperature control and the LCM is the laser current control.

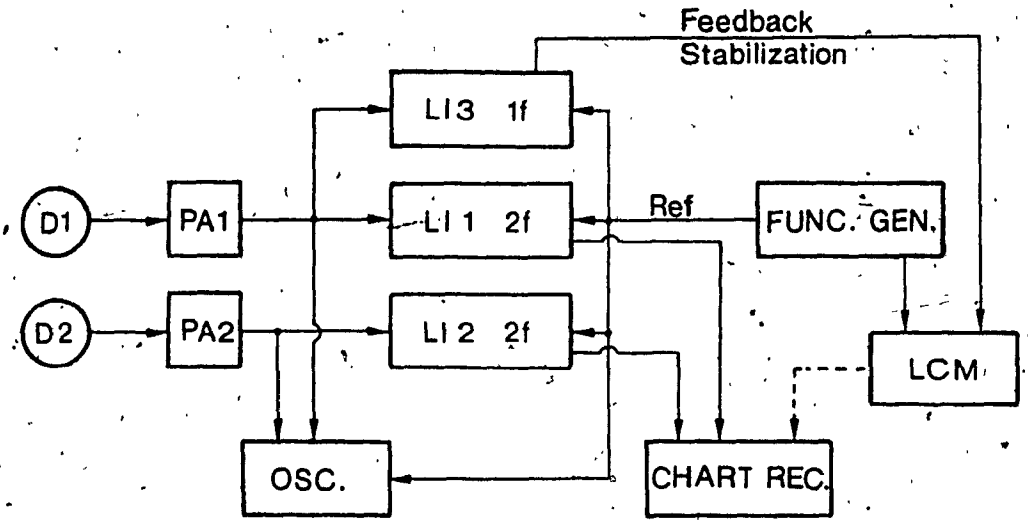


Figure 6-9: Schematic of the System Electronic Connections.

These in fact can be varied in several ways so that the system can operate with a chopper in slow scan modes or with freguency modulation at 1f or 2f. LI1-LI3 are the lock-in amplifiers. In this configuration, LI3 is used for frequency locking while LI1 and LI2 are used for 2f point monitoring of sample and reference signal.

CHAPTER 7

GENERAL CONCLUSIONS AND SUGGESTIONS FOR FUTURE RESEARCH

7.1 Conclusions

7.1.1 The Molecular Constants of Formaldehyde

The simultaneous least-squares fitting of transitions in the ν_3, ν_4 and ν_6 bands yielded excellent results (σ_P=0.00093 cm^{-1}). Both the sixth order (Hamiltonian) and the third order Coriolis interaction constants are reported for the first time. High correlation between some of the rotational constant lead to redundancy in the fitting process. That is to say, different sets of molecular constants yield the same results. Each set, however, may be used to predict with great accuracy all the wavenumbers for transitions up to J'=30 and K_a'=8. Means to reduce the computational redundancies are proposed in section 7.2.

In light of these redundancies as well as the fact that direct measurements of line strengths in the ν_3 band were not available, the dipole moment derivatives obtained in this work should be considered tentative. Similar consideration should be given to the reported band strengths, remembering that these depend both on the dipole moment derivatives and the eigenvectors obtained from the least-squares fittings.

7.1.2 Line Strengths and Foreign-Gas Pressure Broadening

This study reports tunable diode laser measurements of several transitions in the ν_4 and ν_6 bands of H_2CO. Line strengths and foreign-gas (air, N_2, O_2 and H_2) broadening coefficients for these bands are reported for the first time. The Doppler-limited spectra obtained using the diode laser spectrometer facilitated straightforward data analysis and evaluation of absorption parameters. The broadening coefficients for air, N_2, O_2, and H_2 compare favorably with reported microwave and theoretical values.

7.1.3 Analytical

The trace analysis technique developed here is capable of detecting formaldehyde in ambient air at the low ppb levels. The mass based technique allows for analysis in relatively shorter optical path lengths. The lower limits of detection (~7 ppb) for formaldehyde obtained in this work is similar to the results obtained by other workers for N_2O [107,108], NO_2, and SO_2 [18,19,24]. Sampling and calibration problems have been reported for these gases as well, although they are are not as difficult to handle as H_2CO.

Based on existing technology the construction of a mobile TDL "Super Sniffer" system is proposed. This is a multi-faceted system easily modified to suit the particular needs. For the specific application of H_2CO detection the

sniffer may be equipped with several detachable cold traps and a sampling pump (with control for the rate of intake). This will facilitate analysis at locations with difficult access.

7.2 Suggestions for Future Research

From the results and conclusions drawn in this thesis, as well as from the work of other researchers, the scope and range of application of TDL's is obvious. The following suggestions pertain specifically to the study of the H_2CO molecule. In order to close the present stage of work on the 10 μm region of H_2CO we suggest the following additional research.

Line strengths for transitions in the ν_3 band should be measured. This would allow an accurate evaluation of the dipole moment derivative for this band. That in turn, would give a more accurate value of the ν_3 band strength and the extent of its interaction with ν_4 and ν_6. At that point a complete spectrum for the 10 μm region could be generated. This would reduce the problem encountered in the least-squares fitting by pinpointing the most suitable molecular constants for the three bands, i.e. help find the set of constants that yields a calculated spectrum closest to the observed.

Both sets of rotational constants obtained and described in this thesis yielded similar results. For high J values and $K_a > 8$ these sets of constants also differ in their prediction of transition wavenumbers. These are weak transitions and consequently did not appear in the FT-IR spectra studied in this thesis. Thus, we suggest that the spectra of several selected sections of the 10 μm region should be recorded at higher sample (H_2CO) pressur-pathlength. This will facilitate the identification of the weaker transitions and again help to isolate a final set of molecular constants.

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Appendix A

A.1 Least-Squares-Fitting: Results for Fit A

The molecular constants obtained from fit A were described in chapter 5. Consequently, The following pertains only to the comparison of observed and calculated wavenumbers obtained from this fit.

The observed and calculated wavenumbers are listed in Table A-1. The observed transitions were assigned their respective weights as follows: all transitions up to $J'=15$ and $K_a'=5$ were assigned a standard deviation of 0.0005 cm^{-1}, the standard deviation for the higher J and K_a transitions were estimated to be 0.001 cm^{-1}.

Table A-1: Observed vs. Calculated Results From Fit A.

a. Number in bracket is the band identifier.

b. PREC. refers to the standard deviation of the observation.

c. RESID = Observed-Calculated.

d. The symbol * denotes blended transitions. These lines were not included in the fit.

Continues ....

a						b		c											
UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.	UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC														
(4)	21	8	14	-	22	9	14	922.6348	0.001	922.6355	-0.0007	(4)	11	7	5	-	12	8	5	972.8038	0.001	972.8044	-0.0007
(4)	21	8	13	-	22	9	13	922.6348	0.001	922.6355	-0.0007	(4)	11	7	4	-	12	8	4	972.8038	0.001	972.8044	-0.0007
(4)	20	8	13	-	21	9	13	925.1591	0.001	925.1590	0.0001	(4)	20	6	15	-	21	7	15	975.1214	0.001	975.1219	-0.0006
(4)	20	8	12	-	21	9	12	925.1591	0.001	925.1590	0.0001	(4)	20	6	14	-	21	7	14	975.1214	0.001	975.1213	0.0001
(4)	19	8	12	-	20	9	12	927.6804	0.001	927.6802	0.0003	(4)	10	7	4	-	11	8	4	975.2964	0.001	975.2972	-0.0008
(4)	19	8	11	-	20	9	11	927.6804	0.001	927.6802	0.0003	(4)	10	7	3	-	11	8	3	975.2964	0.001	975.2972	-0.0008
(4)	18	8	11	-	19	9	11	930.1990	0.001	930.1987	0.0004	(4)	23	8	16	-	23	9	14	975.6695	0.001	975.6702	-0.0008
(4)	18	8	10	-	19	9	10	930.1990	0.001	930.1987	0.0004	(4)	23	8	15	-	23	9	15	975.6695	0.001	975.6703	-0.0008
(4)	17	8	10	-	18	9	10	932.7145	0.001	932.7141	0.0004	(4)	22	8	15	-	22	9	13	975.7816	0.001	975.7819	-0.0003
(4)	17	8	9	-	18	9	9	932.7145	0.001	932.7141	0.0004	(4)	22	8	14	-	22	9	14	975.7816	0.001	975.7819	-0.0003
(4)	16	8	8	-	17	9	8	935.2267	0.001	935.2263	0.0003	(4)	21	8	14	-	21	9	12	975.8913	0.001	975.8914	-0.0001
(4)	16	8	9	-	17	9	9	935.2267	0.001	935.2263	0.0003	(4)	21	8	13	-	21	9	13	975.8913	0.001	975.8914	-0.0001
(4)	15	8	8	-	16	9	8	937.7353	0.001	937.7349	0.0003	(4)	20	8	13	-	20	9	11	975.9985	0.001	975.9982	0.0003
(4)	15	8	7	-	16	9	7	937.7353	0.001	937.7349	0.0003	(4)	20	8	12	-	20	9	12	975.9985	0.001	975.9982	0.0003
(4)	14	8	7	-	15	9	7	940.2401	0.001	940.2397	0.0004	(4)	19	8	12	-	19	9	10	976.1028	0.001	976.1021	0.0007
(4)	14	8	6	-	15	9	6	940.2401	0.001	940.2397	0.0004	(4)	19	8	11	-	19	9	11	976.1028	0.001	976.1021	0.0007
(4)	13	8	6	-	14	9	6	942.7404	0.001	942.7402	0.0001	(4)	18	8	11	-	18	9	9	976.2034	0.001	976.2028	0.0006
(4)	13	8	5	-	14	9	5	942.7404	0.001	942.7402	0.0001	(4)	18	8	10	-	18	9	10	976.2034	0.001	976.2028	0.0006
(4)	12	8	5	-	13	9	5	945.2364	0.001	945.2364	0.0000	(4)	17	8	10	-	17	9	8	976.3009	0.001	976.3001	0.0008
(4)	12	8	4	-	13	9	4	945.2364	0.001	945.2364	0.0000	(4)	17	8	9	-	17	9	9	976.3009	0.001	976.3001	0.0008
(4)	11	8	4	-	12	9	4	947.7279	0.001	947.7280	0.0000	(4)	16	8	9	-	16	9	7	976.3943	0.001	976.3935	0.0009
(4)	11	8	3	-	12	9	3	947.7279	0.001	947.7280	0.0000	(4)	16	8	8	-	16	9	8	976.3943	0.001	976.3935	0.0009
(4)	10	8	3	-	11	9	3	950.2144	0.001	950.2146	-0.0002	(4)	15	8	8	-	15	9	6	976.4835	0.001	976.4828	0.0007
(4)	10	8	2	-	11	9	2	950.2144	0.001	950.2146	-0.0002	(4)	15	8	7	-	15	9	7	976.4835	0.001	976.4828	0.0007
(4)	9	8	2	-	10	9	2	952.6960	0.001	952.6962	-0.0003	(4)	14	8	7	-	14	9	5	976.5686	0.001	976.5679	0.0007
(4)	9	8	1	-	10	9	1	952.6960	0.001	952.6962	-0.0003	(4)	14	8	6	-	14	9	6	976.5686	0.001	976.5679	0.0007
(4)	19	7	13	-	20	8	13	952.7150	0.001	952.7159	-0.0009	(4)	13	8	6	-	13	9	4	976.6490	0.001	976.6484	0.0006
(4)	19	7	12	-	20	8	12	952.7150	0.001	952.7159	-0.0009	(4)	13	8	5	-	13	9	5	976.6490	0.001	976.6484	0.0006
(4)	8	8	1	-	9	9	1	955.1721	0.001	955.1726	-0.0004	(4)	12	8	5	-	12	9	3	976.7246	0.001	976.7241	0.0004
(4)	8	8	0	-	9	9	0	955.1721	0.001	955.1726	-0.0004	(4)	12	8	4	-	12	9	4	976.7246	0.001	976.7241	0.0004
(4)	18	7	12	-	19	8	12	955.2366	0.001	955.2375	-0.0009	(4)	11	8	4	-	11	9	2	976.7953	0.001	976.7949	0.0004
(4)	18	7	11	-	19	8	11	955.2366	0.001	955.2375	-0.0009	(4)	11	8	3	-	11	9	3	976.7953	0.001	976.7949	0.0004
(4)	17	7	11	-	18	8	11	957.7565	0.001	957.7569	-0.0004	(4)	10	8	3	-	10	9	1	976.8604	0.001	976.8604	0.0000
(4)	17	7	10	-	18	8	10	957.7565	0.001	957.7569	-0.0004	(4)	10	8	2	-	10	9	2	976.8604	0.001	976.8604	0.0000
(4)	16	7	10	-	17	8	10	960.2732	0.001	960.2738	-0.0006	(4)	9	8	2	-	9	9	0	976.9206	0.001	976.9206	0.0000
(4)	16	7	9	-	17	8	9	960.2732	0.001	960.2738	-0.0006	(4)	9	8	1	-	9	9	1	976.9206	0.001	976.9206	0.0000
(4)	15	7	9	-	16	8	9	962.7869	0.001	962.7876	-0.0007	(4)	19	6	14	-	20	7	14	977.6332	0.001	977.6336	-0.0003
(4)	15	7	8	-	16	8	8	962.7869	0.001	962.7876	-0.0007	(4)	19	6	13	-	20	7	13	977.6332	0.001	977.6332	0.0000
(4)	14	7	8	-	15	8	8	965.2974	0.001	965.2980	-0.0006	(4)	9	7	3	-	10	8	3	977.7839	0.001	977.7848	-0.0009
(4)	14	7	7	-	15	8	7	965.2974	0.001	965.2980	-0.0006	(4)	9	7	2	-	10	8	2	977.7839	0.001	977.7848	-0.0009
(4)	23	6	18	-	24	7	18	967.6066	0.001	967.6086	-0.0020	(4)	18	6	13	-	19	7	13	980.1468	0.001	980.1469	-0.0001
(4)	23	6	17	-	24	7	17	967.6066	0.001	967.6053	0.0013	(4)	18	6	12	-	19	7	12	980.1468	0.001	980.1468	0.0000
(4)	13	7	7	-	14	8	7	967.8038	0.001	967.8045	-0.0006	(4)	8	7	2	-	9	8	2	980.2659	0.001	980.2668	-0.0009
(4)	13	7	6	-	14	8	6	967.8038	0.001	967.8045	-0.0006	(4)	8	7	1	-	9	8	1	980.2659	0.001	980.2668	-0.0009
(4)	22	6	17	-	23	7	17	970.1068	0.001	970.1082	-0.0014	(4)	17	6	12	-	18	7	12	982.6609	0.001	982.6610	-0.0001
(4)	22	6	16	-	23	7	16	970.1068	0.001	970.1063	0.0005	(4)	17	6	11	-	18	7	11	982.6609	0.001	982.6610	-0.0001
(4)	12	7	6	-	13	8	6	970.3061	0.001	970.3067	-0.0007	(4)	7	7	1	-	8	8	1	982.7421	0.001	982.7432	-0.0010
(4)	12	7	5	-	13	8	5	970.3061	0.001	970.3067	-0.0007	(4)	7	7	0	-	8	8	0	982.7421	0.001	982.7432	-0.0010
(4)	21	6	16	-	22	7	16	972.6122	0.001	972.6131	-0.0009	(4)	16	6	11	-	17	7	11	985.1749	0.001	985.1750	-0.0001
(4)	21	6	15	-	22	7	15	972.6122	0.001	972.6120	0.0002	(4)	16	6	10	-	17	7	10	985.1749	0.001	985.1750	0.0000

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(4)	15	6	10	-	16	7	10	987.6880	0.001	987.6879	0.0001
(4)	15	6	9	-	16	7	9	987.6880	0.001	987.6879	0.0001
(4)	14	6	9	-	15	7	9	990.1993	0.001	990.1991	0.0002
(4)	14	6	8	-	15	7	8	990.1993	0.001	990.1991	0.0002
(4)	13	6	8	-	14	7	8	992.7078	0.001	992.7078	0.0000
(4)	13	6	7	-	14	7	7	992.7078	0.001	992.7078	0.0000
(4)	12	6	7	-	13	7	7	995.2134	0.001	995.2133	0.0001
(4)	12	6	6	-	13	7	6	995.2134	0.001	995.2133	0.0001
(4)	11	6	6	-	12	7	6	997.7151	0.001	997.7150	0.0001
(4)	11	6	5	-	12	7	5	997.7151	0.001	997.7150	0.0001
(4)	20	5	16	-	21	6	16	1000.2022	0.001	1000.2013	0.0008
(4)	10	6	5	-	11	7	5	1000.2125	0.001	1000.2124	0.0001
(4)	10	6	4	-	11	7	4	1000.2125	0.001	1000.2124	0.0001
(4)	19	7	13	-	19	8	11	1001.1777	0.001	1001.1783	-0.0006
(4)	19	7	12	-	19	8	12	1001.1777	0.001	1001.1784	-0.0006
(4)	18	7	12	-	18	8	10	1001.2789	0.001	1001.2791	-0.0003
(4)	18	7	11	-	18	8	11	1001.2789	0.001	1001.2792	-0.0003
(4)	17	7	11	-	17	8	9	1001.3773	0.001	1001.3775	-0.0002
(4)	17	7	10	-	17	8	10	1001.3773	0.001	1001.3775	-0.0002
(4)	16	7	10	-	16	8	8	1001.4726	0.001	1001.4729	-0.0002
(4)	16	7	9	-	16	8	9	1001.4726	0.001	1001.4729	-0.0002
(4)	15	7	9	-	15	8	7	1001.5646	0.001	1001.5649	-0.0003
(4)	15	7	8	-	15	8	8	1001.5646	0.001	1001.5649	-0.0003
(4)	14	7	8	-	14	8	6	1001.6529	0.001	1001.6531	-0.0002
(4)	14	7	7	-	14	8	7	1001.6529	0.001	1001.6531	-0.0002
(4)	13	7	7	-	13	8	5	1001.7368	0.001	1001.7372	-0.0004
(4)	13	7	6	-	13	8	6	1001.7368	0.001	1001.7372	-0.0004
(4)	12	7	6	-	12	8	4	1001.8163	0.001	1001.8169	-0.0006
(4)	12	7	5	-	12	8	5	1001.8163	0.001	1001.8169	-0.0006
(4)	11	7	5	-	11	8	3	1001.8913	0.001	1001.8916	-0.0003
(4)	11	7	4	-	11	8	4	1001.8913	0.001	1001.8916	-0.0003
(4)	10	7	4	-	10	8	2	1001.9607	0.001	1001.9613	-0.0005
(4)	10	7	3	-	10	8	3	1001.9607	0.001	1001.9613	-0.0005
(4)	9	7	3	-	9	8	1	1002.0250	0.001	1002.0255	-0.0004
(4)	9	7	2	-	9	8	2	1002.0250	0.001	1002.0255	-0.0004
(4)	19	5	14	-	20	6	14	1002.5332	0.001	1002.5328	0.0004
(4)	19	5	15	-	20	6	15	1002.5936	0.001	1002.5933	0.0004
(4)	9	6	4	-	10	7	4	1002.7050	0.001	1002.7049	0.0001
(4)	9	6	3	-	10	7	3	1002.7050	0.001	1002.7049	0.0001
(4)	18	5	13	-	19	6	13	1004.9795	0.001	1004.9795	0.0000
(4)	18	5	14	-	19	6	14	1005.0146	0.001	1005.0144	0.0002
(4)	8	6	3	-	9	7	3	1005.1918	0.001	1005.1921	-0.0003
(4)	8	6	2	-	9	7	2	1005.1918	0.001	1005.1921	-0.0003
(4)	26	4	23	-	27	5	23	1006.6618	0.001	1006.6617	0.0000
(4)	17	5	12	-	18	6	12	1007.4384	0.001	1007.4381	0.0003
(4)	17	5	13	-	18	6	13	1007.4577	0.001	1007.4575	0.0002
(4)	7	6	2	-	8	7	2	1007.6732	0.001	1007.6735	-0.0003
(4)	7	6	1	-	8	7	1	1007.6732	0.001	1007.6735	-0.0003
(4)	25	4	22	-	26	5	22	1009.4046	0.001	1009.4048	-0.0002
(4)	16	5	11	-	17	6	11	1009.9072	0.001	1009.9067	0.0005

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(4)	16	5	12	-	17	6	12	1009.9175	0.001	1009.9172	0.0003
(4)	6	6	1	-	7	7	1	1010.1488	0.001	1010.1488	0.0000
(4)	6	6	0	-	7	7	0	1010.1488	0.001	1010.1488	0.0000
(4)	24	4	21	-	25	5	21	1012.1227	0.001	1012.1229	-0.0002
(4)	15	5	11	-	16	6	11	1012.3855	0.001	1012.3892	-0.0037
(4)	15	5	10	-	16	6	10	1012.3855	0.001	1012.3837	0.0018
(4)	23	4	19	-	24	5	19	1013.0020	0.001	1013.0014	0.0006
(4)	23	4	20	-	24	5	20	1014.8194	0.001	1014.8197	-0.0004
(4)	14	5	10	-	15	6	10	1014.8690	0.001	1014.8698	-0.0008
(4)	14	5	9	-	15	6	9	1014.8690	0.001	1014.8671	0.0019
(4)	22	4	18	-	23	5	18	1016.0448	0.001	1016.0447	0.0002
(4)	13	5	9	-	14	6	9	1017.3561	0.001	1017.3565	-0.0003
(4)	13	5	8	-	14	6	8	1017.3561	0.001	1017.3552	0.0009
(4)	22	4	19	-	23	5	19	1017.4980	0.001	1017.4982	-0.0002
(4)	21	4	17	-	22	5	17	1019.0128	0.001	1019.0126	0.0002
(4)	12	5	8	-	13	6	8	1019.8468	0.001	1019.8467	0.0001
(4)	12	5	7	-	13	6	7	1019.8468	0.001	1019.8461	0.0007
(4)	21	4	18	-	22	5	18	1020.1607	0.001	1020.1610	-0.0003
(4)	20	4	16	-	21	5	16	1021.9158	0.001	1021.9158	0.0001
(4)	11	5	7	-	12	6	7	1022.3388	0.001	1022.3385	0.0003
(4)	11	5	6	-	12	6	6	1022.3388	0.001	1022.3383	0.0005
(4)	20	4	17	-	21	5	17	1022.8101	0.001	1022.8105	-0.0004
(4)	19	4	15	-	20	5	15	1024.7630	0.001	1024.7631	-0.0001
(4)	10	5	6	-	11	6	6	1024.8307	0.001	1024.8303	0.0004
(4)	10	5	5	-	11	6	5	1024.8307	0.001	1024.8302	0.0005
(4)	19	4	16	-	20	5	16	1025.4480	0.001	1025.4483	-0.0003
(4)	23	6	18	-	23	7	16	1025.8066	0.001	1025.8086	-0.0020
(4)	23	6	17	-	23	7	17	1025.8066	0.001	1025.8053	0.0013
(4)	22	6	17	-	22	7	15	1025.8835	0.001	1025.8845	-0.0010
(4)	22	6	16	-	22	7	16	1025.8835	0.001	1025.8826	0.0009
(4)	21	6	16	-	21	7	14	1025.9650	0.001	1025.9656	-0.0006
(4)	21	6	15	-	21	7	15	1025.9650	0.001	1025.9645	0.0005
(4)	20	6	15	-	20	7	13	1026.0504	0.001	1026.0505	-0.0001
(4)	20	6	14	-	20	7	14	1026.0504	0.001	1026.0499	0.0005
(4)	19	6	14	-	19	7	12	1026.1380	0.001	1026.1380	0.0000
(4)	19	6	13	-	19	7	13	1026.1380	0.001	1026.1377	0.0003
(4)	18	6	13	-	18	7	11	1026.2272	0.001	1026.2271	0.0001
(4)	18	6	12	-	18	7	12	1026.2272	0.001	1026.2269	0.0003
(4)	17	6	12	-	17	7	10	1026.3169	0.001	1026.3167	0.0001
(4)	17	6	11	-	17	7	11	1026.3169	0.001	1026.3167	0.0002
(4)	16	6	11	-	16	7	9	1026.4063	0.001	1026.4061	0.0002
(4)	16	6	10	-	16	7	10	1026.4063	0.001	1026.4061	0.0002
(4)	15	6	10	-	15	7	8	1026.4945	0.001	1026.4943	0.0002
(4)	15	6	9	-	15	7	9	1026.4945	0.001	1026.4943	0.0002
(4)	14	6	9	-	14	7	7	1026.5809	0.001	1026.5807	0.0002
(4)	14	6	8	-	14	7	8	1026.5809	0.001	1026.5807	0.0002
(4)	13	6	8	-	13	7	6	1026.6645	0.001	1026.6644	0.0001
(4)	13	6	7	-	13	7	7	1026.6645	0.001	1026.6644	0.0001
(4)	12	6	7	-	12	7	5	1026.7451	0.001	1026.7449	0.0002
(4)	12	6	6	-	12	7	6	1026.7451	0.001	1026.7449	0.0002

UPPER STATE			LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(4)	11	6	6 -	11	7	4	1026.8214	0.001	1026.8214	0.0000
(4)	11	6	5 -	11	7	5	1026.8214	0.001	1026.8214	0.0000
(4)	10	6	5 -	10	7	3	1026.8937	0.001	1026.8936	0.0002
(4)	10	6	4 -	10	7	4	1026.8937	0.001	1026.8936	0.0002
(4)	9	6	4 -	9	7	2	1026.9608	0.001	1026.9608	0.0001
(4)	9	6	3 -	9	7	3	1026.9608	0.001	1026.9608	0.0001
(4)	8	6	3 -	8	7	1	1027.0227	0.001	1027.0226	0.0001
(4)	8	6	2 -	8	7	2	1027.0227	0.001	1027.0226	0.0001
(4)	7	6	2 -	7	7	0	1027.0785	0.001	1027.0786	-0.0001
(4)	7	6	1 -	7	7	1	1027.0785	0.001	1027.0786	-0.0001
(4)	9	5	5 -	11	6	5	1027.3208	0.001	1027.3204	0.0003
(4)	9	5	4 -	11	6	4	1027.3208	0.001	1027.3204	0.0003
(4)	18	4	14 -	19	5	14	1027.5621	0.001	1027.5621	0.0000
(4)	18	4	15 -	19	5	15	1028.0758	0.001	1028.0761	-0.0003
(4)	8	5	4 -	9	6	4	1029.8082	0.001	1029.8077	0.0004
(4)	8	5	3 -	9	6	3	1029.8082	0.001	1029.8077	0.0004
(4)	17	4	13 -	18	5	13	1030.3186	0.001	1030.3187	-0.0001
(4)	17	4	14 -	18	5	14	1030.6945	0.001	1030.6948	-0.0003
(4)	7	5	3 -	8	6	3	1032.2911	0.001	1032.2910	0.0001
(4)	7	5	2 -	8	6	2	1032.2911	0.001	1032.2910	0.0001
(4)	16	4	12 -	17	5	12	1033.0377	0.001	1033.0380	-0.0003
(4)	16	4	13 -	17	5	13	1033.3047	0.001	1033.3051	-0.0003
(4)	6	5	2 -	7	6	2	1034.7696	0.001	1034.7694	0.0002
(4)	6	5	1 -	7	6	1	1034.7696	0.001	1034.7694	0.0002
(4)	15	4	11 -	16	5	11	1035.7238	0.001	1035.7240	-0.0002
(4)	15	4	12 -	16	5	12	1035.9068	0.001	1035.9070	-0.0002
(4)	23	3	21 -	24	4	21	1036.9711	0.001	1036.9701	0.0010
(4)	5	5	1 -	6	6	1	1037.2421	0.001	1037.2419	0.0003
(4)	5	5	0 -	6	6	0	1037.2421	0.001	1037.2419	0.0003
(4)	14	4	10 -	15	5	10	1038.3800	0.001	1038.3803	-0.0002
(4)	14	4	11 -	15	5	11	1038.5006	0.001	1038.5005	0.0001
(4)	22	3	20 -	23	4	20	1039.9180	0.001	1039.9177	0.0003
(4)	13	4	9 -	14	5	9	1041.0093	0.001	1041.0096	-0.0003
(4)	13	4	10 -	14	5	10	1041.0845	0.001	1041.0847	-0.0002
(4)	21	3	19 -	22	4	19	1042.8039	0.001	1042.8038	0.0001
(4)	12	4	8 -	13	5	8	1043.6143	0.001	1043.6145	-0.0002
(4)	22	4	9 -	13	5	9	1043.6589	0.001	1043.6588	0.0001
(4)	21	3	18 -	22	4	18	1044.3918	0.001	1044.3906	0.0012
(4)	25	2	24 -	26	3	24	1045.0218	0.001	1045.0253	-0.0035
(4)	20	3	18 -	21	4	18	1045.6344	0.001	1045.6347	-0.0003
(4)	11	4	7 -	12	5	7	1046.1972	0.001	1046.1973	-0.0001
(4)	11	4	8 -	12	5	8	1046.2216	0.001	1046.2217	-0.0001
(4)	20	3	17 -	21	4	17	1047.0629	0.001	1047.0626	0.0004
(4)	19	3	17 -	20	4	17	1048.4160	0.001	1048.4164	-0.0004
(4)	10	4	6 -	11	5	6	1048.7601	0.001	1048.7600	0.0001
(4)	10	4	7 -	11	5	7	1048.7721	0.001	1048.7723	-0.0002
(4)	9	6	4 -	8	7	2	1048.7721*	0.000	1048.7913	-0.0191
(4)	9	6	3 -	8	7	1	1048.7721*	0.000	1048.7913	-0.0191
(4)	24	2	23 -	25	3	23	1048.9447	0.001	1048.9413	0.0035
(4)	19	3	16 -	20	4	16	1049.5803	0.001	1049.5806	-0.0002
(4)	19	5	14 -	19	6	14	1051.0840	0.001	1051.0846	-0.0005
(4)	18	5	13 -	18	6	13	1051.1030	0.001	1051.1023	0.0007
(4)	22	5	17 -	22	6	17	1051.1173	0.001	1051.1171	0.0002
(4)	18	5	14 -	18	6	12	1051.1335	0.001	1051.1371	-0.0036
(4)	19	5	15 -	19	6	13	1051.1458	0.001	1051.1449	0.0009
(4)	10	6	5 -	9	7	3	1051.1458*	0.000	1051.1495	-0.0037
(4)	10	6	4 -	9	7	2	1051.1458*	0.000	1051.1495	-0.0037
(4)	18	3	16 -	19	4	16	1051.1531	0.001	1051.1546	-0.0016
(4)	17	5	13 -	17	6	11	1051.1531*	0.000	1051.1516	0.0015
(4)	16	5	11 -	16	6	11	1051.1724	0.001	1051.1723	0.0001
(4)	16	5	12 -	16	6	10	1051.1827	0.001	1051.1828	-0.0001
(4)	15	5	11 -	15	6	9	1051.2221	0.001	1051.2264	-0.0042
(4)	15	5	10 -	15	6	10	1051.2221	0.001	1051.2209	0.0012
(4)	21	5	17 -	21	6	15	1051.2580	0.001	1051.2580	0.0000
(4)	14	5	10 -	14	6	8	1051.2779	0.001	1051.2789	-0.0010
(4)	14	5	9 -	14	6	9	1051.2779	0.001	1051.2762	0.0017
(4)	9	4	5 -	10	5	5	1051.3089	0.001	1051.3043	0.0047
(4)	9	4	6 -	10	5	6	1051.3089	0.001	1051.3099	-0.0010
(4)	13	5	9 -	13	6	7	1051.3373	0.001	1051.3375	-0.0002
(4)	13	5	8 -	13	6	8	1051.3373	0.001	1051.3362	0.0011
(4)	22	5	18 -	22	6	16	1051.3858	0.001	1051.3851	0.0007
(4)	12	5	8 -	12	6	6	1051.3999	0.001	1051.3999	0.0001
(4)	12	5	7 -	12	6	7	1051.3999	0.001	1051.3993	0.0007
(4)	11	5	7 -	11	6	5	1051.4644	0.001	1051.4640	0.0004
(4)	11	5	6 -	11	6	6	1051.4644	0.001	1051.4637	0.0006
(4)	10	5	6 -	10	6	4	1051.5284	0.001	1051.5281	0.0002
(4)	10	5	5 -	10	6	5	1051.5284	0.001	1051.5281	0.0003
(4)	9	5	5 -	9	6	3	1051.5911	0.001	1051.5908	0.0003
(4)	9	5	4 -	9	6	4	1051.5911	0.001	1051.5908	0.0003
(4)	8	5	4 -	8	6	2	1051.6511	0.001	1051.6508	0.0004
(4)	8	5	3 -	8	6	3	1051.6511	0.001	1051.6508	0.0004
(4)	7	5	3 -	7	6	1	1051.7070	0.001	1051.7068	0.0002
(4)	7	5	2 -	7	6	2	1051.7070	0.001	1051.7068	0.0002
(4)	6	5	2 -	6	6	0	1051.7585	0.001	1051.7580	0.0005
(4)	6	5	1 -	6	6	1	1051.7585	0.001	1051.7580	0.0005
(4)	18	3	15 -	19	4	15	1052.0558	0.001	1052.0562	-0.0003
(4)	26	0	26 -	27	1	26	1052.2587	0.001	1052.2598	-0.0012
(4)	23	2	22 -	24	3	22	1052.7436	0.001	1052.7418	0.0019
(4)	11	6	6 -	10	7	4	1053.5024	0.001	1053.5026	-0.0003
(4)	11	6	5 -	10	7	3	1053.5024	0.001	1053.5026	-0.0003
(4)	8	4	4 -	9	5	4	1053.8333	0.001	1053.8319	0.0014
(4)	8	4	5 -	9	5	5	1053.8333	0.001	1053.8342	-0.0009
(4)	17	3	15 -	18	4	15	1053.8543	0.001	1053.8547	-0.0004
(4)	27	2	25 -	28	3	25	1054.3082	0.001	1054.3086	-0.0004
(4)	17	3	14 -	18	4	14	1054.5278	0.001	1054.5280	-0.0002
(4)	12	6	7 -	11	7	5	1055.8520	0.001	1055.8513	0.0007
(4)	12	6	6 -	11	7	4	1055.8520	0.001	1055.8513	0.0007
(4)	7	4	3 -	8	5	3	1056.3451	0.001	1056.3443	0.0008
(4)	7	4	4 -	8	5	4	1056.3451	0.001	1056.3451	0.0000
(4)	22	2	21 -	23	3	21	1056.4323	0.001	1056.4305	0.0018

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(4)	16	3	14	-	17	4	14	1056.5214	0.001	1056.5216	-0.0002
(4)	16	3	13	-	17	4	13	1057.0087	0.001	1057.0089	-0.0002
(4)	25	0	25	-	26	1	25	1057.1706	0.001	1057.1713	-0.0007
(4)	26	2	24	-	27	3	24	1057.4903	0.001	1057.4910	-0.0007
(4)	13	6	8	-	12	7	6	1058.1964	0.001	1058.1960	0.0004
(4)	13	6	7	-	12	7	5	1058.1964	0.001	1058.1960	0.0004
(4)	6	4	2	-	7	5	2	1058.8431	0.001	1058.8429	0.0002
(4)	6	4	3	-	7	5	3	1058.8431	0.001	1058.8431	0.0000
(4)	15	3	13	-	16	4	13	1059.1593	0.001	1059.1596	-0.0003
(4)	15	3	12	-	16	4	12	1059.5017	0.001	1059.5019	-0.0002
(4)	21	2	20	-	22	3	20	1060.0122	0.001	1060.0114	0.0008
(4)	25	2	23	-	26	3	23	1060.4739	0.001	1060.4752	-0.0013
(4)	14	6	9	-	13	7	7	1060.5376	0.001	1060.5373	0.0003
(4)	14	6	8	-	13	7	6	1060.5376	0.001	1060.5373	0.0003
(4)	5	4	1	-	6	5	1	1061.3290	0.001	1061.3289	0.0002
(4)	5	4	2	-	6	5	2	1061.3290	0.001	1061.3289	0.0001
(4)	14	3	12	-	15	4	12	1061.7726	0.000	1061.7728	-0.0002
(4)	14	3	11	-	15	4	11	1062.0057	0.000	1062.0058	-0.0001
(4)	24	0	24	-	25	1	24	1062.1064	0.001	1062.1069	-0.0004
(4)	15	6	10	-	14	7	8	1062.8762	0.001	1062.8759	0.0003
(4)	15	6	9	-	14	7	7	1062.8762	0.001	1062.8759	0.0003
(4)	24	2	22	-	25	3	22	1063.2757	0.001	1063.2772	-0.0015
(4)	20	2	19	-	21	3	19	1063.4891	0.001	1063.4885	0.0006
(4)	4	4	0	-	5	5	0	1063.8033	0.001	1063.8034	-0.0001
(4)	4	4	1	-	5	5	1	1063.8033	0.001	1063.8034	-0.0001
(4)	13	3	11	-	14	4	11	1064.3643	0.000	1064.3645	-0.0002
(4)	13	3	10	-	14	4	10	1064.5175	0.000	1064.5178	-0.0003
(4)	16	6	11	-	15	7	9	1065.2128	0.001	1065.2125	0.0003
(4)	16	6	10	-	15	7	8	1065.2128	0.001	1065.2125	0.0003
(4)	23	2	21	-	24	3	21	1065.9137	0.001	1065.9145	-0.0008
(4)	19	2	18	-	20	3	18	1066.8662	0.001	1066.8658	0.0005
(4)	12	3	10	-	13	4	10	1066.9375	0.000	1066.9375	0.0000
(4)	12	3	9	-	13	4	9	1067.0346	0.000	1067.0347	-0.0001
(4)	23	0	23	-	24	1	23	1067.0577	0.001	1067.0576	0.0001
(4)	17	6	12	-	16	7	10	1067.5477	0.001	1067.5479	-0.0002
(4)	17	6	11	-	16	7	9	1067.5477	0.001	1067.5478	-0.0001
(4)	22	2	20	-	23	3	20	1068.4056	0.001	1068.4065	-0.0010
(4)	21	1	21	-	22	2	21	1069.3253	0.001	1069.3260	-0.0007
(4)	11	3	9	-	12	4	9	1069.4941	0.000	1069.4944	-0.0003
(4)	11	3	8	-	12	4	8	1069.5533	0.000	1069.5534	0.0000
(4)	18	6	13	-	17	7	11	1069.8828	0.001	1069.8828	0.0001
(4)	18	6	12	-	17	7	10	1069.8828	0.001	1069.8826	0.0002
(4)	18	2	17	-	19	3	17	1070.1479	0.001	1070.1478	0.0001
(4)	21	2	19	-	22	3	19	1070.7732	0.001	1070.7742	-0.0009
(4)	23	4	19	-	23	5	19	1071.3859	0.001	1071.3848	0.0011
(4)	27	4	24	-	27	5	22	1071.9436	0.001	1071.9426	0.0011
(4)	22	4	18	-	22	5	18	1071.9826	0.001	1071.9821	0.0005
(4)	22	0	22	-	23	1	22	1072.0118	0.001	1072.0118	0.0000
(4)	10	3	8	-	11	4	8	1072.0370	0.000	1072.0370	0.0000
(4)	10	3	7	-	11	4	7	1072.0708	0.000	1072.0710	-0.0003

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(4)	19	6	14	-	18	7	12	1072.2186	0.001	1072.2181	0.0005
(4)	19	6	13	-	18	7	11	1072.2186	0.001	1072.2178	0.0008
(4)	26	4	23	-	26	5	21	1072.2947	0.001	1072.2949	-0.0002
(4)	21	4	17	-	21	5	17	1072.5074	0.001	1072.5072	0.0003
(4)	25	4	22	-	25	5	20	1072.6131	0.001	1072.6128	0.0003
(4)	24	4	21	-	24	5	19	1072.9020	0.001	1072.9019	0.0001
(4)	20	4	16	-	20	5	16	1072.9697	0.001	1072.9699	-0.0002
(4)	20	2	18	-	21	3	18	1073.0390	0.001	1073.0397	-0.0007
(4)	23	4	20	-	23	5	18	1073.1666	0.001	1073.1670	-0.0004
(4)	17	2	16	-	18	3	16	1073.3390	0.001	1073.3391	0.0000
(4)	19	4	15	-	19	5	15	1073.3792	0.001	1073.3786	0.0005
(4)	22	4	19	-	22	5	17	1073.4117	0.001	1073.4121	-0.0003
(4)	21	4	18	-	21	5	16	1073.6401	0.001	1073.6405	-0.0004
(4)	18	4	14	-	18	5	14	1073.7404	0.001	1073.7406	-0.0001
(4)	20	4	17	-	20	5	15	1073.8551	0.001	1073.8551	0.0001
(4)	19	4	16	-	19	5	14	1074.0599	0.001	1074.0580	0.0019
(4)	17	4	13	-	17	5	13	1074.0599	0.001	1074.0614	-0.0015
(4)	18	4	15	-	18	5	13	1074.2509	0.001	1074.2511	-0.0002
(4)	16	4	12	-	16	5	12	1074.3459	0.001	1074.3460	-0.0001
(4)	17	4	14	-	17	5	12	1074.4354	0.001	1074.4355	-0.0001
(4)	20	6	15	-	19	7	13	1074.5547	0.001	1074.5549	-0.0002
(4)	20	6	14	-	19	7	12	1074.5547	0.001	1074.5543	0.0004
(4)	9	3	7	-	10	4	7	1074.5667	0.000	1074.5669	-0.0002
(4)	9	3	6	-	10	4	6	1074.5850	0.000	1074.5853	-0.0003
(4)	15	4	11	-	15	5	11	1074.5980	0.001	1074.5982	-0.0002
(4)	16	4	13	-	16	5	11	1074.6118	0.001	1074.6119	-0.0001
(4)	15	4	12	-	15	5	10	1074.7807	0.001	1074.7806	0.0000
(4)	14	4	10	-	14	5	10	1074.8211	0.001	1074.8214	-0.0003
(4)	14	4	11	-	14	5	9	1074.9411	0.001	1074.9413	-0.0002
(4)	13	4	9	-	13	5	9	1075.0185	0.001	1075.0184	0.0001
(4)	13	4	10	-	13	5	8	1075.0932	0.001	1075.0934	-0.0001
(4)	12	4	8	-	12	5	8	1075.1917	0.001	1075.1917	0.0000
(4)	19	2	17	-	20	3	17	1075.2253	0.001	1075.2261	-0.0008
(4)	12	4	9	-	12	5	7	1075.2359	0.001	1075.2359	0.0000
(4)	11	4	7	-	11	5	7	1075.3435	0.001	1075.3433	0.0001
(4)	11	4	8	-	11	5	6	1075.3677	0.001	1075.3677	0.0001
(4)	10	4	6	-	10	5	6	1075.4755	0.001	1075.4754	0.0001
(4)	10	4	7	-	10	5	5	1075.4875	0.001	1075.4877	-0.0002
(4)	9	4	5	-	9	5	5	1075.5910	0.001	1075.5895	0.0014
(4)	9	4	6	-	9	5	4	1075.5939	0.001	1075.5952	-0.0012
(4)	8	4	4	-	8	5	4	1075.6889	0.001	1075.6874	0.0015
(4)	8	4	5	-	8	5	3	1075.6889	0.001	1075.6897	-0.0008
(4)	7	4	3	-	7	5	3	1075.7709	0.001	1075.7705	0.0004
(4)	7	4	4	-	7	5	2	1075.7709	0.001	1075.7713	-0.0004
(4)	10	5	6	-	9	6	4	1075.7990	0.001	1075.7985	0.0005
(4)	10	5	5	-	9	6	3	1075.7990	0.001	1075.7984	0.0005
(4)	6	4	2	-	6	5	2	1075.8402	0.001	1075.8400	0.0002
(4)	6	4	3	-	6	5	1	1075.8402	0.001	1075.8403	0.0000
(4)	5	4	1	-	5	5	1	1075.8975	0.001	1075.8973	0.0002
(4)	5	4	2	-	5	5	0	1075.8975	0.001	1075.8974	0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(4)	16	2	15	17	3	15	1076.4444	0.001	1076.4446	-0.0002
(4)	21	0	21	22	1	21	1076.9551	0.001	1076.9553	-0.0001
(4)	8	3	6	9	4	6	1077.0850	0.000	1077.0851	-0.0001
(4)	8	3	5	9	4	5	1077.0941	0.000	1077.0944	-0.0002
(4)	18	2	16	19	3	16	1077.3561	0.001	1077.3565	-0.0005
(4)	22	1	21	23	2	21	1077.8221	0.001	1077.8271	-0.0050
(4)	27	4	23	27	5	23	1078.0369	0.001	1078.0402	-0.0033
(4)	11	5	7	10	6	5	1078.1607	0.001	1078.1618	-0.0011
(4)	11	5	6	10	6	4	1078.1607	0.001	1078.1616	-0.0009
(4)	24	4	20	24	5	20	1078.9685	0.001	1078.9700	-0.0015
(4)	22	6	17	21	7	15	1079.2368	0.001	1079.2371	-0.0003
(4)	22	6	16	21	7	14	1079.2368	0.001	1079.2352	0.0017
(4)	17	2	15	18	3	15	1079.4530	0.001	1079.4534	-0.0004
(4)	15	2	14	16	3	14	1079.4691	0.001	1079.4694	-0.0003
(4)	7	3	5	8	4	5	1079.5941	0.000	1079.5924	0.0017
(4)	7	3	4	8	4	4	1079.5941	0.000	1079.5967	-0.0025
(6)	22	2	21	22	5	18	1079.6801	0.001	1079.6807	-0.0006
(6)	21	2	20	21	5	17	1080.0264	0.001	1080.0261	0.0003
(6)	19	2	18	19	5	15	1080.6567	0.001	1080.6572	-0.0005
(6)	18	2	17	18	5	14	1080.9342	0.001	1080.9339	0.0003
(4)	18	1	18	19	2	18	1081.3124	0.001	1081.3130	-0.0006
(4)	16	2	14	17	3	14	1081.5371	0.001	1081.5378	-0.0007
(4)	20	0	20	21	1	20	1081.8711	0.001	1081.8715	-0.0004
(4)	21	1	20	22	2	20	1082.0101	0.001	1082.0088	0.0012
(4)	6	3	4	7	4	4	1082.0901	0.000	1082.0894	0.0007
(4)	6	3	3	7	4	3	1082.0901	0.000	1082.0911	-0.0010
(4)	14	2	13	15	3	13	1082.4185	0.000	1082.4188	-0.0003
(4)	15	2	13	16	3	13	1083.6279	0.001	1083.6284	-0.0005
(4)	5	3	3	6	4	3	1084.5764	0.000	1084.5764	-0.0001
(4)	5	3	2	6	4	2	1084.5764	0.000	1084.5770	-0.0006
(4)	17	1	17	18	2	17	1085.1798	0.001	1085.1805	-0.0007
(4)	13	2	12	14	3	12	1085.2982	0.000	1085.2984	-0.0002
(4)	14	2	12	15	3	12	1085.7409	0.000	1085.7411	-0.0002
(4)	19	0	19	20	1	19	1086.7421	0.001	1086.7424	-0.0003
(4)	4	3	2	5	4	2	1087.0534	0.000	1087.0536	-0.0002
(4)	4	3	1	5	4	1	1087.0534	0.000	1087.0537	-0.0003
(4)	13	2	11	14	3	11	1087.8879	0.000	1087.8880	-0.0001
(4)	12	2	11	13	3	11	1088.1137	0.000	1088.1138	-0.0001
(4)	16	1	16	17	2	16	1088.9781	0.001	1088.9780	0.0001
(4)	3	3	1	4	4	1	1089.5205	0.000	1089.5210	-0.0005
(4)	3	3	0	4	4	0	1089.5205	0.000	1089.5210	-0.0005
(4)	16	2	14	17	3	14	1081.5371	0.001	1081.5378	-0.0007
(4)	14	2	13	15	3	13	1082.4185	0.000	1082.4188	-0.0003
(4)	15	2	13	16	3	13	1083.6279	0.001	1083.6284	-0.0005
(4)	17	1	17	18	2	17	1085.1798	0.001	1085.1805	-0.0007
(4)	13	2	12	14	3	12	1085.2982	0.000	1085.2984	-0.0002
(4)	14	2	12	15	3	12	1085.7409	0.000	1085.7411	-0.0002
(4)	13	2	11	14	3	11	1087.8879	0.000	1087.8880	-0.0001
(4)	12	2	11	13	3	11	1088.1137	0.000	1088.1138	-0.0001
(4)	16	1	16	17	2	16	1088.9781	0.001	1088.9780	0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(4)	19	1	18	20	2	18	1089.7630	0.001	1089.7629	0.0001
(4)	12	2	10	13	3	10	1090.0776	0.000	1090.0777	-0.0001
(4)	11	2	10	12	3	10	1090.8706	0.000	1090.8707	0.0000
(4)	18	0	18	19	1	18	1091.5491	0.001	1091.5490	0.0001
(4)	11	2	9	12	3	9	1092.3145	0.000	1092.3144	0.0001
(4)	15	1	15	16	2	15	1092.7022	0.001	1092.7025	-0.0003
(4)	7	4	3	6	5	1	1092.7688	0.001	1092.7676	0.0012
(4)	7	4	4	6	5	2	1092.7688	0.001	1092.7684	0.0004
(4)	18	1	17	19	2	17	1093.3476	0.001	1093.3474	0.0002
(4)	10	2	9	11	3	9	1093.5748	0.000	1093.5748	0.0001
(4)	10	2	8	11	3	8	1094.5988	0.000	1094.5989	0.0000
(4)	23	3	21	23	4	19	1095.0876	0.001	1095.0867	0.0009
(4)	8	4	4	7	5	2	1095.1151	0.001	1095.1136	0.0016
(4)	8	4	5	7	5	3	1095.1151	0.001	1095.1159	-0.0007
(4)	22	3	20	22	4	18	1095.6928	0.001	1095.6920	0.0007
(4)	21	3	19	21	4	17	1096.2092	0.001	1096.2092	0.0000
(4)	9	2	8	10	3	8	1096.2318	0.000	1096.2318	0.0000
(4)	17	0	17	18	1	17	1096.2723	0.001	1096.2724	-0.0001
(4)	14	1	14	15	2	14	1096.3512	0.000	1096.3514	-0.0001
(4)	20	3	18	20	4	16	1096.6510	0.001	1096.6508	0.0002
(4)	17	1	16	18	2	16	1096.7474	0.001	1096.7473	0.0001
(4)	9	2	7	10	3	7	1096.9287	0.000	1096.9285	0.0002
(4)	19	3	17	19	4	15	1097.0279	0.001	1097.0280	-0.0001
(4)	18	3	16	18	4	14	1097.3502	0.001	1097.3505	-0.0002
(4)	9	4	5	8	5	3	1097.4470	0.001	1097.4450	0.0019
(4)	9	4	6	8	5	4	1097.4470	0.001	1097.4507	-0.0037
(4)	17	3	15	17	4	13	1097.6274	0.001	1097.6270	0.0004
(4)	16	3	14	16	4	12	1097.8646	0.001	1097.8649	-0.0003
(4)	15	3	13	15	4	11	1098.0707	0.000	1098.0706	0.0001
(4)	21	3	18	21	4	18	1098.2143	0.001	1098.2130	0.0013
(4)	14	3	12	14	4	10	1098.2492	0.000	1098.2495	-0.0003
(4)	20	3	17	20	4	17	1098.3682	0.001	1098.3675	0.0008
(4)	19	3	16	19	4	16	1098.3844*	0.000	1098.3882	-0.0038
(4)	18	3	15	18	4	15	1098.3844*	0.000	1098.3824	0.0021
(4)	17	3	14	17	4	14	1098.3844*	0.000	1098.3849	-0.0004
(4)	16	3	13	16	4	13	1098.4058*	0.000	1098.4058	0.0001
(4)	13	3	11	13	4	9	1098.4058*	0.000	1098.4060	-0.0001
(4)	15	3	12	15	4	12	1098.4455	0.000	1098.4457	-0.0002
(4)	14	3	11	14	4	11	1098.5019	0.000	1098.5020	-0.0001
(4)	12	3	10	12	4	8	1098.5436	0.000	1098.5437	0.0000
(4)	13	3	10	13	4	10	1098.5704	0.000	1098.5704	0.0000
(4)	12	3	9	12	4	9	1098.6467	0.000	1098.6469	-0.0002
(4)	11	3	9	11	4	7	1098.6655	0.000	1098.6655	0.0000
(4)	11	3	8	11	4	8	1098.7275	0.000	1098.7276	-0.0001
(4)	10	3	8	10	4	6	1098.7735	0.000	1098.7735	0.0000
(4)	10	3	7	10	4	7	1098.8091	0.000	1098.8091	0.0000
(4)	8	2	7	9	3	7	1098.8471	0.000	1098.8473	-0.0002
(4)	9	3	7	9	4	5	1098.8697	0.000	1098.8696	0.0001
(4)	9	3	6	9	4	6	1098.8887	0.000	1098.8887	-0.0001
(4)	8	3	6	8	4	4	1098.9547	0.000	1098.9548	-0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(4)	8	3	5	8	4	5	1098.9642	0.000	1098.9644	-0.0001
(4)	7	3	5	7	4	3	1099.0322	0.000	1099.0299	0.0023
(4)	7	3	4	7	4	4	1099.0322	0.000	1099.0343	-0.0020
(4)	6	3	4	6	4	2	1099.0963	0.000	1099.0955	0.0008
(4)	6	3	3	6	4	3	1099.0963	0.000	1099.0972	-0.0009
(4)	5	3	3	5	4	1	1099.1518	0.000	1099.1517	0.0001
(4)	5	3	2	5	4	2	1099.1518	0.000*	1099.1523	-0.0005
(4)	4	3	2	4	4	0	1099.1988	0.000	1099.1988	0.0000
(4)	4	3	1	4	4	1	1099.1988	0.000	1099.1989	-0.0001
(4)	8	2	6	9	3	6	1099.2979	0.000	1099.2980	-0.0002
(4)	10	4	6	9	5	4	1099.7607	0.001	1099.7606	0.0001
(4)	10	4	7	9	5	5	1099.7730	0.001	1099.7729	0.0001
(4)	13	1	13	14	2	13	1099.9226	0.000	1099.9225	0.0002
(4)	16	1	15	17	2	15	1099.9720	0.001	1099.9718	0.0002
(4)	16	0	16	17	1	16	1100.8943	0.001	1100.8945	-0.0001
(4)	7	2	6	8	3	6	1101.4265	0.000	1101.4265	0.0000
(4)	7	2	5	8	3	5	1101.7005	0.000	1101.7006	-0.0002
(4)	11	4	7	10	5	5	1102.0592	0.001	1102.0587	0.0005
(4)	11	4	8	10	5	6	1102.0828	0.001	1102.0831	-0.0002
(4)	15	1	14	16	2	14	1103.0307	0.001	1103.0306	0.0001
(4)	12	1	12	13	2	12	1103.4143	0.000	1103.4142	0.0001
(4)	6	2	5	7	3	5	1103.9744	0.000	1103.9746	-0.0002
(4)	6	2	4	7	3	4	1104.1283	0.000	1104.1285	-0.0002
(4)	12	4	8	11	5	6	1104.3380	0.001	1104.3376	0.0004
(4)	24	2	23	24	3	21	1104.3695	0.001	1104.3663	0.0032
(4)	12	4	9	11	5	7	1104.3818	0.001	1104.3819	-0.0001
(4)	15	0	15	16	1	15	1105.3990	0.001	1105.3989	0.0000
(4)	14	1	13	15	2	13	1105.9346	0.000	1105.9346	0.0000
(4)	5	2	4	6	3	4	1106.4959	0.000	1106.4960	-0.0001
(4)	5	2	3	6	3	3	1106.5737	0.000	1106.5737	0.0000
(4)	13	4	9	12	5	7	1106.5955	0.001	1106.5955	0.0000
(4)	13	4	10	12	5	8	1106.6706	0.001	1106.6705	0.0000
(4)	23	2	22	23	3	20	1106.8183	0.001	1106.8157	0.0026
(4)	11	1	11	12	2	11	1106.8253	0.000	1106.8252	0.0001
(4)	13	1	12	14	2	12	1108.6958	0.000	1108.6957	0.0001
(4)	14	4	10	13	5	8	1108.8299	0.001	1108.8301	-0.0002
(4)	14	4	11	13	5	9	1108.9501	0.001	1108.9502	-0.0001
(4)	22	2	21	22	3	19	1108.9947*	0.000	1108.9892	0.0055
(4)	4	2	3	5	3	3	1108.9947	0.000	1108.9951	-0.0004
(4)	4	2	2	5	3	2	1109.0285	0.000	1109.0286	-0.0002
(4)	14	0	14	15	1	14	1109.7722	0.000	1109.7720	0.0002
(4)	10	1	10	11	2	10	1110.1544	0.000	1110.1546	-0.0001
(4)	21	2	20	21	3	18	1110.9045	0.001	1110.9032	0.0012
(4)	15	4	11	14	5	9	1111.0390	0.001	1111.0391	0.0000
(4)	15	4	12	14	5	10	1111.2215	0.001	1111.2218	-0.0003
(4)	12	1	11	13	2	11	1111.3272	0.000	1111.3272	0.0001
(4)	3	2	2	4	3	2	1111.4755	0.000	1111.4755	0.0000
(4)	3	2	1	4	3	1	1111.4864	0.000	1111.4867	-0.0003
(4)	20	2	19	20	3	17	1112.5769	0.001	1112.5763	0.0006
(4)	16	4	12	15	5	10	1113.2194	0.001	1113.2196	-0.0002
(4)	9	1	9	10	2	9	1113.4016	0.000	1113.4018	-0.0002
(4)	16	4	13	15	5	11	1113.4860	0.001	1113.4861	-0.0001
(4)	6	3	4	5	4	2	1113.6717	0.000	1113.6708	0.0008
(4)	6	3	3	5	4	1	1113.6717	0.000	1113.6726	-0.0009
(4)	11	1	10	12	2	10	1113.8438	0.000	1113.8438	0.0000
(4)	2	2	1	3	3	1	1113.9411	0.000	1113.9402	0.0009
(4)	2	2	0	3	3	0	1113.9411	0.000	1113.9424	-0.0013
(4)	13	0	13	14	1	13	1114.0030	0.000	1114.0030	0.0000
(4)	19	2	18	19	3	16	1114.0284	0.001	1114.0280	0.0004
(4)	19	1	19	19	2	17	1114.4987	0.001	1114.4984	0.0003
(4)	18	2	17	18	3	15	1115.2789	0.001	1115.2787	0.0002
(4)	17	4	13	16	5	11	1115.3683	0.001	1115.3683	0.0000
(4)	17	4	14	16	5	12	1115.7432	0.001	1115.7435	-0.0003
(4)	7	3	5	6	4	3	1116.0377	0.000	1116.0360	0.0017
(4)	7	3	4	6	4	2	1116.0377	0.000	1116.0404	-0.0027
(4)	10	1	9	11	2	9	1116.2623	0.000	1116.2622	0.0001
(4)	17	2	16	17	3	14	1116.3487	0.001	1116.3486	0.0000
(4)	8	1	8	9	2	8	1116.5665	0.000	1116.5667	-0.0002
(4)	16	2	15	16	3	13	1117.2576	0.001	1117.2576	0.0000
(4)	18	4	14	17	5	12	1117.4815	0.001	1117.4813	0.0003
(4)	18	1	18	18	2	16	1117.8185	0.001	1117.8187	-0.0002
(4)	18	4	15	17	5	13	1117.9935	0.001	1117.9938	-0.0003
(4)	15	2	14	15	3	12	1118.0245	0.000	1118.0246	-0.0001
(4)	12	0	12	13	1	12	1118.0853	0.000	1118.0851	0.0002
(4)	8	3	6	7	4	4	1118.3921	0.000	1118.3924	-0.0003
(4)	8	3	5	7	4	3	1118.4012	0.000	1118.4019	-0.0007
(4)	9	1	8	10	2	8	1118.5998	0.000	1118.5999	-0.0001
(4)	14	2	13	14	3	11	1118.6668	0.000	1118.6672	-0.0003
(4)	13	2	12	13	3	10	1119.2014	0.000	1119.2018	-0.0003
(4)	19	4	15	18	5	13	1119.5536	0.001	1119.5537	-0.0001
(4)	12	2	11	12	3	9	1119.6433	0.000	1119.6432	0.0001
(4)	7	1	7	8	2	7	1119.6433*	0.000	1119.6491	-0.0058
(4)	11	2	10	11	3	8	1120.0048	0.000	1120.0049	-0.0001
(4)	19	4	16	18	5	14	1120.2367	0.001	1120.2365	0.0001
(4)	10	2	9	10	3	7	1120.2987	0.000	1120.2989	-0.0002
(4)	9	2	8	9	3	6	1120.5353	0.000	1120.5357	-0.0003
(4)	8	2	7	8	3	5	1120.7243	0.000	1120.7245	-0.0002
(4)	9	3	7	8	4	5	1120.7394	0.000	1120.7396	-0.0002
(4)	9	3	6	8	4	4	1120.7585	0.000	1120.7585	0.0000
(4)	7	2	6	7	3	4	1120.8737	0.000	1120.8736	0.0002
(4)	8	1	7	9	2	7	1120.8737*	0.000	1120.8757	-0.0020
(4)	17	1	17	17	2	15	1120.8979	0.001	1120.8982	-0.0004
(4)	6	2	5	6	3	3	1120.9894	0.000	1120.9897	-0.0003
(4)	5	2	4	5	3	2	1121.0787	0.000	1121.0788	-0.0001
(4)	6	2	4	6	3	4	1121.1490*	0.000	1121.1500	-0.0011
(4)	4	2	3	4	3	1	1121.1490*	0.000	1121.1459	0.0031
(4)	7	2	5	7	3	5	1121.1605*	0.000	1121.1623	-0.0018
(4)	5	2	3	5	3	3	1121.1605*	0.000	1121.1589	0.0016
(4)	4	2	2	4	3	2	1121.1799	0.000	1121.1802	-0.0003
(4)	3	2	2	3	3	0	1121.1951	0.000	1121.1949	0.0003

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(4)	8	2	6	-	8	3	6	1121.2053*	0.000	1121.2054	0.0000
(4)	3	2	1	-	3	3	1	1121.2053*	0.000	1121.2063	-0.0009
(4)	9	2	7	-	9	3	7	1121.2895	0.000	1121.2895	0.0000
(4)	10	2	8	-	10	3	8	1121.4248	0.000	1121.4249	-0.0001
(4)	20	4	16	-	19	5	14	1121.5797	0.001	1121.5796	0.0002
(4)	11	2	9	-	11	3	9	1121.6207	0.000	1121.6211	-0.0003
(4)	12	2	10	-	12	3	10	1121.8859	0.000	1121.8860	-0.0002
(4)	11	0	11	-	12	1	11	1122.0151	0.000	1122.0149	0.0002
(4)	13	2	11	-	13	3	11	1122.2258	0.000	1122.2260	-0.0002
(4)	20	4	17	-	19	5	15	1122.4704	0.001	1122.4706	-0.0002
(4)	14	2	12	-	14	3	12	1122.6449	0.000	1122.6447	0.0002
(4)	6	1	6	-	7	2	6	1122.6449*	0.000	1122.6492	-0.0043
(4)	10	3	8	-	9	4	6	1123.0767	0.000	1123.0770	-0.0003
(4)	10	3	7	-	9	4	5	1123.1094*	0.000	1123.1118	-0.0024
(4)	7	1	6	-	8	2	6	1123.1094*	0.000	1123.1088	0.0006
(4)	15	2	13	-	15	3	13	1123.1432	0.000	1123.1436	-0.0005
(4)	21	4	17	-	20	5	15	1123.5521	0.001	1123.5518	0.0004
(4)	25	2	23	-	26	1	25	1123.6249	0.001	1123.6255	-0.0006
(4)	16	2	14	-	16	3	14	1123.7211	0.001	1123.7217	-0.0005
(4)	16	1	16	-	16	2	14	1123.7315	0.001	1123.7320	-0.0005
(4)	17	2	15	-	17	3	15	1124.3752	0.001	1124.3756	-0.0004
(4)	21	4	18	-	20	5	16	1124.6945	0.001	1124.6946	-0.0001
(4)	18	2	16	-	18	3	16	1125.0998	0.001	1125.1004	-0.0006
(4)	6	1	5	-	7	2	5	1125.3179	0.000	1125.3179	0.0000
(4)	11	3	9	-	10	4	7	1125.4035	0.000	1125.4035	0.0000
(4)	22	4	18	-	21	5	16	1125.4550	0.001	1125.4616	-0.0066
(4)	11	3	8	-	10	4	6	1125.4631	0.000	1125.4641	-0.0010
(4)	5	1	5	-	6	2	5	1125.5676	0.000	1125.5674	0.0002
(4)	10	0	10	-	11	1	10	1125.7928	0.000	1125.7927	0.0001
(4)	23	2	21	-	24	1	23	1125.8281	0.001	1125.8296	-0.0015
(4)	19	2	17	-	19	3	17	1125.8888	0.001	1125.8894	-0.0006
(4)	15	1	15	-	15	2	13	1126.3173	0.000	1126.3176	-0.0003
(4)	20	2	18	-	20	3	18	1126.7342	0.001	1126.7350	-0.0007
(4)	22	4	19	-	21	5	17	1126.9068	0.001	1126.9066	0.0002
(4)	22	2	20	-	23	1	22	1127.1860	0.001	1127.1864	-0.0004
(4)	23	4	19	-	22	5	17	1127.2997	0.001	1127.2986	0.0011
(4)	5	1	4	-	6	2	4	1127.5208	0.000	1127.5208	0.0000
(4)	21	2	19	-	21	3	19	1127.6273	0.001	1127.6281	-0.0008
(4)	12	3	10	-	11	4	8	1127.7184	0.000	1127.7179	0.0005
(4)	12	3	9	-	11	4	7	1127.8178	0.000	1127.8180	-0.0001
(4)	4	1	4	-	5	2	4	1128.4039	0.000	1128.4038	0.0001
(4)	22	2	20	-	22	3	20	1128.5586	0.001	1128.5593	-0.0007
(4)	14	1	14	-	14	2	12	1128.6553	0.000	1128.6553	0.0000
(4)	21	2	19	-	22	1	21	1128.7187	0.001	1128.7190	-0.0003
(4)	23	4	20	-	22	5	18	1129.1045	0.001	1129.1045	0.0000
(4)	9	0	9	-	10	1	9	1129.4222	0.000	1129.4219	0.0003
(4)	23	2	21	-	23	3	21	1129.5171	0.001	1129.5178	-0.0008
(4)	4	1	3	-	5	2	3	1129.7337	0.000	1129.7337	-0.0001
(4)	13	3	11	-	12	4	9	1130.0181	0.000	1130.0182	-0.0001
(4)	13	3	10	-	12	4	8	1130.1763	0.000	1130.1766	-0.0003

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(4)	20	2	18	-	21	1	20	1130.4268	0.001	1130.4272	-0.0005
(4)	24	2	22	-	24	3	22	1130.4913	0.001	1130.4923	-0.0011
(4)	13	1	13	-	13	2	11	1130.7486	0.000	1130.7487	-0.0001
(4)	4	2	3	-	3	3	1	1130.8649	0.000	1130.8655	-0.0005
(4)	3	1	3	-	4	2	3	1131.1590	0.000	1131.1588	0.0003
(4)	24	4	21	-	23	5	19	1131.2853	0.001	1131.2854	0.0000
(4)	25	2	23	-	25	3	23	1131.4698	0.001	1131.4704	-0.0006
(4)	3	1	2	-	4	2	2	1131.9711	0.000	1131.9710	0.0002
(4)	14	3	12	-	13	4	10	1132.3068	0.000	1132.3022	0.0046
(4)	19	2	17	-	20	1	19	1132.3068*	0.000	1132.3078	-0.0010
(4)	26	2	24	-	26	3	24	1132.4385	0.001	1132.4388	-0.0003
(4)	14	3	11	-	13	4	9	1132.5436	0.000	1132.5435	0.0000
(4)	12	1	12	-	12	2	10	1132.6047	0.000	1132.6045	0.0003
(4)	8	0	8	-	9	1	8	1132.9085	0.000	1132.9084	0.0001
(4)	5	2	4	-	4	3	2	1133.2305	0.000	1133.2304	0.0002
(4)	5	2	3	-	4	3	1	1133.3097	0.000	1133.3097	0.0001
(4)	27	2	25	-	27	3	25	1133.3832	0.001	1133.3831	0.0000
(4)	25	4	22	-	24	5	20	1133.4468	0.001	1133.4461	0.0007
(4)	2	1	2	-	3	2	2	1133.8326	0.000	1133.8325	0.0001
(4)	11	1	11	-	11	2	9	1134.2328	0.000	1134.2327	0.0001
(4)	2	1	1	-	3	2	1	1134.2446	0.000	1134.2446	0.0000
(4)	28	2	26	-	28	3	26	1134.2890	0.001	1134.2881	0.0009
(4)	18	2	16	-	19	1	18	1134.3544	0.001	1134.3550	-0.0005
(4)	15	3	13	-	14	4	11	1134.5670	0.000	1134.5668	0.0002
(4)	15	3	12	-	14	4	10	1134.9227	0.000	1134.9225	0.0003
(4)	20	3	17	-	21	2	19	1134.9694	0.001	1134.9693	0.0001
(4)	6	2	5	-	5	3	3	1135.5749	0.000	1135.5749	-0.0001
(4)	10	1	10	-	10	2	8	1135.6460	0.000	1135.6460	0.0000
(4)	6	2	4	-	5	3	2	1135.7327	0.000	1135.7328	-0.0001
(4)	7	0	7	-	8	1	7	1136.2596	0.000	1136.2594	0.0002
(4)	1	1	1	-	2	2	1	1136.4251	0.000	1136.4251	0.0000
(4)	1	1	0	-	2	2	0	1136.5622	0.000	1136.5640	-0.0018
(4)	17	2	15	-	18	1	17	1136.5622*	0.000	1136.5606	0.0016
(4)	16	3	14	-	15	4	12	1136.8083	0.000	1136.8087	-0.0005
(4)	9	1	9	-	9	2	7	1136.8595	0.000	1136.8595	0.0001
(4)	16	3	13	-	15	4	11	1137.3167	0.000	1137.3167	-0.0001
(4)	7	2	6	-	6	3	4	1137.8904*	0.000	1137.8951	-0.0047
(4)	8	1	8	-	8	2	6	1137.8904	0.000	1137.8895	0.0009
(4)	7	2	5	-	6	3	3	1138.1776	0.000	1138.1774	0.0002
(6)	21	4	17	-	22	5	18	1138.3144	0.001	1138.3147	-0.0003
(4)	19	3	16	-	20	4	18	1138.7152	0.001	1138.7152	-0.0001
(4)	7	1	7	-	7	2	5	1138.7534	0.000	1138.7532	0.0002
(4)	16	2	14	-	17	1	16	1138.9147	0.001	1138.9150	-0.0003
(4)	17	3	15	-	16	4	13	1139.0239	0.001	1139.0238	0.0002
(4)	6	1	6	-	6	2	4	1139.4673	0.000	1139.4673	0.0003
(4)	6	0	6	-	7	1	6	1139.4834	0.000	1139.4832	0.0002
(4)	17	3	14	-	16	4	12	1139.7286	0.001	1139.7282	0.0005
(4)	5	1	5	-	5	2	3	1140.0476	0.000	1140.0475	0.0001
(4)	8	2	7	-	7	3	5	1140.1861	0.000	1140.1862	-0.0001
(4)	4	1	4	-	4	2	2	1140.5084	0.000	1140.5082	0.0003

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(4)	8	2	6	-	7	3	4	1140.6523	0.000	1140.6524	-0.0001
(6)	20	4	17	-	21	5	16	1140.7294	0.001	1140.7289	0.0005
(4)	3	1	3	-	3	2	1	1140.8618	0.000	1140.8616	0.0002
(4)	2	1	2	-	2	2	0	1141.1179	0.000	1141.1177	0.0002
(4)	18	3	16	-	17	4	14	1141.2076	0.001	1141.2073	0.0003
(4)	15	2	13	-	16	1	15	1141.4066	0.001	1141.4068	-0.0002
(4)	2	1	1	-	2	2	1	1141.5440	0.000	1141.5440	0.0000
(4)	3	1	2	-	3	2	2	1141.7215	0.000	1141.7212	0.0003
(4)	4	1	3	-	4	2	3	1141.9566	0.000	1141.9565	0.0002
(4)	18	3	15	-	17	4	13	1142.1543	0.001	1142.1546	-0.0003
(6)	16	5	12	-	17	6	11	1142.1914	0.001	1142.1908	0.0006
(4)	5	1	4	-	5	2	4	1142.2490	0.000	1142.2490	0.0000
(4)	9	2	8	-	8	3	6	1142.4431	0.000	1142.4430	0.0001
(4)	5	0	5	-	6	1	5	1142.5884	0.000	1142.5880	0.0004
(4)	6	1	5	-	6	2	5	1142.5977	0.000	1142.5976	0.0001
(4)	7	1	6	-	7	2	6	1143.0009	0.000	1143.0005	0.0004
(4)	9	2	7	-	8	3	5	1143.1669	0.000	1143.1668	0.0001
(6)	19	4	16	-	20	5	15	1143.2709	0.001	1143.2707	0.0002
(4)	19	3	17	-	18	4	15	1143.3545	0.001	1143.3541	0.0004
(4)	8	1	7	-	8	2	7	1143.4561	0.000	1143.4559	0.0002
(4)	9	1	8	-	9	2	8	1143.9613	0.000	1143.9610	0.0003
(4)	14	2	12	-	15	1	14	1144.0230	0.000	1144.0232	-0.0001
(6)	12	6	6	-	13	7	7	1144.4157	0.001	1144.4152	0.0005
(4)	10	1	9	-	10	2	9	1144.5129	0.000	1144.5127	0.0002
(4)	19	3	16	-	18	4	14	1144.5839	0.001	1144.5841	-0.0001
(4)	10	2	9	-	9	3	7	1144.6598	0.000	1144.6599	-0.0002
(4)	23	4	20	-	24	3	22	1144.7294	0.001	1144.7307	-0.0013
(4)	11	1	10	-	11	2	10	1145.1072	0.000	1145.1070	0.0002
(4)	20	3	18	-	19	4	16	1145.4587	0.001	1145.4585	0.0002
(4)	4	0	4	-	5	1	4	1145.5818	0.000	1145.5814	0.0005
(6)	23	2	22	-	24	3	21	1145.5818*	0.000	1145.5866	-0.0048
(4)	10	2	8	-	9	3	6	1145.7289	0.000	1145.7288	0.0001
(4)	12	1	11	-	12	2	11	1145.7393	0.000	1145.7390	0.0003
(6)	18	4	15	-	19	5	14	1145.8062	0.001	1145.8057	0.0005
(6)	18	4	14	-	19	5	15	1145.8459	0.001	1145.8457	0.0002
(4)	13	1	12	-	13	2	12	1146.4029	0.000	1146.4028	0.0002
(4)	16	1	15	-	17	0	17	1146.4707	0.001	1146.4705	0.0002
(4)	13	2	11	-	14	1	13	1146.7498	0.000	1146.7499	-0.0001
(4)	11	2	10	-	10	3	8	1146.8308	0.000	1146.8310	-0.0002
(6)	11	6	5	-	12	7	6	1146.8986	0.001	1146.8956	0.0030
(4)	20	3	17	-	19	4	15	1146.9796	0.001	1146.9790	0.0006
(4)	14	1	13	-	14	2	13	1147.0914	0.000	1147.0913	0.0001
(6)	14	5	10	-	15	6	9	1147.2615	0.001	1147.2614	0.0001
(4)	21	3	19	-	20	4	17	1147.5139	0.001	1147.5142	-0.0002
(4)	14	1	13	-	15	0	15	1147.7163	0.000	1147.7160	0.0002
(4)	15	1	14	-	15	2	14	1147.7966	0.000	1147.7963	0.0002
(6)	17	4	14	-	18	5	13	1148.3351	0.001	1148.3347	0.0004
(4)	11	2	9	-	10	3	7	1148.3452	0.000	1148.3452	0.0000
(6)	17	4	13	-	18	5	14	1148.3600	0.081	1148.3602	-0.0001
(4)	3	0	3	-	4	1	3	1148.4704	0.000	1148.4702	0.0002
(4)	16	1	15	-	16	2	15	1148.5085	0.001	1148.5083	0.0002
(4)	13	1	12	-	14	0	14	1148.5525	0.000	1148.5529	-0.0005
(4)	12	2	11	-	11	3	9	1148.9498	0.000	1148.9499	-0.0001
(4)	17	1	16	-	17	2	16	1149.2168	0.001	1149.2167	0.0002
(6)	22	2	21	-	23	3	20	1149.3801*	0.000	1149.3809	-0.0007
(4)	12	1	11	-	13	0	13	1149.5434	0.000	1149.5431	0.0003
(4)	12	2	10	-	13	1	12	1149.5710	0.000	1149.5712	-0.0002
(6)	13	5	9	-	14	6	8	1149.7877	0.001	1149.7876	0.0001
(6)	13	5	8	-	14	6	9	1149.7877	0.001	1149.7876	0.0000
(4)	18	1	17	-	18	2	17	1149.9094	0.001	1149.9094	0.0001
(4)	4	1	4	-	3	2	2	1150.2590*	0.000	1150.2584	0.0006
(4)	19	1	18	-	19	2	18	1150.5740	0.001	1150.5737	0.0003
(4)	11	1	10	-	12	0	12	1150.6899	0.000	1150.6895	0.0004
(6)	16	4	13	-	17	5	12	1150.8578	0.001	1150.8582	-0.0004
(6)	16	4	12	-	17	5	13	1150.8736	0.001	1150.8740	-0.0004
(4)	13	2	12	-	12	3	10	1151.0101	0.000	1151.0101	0.0000
(4)	12	2	10	-	11	3	8	1151.0202	0.000	1151.0203	-0.0001
(4)	20	1	19	-	20	2	19	1151.1969	0.001	1151.1963	0.0005
(4)	2	0	2	-	3	1	2	1151.2602	0.000	1151.2599	0.0003
(4)	23	3	21	-	22	4	19	1151.4532	0.001	1151.4524	0.0008
(4)	4	1	3	-	3	2	1	1151.6593	0.000	1151.6593	0.0000
(4)	21	1	20	-	21	2	20	1151.7645	0.001	1151.7638	0.0007
(4)	10	1	9	-	11	0	11	1151.9912	0.000	1151.9911	0.0001
(4)	5	1	5	-	4	2	3	1152.2644R	0.000	1152.2703	-0.0058
(6)	12	5	8	-	13	6	7	1152.3073	0.001	1152.3075	-0.0002
(6)	12	5	7	-	13	6	8	1152.3073	0.001	1152.3075	-0.0002
(4)	11	2	9	-	12	1	11	1152.4695	0.000	1152.4695	0.0000
(4)	23	1	22	-	23	2	22	1152.6724	0.001	1152.6820	-0.0096
(4)	20	4	17	-	21	3	19	1152.6836	0.001	1152.6794	0.0042
(4)	15	3	12	-	16	2	14	1152.9720	0.001	1152.9727	-0.0007
(4)	14	2	13	-	13	3	11	1153.0050	0.000	1153.0051	-0.0001
(6)	21	2	20	-	22	3	19	1153.0408	0.001	1153.0411	-0.0003
(6)	15	4	12	-	16	5	11	1153.3765	0.001	1153.3766	-0.0001
(6)	15	4	11	-	16	5	12	1153.3860	0.001	1153.3860	0.0000
(4)	13	2	11	-	12	3	9	1153.7554	0.000	1153.7554	0.0000
(4)	1	0	1	-	2	1	1	1153.9546	0.000	1153.9544	0.0002
(4)	6	1	6	-	5	2	4	1154.1957	0.000	1154.1955	0.0002
(4)	5	1	4	-	4	2	2	1154.3533	0.000	1154.3534	-0.0001
(4)	15	2	14	-	14	3	12	1154.9282	0.000	1154.9282	0.0000
(4)	8	1	7	-	9	0	9	1155.0388	0.000	1155.0386	0.0002
(4)	10	2	8	-	11	1	10	1155.4261	0.000	1155.4263	-0.0002
(4)	17	2	16	-	18	1	18	1155.6935*	0.000	1155.6926	0.0009
(6)	14	4	11	-	15	5	10	1155.8908	0.001	1155.8899	0.0009
(6)	14	4	10	-	15	5	11	1155.8908	0.001	1155.8953	-0.0045
(4)	7	1	7	-	6	2	5	1156.0328	0.000	1156.0329	-0.0001
(4)	14	2	12	-	13	3	10	1156.5479	0.000	1156.5480	-0.0001
(4)	0	0	0	-	1	1	0	1156.5566	0.000	1156.5564	0.0002
(4)	16	2	15	-	15	3	13	1156.7724	0.000	1156.7728	-0.0004
(4)	16	2	15	-	17	1	17	1156.7724*	0.000	1156.7989	-0.0265
(4)	6	1	5	-	5	2	3	1157.0778	0.000	1157.0777	0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(6)	10	5	5	-	11	6	6	1157.3275	0.001	1157.3278	-0.0002
(6)	10	5	6	-	11	6	5	1157.3275	0.001	1157.3278	-0.0002
(4)	8	1	8	-	7	2	6	1157.7813	0.000	1157.7812	0.0001
(4)	15	2	14	-	16	1	16	1157.9701	0.001	1157.9699	0.0002
(6)	17	3	14	-	18	4	15	1158.2586	0.001	1158.2585	0.0001
(6)	13	4	10	-	14	5	9	1158.3998	0.001	1158.3983	0.0015
(6)	13	4	9	-	14	5	10	1158.3998	0.001	1158.4013	-0.0015
(4)	9	2	7	-	10	1	9	1158.4218	0.000	1158.4221	-0.0002
(4)	17	2	16	-	18	3	14	1158.5324	0.001	1158.5325	-0.0001
(4)	6	1	5	-	7	0	7	1158.6179	0.000	1158.6177	0.0002
(4)	1	0	1	-	1	1	1	1159.1358	0.000	1159.1356	0.0002
(4)	14	2	13	-	15	1	15	1159.2086	0.000	1159.2089	-0.0003
(4)	2	0	2	-	2	1	2	1159.2716	0.000	1159.2716	0.0000
(4)	15	2	13	-	14	3	11	1159.3916	0.000	1159.3920	-0.0004
(4)	9	1	9	-	8	2	7	1159.4395	0.000	1159.4396	-0.0001
(4)	3	0	3	-	3	1	3	1159.4718	0.000	1159.4715	0.0003
(4)	4	0	4	-	4	1	4	1159.7307	0.000	1159.7304	0.0003
(4)	7	1	6	-	6	2	4	1159.8184	0.000	1159.8185	-0.0001
(6)	9	5	4	-	10	6	5	1159.8277	0.001	1159.8278	-0.0001
(6)	9	5	5	-	10	6	4	1159.8277	0.001	1159.8278	-0.0001
(6)	19	2	18	-	20	3	17	1159.9540	0.001	1159.9539	0.0001
(6)	5	0	5	-	5	1	5	1160.0421	0.000	1160.0418	0.0003
(6)	16	3	14	-	17	4	13	1160.1758	0.001	1160.1763	-0.0005
(4)	18	2	17	-	17	3	15	1160.2012	0.001	1160.2009	0.0003
(6)	17	1	17	-	18	2	16	1160.2434	0.001	1160.2452	-0.0018
(4)	6	0	6	-	6	1	6	1160.3979	0.000	1160.3976	0.0003
(4)	13	2	12	-	14	1	14	1160.5185	0.000	1160.5188	-0.0004
(4)	5	1	4	-	6	0	6	1160.5791	0.000	1160.5790	0.0001
(6)	16	3	13	-	17	4	14	1160.6636	0.001	1160.6634	0.0002
(4)	7	0	7	-	7	1	7	1160.7885	0.000	1160.7884	0.0001
(6)	12	4	9	-	13	5	8	1160.9021	0.001	1160.9016	0.0005
(6)	12	4	8	-	13	5	9	1160.9021	0.001	1160.9032	-0.0010
(4)	10	1	10	-	9	2	8	1161.0071	0.000	1161.0072	0.0000
(4)	8	0	8	-	8	1	8	1161.2039	0.000	1161.2037	0.0003
(4)	8	2	6	-	9	1	8	1161.4367	0.000	1161.4370	-0.0002
(4)	9	0	9	-	9	1	9	1161.6324	0.000	1161.6322	0.0002
(4)	19	2	18	-	18	3	16	1161.7724	0.001	1161.7719	0.0005
(4)	12	2	11	-	13	1	13	1161.9015	0.000	1161.9019	-0.0003
(4)	10	0	10	-	10	1	10	1162.0629	0.000	1162.0629	0.0000
(4)	16	2	14	-	15	3	12	1162.2766	0.000	1162.2768	-0.0003
(6)	8	5	4	-	9	6	3	1162.3204	0.001	1162.3209	-0.0005
(6)	8	5	3	-	9	6	4	1162.3204	0.001	1162.3209	-0.0005
(4)	11	1	11	-	10	2	9	1162.4850*	0.000	1162.4833	0.0017
(4)	11	0	11	-	11	1	11	1162.4850	0.000	1162.4850	0.0000
(4)	8	1	7	-	7	2	5	1162.5601	0.000	1162.5600	0.0002
(4)	4	1	3	-	3	0	3	1162.6397	0.000	1162.6397	0.0000
(4)	12	0	12	-	12	1	12	1162.8889	0.000	1162.8889	-0.0001
(6)	15	3	12	-	16	4	13	1163.0899	0.001	1163.0902	-0.0003
(6)	18	2	17	-	19	3	16	1163.2146	0.001	1163.2144	0.0002
(4)	20	2	19	-	19	3	17	1163.2403	0.001	1163.2396	0.0007

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(4)	13	0	13	-	13	1	13	1163.2672	0.000	1163.2671	0.0000
(4)	11	2	10	-	12	1	12	1163.3595	0.000	1163.3596	-0.0001
(6)	11	4	8	-	12	5	7	1163.3999	0.001	1163.3998	0.0001
(6)	11	4	7	-	12	5	8	1163.3999	0.001	1163.4006	-0.0007
(4)	14	0	14	-	14	1	14	1163.6140	0.000	1163.6139	0.0001
(4)	2	0	2	-	1	1	0	1163.8087	0.000	1163.8084	0.0003
(4)	12	1	12	-	11	2	10	1163.8676	0.000	1163.8677	-0.0001
(4)	15	0	15	-	15	1	15	1163.9258	0.000	1163.9259	-0.0001
(4)	16	0	16	-	16	1	16	1164.2018	0.001	1164.2017	0.0001
(4)	17	0	17	-	17	1	17	1164.4417	0.001	1164.4418	-0.0001
(4)	7	2	5	-	8	1	7	1164.4507	0.000	1164.4515	-0.0008
(4)	21	2	20	-	20	3	18	1164.5994	0.001	1164.5985	0.0009
(4)	18	0	18	-	18	1	18	1164.6479	0.001	1164.6480	-0.0001
(4)	3	1	2	-	4	0	4	1164.7896	0.000	1164.7893	0.0003
(6)	7	5	3	-	8	6	2	1164.8067	0.001	1164.8070	-0.0003
(6)	7	5	2	-	8	6	3	1164.8067	0.001	1164.8070	-0.0003
(4)	19	0	19	-	19	1	19	1164.8229	0.001	1164.8231	-0.0002
(4)	10	2	9	-	11	1	11	1164.8933	0.000	1164.8933	0.0001
(4)	20	0	20	-	20	1	20	1164.9702	0.001	1164.9704	-0.0002
(4)	21	0	21	-	21	1	21	1165.0932	0.001	1165.0935	-0.0003
(4)	13	1	13	-	12	2	11	1165.1607	0.000	1165.1606	0.0001
(4)	17	2	15	-	16	3	13	1165.1888	0.001	1165.1887	0.0001
(4)	22	0	22	-	22	1	22	1165.1956	0.001	1165.1960	-0.0004
(4)	9	1	8	-	8	2	6	1165.2815*	0.000	1165.2839	-0.0024
(4)	23	0	23	-	23	1	23	1165.2815	0.001	1165.2812	0.0003
(6)	14	3	12	-	15	4	11	1165.3091	0.000	1165.3099	-0.0008
(4)	24	0	24	-	24	1	24	1165.3523	0.001	1165.3523	0.0000
(4)	25	0	25	-	25	1	25	1165.4121	0.001	1165.4121	0.0000
(4)	26	0	26	-	26	1	26	1165.4631	0.001	1165.4630	0.0001
(4)	27	0	27	-	27	1	27	1165.5078	0.001	1165.5072	0.0006
(6)	14	3	11	-	15	4	12	1165.5337	0.000	1165.5338	-0.0001
(4)	28	0	28	-	28	1	28	1165.5473	0.001	1165.5464	0.0009
(4)	29	0	29	-	29	1	29	1165.5831	0.001	1165.5822	0.0009
(4)	22	2	21	-	21	3	19	1165.8449	0.001	1165.8432	0.0018
(4)	28	1	28	-	28	0	28	1165.8530	0.001	1165.8525	0.0005
(4)	27	1	27	-	27	0	27	1165.8921*	0.000	1165.8896	0.0025
(6)	10	4	7	-	11	5	6	1165.8921	0.001	1165.8929	-0.0007
(6)	10	4	6	-	11	5	7	1165.8921	0.001	1165.8932	-0.0011
(4)	26	1	26	-	26	0	26	1165.9394	0.001	1165.9397	-0.0003
(4)	25	1	25	-	25	0	25	1166.0046	0.001	1166.0047	-0.0002
(4)	3	0	3	-	2	1	1	1166.0336	0.000	1166.0335	0.0002
(4)	24	1	24	-	24	0	24	1166.0866	0.001	1166.0870	-0.0004
(4)	23	1	23	-	23	0	23	1166.1888	0.001	1166.1891	-0.0004
(4)	22	1	22	-	22	0	22	1166.3139	0.001	1166.3141	-0.0002
(4)	14	1	14	-	13	2	12	1166.3556*	0.000	1166.3624	-0.0068
(6)	17	2	16	-	18	3	15	1166.3556	0.001	1166.3551	0.0005
(4)	21	1	21	-	21	0	21	1166.4646	0.001	1166.4650	-0.0004
(4)	9	2	8	-	10	1	10	1166.5030	0.000	1166.5033	-0.0003
(4)	20	1	20	-	20	0	20	1166.6450	0.001	1166.6454	-0.0004
(4)	19	1	19	-	19	0	19	1166.8584	0.001	1166.8587	-0.0003

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(4)	22	2	21	-	22	1	21	1166.9357	0.001	1166.9340	0.0017
(4)	23	2	22	-	22	3	20	1166.9707	0.001	1166.9685	0.0023
(4)	2	1	1	-	3	0	3	1167.0188	0.000	1167.0187	0.0001
(4)	18	1	18	-	18	0	18	1167.1079	0.001	1167.1082	-0.0004
(6)	6	5	1	-	7	6	1	1167.2857	0.001	1167.2859	-0.0002
(6)	6	5	2	-	7	6	2	1167.2857	0.001	1167.2859	-0.0002
(4)	17	1	17	-	17	0	17	1167.3966	0.001	1167.3970	-0.0003
(4)	6	2	4	-	7	1	6	1167.4472	0.000	1167.4472	0.0000
(6)	23	2	21	-	24	3	22	1167.4578	0.001	1167.4574	0.0004
(4)	15	1	15	-	14	2	13	1167.4743	0.000	1167.4743	0.0000
(4)	16	1	16	-	16	0	16	1167.7267	0.001	1167.7269	-0.0002
(6)	13	3	11	-	14	4	10	1167.8444	0.000	1167.8447	-0.0003
(4)	24	2	23	-	23	3	21	1167.9710*	0.000	1167.9696	0.0014
(4)	10	1	9	-	9	2	7	1167.9710	0.000	1167.9704	0.0006
(6)	13	3	10	-	14	4	11	1167.9898	0.000	1167.9898	0.0000
(4)	15	1	15	-	15	0	15	1168.0988	0.000	1168.0991	-0.0002
(4)	18	2	16	-	17	3	14	1168.1093	0.001	1168.1099	-0.0006
(4)	4	0	4	-	3	1	2	1168.1548	0.000	1168.1547	0.0001
(4)	8	2	7	-	9	1	9	1168.1899	0.000	1168.1901	-0.0002
(4)	21	2	20	-	21	1	20	1168.2917	0.001	1168.2908	0.0009
(6)	22	2	20	-	23	3	21	1168.3370	0.001	1168.3365	0.0005
(6)	9	4	6	-	10	5	5	1168.3800	0.001	1168.3805	-0.0005
(6)	9	4	5	-	10	5	6	1168.3800	0.001	1168.3806	-0.0006
(4)	16	1	16	-	15	2	14	1168.4975	0.000	1168.4977	-0.0002
(4)	14	1	14	-	14	0	14	1168.5124	0.000	1168.5126	-0.0001
(4)	13	1	13	-	13	0	13	1168.9646	0.000	1168.9646	-0.0001
(6)	21	2	19	-	22	3	20	1169.3058	0.001	1169.3053	0.0005
(6)	16	2	15	-	17	3	14	1169.3865	0.001	1169.3862	0.0003
(4)	17	1	17	-	16	2	15	1169.4343	0.001	1169.4348	-0.0005
(4)	12	1	12	-	12	0	12	1169.4500	0.000	1169.4502	-0.0002
(4)	20	2	19	-	20	1	19	1169.6585	0.001	1169.6580	0.0005
(6)	5	5	1	-	6	6	0	1169.7573	0.001	1169.7575	-0.0002
(6)	5	5	0	-	6	6	1	1169.7573	0.001	1169.7575	-0.0002
(4)	7	2	6	-	8	1	8	1169.9547	0.000	1169.9534	0.0013
(4)	11	1	11	-	11	0	11	1169.9615	0.000	1169.9616	-0.0001
(4)	5	0	5	-	4	1	3	1170.1651	0.000	1170.1650	0.0002
(4)	18	1	18	-	17	2	16	1170.2876	0.001	1170.2880	-0.0004
(6)	12	3	10	-	13	4	9	1170.3630	0.000	1170.3633	-0.0004
(6)	20	2	18	-	21	3	19	1170.3710	0.001	1170.3707	0.0003
(4)	5	2	3	-	6	1	5	1170.4069	0.000	1170.4070	-0.0001
(6)	12	3	9	-	13	4	10	1170.4540	0.000	1170.4540	0.0000
(4)	10	1	10	-	10	0	10	1170.4895	0.000	1170.4895	0.0001
(4)	11	1	10	-	10	2	8	1170.5985	0.000	1170.5985	0.0001
(6)	8	4	5	-	9	5	4	1170.8621	0.001	1170.8626	-0.0005
(6)	8	4	4	-	9	5	5	1170.8621	0.001	1170.8626	-0.0005
(4)	19	2	17	-	18	3	15	1171.0226*	0.000	1171.0204	0.0023
(4)	19	2	18	-	19	1	18	1171.0226*	0.000	1171.0265	-0.0038
(4)	9	1	9	-	9	0	9	1171.0226*	0.000	1171.0223	0.0003
(4)	19	1	19	-	18	2	17	1171.0601	0.001	1171.0604	-0.0002
(6)	19	2	17	-	20	3	18	1171.5396	0.001	1171.5386	0.0010

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(4)	8	1	8	-	8	0	8	1171.5478	0.000	1171.5478	0.0000
(4)	20	1	20	-	19	2	18	1171.7553	0.001	1171.7554	-0.0001
(4)	6	2	5	-	7	1	7	1171.7922	0.000	1171.7928	-0.0006
(4)	6	0	6	-	5	1	4	1172.0547*	0.000	1172.0561	-0.0014
(4)	7	1	7	-	7	0	7	1172.0547*	0.000	1172.0530	0.0016
(6)	15	2	14	-	16	3	13	1172.3194	0.001	1172.3192	0.0002
(4)	21	1	21	-	20	2	19	1172.3777	0.001	1172.3770	0.0007
(4)	18	2	17	-	18	1	17	1172.3860	0.001	1172.3859	0.0002
(4)	6	1	6	-	6	0	6	1172.5255	0.000	1172.5255	0.0000
(6)	18	2	16	-	19	3	17	1172.8146	0.001	1172.8140	0.0007
(6)	11	3	9	-	12	4	8	1172.8685	0.000	1172.8688	-0.0003
(6)	11	3	8	-	12	4	9	1172.9233	0.000	1172.9232	0.0001
(4)	5	1	5	-	5	0	5	1172.9535	0.000	1172.9535	0.0000
(4)	12	1	11	-	11	2	9	1173.1466	0.000	1173.1465	0.0001
(4)	4	2	2	-	5	1	4	1173.3157	0.000	1173.3158	-0.0001
(4)	4	1	4	-	4	0	4	1173.3266	0.000	1173.3265	0.0001
(6)	7	4	4	-	8	5	3	1173.3384	0.001	1173.3390	-0.0006
(6)	7	4	3	-	8	5	4	1173.3384	0.001	1173.3390	-0.0006
(4)	3	1	3	-	3	0	3	1173.6357	0.000	1173.6357	-0.0001
(4)	5	2	4	-	6	1	6	1173.7075	0.000	1173.7076	-0.0001
(4)	17	2	16	-	17	1	16	1173.7257	0.001	1173.7258	-0.0001
(4)	7	0	7	-	6	1	5	1173.8187	0.000	1173.8186	0.0001
(4)	2	1	2	-	2	0	2	1173.8741	0.000	1173.8739	0.0001
(4)	20	2	18	-	19	3	16	1173.8965	0.001	1173.8972	-0.0007
(4)	1	1	1	-	1	0	1	1174.0360	0.000	1174.0357	0.0003
(6)	17	2	15	-	18	3	16	1174.2011	0.001	1174.2007	0.0005
(4)	16	2	15	-	16	1	15	1175.0358	0.001	1175.0360	-0.0001
(6)	14	2	13	-	15	3	12	1175.1662	0.000	1175.1657	0.0005
(6)	10	3	8	-	11	4	7	1175.3634	0.000	1175.3635	-0.0001
(6)	10	3	7	-	11	4	8	1175.3943	0.000	1175.3945	-0.0002
(4)	8	0	8	-	7	1	6	1175.4426	0.000	1175.4425	0.0001
(4)	13	1	12	-	12	2	10	1175.5930	0.000	1175.5931	0.0000
(4)	4	2	3	-	5	1	5	1175.7009	0.000	1175.6970	0.0038
(6)	16	2	14	-	17	3	15	1175.7009*	0.000	1175.7011	-0.0003
(6)	6	4	3	-	7	5	2	1175.8091	0.001	1175.8096	-0.0005
(6)	6	4	2	-	7	5	3	1175.8091	0.001	1175.8096	-0.0005
(6)	12	6	6	-	12	7	5	1175.9478	0.001	1175.9468	0.0010
(6)	11	6	5	-	11	7	4	1176.0044	0.001	1176.0020	0.0024
(4)	3	2	1	-	4	1	3	1176.1607	0.000	1176.1610	-0.0003
(4)	15	2	14	-	15	1	14	1176.3065	0.000	1176.3067	-0.0002
(4)	1	1	0	-	0	0	0	1176.6069	0.000	1176.6066	0.0002
(4)	21	2	19	-	20	3	17	1176.7152	0.001	1176.7160	-0.0008
(4)	9	0	9	-	8	1	7	1176.9177	0.000	1176.9175	0.0002
(6)	15	2	13	-	16	3	14	1177.3165	0.001	1177.3161	0.0004
(4)	14	2	13	-	14	1	13	1177.5290	0.000	1177.5291	0.0000
(4)	3	2	2	-	4	1	4	1177.7599	0.000	1177.7602	-0.0003
(6)	9	3	7	-	10	4	6	1177.8490	0.000	1177.8492	-0.0002
(6)	9	3	6	-	10	4	7	1177.8657	0.000	1177.8659	-0.0002
(4)	14	1	13	-	13	2	11	1177.9174	0.000	1177.9175	-0.0001
(6)	13	2	12	-	14	3	11	1177.9375	0.000	1177.9372	0.0003

UPPER STATE J KA KC			LOWER STATE J KA KC			OBSERVATION	PREC.	CALCULATION	RESID.
(4)	10	0	10 - 9	1	8	1178.2343	0.000	1178.2341	0.0002
(6)	5	4	2 - 6	5	1	1178.2739	0.001	1178.2743	-0.0004
(6)	5	4	1 - 6	5	2	1178.2739	0.001	1178.2743	-0.0004
(4)	24	3	22 - 24	2	22	1178.5485	0.001	1178.5469	0.0016
(4)	13	2	12 - 13	1	12	1178.6952	0.000	1178.6953	0.0000
(6)	14	2	12 - 15	3	13	1179.0447	0.000	1179.0445	0.0003
(4)	2	1	1 - 1	0	1	1179.1546	0.000	1179.1546	0.0000
(4)	11	0	11 - 10	1	9	1179.3843	0.000	1179.3842	0.0001
(4)	22	2	20 - 21	3	18	1179.4503	0.001	1179.4511	-0.0008
(4)	12	2	11 - 12	1	11	1179.7982	0.000	1179.7983	-0.0001
(4)	2	2	1 - 3	1	3	1179.8958	0.000	1179.8962	-0.0004
(4)	26	0	26 - 25	1	24	1179.9082	0.001	1179.9083	0.0000
(4)	15	1	14 - 14	2	12	1180.1002	0.000	1180.1003	0.0000
(6)	13	1	13 - 14	2	12	1180.2236	0.000	1180.2236	0.0000
(6)	8	3	6 - 9	4	5	1180.3275	0.000	1180.3273	0.0002
(6)	8	3	5 - 9	4	6	1180.3353	0.000	1180.3356	-0.0003
(4)	12	0	12 - 11	1	10	1180.3617*	0.000	1180.3617	0.0001
(4)	25	0	25 - 24	1	23	1180.3617*	0.000	1180.3563	0.0054
(4)	23	3	21 - 23	2	21	1180.4893	0.001	1180.4883	0.0010
(6)	12	2	11 - 13	3	10	1180.6446	0.000	1180.6443	0.0003
(6)	4	4	1 - 5	5	0	1180.7325	0.001	1180.7330	-0.0005
(6)	4	4	0 - 5	5	1	1180.7325	0.001	1180.7330	-0.0005
(4)	24	0	24 - 23	1	22	1180.8080	0.001	1180.8080	0.0000
(4)	11	2	10 - 11	1	10	1180.8321	0.000	1180.8324	-0.0002
(6)	13	2	11 - 14	3	12	1180.8832	0.000	1180.8831	0.0002
(4)	13	0	13 - 12	1	11	1181.1638	0.000	1181.1636	0.0002
(4)	23	0	23 - 22	1	21	1181.2496	0.001	1181.2494	0.0002
(4)	22	0	22 - 21	1	20	1181.6639	0.001	1181.6641	-0.0002
(4)	3	1	2 - 2	0	2	1181.7626	0.000	1181.7626	0.0000
(4)	14	0	14 - 13	1	12	1181.7916*	0.000	1181.7903	0.0012
(4)	10	2	9 - 10	1	9	1181.7916*	0.000	1181.7925	-0.0009
(4)	21	0	21 - 20	1	19	1182.0336	0.001	1182.0340	-0.0004
(4)	23	2	21 - 22	3	19	1182.0756	0.001	1182.0765	-0.0009
(4)	16	1	15 - 15	2	13	1182.1235	0.000	1182.1235	0.0000
(4)	15	0	15 - 14	1	13	1182.2461	0.000	1182.2461	0.0000
(4)	20	0	20 - 19	1	18	1182.3398	0.001	1182.3399	-0.0001
(4)	22	3	20 - 22	2	20	1182.3485*	0.000	1182.3476	0.0009
(4)	16	0	16 - 15	1	14	1182.5385	0.000	1182.5385	0.0001
(4)	19	0	19 - 18	1	17	1182.5619	0.001	1182.5621	-0.0002
(4)	17	0	17 - 16	1	15	1182.6760*	0.000	1182.6788	-0.0028
(4)	9	2	8 - 9	1	8	1182.6760*	0.000	1182.6746	0.0014
(4)	18	0	18 - 17	1	16	1182.6760*	0.000	1182.6812	-0.0051
(6)	7	3	5 - 8	4	4	1182.8004	0.000	1182.7987	0.0017
(6)	7	3	4 - 8	4	5	1182.8004	0.000	1182.8024	-0.0020
(6)	12	2	10 - 13	3	11	1182.8267	0.000	1182.8266	0.0001
(6)	19	5	15 - 19	6	14	1183.0946	0.001	1183.0938	0.0008
(6)	19	5	14 - 19	6	13	1183.0946	0.001	1183.0965	-0.0019
(6)	18	5	14 - 18	6	13	1183.2207	0.001	1183.2200	0.0007
(6)	18	5	13 - 18	6	12	1183.2207	0.001	1183.2215	-0.0008
(6)	11	2	10 - 12	3	9	1183.2972	0.000	1183.2970	0.0003
(6)	17	5	13 - 17	6	12	1183.3413	0.001	1183.3409	0.0005
(6)	17	5	12 - 17	6	11	1183.3413	0.001	1183.3417	-0.0004
(6)	26	1	25 - 27	2	26	1183.4054	0.001	1183.4085	-0.0031
(6)	16	5	12 - 16	6	11	1183.4568	0.001	1183.4563	0.0004
(6)	16	5	11 - 16	6	10	1183.4568	0.001	1183.4568	0.0000
(4)	8	2	7 - 8	1	7	1183.4753	0.000	1183.4754	-0.0001
(6)	15	5	11 - 15	6	10	1183.5664	0.001	1183.5663	0.0001
(6)	15	5	10 - 15	6	9	1183.5664	0.001	1183.5665	-0.0001
(6)	14	5	10 - 14	6	9	1183.6704	0.001	1183.6704	0.0000
(6)	14	5	9 - 14	6	8	1183.6704	0.001	1183.6705	-0.0001
(6)	13	5	9 - 13	6	8	1183.7685	0.001	1183.7686	-0.0001
(6)	13	5	8 - 13	6	7	1183.7685	0.001	1183.7687	-0.0002
(6)	12	5	8 - 12	6	7	1183.8605	0.001	1183.8607	-0.0002
(6)	12	5	7 - 12	6	6	1183.8605	0.001	1183.8607	-0.0002
(6)	11	5	7 - 11	6	6	1183.9462	0.001	1183.9464	-0.0001
(6)	11	5	6 - 11	6	5	1183.9462	0.001	1183.9464	-0.0002
(4)	17	1	16 - 16	2	14	1183.9708	0.001	1183.9707	0.0001
(6)	10	5	6 - 10	6	5	1184.0255	0.001	1184.0256	-0.0002
(6)	10	5	5 - 10	6	4	1184.0255	0.001	1184.0256	-0.0002
(6)	9	5	5 - 9	6	4	1184.0982	0.001	1184.0982	0.0000
(6)	9	5	4 - 9	6	3	1184.0982	0.001	1184.0982	0.0000
(4)	21	3	19 - 21	2	19	1184.1162	0.001	1184.1160	0.0002
(6)	8	5	4 - 8	6	3	1184.1636	0.001	1184.1640	-0.0003
(6)	8	5	3 - 8	6	2	1184.1636	0.001	1184.1640	-0.0003
(4)	7	2	6 - 7	1	6	1184.1922	0.000	1184.1922	0.0000
(6)	7	5	3 - 7	6	2	1184.2223	0.001	1184.2228	-0.0005
(6)	7	5	2 - 7	6	1	1184.2223	0.001	1184.2228	-0.0005
(6)	6	5	2 - 6	6	1	1184.2737	0.001	1184.2745	-0.0008
(6)	6	5	1 - 6	6	0	1184.2737	0.001	1184.2745	-0.0008
(4)	4	1	3 - 3	0	3	1184.4334	0.000	1184.4334	0.0000
(4)	24	2	22 - 23	3	20	1184.5656	0.001	1184.5663	-0.0007
(6)	12	1	12 - 13	2	11	1184.6395	0.000	1184.6395	0.0000
(4)	6	2	5 - 6	1	5	1184.8228	0.000	1184.8230	-0.0001
(6)	11	2	9 - 12	3	10	1184.8677	0.000	1184.8677	0.0001
(6)	6	3	4 - 7	4	3	1185.2651	0.000	1185.2640	0.0012
(6)	6	3	3 - 7	4	4	1185.2651	0.000	1185.2655	-0.0003
(4)	5	2	4 - 5	1	4	1185.3659	0.000	1185.3660	-0.0001
(4)	18	1	17 - 17	2	15	1185.6273	0.001	1185.6271	0.0002
(4)	20	3	18 - 20	2	18	1185.7854	0.001	1185.7855	0.0000
(4)	4	2	3 - 4	1	3	1185.8201	0.000	1185.8202	-0.0001
(6)	24	1	23 - 25	2	24	1185.8781	0.001	1185.8799	-0.0018
(6)	10	2	9 - 11	3	8	1185.9041	0.000	1185.9040	0.0001
(6)	6	3	4 - 7	4	3	1185.2651	0.000	1185.2640	0.0012
(4)	3	2	2 - 3	1	2	1186.1844	0.000	1186.1845	-0.0001
(4)	2	2	1 - 2	1	1	1186.4583	0.000	1186.4582	0.0001
(4)	25	2	23 - 24	3	21	1186.8949	0.001	1186.8954	-0.0005
(4)	2	2	0 - 2	1	2	1186.9438	0.000	1186.9438	0.0001
(6)	10	2	8 - 11	3	9	1186.9973	0.000	1186.9971	0.0003
(6)	27	2	26 - 28	1	27	1187.0190	0.001	1187.0156	0.0035
(6)	23	1	22 - 24	2	23	1187.0564	0.001	1187.0579	-0.0015

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(4)	19	1	18	-	18	2	16	1187.0796	0.001	1187.0793	0.0003
(4)	3	2	1	-	3	1	3	1187.1625	0.000	1187.1623	0.0002
(4)	5	1	4	-	4	0	4	1187.1720	0.000	1187.1717	0.0002
(6)	26	0	26	-	27	1	27	1187.3169	0.001	1187.3179	-0.0010
(4)	19	3	17	-	19	2	17	1187.3480	0.001	1187.3484	-0.0004
(4)	4	2	2	-	4	1	4	1187.4649	0.000	1187.4649	0.0000
(6)	5	3	3	-	6	4	2	1187.7238	0.000	1187.7237	0.0001
(6)	5	3	2	-	6	4	3	1187.7238	0.000	1187.7242	-0.0004
(4)	5	2	3	-	5	1	5	1187.8609	0.000	1187.8608	0.0001
(6)	22	1	21	-	23	2	22	1188.2068	0.001	1188.2080	-0.0013
(4)	20	1	19	-	19	2	17	1188.3165	0.001	1188.3158	0.0007
(4)	6	2	4	-	6	1	6	1188.3616	0.000	1188.3616	0.0000
(6)	9	2	8	-	10	3	7	1188.4734	0.000	1188.4733	0.0001
(6)	11	1	11	-	12	2	10	1188.8270	0.000	1188.8273	-0.0003
(4)	7	2	5	-	7	1	7	1188.9805	0.000	1188.9805	0.0000
(4)	26	2	24	-	25	3	22	1189.0399	0.001	1189.0401	-0.0002
(6)	9	2	7	-	10	3	8	1189.2043	0.000	1189.2041	0.0002
(6)	25	1	25	-	26	0	26	1189.2597	0.001	1189.2559	0.0038
(4)	21	1	20	-	20	2	18	1189.3275	0.001	1189.3265	0.0010
(6)	21	1	20	-	22	2	21	1189.3388	0.001	1189.3401	-0.0013
(6)	25	0	25	-	26	1	26	1189.3840	0.001	1189.3847	-0.0008
(6)	26	2	25	-	27	1	26	1189.5012	0.001	1189.4987	0.0025
(4)	8	2	6	-	8	1	8	1189.7321	0.000	1189.7323	-0.0002
(4)	6	1	5	-	5	0	5	1189.9838	0.000	1189.9837	0.0002
(4)	17	3	15	-	17	2	15	1190.1284	0.001	1190.1287	-0.0003
(6)	4	3	2	-	5	4	1	1190.1779	0.000	1190.1780	-0.0001
(6)	4	3	1	-	5	4	2	1190.1779	0.000	1190.1781	-0.0002
(4)	12	6	6	-	13	5	8	1190.3879	0.001	1190.3887	-0.0007
(4)	12	6	7	-	13	5	9	1190.3879	0.001	1190.3887	-0.0008
(6)	20	1	19	-	21	2	20	1190.4641	0.001	1190.4649	-0.0009
(4)	9	2	7	-	9	1	9	1190.6323	0.000	1190.6324	0.0000
(6)	27	4	24	-	27	5	23	1190.8174	0.001	1190.8195	-0.0022
(4)	27	2	25	-	26	3	23	1190.9784	0.001	1190.9781	0.0003
(6)	26	4	23	-	26	5	22	1190.9927	0.001	1190.9950	-0.0023
(6)	8	2	7	-	9	3	6	1191.0119	0.000	1191.0117	0.0001
(6)	25	4	22	-	25	5	21	1191.1530	0.001	1191.1541	-0.0011
(6)	24	1	24	-	25	0	25	1191.2079	0.001	1191.2044	0.0035
(6)	24	4	21	-	24	5	20	1191.2988	0.001	1191.2996	-0.0008
(4)	16	3	14	-	16	2	14	1191.3356	0.001	1191.3357	0.0000
(6)	23	4	20	-	23	5	19	1191.4330	0.001	1191.4335	-0.0005
(6)	24	0	24	-	25	1	25	1191.4613	0.001	1191.4618	-0.0005
(4)	2	2	0	-	1	1	0	1191.4780	0.000	1191.4806	-0.0026
(6)	8	2	6	-	9	3	7	1191.4780	0.000	1191.4771	0.0009
(6)	22	4	19	-	22	5	18	1191.5574	0.001	1191.5577	-0.0003
(6)	19	1	18	-	20	2	19	1191.5936	0.001	1191.5937	-0.0001
(6)	27	4	23	-	27	5	22	1191.6150	0.001	1191.6169	-0.0019
(4)	2	2	1	-	1	1	1	1191.6393	0.000	1191.6394	-0.0001
(6)	21	4	18	-	21	5	17	1191.6740	0.001	1191.6738	0.0003
(4)	10	2	8	-	10	1	10	1191.6965	0.000	1191.6965	0.0000
(6)	22	4	18	-	22	5	17	1191.7290	0.001	1191.7295	-0.0006

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(6)	20	4	17	-	20	5	16	1191.7828	0.001	1191.7830	-0.0001
(6)	21	4	17	-	21	5	16	1191.7940	0.001	1191.7941	-0.0001
(6)	20	4	16	-	20	5	15	1191.8655	0.001	1191.8657	-0.0002
(6)	19	4	16	-	19	5	15	1191.8860	0.001	1191.8862	-0.0002
(6)	19	4	15	-	19	5	14	1191.9417	0.001	1191.9418	-0.0001
(6)	18	4	15	-	18	5	14	1191.9841	0.001	1191.9842	-0.0001
(6)	18	4	14	-	18	5	13	1192.0208	0.001	1192.0208	0.0001
(6)	17	4	14	-	17	5	13	1192.0776	0.001	1192.0774	0.0002
(6)	17	4	13	-	17	5	12	1192.1010	0.001	1192.1009	0.0001
(6)	16	4	13	-	16	5	12	1192.1664	0.001	1192.1662	0.0001
(6)	16	4	12	-	16	5	11	1192.1807	0.001	1192.1808	-0.0001
(6)	15	4	12	-	15	5	11	1192.2510	0.001	1192.2508	0.0002
(6)	15	4	11	-	15	5	10	1192.2593	0.001	1192.2596	-0.0003
(6)	14	4	11	-	14	5	10	1192.3327	0.001	1192.3311	0.0016
(6)	14	4	11	-	14	5	10	1192.3327	0.001	1192.3311	0.0016
(6)	14	4	10	-	14	5	9	1192.3327	0.001	1192.3362	-0.0035
(6)	13	4	10	-	13	5	9	1192.4085	0.001	1192.4071	0.0014
(6)	13	4	9	-	13	5	8	1192.4085	0.001	1192.4100	-0.0014
(6)	12	4	9	-	12	5	8	1192.4793	0.001	1192.4787	0.0005
(6)	12	4	8	-	12	5	7	1192.4793	0.001	1192.4803	-0.0010
(6)	11	4	8	-	11	5	7	1192.5461	0.001	1192.5459	0.0002
(6)	11	4	7	-	11	5	6	1192.5461	0.001	1192.5466	-0.0005
(6)	10	4	7	-	10	5	6	1192.6083	0.001	1192.6082	0.0001
(6)	10	4	6	-	10	5	5	1192.6083	0.001	1192.6086	-0.0003
(6)	3	3	1	-	4	4	0	1192.6268	0.000	1192.6270	-0.0002
(6)	3	3	0	-	4	4	1	1192.6268	0.000	1192.6270	-0.0003
(6)	9	4	6	-	9	5	5	1192.6657	0.001	1192.6657	-0.0001
(6)	9	4	5	-	9	5	4	1192.6657	0.001	1192.6659	-0.0002
(4)	28	2	26	-	27	3	24	1192.6896	0.001	1192.6891	0.0006
(6)	8	4	5	-	8	5	4	1192.7177	0.001	1192.7181	-0.0004
(6)	8	4	4	-	8	5	3	1192.7177	0.001	1192.7182	-0.0004
(6)	18	1	17	-	19	2	18	1192.7369	0.001	1192.7374	-0.0005
(6)	7	4	4	-	7	5	3	1192.7648	0.001	1192.7652	-0.0004
(6)	7	4	3	-	7	5	2	1192.7648	0.001	1192.7652	-0.0004
(6)	10	1	10	-	11	2	9	1192.7955	0.000	1192.7954	0.0000
(6)	6	4	3	-	6	5	2	1192.8064	0.001	1192.8068	-0.0004
(6)	6	4	2	-	6	5	1	1192.8064	0.001	1192.8068	-0.0004
(6)	5	4	2	-	5	5	1	1192.8424	0.001	1192.8428	-0.0004
(6)	5	4	1	-	5	5	0	1192.8424	0.001	1192.8428	-0.0004
(4)	7	1	6	-	6	0	6	1192.8665R	0.000	1192.8768	-0.0103
(4)	27	4	24	-	27	3	24	1192.8770	0.001	1192.8803	-0.0033
(4)	11	2	9	-	11	1	11	1192.9394	0.000	1192.9396	-0.0001
(4)	14	3	12	-	14	2	12	1193.3694	0.000	1193.3694	0.0000
(6)	7	2	6	-	8	3	5	1193.5251	0.000	1193.5250	0.0002
(6)	23	0	23	-	24	1	24	1193.5414	0.001	1193.5418	-0.0004
(4)	3	2	1	-	2	1	1	1193.7243	0.000	1193.7243	0.0000
(6)	7	2	5	-	8	3	6	1193.8041	0.000	1193.8039	0.0002
(6)	22	1	22	-	23	0	23	1193.8717	0.001	1193.8693	0.0024
(6)	17	1	16	-	18	2	17	1193.9063	0.001	1193.9067	-0.0003
(4)	29	2	27	-	28	3	25	1194.1564	0.001	1194.1549	0.0016

	UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(4)	3	2	2	-	2	1	2	1194.1964	0.000	1194.1962	0.0002
(4)	12	2	10	-	12	1	12	1194.3750	0.000	1194.3750	0.0000
(4)	26	4	23	-	26	3	23	1194.5876	0.001	1194.5868	0.0008
(6)	24	2	23	-	25	1	24	1194.7691	0.001	1194.7676	0.0015
(4)	12	3	10	-	12	2	10	1194.9021	0.000	1194.9022	0.0000
(6)	16	1	15	-	17	2	16	1195.1107	0.001	1195.1112	-0.0004
(4)	11	3	9	-	11	2	9	1195.4921	0.000	1195.4923	-0.0001
(6)	22	0	22	-	23	1	23	1195.6175	0.001	1195.6176	-0.0001
(4)	8	1	7	-	7	0	7	1195.8600	0.000	1195.8598	0.0001
(4)	4	2	2	-	3	1	2	1195.8892	0.000	1195.8891	0.0001
(4)	10	3	8	-	10	2	8	1195.9761	0.000	1195.9759	0.0002
(4)	13	2	11	-	13	1	13	1196.0177*	0.000	1196.0140	0.0037
(6)	6	2	5	-	7	3	4	1196.0177	0.000	1196.0180	-0.0003
(4)	25	4	22	-	25	3	22	1196.1422	0.001	1196.1420	0.0003
(6)	6	2	4	-	7	3	5	1196.1727	0.000	1196.1726	0.0001
(6)	15	1	14	-	16	2	15	1196.3600	0.001	1196.3596	0.0004
(6)	9	1	9	-	10	2	8	1196.5550	0.000	1196.5551	-0.0002
(4)	8	3	6	-	8	2	6	1196.6683	0.000	1196.6681	0.0002
(4)	4	2	3	-	3	1	3	1196.8215	0.000	1196.8215	0.0000
(4)	7	3	5	-	7	2	5	1196.9010	0.000	1196.9010	0.0000
(4)	6	3	4	-	6	2	4	1197.0751	0.000	1197.0748	0.0003
(4)	10	3	7	-	10	2	9	1197.1486	0.000	1197.1484	0.0002
(4)	8	3	5	-	8	2	7	1197.1694	0.000	1197.1688	0.0006
(4)	5	3	3	-	5	2	3	1197.2015	0.000	1197.2011	0.0003
(4)	12	3	9	-	12	2	11	1197.2384	0.000	1197.2373	0.0012
(4)	5	3	2	-	5	2	4	1197.2850	0.000	1197.2846	0.0005
(4)	4	3	1	-	4	2	3	1197.3264	0.000	1197.3259	0.0005
(4)	13	3	10	-	13	2	12	1197.3446	0.000	1197.3448	-0.0002
(6)	28	2	27	-	28	3	26	1197.4921	0.001	1197.4899	0.0022
(4)	14	3	11	-	14	2	13	1197.5081	0.000	1197.5081	0.0000
(4)	24	4	21	-	24	3	21	1197.5474	0.001	1197.5468	0.0007
(6)	14	1	13	-	15	2	14	1197.6595	0.000	1197.6598	-0.0002
(6)	21	0	21	-	22	1	22	1197.6826	0.001	1197.6827	-0.0001
(4)	15	3	12	-	15	2	14	1197.7384	0.000	1197.7384	0.0000
(4)	14	2	12	-	14	1	14	1197.8647	0.000	1197.8651	-0.0004
(4)	5	2	3	-	4	1	3	1197.9840	0.000	1197.9840	0.0001
(4)	16	3	13	-	16	2	15	1198.0472	0.001	1198.0472	0.0000
(6)	27	2	26	-	27	3	25	1198.3689	0.001	1198.3667	0.0022
(4)	17	3	14	-	17	2	16	1198.4451	0.001	1198.4449	0.0001
(6)	5	2	4	-	6	3	3	1198.4951	0.000	1198.4950	0.0001
(6)	5	2	3	-	6	3	4	1198.5720	0.000	1198.5720	0.0000
(4)	23	4	20	-	23	3	20	1198.8050	0.001	1198.8047	0.0004
(6)	25	3	23	-	25	4	22	1198.9314	0.001	1198.9324	-0.0010
(6)	13	1	12	-	14	2	13	1199.0177	0.000	1199.0181	-0.0003
(4)	5	2	4	-	4	1	4	1199.5149	0.000	1199.5151	-0.0002
(6)	20	0	20	-	21	1	21	1199.7307	0.001	1199.7308	-0.0001
(4)	22	4	19	-	22	3	19	1199.9219	0.001	1199.9216	0.0003
(4)	15	2	13	-	15	1	15	1199.9281*	0.000	1199.9337	-0.0056
(4)	6	2	4	-	5	1	4	1200.0200	0.000	1200.0200	0.0000
(6)	8	1	8	-	9	2	7	1200.1200	0.000	1200.1202	-0.0002

	UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(6)	12	1	11	-	13	2	12	1200.4401*	0.000	1200.4400	0.0001
(4)	21	4	18	-	21	3	18	1200.9062	0.001	1200.9058	0.0004
(6)	4	2	3	-	5	3	2	1200.9591	0.000	1200.9591	0.0000
(6)	4	2	2	-	5	3	3	1200.9918	0.000	1200.9920	-0.0002
(4)	23	4	19	-	23	3	21	1201.2500	0.001	1201.2495	0.0005
(6)	15	3	13	-	15	4	12	1201.6991	0.000	1201.6991	-0.0001
(6)	19	0	19	-	20	1	20	1201.7562	0.001	1201.7563	-0.0001
(4)	20	4	17	-	20	3	17	1201.7672	0.001	1201.7672	0.0000
(6)	14	3	12	-	14	4	11	1201.8061	0.000	1201.8062	-0.0001
(4)	22	4	18	-	22	3	20	1201.8363	0.001	1201.8351	0.0012
(6)	13	3	11	-	13	4	10	1201.8974	0.000	1201.8974	0.0000
(6)	11	1	10	-	12	2	11	1201.9299	0.000	1201.9301	-0.0002
(6)	12	3	10	-	12	4	9	1201.9754	0.000	1201.9756	-0.0002
(4)	7	2	5	-	6	1	5	1202.0102	0.000	1202.0107	-0.0005
(6)	14	3	11	-	14	4	10	1202.0102	0.000	1202.0106	-0.0003
(6)	15	3	12	-	15	4	11	1202.0102*	0.000	1202.0012	0.0091
(6)	13	3	10	-	13	4	9	1202.0311	0.000	1202.0313	-0.0002
(6)	11	3	9	-	11	4	8	1202.0430	0.000	1202.0430	0.0000
(6)	12	3	9	-	12	4	8	1202.0600	0.000	1202.0601	-0.0002
(6)	11	3	8	-	11	4	7	1202.0945	0.000	1202.0942	0.0003
(6)	10	3	8	-	10	4	7	1202.1011	0.000	1202.1016	-0.0004
(6)	10	3	7	-	10	4	6	1202.1322	0.000	1202.1310	0.0012
(6)	9	3	7	-	9	4	6	1202.1520	0.000	1202.1526	-0.0006
(6)	9	3	6	-	9	4	5	1202.1682	0.000	1202.1686	-0.0003
(6)	8	3	6	-	8	4	5	1202.1973	0.000	1202.1973	0.0001
(6)	8	3	5	-	8	4	4	1202.2050	0.000	1202.2053	-0.0003
(4)	16	2	14	-	16	1	16	1202.2217	0.001	1202.2222	-0.0004
(6)	7	3	5	-	7	4	4	1202.2389*	0.000	1202.2363	0.0026
(6)	7	3	4	-	7	4	3	1202.2389*	0.000	1202.2399	-0.0011
(6)	6	3	4	-	6	4	3	1202.2716	0.000	1202.2701	0.0015
(6)	6	3	3	-	6	4	2	1202.2716	0.000	1202.2716	0.0001
(4)	6	2	5	-	5	1	5	1202.2761	0.000	1202.2768	-0.0008
(6)	5	3	3	-	5	4	2	1202.2990	0.000	1202.2990	0.0000
(6)	5	3	2	-	5	4	1	1202.2990	0.000	1202.2995	-0.0005
(6)	4	3	2	-	4	4	1	1202.3230	0.000	1202.3231	-0.0002
(6)	4	3	1	-	4	4	0	1202.3230	0.000	1202.3233	-0.0003
(4)	21	4	17	-	21	3	19	1202.3767	0.001	1202.3761	0.0006
(4)	19	4	16	-	19	3	16	1202.5171	0.001	1202.5171	0.0001
(4)	20	4	16	-	20	3	18	1202.8768	0.001	1202.8763	0.0005
(4)	18	4	15	-	18	3	15	1203.1669	0.001	1203.1670	-0.0001
(4)	19	4	15	-	19	3	17	1203.3389	0.001	1203.3386	0.0003
(6)	3	2	2	-	4	3	1	1203.4132	0.000	1203.4131	0.0001
(6)	3	2	1	-	4	3	2	1203.4238	0.000	1203.4240	-0.0002
(6)	10	1	9	-	11	2	10	1203.4917	0.000	1203.4919	-0.0002
(6)	7	1	7	-	8	2	6	1203.5056	0.000	1203.5058	-0.0002
(4)	17	4	14	-	17	3	14	1203.7287	0.001	1203.7287	0.0000
(6)	18	0	18	-	19	1	19	1203.7540	0.001	1203.7543	-0.0003
(4)	18	4	14	-	18	3	16	1203.7650	0.001	1203.7650	0.0000
(6)	25	0	25	-	25	1	24	1203.8289	0.001	1203.8300	-0.0011
(4)	8	2	6	-	7	1	6	1203.9710	0.000	1203.9711	0.0000

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(4)	17	4	13	-	17	3	15	1204.1568	0.001	1204.1568	0.0000
(4)	16	4	13	-	16	3	13	1204.2133	0.001	1204.2134	-0.0001
(4)	16	4	12	-	16	3	14	1204.5148	0.001	1204.5151	-0.0002
(4)	15	4	12	-	15	3	12	1204.6312	0.000	1204.6313	-0.0001
(4)	15	4	11	-	15	3	13	1204.8407	0.000	1204.8407	-0.0001
(4)	14	4	11	-	14	3	11	1204.9913	0.000	1204.9913	0.0000
(4)	7	2	6	-	6	1	6	1205.1066	0.000	1205.1066	-0.0001
(6)	9	1	8	-	10	2	9	1205.1284	0.000	1205.1282	0.0002
(4)	14	4	10	-	14	3	12	1205.1340	0.000	1205.1346	-0.0006
(4)	13	4	10	-	13	3	10	1205.3011	0.000	1205.3012	-0.0001
(4)	13	4	9	-	13	3	11	1205.3974	0.000	1205.3975	-0.0001
(6)	23	2	22	-	24	1	23	1205.5007	0.001	1205.5017	-0.0010
(4)	12	4	9	-	12	3	9	1205.5672	0.000	1205.5673	-0.0001
(4)	12	4	8	-	12	3	10	1205.6307	0.000	1205.6307	0.0001
(6)	17	0	17	-	18	1	18	1205.7207	0.001	1205.7210	-0.0004
(4)	11	4	8	-	11	3	8	1205.7949	0.000	1205.7949	-0.0001
(4)	11	4	7	-	11	3	9	1205.8355	0.000	1205.8354	0.0001
(6)	2	2	1	-	3	3	0	1205.8599	0.000	1205.8591	0.0008
(6)	2	2	0	-	3	3	1	1205.8599	0.000	1205.8613	-0.0014
(4)	9	2	7	-	8	1	7	1205.9175	0.000	1205.9177	-0.0001
(4)	10	4	7	-	10	3	7	1205.9887	0.000	1205.9885	0.0002
(4)	10	4	6	-	10	3	8	1206.0134	0.000	1206.0133	0.0001
(4)	9	4	6	-	9	3	6	1206.1519	0.000	1206.1518	0.0002
(4)	9	4	5	-	9	3	7	1206.1662	0.000	1206.1661	0.0000
(4)	8	4	5	-	8	3	5	1206.2884	0.000	1206.2881	0.0004
(4)	8	4	4	-	8	3	6	1206.2955	0.000	1206.2958	-0.0003
(4)	7	4	4	-	7	3	4	1206.4031	0.000	1206.4005	0.0025
(4)	7	4	3	-	7	3	5	1206.4031	0.000	1206.4043	-0.0012
(6)	24	0	24	-	24	1	23	1206.4031*	0.000	1206.4060	-0.0030
(4)	6	4	3	-	6	3	3	1206.4929	0.000	1206.4921	0.0008
(4)	6	4	2	-	6	3	4	1206.4929	0.000	1206.4937	-0.0008
(4)	5	4	2	-	5	3	2	1206.5660	0.000	1206.5654	0.0006
(4)	5	4	1	-	5	3	3	1206.5660	0.000	1206.5659	0.0001
(4)	4	4	1	-	4	3	1	1206.6229	0.000	1206.6228	0.0002
(4)	4	4	0	-	4	3	2	1206.6229	0.000	1206.6229	0.0000
(6)	6	1	6	-	7	2	5	1206.7278	0.000	1206.7278	0.0000
(6)	8	1	7	-	9	2	8	1206.8409	0.000	1206.8411	-0.0002
(6)	16	0	16	-	17	1	17	1207.6537	0.001	1207.6542	-0.0005
(4)	10	2	8	-	9	1	8	1207.8674	0.000	1207.8677	-0.0002
(4)	8	2	7	-	7	1	7	1208.0042	0.000	1208.0044	-0.0002
(6)	22	2	21	-	23	1	22	1208.1603	0.001	1208.1608	-0.0005
(6)	7	1	6	-	8	2	7	1208.6320	0.000	1208.6321	-0.0001
(6)	23	0	23	-	23	1	22	1208.9972	0.001	1208.9975	-0.0003
(6)	23	2	22	-	23	3	21	1209.1882	0.001	1209.1899	-0.0017
(6)	22	2	21	-	22	3	20	1209.5347*	0.000	1209.5337	0.0010
(6)	15	0	15	-	16	1	16	1209.5529	0.001	1209.5532	-0.0003
(6)	5	1	5	-	6	2	4	1209.8012*	0.000	1209.8018	-0.0006
(4)	11	2	9	-	10	1	9	1209.8385	0.000	1209.8388	-0.0003
(6)	21	2	20	-	21	3	19	1209.8948	0.001	1209.8950	-0.0002
(6)	20	2	19	-	20	3	18	1210.2598	0.001	1210.2600	-0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(6)	6	1	5	-	7	2	6	1210.5022	0.000	1210.5022	0.0000
(6)	19	2	18	-	19	3	17	1210.6173	0.001	1210.6172	0.0001
(6)	18	2	17	-	18	3	16	1210.9587	0.001	1210.9583	0.0004
(4)	9	2	8	-	8	1	8	1210.9697	0.000	1210.9699	-0.0002
(6)	21	2	20	-	22	1	21	1210.9855	0.001	1210.9859	-0.0004
(6)	18	1	18	-	18	2	17	1211.2668	0.001	1211.2666	0.0001
(6)	17	2	16	-	17	3	15	1211.2776	0.001	1211.2773	0.0004
(6)	14	0	14	-	15	1	15	1211.4191	0.000	1211.4194	-0.0002
(6)	16	2	15	-	16	3	14	1211.5704	0.001	1211.5701	0.0003
(6)	22	0	22	-	22	1	21	1211.5852	0.001	1211.5858	-0.0006
(6)	15	2	14	-	15	3	13	1211.8347	0.000	1211.8344	0.0003
(4)	12	2	10	-	11	1	10	1211.8475	0.000	1211.8477	-0.0002
(6)	14	2	13	-	14	3	12	1212.0697	0.000	1212.0694	0.0004
(6)	8	4	5	-	7	5	2	1212.1438	0.001	1212.1443	-0.0005
(6)	8	4	4	-	7	5	3	1212.1438	0.001	1212.1443	-0.0005
(6)	13	2	12	-	13	3	11	1212.2753	0.000	1212.2751	0.0002
(6)	5	1	4	-	6	2	5	1212.4525	0.000	1212.4522	0.0003
(6)	12	2	11	-	12	3	10	1212.4525*	0.000	1212.4527	-0.0002
(6)	11	2	10	-	11	3	9	1212.6037	0.000	1212.6036	0.0001
(6)	17	1	17	-	17	2	16	1212.7149	0.001	1212.7145	0.0004
(6)	10	2	9	-	10	3	8	1212.7301	0.000	1212.7301	0.0000
(6)	4	1	4	-	5	2	3	1212.7421	0.000	1212.7424	-0.0003
(6)	9	2	8	-	9	3	7	1212.8342	0.000	1212.8344	-0.0002
(6)	8	2	7	-	8	3	6	1212.9189	0.000	1212.9191	-0.0002
(6)	7	2	6	-	7	3	5	1212.9867	0.000	1212.9866	0.0001
(6)	6	2	5	-	6	3	4	1213.0395	0.000	1213.0396	0.0000
(6)	5	2	4	-	5	3	3	1213.0800	0.000	1213.0802	-0.0002
(6)	4	2	3	-	4	3	2	1213.1106	0.000	1213.1106	0.0000
(6)	3	2	2	-	3	3	1	1213.1328	0.000	1213.1327	0.0001
(6)	3	2	1	-	3	3	0	1213.1427	0.000	1213.1434	-0.0007
(6)	4	2	2	-	4	3	1	1213.1427*	0.000	1213.1428	0.0000
(6)	5	2	3	-	5	3	2	1213.1545	0.000	1213.1548	-0.0003
(6)	6	2	4	-	6	3	3	1213.1876	0.000	1213.1878	-0.0001
(6)	13	0	13	-	14	1	14	1213.2550	0.000	1213.2564	-0.0014
(6)	7	2	5	-	7	3	4	1213.2550*	0.000	1213.2510	0.0040
(6)	8	2	6	-	8	3	5	1213.3543	0.000	1213.3544	0.0000
(6)	9	2	7	-	9	3	6	1213.5080	0.000	1213.5080	0.0001
(6)	10	2	8	-	10	3	7	1213.7211	0.000	1213.7212	-0.0001
(4)	13	2	11	-	12	1	11	1213.9101	0.000	1213.9105	-0.0003
(6)	20	2	19	-	21	1	20	1213.9522	0.001	1213.9522	0.0000
(6)	11	2	9	-	11	3	8	1214.0021	0.000	1214.0019	0.0001
(6)	16	1	16	-	16	2	15	1214.1163	0.001	1214.1162	0.0001
(6)	21	0	21	-	21	1	20	1214.1504	0.001	1214.1508	-0.0005
(6)	12	2	10	-	12	3	9	1214.3561	0.000	1214.3560	0.0001
(6)	4	1	3	-	5	2	4	1214.4822	0.000	1214.4824	-0.0002
(6)	9	4	6	-	8	5	3	1214.5210	0.001	1214.5212	-0.0003
(6)	9	4	5	-	8	5	4	1214.5210	0.001	1214.5214	-0.0004
(6)	15	1	15	-	16	0	16	1214.6872	0.001	1214.6873	0.0000
(6)	13	2	11	-	13	3	10	1214.7867	0.000	1214.7864	0.0003
(6)	12	0	12	-	13	1	13	1215.0698	0.000	1215.0701	-0.0003

UPPER STATE			LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(6)	14	2	12	14	3	11	1215.2929	0.000	1215.2928	0.0001
(6)	15	1	15	15	2	14	1215.4582	0.000	1215.4581	0.0001
(6)	3	1	3	4	2	2	1215.5629	0.000	1215.5629	0.0000
(6)	15	2	13	15	3	12	1215.8714	0.000	1215.8713	0.0001
(4)	14	2	12	13	1	12	1216.0413	0.000	1216.0415	-0.0002
(4)	4	4	0	3	3	0	1216.3424	0.000	1216.3423	0.0001
(4)	4	4	1	3	3	1	1216.3424	0.000	1216.3423	0.0000
(6)	16	2	14	16	3	13	1216.5144	0.001	1216.5142	0.0003
(6)	3	1	2	4	2	3	1216.5928	0.000	1216.5929	0.0000
(6)	20	0	20	20	1	19	1216.6710	0.001	1216.6713	-0.0003
(6)	14	1	14	14	2	13	1216.7315	0.000	1216.7315	0.0000
(6)	11	0	11	12	1	12	1216.8681	0.000	1216.8686	-0.0005
(6)	10	4	7	9	5	4	1216.8936	0.001	1216.8935	0.0001
(6)	10	4	6	9	5	5	1216.8936	0.001	1216.8938	-0.0003
(6)	19	2	18	20	1	19	1217.0356	0.001	1217.0356	0.0000
(4)	11	2	10	10	1	10	1217.1023	0.000	1217.1025	-0.0002
(6)	17	2	15	17	3	14	1217.2105	0.001	1217.2102	0.0003
(6)	14	1	14	15	0	15	1217.3562	0.000	1217.3563	-0.0001
(6)	13	1	13	13	2	12	1217.9307	0.000	1217.9307	0.0000
(6)	18	2	16	18	3	15	1217.9454	0.001	1217.9449	0.0005
(4)	15	2	13	14	1	13	1218.2536	0.000	1218.2539	-0.0003
(6)	10	0	10	11	1	11	1218.6611	0.000	1218.6613	-0.0003
(6)	19	2	17	19	3	16	1218.7012	0.001	1218.7008	0.0004
(4)	5	4	1	4	3	1	1218.7170	0.000	1218.7167	0.0003
(4)	5	4	2	4	3	2	1218.7170	0.000	1218.7169	0.0001
(6)	12	1	12	12	2	11	1219.0510	0.000	1219.0514	-0.0003
(6)	19	0	19	19	1	18	1219.1255	0.001	1219.1258	-0.0003
(6)	11	4	8	10	5	5	1219.2614	0.001	1219.2612	0.0002
(6)	11	4	7	10	5	6	1219.2614	0.001	1219.2620	-0.0006
(6)	20	2	18	20	3	17	1219.4592	0.001	1219.4585	0.0007
(6)	13	1	13	14	0	14	1220.0809	0.000	1220.0809	0.0000
(6)	11	1	11	11	2	10	1220.0904	0.000	1220.0905	-0.0002
(6)	21	2	19	21	3	18	1220.1978	0.001	1220.1971	0.0007
(6)	18	2	17	19	1	18	1220.2132	0.001	1220.2129	0.0003
(4)	12	2	11	11	1	11	1220.2683	0.000	1220.2684	-0.0001
(6)	9	0	9	10	1	10	1220.4590	0.000	1220.4593	-0.0003
(4)	16	2	14	15	1	14	1220.5586	0.000	1220.5589	-0.0003
(6)	22	2	20	22	3	19	1220.8959	0.001	1220.8951	0.0008
(6)	10	1	10	10	2	9	1221.0462	0.000	1221.0460	0.0002
(4)	6	4	2	5	3	2	1221.0770	0.000	1221.0765	0.0006
(4)	6	4	3	5	3	3	1221.0770	0.000	1221.0773	-0.0003
(6)	18	0	18	18	1	17	1221.4931	0.001	1221.4933	-0.0002
(6)	23	2	21	23	3	20	1221.5323	0.001	1221.5313	0.0009
(6)	12	4	9	11	5	6	1221.6253	0.001	1221.6247	0.0006
(6)	12	4	8	11	5	7	1221.6253	0.001	1221.6263	-0.0009
(6)	9	1	9	9	2	8	1221.9162	0.000	1221.9163	-0.0001
(6)	24	2	22	24	3	21	1222.0861	0.001	1222.0854	0.0007
(6)	25	1	24	25	2	23	1222.1067	0.001	1222.1095	-0.0028
(6)	8	0	8	9	1	9	1222.2735	0.000	1222.2738	-0.0003
(6)	25	2	23	25	3	22	1222.5395	0.001	1222.5384	0.0010

UPPER STATE			LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(6)	8	1	8	8	2	7	1222.7001	0.000	1222.7003	-0.0002
(6)	4	2	3	3	3	0	1222.8298	0.000	1222.8300	-0.0002
(6)	12	1	12	13	0	13	1222.8554	0.000	1222.8555	-0.0001
(6)	4	2	2	3	3	1	1222.8554*	0.000	1222.8623	-0.0069
(4)	17	2	15	16	1	15	1222.9667	0.001	1222.9670	-0.0003
(6)	7	1	7	7	2	6	1223.3974	0.000	1223.3975	-0.0001
(4)	7	4	3	6	3	3	1223.4209	0.000	1223.4194	0.0014
(4)	7	4	4	6	3	4	1223.4209	0.000	1223.4221	-0.0012
(6)	17	2	16	18	1	17	1223.4626	0.001	1223.4622	0.0003
(4)	13	2	12	12	1	12	1223.4990	0.000	1223.4991	-0.0001
(6)	24	1	23	24	2	22	1223.6285	0.001	1223.6307	-0.0022
(6)	17	0	17	17	1	16	1223.7538	0.001	1223.7542	-0.0004
(6)	13	4	10	12	5	7	1223.9855	0.001	1223.9842	0.0013
(6)	13	4	9	12	5	8	1223.9855	0.001	1223.9871	-0.0016
(6)	6	1	6	6	2	5	1224.0074	0.000	1224.0074	-0.0001
(4)	10	2	9	9	1	9	1214.0021*	0.000	1214.0028	-0.0007
(6)	7	0	7	8	1	8	1224.1159	0.000	1224.1163	-0.0003
(6)	5	1	5	5	2	4	1224.5300	0.000	1224.5300	0.0000
(6)	4	1	4	4	2	3	1224.9652	0.000	1224.9652	0.0000
(6)	23	1	22	23	2	21	1224.9819	0.001	1224.9837	-0.0018
(6)	5	2	4	4	3	1	1225.2308	0.000	1225.2310	-0.0001
(6)	3	1	3	3	2	2	1225.3130	0.000	1225.3131	-0.0001
(6)	5	2	3	4	3	2	1225.3130*	0.000	1225.3063	0.0067
(4)	18	2	16	17	1	16	1225.4866	0.001	1225.4871*	-0.0005
(6)	11	1	11	12	0	12	1225.6730	0.000	1225.6730	0.0000
(4)	8	4	4	7	3	4	1225.7436	0.000	1225.7428	0.0008
(4)	8	4	5	7	3	5	1225.7496	0.000	1225.7497	-0.0001
(6)	16	0	16	16	1	15	*1225.8910	0.001	1225.8912	-0.0002
(6)	6	0	6	7	1	7	1225.9975	0.000	1225.9976	0.0000
(6)	22	1	21	22	2	20	1226.1652	0.001	1226.1667	-0.0015
(6)	3	1	2	3	2	1	1226.2957	0.000	1226.2957	0.0001
(6)	14	4	11	13	5	8	1226.3419	0.001	1226.3398	0.0022
(6)	14	4	10	13	5	9	1226.3419	0.001	1226.3450	-0.0031
(6)	10	3	8	9	4	5	1226.4042	0.000	1226.4043	0.0000
(6)	10	3	7	9	4	6	1226.4346	0.000	1226.4344	0.0002
(6)	4	1	3	4	2	2	1226.5867	0.000	1226.5868	0.0000
(6)	16	2	15	17	1	16	1226.7638	0.001	1226.7633	0.0004
(4)	14	2	13	13	1	13	1226.7931	0.000	1226.7932	-0.0001
(6)	5	1	4	5	2	3	1226.9323	0.000	1226.9323	-0.0001
(6)	21	1	20	21	2	19	1227.1794	0.001	1227.1803	-0.0010
(6)	6	1	5	6	2	4	1227.3201	0.000	1227.3203	-0.0001
(6)	6	2	5	5	3	2	1227.6224	0.000	1227.6224	0.0000
(6)	7	1	6	7	2	5	1227.7362	0.000	1227.7362	0.0000
(6)	6	2	4	5	3	3	1227.7731	0.000	1227.7730	0.0001
(6)	15	0	15	15	1	14	1227.8897	0.000	1227.8900	-0.0002
(6)	5	0	5	6	1	6	1227.9273	0.000	1227.9275	-0.0002
(6)	20	1	19	20	2	18	1228.0269	0.001	1228.0276	-0.0007
(4)	9	4	5	8	3	5	1228.0435	0.000	1228.0434	0.0001
(4)	9	4	6	8	3	6	1228.0593	0.000	1228.0591	0.0002
(4)	19	2	17	18	1	17	1228.1270	0.001	1228.1275	-0.0005

UPPER STATE J KA KC			LOWER STATE J KA KC			OBSERVATION	PREC.	CALCULATION	RESID.
(6)	8	1	7	8	2	6	1228.1637	0.000	1228.1639	-0.0002
(6)	10	1	10	11	0	11	1228.5244	0.000	1228.5244	0.0000
(6)	9	1	8	9	2	7	1228.5858	0.000	1228.5858	0.0000
(6)	15	4	12	14	5	9	1228.6921	0.001	1228.6916	0.0004
(6)	15	4	12	14	5	10	1228.7007	0.001	1228.6917	0.0089
(6)	19	1	18	19	2	17	1228.7125	0.001	1228.7132	-0.0007
(6)	11	3	9	10	4	6	1228.7796	0.000	1228.7795	0.0001
(6)	11	3	8	10	4	7	1228.8325	0.000	1228.8322	0.0003
(6)	10	1	9	10	2	8	1228.9832	0.000	1228.9833	-0.0001
(6)	18	1	17	18	2	16	1229.2426	0.001	1229.2431	-0.0005
(6)	11	1	10	11	2	9	1229.3374	0.000	1229.3376	-0.0002
(6)	17	1	16	17	2	15	1229.6249	0.001	1229.6244	0.0005
(6)	12	1	11	12	2	10	1229.6300	0.000	1229.6303	-0.0003
(6)	14	0	14	14	1	13	1229.7391	0.000	1229.7395	-0.0004
(6)	13	1	12	13	2	11	1229.8442	0.000	1229.8443	-0.0001
(6)	16	1	15	16	2	14	1229.8647	0.001	1229.8652	-0.0005
(6)	4	0	4	5	1	5	1229.9147	0.000	1229.9147	0.0000
(6)	14	1	13	14	2	12	1229.9635	0.000	1229.9637	-0.0002
(6)	15	1	14	15	2	13	1229.9744	0.000	1229.9748	-0.0004
(6)	7	2	6	6	3	3	1230.0018	0.000	1230.0018	0.0000
(6)	15	2	14	16	1	15	1230.0980	0.001	1230.0975	0.0005
(4)	15	2	14	14	1	14	1230.1485	0.000	1230.1486	-0.0001
(6)	7	2	5	6	3	4	1230.2725	0.000	1230.2725	0.0000
(4)	10	4	6	9	3	6	1230.3172	0.000	1230.3172	0.0000
(4)	10	4	7	9	3	7	1230.3496	0.000	1230.3496	0.0000
(4)	20	2	18	19	1	18	1230.8951	0.001	1230.8957	-0.0006
(6)	16	4	13	15	5	10	1231.0397	0.001	1231.0398	-0.0001
(6)	16	4	12	15	5	11	1231.0549	0.001	1231.0550	-0.0001
(6)	12	3	10	11	4	7	1231.1466	0.000	1231.1466	0.0000
(6)	12	3	9	11	4	8	1231.2340	0.000	1231.2343	-0.0003
(6)	9	1	9	10	0	10	1231.3986	0.000	1231.3986	0.0000
(6)	13	0	13	13	1	12	1231.4323	0.000	1231.4328	-0.0005
(6)	3	0	3	4	1	4	1231.9665	0.000	1231.9664	0.0001
(6)	8	2	7	7	3	4	1232.3662	0.000	1232.3661	0.0001
(4)	11	4	7	10	3	7	1232.5594	0.000	1232.5595	-0.0001
(4)	11	4	8	10	3	8	1232.6213	0.000	1232.6210	0.0003
(6)	8	2	6	7	3	5	1232.8162	0.000	1232.8160	0.0002
(6)	12	0	12	12	1	11	1232.9663	0.000	1232.9666	-0.0003
(6)	17	4	14	16	5	11	1233.3845	0.001	1233.3843	0.0002
(6)	17	4	13	16	5	12	1233.4090	0.001	1233.4089	0.0001
(6)	14	2	13	15	1	14	1233.4482	0.000	1233.4478	0.0003
(6)	13	3	11	12	4	8	1233.5037	0.000	1233.5035	0.0002
(4)	16	2	15	15	1	15	1233.5631	0.000	1233.5629	0.0002
(6)	13	3	10	12	4	9	1233.6436	0.000	1233.6436	0.0000
(4)	21	2	19	20	1	19	1233.7974	0.001	1233.7977	-0.0004
(6)	2	0	2	3	1	3	1234.0878	0.000	1234.0880	-0.0002
(6)	8	1	8	9	0	9	1234.2830	0.000	1234.2831	0.0000
(6)	11	0	11	11	1	10	1234.3410	0.000	1234.3413	-0.0003
(6)	4	1	4	3	2	1	1234.6679	0.000	1234.6680	-0.0001
(6)	9	2	8	8	3	5	1234.7119	0.000	1234.7117	0.0002

UPPER STATE J KA KC			LOWER STATE J KA KC			OBSERVATION	PREC.	CALCULATION	RESID.
(4)	12	4	8	11	3	8	1234.7652	0.000	1234.7649	0.0003
(4)	12	4	9	11	3	9	1234.8741	0.000	1234.8740	0.0001
(6)	9	2	7	8	3	6	1235.4155	0.000	1235.4153	0.0002
(6)	10	0	10	10	1	9	1235.5604	0.000	1235.5606	-0.0001
(6)	18	4	15	17	5	12	1235.7251	0.001	1235.7249	0.0002
(6)	18	4	14	17	5	13	1235.7636	0.001	1235.7635	0.0001
(6)	14	3	12	13	4	9	1235.8475	0.000	1235.8477	-0.0002
(6)	14	3	11	13	4	10	1236.0637	0.000	1236.0632	0.0004
(6)	1	0	1	2	1	2	1236.2836	0.000	1236.2835	0.0001
(6)	4	1	3	3	2	2	1236.3371	0.000	1236.3370	0.0001
(6)	9	0	9	9	1	8	1236.6304	0.000	1236.6305	-0.0001
(6)	5	1	5	4	2	2	1236.6304*	0.000	1236.6344	-0.0040
(6)	13	2	12	14	1	13	1236.7995	0.000	1236.7991	0.0004
(4)	22	2	20	21	1	20	1236.8382	0.001	1236.8387	-0.0005
(4)	13	4	9	12	3	9	1236.9272	0.000	1236.9269	0.0003
(4)	17	2	16	16	1	16	1237.0341*	0.000	1237.0330	0.0011
(6)	10	2	9	9	3	6	1237.0341	0.000	1237.0340	0.0001
(4)	13	4	10	12	3	10	1237.1097	0.000	1237.1095	0.0001
(6)	7	1	7	8	0	8	1237.1639	0.000	1237.1641	-0.0001
(6)	8	0	8	8	1	7	1237.5588	0.000	1237.5591	-0.0003
(6)	19	4	16	18	5	13	1238.0611	0.001	1238.0612	-0.0001
(6)	10	2	8	9	3	7	1238.0823	0.000	1238.0822	0.0001
(6)	19	4	15	18	5	14	1238.1203	0.001	1238.1203	0.0000
(6)	15	3	13	14	4	10	1238.1760	0.000	1238.1758	0.0002
(6)	7	0	7	7	1	6	1238.3551	0.000	1238.3551	0.0001
(6)	6	1	6	5	2	3	1238.4877	0.000	1238.4876	0.0001
(6)	15	3	12	14	4	11	1238.4976	0.000	1238.4974	0.0002
(6)	6	0	6	6	1	5	1239.0278	0.000	1239.0278	0.0001
(6)	5	1	4	4	2	3	1239.1551	0.000	1239.1551	0.0000
(4)	14	4	11	13	3	11	1239.3282*	0.000	1239.3292	-0.0011
(6)	11	2	10	10	3	7	1239.3282	0.000	1239.3278	0.0004
(6)	5	0	5	5	1	4	1239.5861	0.000	1239.5860	0.0001
(4)	23	2	21	22	1	21	1240.0279	0.001	1240.0213	0.0066
(6)	6	1	6	7	0	7	1240.0279	0.000	1240.0276	0.0003
(6)	4	0	4	4	1	3	1240.0376	0.000	1240.0379	-0.0002
(6)	12	2	11	13	1	12	1240.1380	0.000	1240.1378	0.0002
(6)	7	1	7	6	2	4	1240.2155	0.000	1240.2155	0.0000
(6)	3	0	3	3	1	2	1240.3907	0.000	1240.3906	0.0001
(6)	20	4	17	19	5	14	1240.3907*	0.000	1240.3927	-0.0020
(6)	20	4	16	19	5	15	1240.4825*	0.000	1240.4812	0.0013
(6)	2	0	2	2	1	1	1240.6500	0.000	1240.6499	0.0001
(6)	1	0	1	1	1	0	1240.8203	0.000	1240.8203	0.0000
(6)	11	2	9	10	3	8	1240.8276	0.000	1240.8280	-0.0004
(6)	12	2	11	11	3	8	1241.5871	0.000	1241.5870	0.0002
(6)	8	1	8	7	2	5	1241.8043	0.000	1241.8045	-0.0002
(6)	6	1	5	5	2	4	1242.0485	0.000	1242.0485	0.0000
(6)	21	4	18	20	5	15	1242.7182	0.001	1242.7184	-0.0002
(6)	21	4	17	20	5	16	1242.8487	0.001	1242.8482	0.0005
(6)	5	1	5	6	0	6	1242.8599*	0.000	1242.8600	-0.0001
(6)	9	1	9	8	2	6	1243.2390	0.000	1243.2392	-0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(6)	11	2	10	-	12	1	11	1243.4522	0.000	1243.4521	0.0001
(6)	12	2	10	-	11	3	9	1243.6629	0.000	1243.6627	0.0003
(6)	13	2	12	-	12	3	9	1243.8048	0.000	1243.8046	0.0003
(6)	10	1	10	-	9	2	7	1244.5035	0.000	1244.5037	-0.0001
(6)	7	1	6	-	6	2	5	1245.0160	0.000	1245.0159	0.0001
(6)	22	4	19	-	21	5	16	1245.0367	0.001	1245.0371	-0.0004
(6)	22	4	18	-	21	5	17	1245.2236	0.001	1245.2241	-0.0005
(6)	11	1	11	-	10	2	8	1245.5818	0.000	1245.5819	-0.0001
(6)	4	1	4	-	5	0	5	1245.6483	0.000	1245.6484	-0.0001
(6)	2	0	2	-	1	1	1	1245.8311	0.000	1245.8311	0.0000
(6)	14	2	13	-	13	3	10	1245.9729	0.000	1245.9727	0.0002
(6)	12	1	12	-	11	2	9	1246.4587	0.000	1246.4588	-0.0001
(6)	13	2	11	-	12	3	10	1246.5950	0.000	1246.5948	0.0002
(6)	10	2	9	-	11	1	10	1246.7317	0.000	1246.7315	0.0002
(6)	13	1	13	-	12	2	10	1247.1208	0.000	1247.1210	-0.0002
(6)	17	1	17	-	16	2	14	1247.4690	0.001	1247.4685	0.0005
(6)	14	1	14	-	13	2	11	1247.5579	0.000	1247.5577	0.0001
(6)	16	1	16	-	15	2	13	1247.7313	0.000	1247.7313	0.0000
(6)	15	1	15	-	14	2	12	1247.7623	0.000	1247.7621	0.0003
(6)	8	1	7	-	7	2	6	1248.0556	0.000	1248.0557	-0.0001
(6)	15	2	14	-	14	3	11	1248.0831	0.000	1248.0827	0.0004
(6)	3	1	3	-	4	0	4	1248.3811	0.000	1248.3813	-0.0002
(6)	3	0	3	-	2	1	2	1248.4022	0.000	1248.4023	-0.0002
(6)	14	2	12	-	13	3	11	1249.6310	0.000	1249.6307	0.0003
(6)	9	2	8	-	10	1	9	1249.9670	0.000	1249.9669	0.0001
(6)	16	2	15	-	15	3	12	1250.1255	0.000	1250.1252	0.0003
(6)	4	0	4	-	3	1	3	1251.0392	0.000	1251.0392	0.0000
(6)	2	1	2	-	3	0	3	1251.0483	0.000	1251.0486	-0.0003
(6)	9	1	8	-	8	2	7	1251.1658	0.000	1251.1660	-0.0002
(6)	17	2	16	-	16	3	13	1252.0905	0.001	1252.0903	0.0002
(6)	15	2	13	-	14	3	12	1252.7752	0.000	1252.7749	0.0003
(6)	8	2	7	-	9	1	8	1253.1506	0.000	1253.1507	-0.0001
(6)	1	1	1	-	2	0	2	1253.6421	0.000	1253.6424	-0.0003
(6)	5	0	5	-	4	1	4	1253.7347	0.000	1253.7350	-0.0003
(6)	18	2	17	-	17	3	14	1253.9680	0.001	1253.9679	0.0001
(6)	10	1	9	-	9	2	8	1254.3442	0.000	1254.3445	-0.0002
(6)	19	2	18	-	18	3	15	1255.7482	0.001	1255.7481	0.0001
(6)	15	2	13	-	16	1	16	1255.8169	0.001	1255.8166	0.0003
(6)	14	2	12	-	15	1	15	1255.8347	0.000	1255.8346	0.0001
(6)	16	2	14	-	15	3	13	1256.0296	0.000	1256.0294	0.0002
(6)	16	2	14	-	17	1	17	1256.0557	0.001	1256.0555	0.0002
(6)	13	2	11	-	14	1	14	1256.1038	0.000	1256.1035	0.0003
(6)	7	2	6	-	8	1	7	1256.2757	0.000	1256.2758	-0.0001
(6)	6	0	6	-	5	1	5	1256.4814	0.000	1256.4816	-0.0002
(6)	17	2	15	-	18	1	18	1256.5547	0.001	1256.5542	0.0005
(6)	12	2	10	-	13	1	13	1256.6148	0.000	1256.6147	0.0002
(6)	18	2	16	-	19	1	19	1257.3137	0.001	1257.3131	0.0006
(6)	11	2	9	-	12	1	12	1257.3567	0.000	1257.3566	0.0001
(6)	20	2	19	-	19	3	16	1257.4220	0.001	1257.4222	-0.0002
(6)	11	1	10	-	10	2	9	1257.5887	0.000	1257.5882	-0.0005

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(6)	23	4	20	-	24	3	21	1257.6987	0.001	1257.6949	0.0038
(6)	10	2	8	-	11	1	11	1258.3155	0.000	1258.3155	0.0000
(6)	19	2	17	-	20	1	20	1258.3300	0.001	1258.3298	0.0003
(6)	1	1	0	-	1	0	1	1258.6649	0.000	1258.6649	0.0000
(6)	2	1	1	-	2	0	2	1258.8248	0.000	1258.8250	-0.0002
(6)	21	2	20	-	20	3	17	1258.9826	0.001	1258.9829	-0.0003
(6)	3	1	2	-	3	0	3	1259.0697	0.000	1259.0698	-0.0001
(6)	7	0	7	-	6	1	6	1259.2690	0.000	1259.2695	-0.0005
(6)	6	2	5	-	7	1	6	1259.3366	0.000	1259.3367	-0.0001
(6)	17	2	15	-	16	3	14	1259.3946	0.001	1259.3941	0.0005
(6)	4	1	3	-	4	0	4	1259.4049	0.000	1259.4051	-0.0002
(6)	9	2	7	-	10	1	10	1259.4755	0.000	1259.4757	-0.0001
(6)	5	1	4	-	5	0	5	1259.8383	0.000	1259.8383	0.0000
(6)	6	1	5	-	6	0	6	1260.3782	0.000	1260.3785	-0.0003
(6)	22	2	21	-	21	3	18	1260.4246*	0.000	1260.4255	-0.0009
(6)	8	2	6	-	9	1	9	1260.8200	0.000	1260.8199	0.0001
(6)	24	4	20	-	25	3	23	1260.8507	0.001	1260.8519	-0.0012
(6)	12	1	11	-	11	2	10	1260.8932	0.000	1260.8935	-0.0003
(6)	7	1	6	-	7	0	7	1261.0358	0.000	1261.0360	-0.0003
(6)	22	4	19	-	23	3	20	1261.2576	0.001	1261.2579	-0.0002
(6)	23	2	22	-	22	3	19	1261.7480	0.001	1261.7486	-0.0006
(6)	8	1	7	-	8	0	8	1261.8219	0.000	1261.8222	-0.0003
(6)	8	0	8	-	7	1	7	1262.0876	0.000	1262.0881	-0.0005
(6)	5	2	4	-	6	1	5	1262.3293	0.000	1262.3282	0.0011
(6)	7	2	5	-	8	1	8	1262.3293*	0.000	1262.3308	-0.0015
(6)	9	1	8	-	9	0	9	1262.7484	0.000	1262.7487	-0.0003
(6)	18	2	16	-	17	3	15	1262.8677	0.001	1262.8671	0.0006
(6)	2	1	2	-	1	0	1	1263.1844	0.000	1263.1845	-0.0001
(6)	23	4	19	-	24	3	22	1263.2377	0.001	1263.2382	-0.0005
(6)	10	1	9	-	10	0	10	1263.8265	0.000	1263.8268	-0.0003
(6)	6	2	4	-	7	1	7	1263.9908	0.000	1263.9908	0.0000
(6)	13	1	12	-	12	2	11	1264.2558	0.000	1264.2561	-0.0003
(6)	21	4	18	-	22	3	19	1264.6886	0.001	1264.6887	-0.0001
(6)	9	0	9	-	8	1	8	1264.9254	0.000	1264.9258	-0.0004
(6)	11	1	10	-	11	0	11	1265.0663	0.000	1265.0666	-0.0002
(6)	4	2	3	-	5	1	4	1265.2462	0.000	1265.2463	-0.0001
(6)	3	1	3	-	2	0	2	1265.3543	0.000	1265.3545	-0.0002
(6)	22	4	18	-	23	3	21	1265.6806	0.001	1265.6804	0.0002
(6)	5	2	3	-	6	1	6	1265.7834	0.000	1265.7836	-0.0001
(6)	19	2	17	-	18	3	16	1266.4453	0.001	1266.4447	0.0006
(6)	12	1	11	-	12	0	12	1266.4755	0.000	1266.4760	-0.0005
(6)	4	1	4	-	3	0	3	1267.4421	0.000	1267.4421	-0.0001
(6)	14	1	13	-	13	2	12	1267.6706	0.000	1267.6708	-0.0002
(6)	4	2	2	-	5	1	5	1267.6937	0.000	1267.6939	-0.0002
(6)	10	0	10	-	9	1	9	1267.7705	0.000	1267.7709	-0.0003
(6)	20	4	17	-	21	3	18	1267.9943	0.001	1267.9942	0.0001
(6)	13	1	12	-	13	0	13	1268.0600	0.000	1268.0602	-0.0002
(6)	3	2	2	-	4	1	3	1268.0874	0.000	1268.0874	0.0000
(6)	21	4	17	-	22	3	20	1268.1677	0.001	1268.1677	0.0000
(6)	5	1	5	-	4	0	4	1269.4526	0.000	1269.4527	-0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(6)	3	2	1	-	4	1	4	1269.7086	0.000	1269.7088	-0.0001
(6)	14	1	13	-	14	0	14	1269.8206	0.000	1269.8210	-0.0004
(6)	20	2	18	-	19	3	17	1270.1225	0.001	1270.1219	0.0007
(6)	11	0	11	-	10	1	10	1270.6112	0.000	1270.6115	-0.0003
(6)	20	4	16	-	21	3	19	1270.6901	0.001	1270.6900	0.0002
(6)	2	2	1	-	3	1	2	1270.8486	0.000	1270.8487	-0.0001
(6)	15	1	14	-	14	2	13	1271.1311	0.000	1271.1315	-0.0004
(6)	19	4	16	-	20	3	17	1271.1831	0.001	1271.1828	0.0003
(6)	6	1	6	-	5	0	5	1271.3935	0.000	1271.3935	0.0000
(6)	15	1	14	-	15	0	15	1271.7559	0.000	1271.7562	-0.0003
(6)	2	2	0	-	3	1	3	1271.8174	0.000	1271.8173	0.0001
(6)	19	4	15	-	20	3	18	1273.2387	0.001	1273.2386	0.0001
(6)	7	1	7	-	6	0	6	1273.2738	0.000	1273.2738	0.0000
(6)	12	0	12	-	11	1	11	1273.4363	0.000	1273.4366	-0.0003
(6)	16	1	15	-	16	0	16	1273.8599	0.001	1273.8601	-0.0002
(6)	21	2	19	-	20	3	18	1273.8931	0.001	1273.8924	0.0007
(6)	14	2	12	-	14	1	13	1274.1546	0.000	1274.1547	-0.0001
(6)	15	2	13	-	15	1	14	1274.1546*	0.000	1274.1534	0.0012
(6)	18	4	15	-	19	3	16	1274.2653	0.001	1274.2647	0.0005
(6)	13	2	11	-	13	1	12	1274.2803	0.000	1274.2799	0.0004
(6)	16	2	14	-	16	1	15	1274.2930	0.001	1274.2925	0.0005
(6)	12	2	10	-	12	1	11	1274.5115	0.000	1274.5111	0.0004
(6)	17	2	15	-	17	1	16	1274.5880	0.001	1274.5874	0.0007
(6)	16	1	15	-	15	2	14	1274.6306	0.000	1274.6309	-0.0003
(6)	11	2	9	-	11	1	10	1274.8297	0.000	1274.8294	0.0003
(6)	18	2	16	-	18	1	17	1275.0526	0.001	1275.0521	0.0005
(6)	8	1	8	-	7	0	7	1275.1043	0.000	1275.1043	0.0000
(6)	10	2	8	-	10	1	9	1275.2150	0.000	1275.2148	0.0003
(6)	9	2	7	-	9	1	8	1275.6471	0.000	1275.6469	0.0002
(6)	19	2	17	-	19	1	18	1275.6995	0.001	1275.6993	0.0002
(6)	18	4	14	-	19	3	17	1275.8060	0.001	1275.8057	0.0003
(6)	8	2	6	-	8	1	7	1276.1049	0.000	1276.1052	-0.0003
(6)	13	0	13	-	12	1	12	1276.2365	0.000	1276.2366	-0.0001
(6)	20	2	18	-	20	1	19	1276.5411	0.001	1276.5403	0.0008
(6)	7	2	5	-	7	1	6	1276.5692	0.000	1276.5696	-0.0004
(6)	9	1	9	-	8	0	8	1276.8981*	0.000	1276.8974	0.0007
(6)	6	2	4	-	6	1	5	1277.0213	0.000	1277.0210	0.0002
(6)	17	4	14	-	18	3	15	1277.2510	0.001	1277.2506	0.0004
(6)	5	2	3	-	5	1	4	1277.4422	0.000	1277.4420	0.0002
(6)	21	2	19	-	21	1	20	1277.5857	0.001	1277.5847	0.0010
(6)	22	2	20	-	21	3	19	1277.7503	0.001	1277.7491	0.0012
(6)	4	2	2	-	4	1	3	1277.8175	0.000	1277.8170	0.0005
(6)	3	2	1	-	3	1	2	1278.4332	0.000	1278.1330	0.0002
(6)	17	1	16	-	16	2	15	1278.1608	0.001	1278.1609	-0.0002
(6)	17	4	13	-	18	3	16	1278.3801*	0.000	1278.3845	-0.0044
(6)	2	2	0	-	2	1	1	1278.3801*	0.000	1278.3793	0.0008
(6)	10	1	10	-	9	0	9	1278.6668	0.000	1278.6665	0.0003
(6)	22	2	20	-	22	1	21	1278.8406	0.001	1278.8400	0.0006
(6)	2	2	1	-	2	1	2	1278.8613	0.000	1278.8604	0.0009
(6)	14	0	14	-	13	1	13	1279.0037	0.000	1279.0036	0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(6)	3	2	2	-	3	1	3	1279.0891	0.000	1279.0887	0.0004
(6)	4	2	3	-	4	1	4	1279.3957	0.000	1279.3954	0.0004
(6)	5	2	4	-	5	1	5	1279.7826	0.000	1279.7821	0.0005
(6)	16	4	13	-	17	3	14	1280.1518	0.001	1280.1515	0.0003
(6)	6	2	5	-	6	1	6	1280.2514	0.000	1280.2511	0.0003
(6)	23	2	21	-	23	1	22	1280.3124	0.001	1280.3112	0.0012
(6)	11	1	11	-	10	0	10	1280.4254	0.000	1280.4254	-0.0001
(6)	7	2	6	-	7	1	7	1280.8050	0.000	1280.8048	0.0001
(6)	16	4	12	-	17	3	15	1280.9696	0.001	1280.9693	0.0003
(6)	8	2	7	-	8	1	8	1281.4460	0.000	1281.4459	0.0001
(6)	23	2	21	-	22	3	20	1281.6849	0.001	1281.6841	0.0008
(6)	18	1	17	-	17	2	16	1281.7121	0.001	1281.7124	-0.0002
(6)	15	0	15	-	14	1	14	1281.7320	0.000	1281.7319	0.0001
(6)	24	2	22	-	24	1	23	1282.0017	0.001	1282.0005	0.0012
(6)	9	2	8	-	9	1	9	1282.1777	0.000	1282.1772	0.0005
(6)	12	1	12	-	11	0	11	1282.1880	0.000	1282.1878	0.0002
(6)	15	4	12	-	16	3	13	1282.9781	0.001	1282.9781	0.0000
(6)	10	2	9	-	10	1	10	1283.0020	0.000	1283.0016	0.0004
(6)	2	2	1	-	1	1	0	1283.3976	0.000	1283.3972	0.0004
(6)	2	2	0	-	1	1	1	1283.5608	0.000	1283.5605	0.0003
(6)	15	4	11	-	16	3	14	1283.5608*	0.000	1283.5551	0.0057
(6)	25	2	23	-	25	1	24	1283.9076	0.001	1283.9063	0.0013
(6)	11	2	10	-	11	1	11	1283.9226	0.000	1283.9221	0.0004
(6)	13	1	13	-	12	0	12	1283.9670	0.000	1283.9667	0.0003
(6)	16	0	16	-	15	1	15	1284.4182	0.000	1284.4182	0.0000
(6)	12	2	11	-	12	1	12	1284.9422	0.000	1284.9416	0.0006
(6)	19	1	18	-	18	2	17	1285.2747	0.001	1285.2751	-0.0004
(6)	3	2	2	-	2	1	1	1285.6509	0.000	1285.6507	0.0002
(6)	24	2	22	-	23	3	21	1285.6900	0.001	1285.6887	0.0013
(6)	14	4	11	-	15	3	12	1285.7406	0.000	1285.7406	0.0000
(6)	14	1	14	-	13	0	13	1285.7741	0.000	1285.7737	0.0004
(6)	25	3	22	-	25	2	23	1285.8484	0.001	1285.8471	0.0013
(6)	26	2	24	-	26	1	25	1286.0252	0.001	1286.0238	0.0014
(6)	13	2	12	-	13	1	13	1286.0636	0.000	1286.0632	0.0004
(6)	14	4	10	-	15	3	13	1286.1382	0.000	1286.1378	0.0004
(6)	3	2	1	-	2	1	2	1286.1448	0.000	1286.1447	0.0001
(6)	24	3	21	-	24	2	22	1286.9418	0.001	1286.9406	0.0012
(6)	17	0	17	-	16	1	16	1287.0616	0.001	1287.0614	0.0002
(6)	14	2	13	-	14	1	14	1287.2905	0.000	1287.2898	0.0007
(6)	15	1	15	-	14	0	14	1287.6194	0.000	1287.6193	0.0001
(6)	4	2	3	-	3	1	2	1287.8199	0.000	1287.8196	0.0004
(6)	23	3	20	-	23	2	21	1288.0433	0.001	1288.0424	0.0009
(6)	27	2	25	-	27	1	26	1288.3457	0.001	1288.3443	0.0015
(6)	13	4	10	-	14	3	11	1288.4484	0.000	1288.4482	0.0001
(6)	15	2	14	-	15	1	15	1288.6250	0.000	1288.6245	0.0005
(6)	13	4	9	-	14	3	12	1288.7144	0.000	1288.7144	0.0000
(6)	4	2	2	-	3	1	3	1288.8187	0.000	1288.8184	0.0004
(6)	20	1	19	-	19	2	18	1288.8377	0.001	1288.8384	-0.0007
(6)	22	3	19	-	22	2	20	1289.1538	0.001	1289.1531	0.0008
(6)	16	1	16	-	15	0	15	1289.5133	0.000	1289.5128	0.0006

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(6)	18	0	18	-	17	1	17	1289.6628	0.001	1289.6627	0.0002
(6)	5	2	4	-	4	1	3	1289.9056	0.000	1289.9052	0.0004
(6)	16	2	15	-	16	1	16	1290.0711	0.001	1290.0705	0.0006
(6)	21	3	18	-	21	2	19	1290.2684	0.001	1290.2677	0.0007
(6)	28	2	26	-	28	1	27	1290.8571	0.001	1290.8555	0.0016
(6)	12	4	9	-	13	3	10	1291.1096	0.000	1291.1094	0.0002
(6)	12	4	8	-	13	3	11	1291.2823	0.000	1291.2823	0.0001
(6)	20	3	17	-	20	2	18	1291.3774	0.001	1291.3768	0.0006
(6)	17	1	17	-	16	0	16	1291.4640	0.001	1291.4634	0.0006
(6)	5	2	3	-	4	1	4	1291.5914	0.000	1291.5911	0.0003
(6)	17	2	16	-	17	1	17	1291.6322	0.001	1291.6316	0.0006
(6)	6	2	5	-	5	1	4	1291.9099	0.000	1291.9096	0.0003
(6)	19	0	19	-	18	1	18	1292.2246	0.001	1292.2248	-0.0001
(6)	21	1	20	-	20	2	19	1292.3901	0.001	1292.3910	-0.0009
(6)	19	3	16	-	19	2	17	1292.4677	0.001	1292.4673	0.0004
(6)	18	2	17	-	18	1	18	1293.3126	0.001	1293.3119	0.0007
(6)	18	1	18	-	17	0	17	1293.4836	0.001	1293.4831	0.0006
(6)	18	3	15	-	18	2	16	1293.5246	0.001	1293.5243	0.0004
(6)	11	4	8	-	12	3	9	1293.7312	0.000	1293.7313	0.0000
(6)	7	2	6	-	6	1	5	1293.8355	0.000	1293.8350	0.0005
(6)	11	4	7	-	12	3	10	1293.8355*	0.000	1293.8396	-0.0041
(6)	6	2	4	-	5	1	5	1294.4752	0.000	1294.4749	0.0003
(6)	17	3	14	-	17	2	15	1294.5329	0.001	1294.5325	0.0004
(6)	20	0	20	-	19	1	19	1294.7520	0.001	1294.7520	0.0000
(6)	19	2	18	-	19	1	19	1295.1166	0.001	1295.1163	0.0003
(6)	16	3	13	-	16	2	14	1295.4780	0.001	1295.4775	0.0005
(6)	19	1	19	-	18	0	18	1295.5923	0.001	1295.5920	0.0003
(6)	8	2	7	-	7	1	6	1295.6852	0.000	1295.6848	0.0004
(6)	22	1	21	-	21	2	20	1295.9205	0.001	1295.9217	-0.0012
(6)	10	4	7	-	11	3	8	1296.3201	0.000	1296.3201	0.0000
(6)	15	3	12	-	15	2	13	1296.3471	0.000	1296.3468	0.0003
(6)	10	4	6	-	11	3	9	1296.3855	0.000	1296.3853	0.0002
(6)	20	2	19	-	20	1	20	1297.0514	0.001	1297.0511	0.0002
(6)	14	3	11	-	14	2	12	1297.1306	0.000	1297.1305	0.0001
(6)	21	0	21	-	20	1	20	1297.2497	0.001	1297.2497	0.0000
(6)	9	2	8	-	8	1	7	1297.4627	0.000	1297.4625	0.0002
(6)	7	2	5	-	6	1	6	1297.4843	0.000	1297.4840	0.0003
(6)	13	3	10	-	13	2	11	1297.8225	0.000	1297.8221	0.0004
(6)	20	1	20	-	19	0	19	1297.8347	0.001	1297.8345	0.0003
(6)	12	3	9	-	12	2	10	1298.4189	0.000	1298.4186	0.0002
(6)	9	4	6	-	10	3	7	1298.8813	0.000	1298.8813	0.0000
(6)	11	3	8	-	11	2	9	1298.9206	0.000	1298.9210	-0.0004
(6)	9	4	5	-	10	3	8	1298.9206*	0.000	1298.9186	0.0020
(6)	21	2	20	-	21	1	21	1299.1242	0.001	1299.1241	0.0001
(6)	10	2	9	-	9	1	8	1299.1734	0.000	1299.1729	0.0005
(6)	10	3	7	-	10	2	8	1299.3335	0.000	1299.3334	0.0001
(6)	23	1	22	-	22	2	21	1299.4185	0.001	1299.4198	-0.0013
(6)	9	3	6	-	9	2	7	1299.6631	0.000	1299.6629	0.0003
(6)	22	0	22	-	21	1	21	1299.7239	0.001	1299.7240	-0.0002
(6)	8	3	5	-	8	2	6	1299.9186	0.000	1299.9186	0.0000

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(6)	7	3	4	-	7	2	5	1300.1112	0.000	1300.1110	0.0002
(6)	6	3	3	-	6	2	4	1300.2509	0.000	1300.2509	0.0000
(6)	5	3	2	-	5	2	3	1300.3488	0.000	1300.3489	-0.0001
(6)	7	3	5	-	7	2	6	1300.4026*	0.000	1300.4037	-0.0011
(6)	8	3	6	-	8	2	7	1300.4026*	0.000	1300.4017	0.0009
(6)	4	3	1	-	4	2	2	1300.4139*	0.000	1300.4147	-0.0008
(6)	6	3	4	-	6	2	5	1300.4139*	0.000	1300.4147	-0.0008
(6)	9	3	7	-	9	2	8	1300.4139*	0.000	1300.4128	0.0012
(6)	5	3	3	-	5	2	4	1300.4313	0.000	1300.4312	0.0001
(6)	4	3	2	-	4	2	3	1300.4502	0.000	1300.4501	0.0001
(6)	10	3	8	-	10	2	9	1300.4502*	0.000	1300.4409	0.0093
(6)	3	3	0	-	3	2	1	1300.4567	0.000	1300.4568	-0.0001
(6)	3	3	1	-	3	2	2	1300.4684	0.000	1300.4686	-0.0002
(6)	11	3	9	-	11	2	10	1300.4907	0.000	1300.4905	0.0002
(6)	12	3	10	-	12	2	11	1300.5661	0.000	1300.5659	0.0001
(6)	8	2	6	-	7	1	7	1300.6346	0.000	1300.6342	0.0004
(6)	13	3	11	-	13	2	12	1300.6720	0.000	1300.6717	0.0003
(6)	14	3	12	-	14	2	13	1300.8123	0.000	1300.8122	0.0001
(6)	11	2	10	-	10	1	9	1300.8218	0.000	1300.8213	0.0005
(6)	15	3	13	-	15	2	14	1300.9920	0.000	1300.9918	0.0002
(6)	16	3	14	-	16	2	15	1301.2147	0.001	1301.2145	0.0001
(6)	22	2	21	-	22	1	22	1301.3448	0.001	1301.3449	-0.0001
(6)	8	4	5	-	9	3	6	1301.4189	0.000	1301.4192	-0.0002
(6)	8	4	4	-	9	3	7	1301.4390	0.000	1301.4393	-0.0002
(6)	17	3	15	-	17	2	16	1301.4846	0.001	1301.4845	0.0002
(6)	23	1	23	-	22	0	22	1301.7221	0.001	1301.7185	0.0035
(6)	18	3	16	-	18	2	17	1301.8054	0.001	1301.8053	0.0001
(6)	19	3	17	-	19	2	18	1302.1813*	0.000	1302.1808	0.0005
(6)	23	0	23	-	22	1	22	1302.1813*	0.000	1302.1816	-0.0003
(6)	12	2	11	-	11	1	10	1302.4146	0.000	1302.4144	0.0002
(6)	20	3	18	-	20	2	19	1302.6144	0.001	1302.6142	0.0002
(6)	24	1	23	-	23	2	22	1302.8738	0.001	1302.8756	-0.0017
(6)	21	3	19	-	21	2	20	1303.1090	0.001	1303.1092	-0.0002
(6)	22	3	20	-	22	2	21	1303.6682	0.001	1303.6690	-0.0008
(6)	23	2	22	-	23	1	23	1303.7252	0.001	1303.7253	-0.0001
(6)	9	2	7	-	8	1	8	1303.9426	0.000	1303.9422	0.0004
(6)	7	4	4	-	8	3	5	1303.9426	0.000	1303.9374	0.0052
(6)	7	4	3	-	8	3	6	1303.9426	0.000	1303.9474	-0.0049
(6)	13	2	12	-	12	1	11	1303.9602	0.000	1303.9596	0.0006
(6)	23	3	21	-	23	2	22	1304.2968	0.001	1304.2972	-0.0004
(6)	24	0	24	-	23	1	23	1304.6293	0.001	1304.6296	-0.0003
(6)	24	3	22	-	24	2	23	1304.9969	0.001	1304.9976	-0.0008
(6)	14	2	13	-	13	1	12	1305.4668	0.000	1305.4662	0.0006
(6)	6	4	3	-	7	3	4	1306.4409	0.000	1306.4389	0.0020
(6)	6	4	2	-	7	3	5	1306.4409	0.000	1306.4435	-0.0025
(6)	15	2	14	-	14	1	13	1306.9454	0.000	1306.9446	0.0007
(6)	25	0	25	-	24	1	24	1307.0751	0.001	1307.0754	-0.0003
(6)	10	2	8	-	9	1	9	1307.4254	0.000	1307.4251	0.0003
(6)	3	3	1	-	2	2	0	1307.7550	0.000	1307.7538	0.0011
(6)	3	3	0	-	2	2	1	1307.7950	0.000	1307.7562	-0.0013

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(6)	16	2	15	15	1	14	1308.4080	0.000	1308.4073	0.0007
(6)	5	4	2	6	3	3	1308.9268	0.000	1308.9261	0.0006
(6)	5	4	1	6	3	4	1308.9268	0.000	1308.9280	-0.0012
(6)	26	0	26	25	1	25	1309.5260	0.001	1309.5266	-0.0006
(6)	17	2	16	16	1	15	1309.8692	0.001	1309.8686	0.0006
(6)	4	3	2	3	2	1	1310.1530	0.000	1310.1529	0.0001
(6)	4	3	1	3	2	2	1310.1649	0.000	1310.1649	0.0000
(6)	11	2	9	10	1	10	1311.0998	0.000	1311.0995	0.0002
(6)	18	2	17	17	1	16	1311.3457	0.001	1311.3458	0.0006
(6)	4	4	1	5	3	2	1311.4011	0.000	1311.4010	0.0001
(6)	4	4	0	5	3	3	1311.4011	0.000	1311.4016	-0.0005
(6)	27	0	27	26	1	26	1311.9904	0.001	1311.9913	-0.0009
(6)	5	3	3	4	2	2	1312.5357	0.000	1312.5356	0.0001
(6)	5	3	2	4	2	3	1312.5718	0.000	1312.5717	0.0002
(6)	19	2	18	18	1	17	1312.8559	0.001	1312.8553	0.0006
(6)	26	4	22	26	3	23	1313.8906	0.001	1313.8911	-0.0005
(6)	20	2	19	19	1	18	1314.4208	0.001	1314.4207	0.0001
(6)	28	0	28	27	1	27	1314.4764	0.001	1314.4778	-0.0014
(6)	6	3	4	5	2	3	1314.8947	0.000	1314.8948	-0.0001
(6)	6	3	3	5	2	4	1314.9805*	0.000	1314.9791	0.0013
(6)	12	2	10	11	1	11	1314.9805*	0.000	1314.9812	-0.0007
(6)	25	4	21	25	3	22	1315.1346	0.001	1315.1348	-0.0003
(6)	21	2	20	20	1	19	1316.0646	0.001	1316.0646	0.0000
(6)	24	4	20	24	3	21	1316.2769	0.001	1316.2769	0.0000
(6)	7	3	5	6	2	4	1317.2217	0.000	1317.2217	0.0000
(6)	23	4	19	23	3	20	1317.3123	0.001	1317.3122	0.0001
(6)	7	3	4	6	2	5	1317.3906	0.000	1317.3906	-0.0001
(6)	22	2	21	21	1	20	1317.8127	0.001	1317.8130	-0.0003
(6)	22	4	18	22	3	19	1318.2394	0.001	1318.2391	0.0003
(6)	21	4	17	21	3	18	1319.0597	0.001	1319.0594	0.0003
(6)	13	2	11	12	1	12	1319.0841	0.000	1319.0837	0.0003
(6)	8	3	6	7	2	5	1319.5059	0.000	1319.5059	0.0000
(6)	23	2	22	22	1	21	1319.6927	0.001	1319.6934	-0.0007
(6)	20	4	16	20	3	17	1319.7782	0.001	1319.7778	0.0004
(6)	8	3	5	7	2	6	1319.8104	0.000	1319.8103	0.0000
(6)	19	4	15	19	3	16	1320.4012	0.001	1320.4003	0.0003
(6)	18	4	14	18	3	15	1320.9369	0.001	1320.9366	0.0002
(6)	25	4	22	25	3	23	1321.1515	0.001	1321.1530	-0.0015
(6)	24	4	21	24	3	22	1321.2109	0.001	1321.2105	0.0003
(6)	23	4	20	23	3	21	1321.2985	0.001	1321.2982	0.0003
(6)	17	4	13	17	3	14	1321.3944	0.001	1321.3941	0.0002
(6)	22	4	19	22	3	20	1321.4107	0.001	1321.4106	0.0001
(6)	21	4	18	21	3	19	1321.5431	0.001	1321.5427	0.0004
(6)	20	4	17	20	3	18	1321.6898	0.001	1321.6895	0.0003
(6)	9	3	7	8	2	6	1321.7352*	0.000	1321.7356	-0.0005
(6)	16	4	12	16	3	13	1321.7825	0.001	1321.7823	0.0002
(6)	19	4	16	19	3	17	1321.8464	0.001	1321.8462	0.0003
(6)	18	4	15	18	3	16	1322.0090	0.001	1322.0086	0.0004
(6)	15	4	11	15	3	12	1322.1106	0.000	1322.1103	0.0003
(6)	17	4	14	17	3	15	1322.1729	0.001	1322.1728	0.0001
(6)	9	3	6	8	2	7	1322.2432	0.000	1322.2430	0.0001
(6)	16	4	13	16	3	14	1322.3356	0.001	1322.3353	0.0002
(6)	14	4	10	14	3	11	1322.3862	0.000	1322.3862	0.0001
(6)	15	4	12	15	3	13	1322.4934	0.000	1322.4933	0.0001
(6)	13	4	9	13	3	10	1322.6180	0.000	1322.6177	0.0002
(6)	14	4	11	14	3	12	1322.6443	0.000	1322.6442	0.0000
(6)	13	4	10	13	3	11	1322.7861	0.000	1322.7862	0.0000
(6)	12	4	8	12	3	9	1322.8115	0.000	1322.8117	-0.0001
(6)	12	4	9	12	3	10	1322.9178	0.000	1322.9177	0.0001
(6)	11	4	7	11	3	8	1322.9741	0.000	1322.9739	0.0002
(6)	11	4	8	11	3	9	1323.0380	0.000	1323.0379	0.0001
(6)	10	4	6	10	3	7	1323.1095	0.000	1323.1094	0.0001
(6)	10	4	7	10	3	8	1323.1460	0.000	1323.1462	-0.0002
(6)	9	4	5	9	3	6	1323.2224	0.000	1323.2225	-0.0001
(6)	9	4	6	9	3	7	1323.2422	0.000	1323.2423	-0.0001
(6)	8	4	4	8	3	5	1323.3165	0.000	1323.3165	0.0000
(6)	8	4	5	8	3	6	1323.3265	0.000	1323.3265	0.0000
(6)	7	4	3	7	3	4	1323.3954	0.000	1323.3945	0.0009
(6)	7	4	4	7	3	5	1323.3954	0.000	1323.3990	-0.0036
(6)	14	2	12	13	1	13	1323.4194	0.000	1323.4188	0.0007
(6)	6	4	2	6	3	3	1323.4594	0.000	1323.4586	0.0007
(6)	6	4	3	6	3	4	1323.4594	0.000	1323.4604	-0.0011
(6)	5	4	1	5	3	2	1323.5107	0.000	1323.5108	0.0000
(6)	5	4	2	5	3	3	1323.5107	0.000	1323.5114	-0.0006
(6)	4	4	0	4	3	1	1323.5520	0.000	1323.5523	-0.0004
(6)	4	4	1	4	3	2	1323.5520	0.000	1323.5525	-0.0005
(6)	10	3	8	9	2	7	1323.8986	0.000	1323.8986	0.0001
(6)	10	3	7	9	2	8	1324.6946	0.000	1324.6946	0.0000
(6)	11	3	9	10	2	8	1325.9819	0.000	1325.9819	0.0000
(6)	11	3	8	10	2	9	1327.1718	0.000	1327.1716	0.0002
(6)	12	3	10	11	2	9	1327.9736	0.000	1327.9734	0.0002
(6)	15	2	13	14	1	14	1327.9959	0.000	1327.9953	0.0005
(6)	12	3	9	11	2	10	1329.6819	0.000	1329.6818	0.0001
(6)	13	3	11	12	2	10	1329.8623	0.000	1329.8620	0.0003
(6)	14	3	12	13	2	11	1331.6387	0.000	1331.6384	0.0002
(6)	13	3	10	12	2	11	1332.2342	0.000	1332.2339	0.0003
(6)	16	2	14	15	1	15	1332.8200	0.000	1332.8195	0.0006
(6)	4	4	1	3	3	0	1333.2716	0.000	1333.2719	-0.0003
(6)	4	4	0	3	3	1	1333.2716	0.000	1333.2719	-0.0003
(6)	15	3	13	14	2	12	1333.2958	0.000	1333.2958	0.0001
(6)	14	3	11	13	2	12	1334.8298R	0.000	1334.8376	-0.0078
(6)	16	3	14	15	2	13	1334.8379R	0.000	1334.8297	0.0082
(6)	5	4	2	4	3	1	1335.6618	0.000	1335.6621	-0.0003
(6)	5	4	1	4	3	2	1335.6618	0.000	1335.6623	-0.0004
(6)	17	3	15	16	2	14	1336.2387	0.001	1336.2385	0.0002
(6)	15	3	12	14	2	13	1337.5038	0.000	1337.5035	0.0003
(6)	18	3	16	17	2	15	1337.5231	0.001	1337.5230	0.0000
(6)	17	2	15	16	1	16	1337.8953	0.001	1337.8946	0.0007
(6)	6	4	3	5	3	2	1338.0435	0.000	1338.0432	0.0002
(6)	6	4	2	5	3	3	1338.0435	0.000	1338.0439	-0.0004

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(6)	19	3	17 -	18	2	16	1338.6865	0.001	1338.6864	0.0001
(6)	20	3	18 -	19	2	17	1339.7337	0.001	1339.7337	0.0000
(6)	16	3	13 -	15	2	14	1340.2435	0.000	1340.2432	0.0003
(6)	7	4	4 -	6	3	3	1340.4146	0.000	1340.4142	0.0004
(6)	7	4	3 -	6	3	4	1340.4146	0.000	1340.4160	-0.0014
(6)	21	3	19 -	20	2	18	1340.6716	0.001	1340.6718	-0.0002
(6)	22	3	20 -	21	2	19	1341.5090	0.001	1341.5092	-0.0002
(6)	23	3	21 -	22	2	20	1342.2555	0.001	1342.2559	-0.0005
(6)	8	4	5 -	7	3	4	1342.7752	0.000	1342.7736	0.0016
(6)	8	4	4 -	7	3	5	1342.7752	0.000	1342.7782	-0.0030
(6)	24	3	22 -	23	2	21	1342.9230	0.001	1342.9234	-0.0004
(6)	17	3	14 -	16	2	15	1343.0694	0.001	1343.0690	0.0004
(6)	18	2	16 -	17	1	17	1343.2223	0.001	1343.2214	0.0009
(6)	23	5	19 -	23	4	20	1344.1808	0.001	1344.1817	-0.0010
(6)	22	5	17 -	22	4	18	1344.2918	0.001	1344.2917	0.0001
(6)	22	5	18 -	22	4	19	1344.5204	0.001	1344.5209	-0.0005
(6)	21	5	16 -	21	4	17	1344.6688*	0.000	1344.6697	-0.0009
(6)	21	5	17 -	21	4	18	1344.8321	0.001	1344.8324	-0.0002
(6)	20	5	15 -	20	4	16	1345.0099	0.001	1345.0100	-0.0001
(6)	9	4	6 -	8	3	5	1345.1194	0.000	1345.1196	-0.0002
(6)	9	4	5 -	8	3	6	1345.1295	0.000	1345.1298	-0.0003
(6)	19	5	14 -	19	4	15	1345.3168	0.001	1345.3167	0.0000
(6)	19	5	15 -	19	4	16	1345.3928	0.001	1345.3927	0.0001
(6)	18	5	13 -	18	4	14	1345.5937	0.001	1345.5935	0.0002
(6)	18	5	14 -	18	4	15	1345.6437	0.001	1345.6436	0.0001
(6)	17	5	12 -	17	4	13	1345.8436	0.001	1345.8436	0.0000
(6)	17	5	13 -	17	4	14	1345.8757	0.001	1345.8757	0.0000
(6)	18	3	15 -	17	2	16	1345.9941	0.001	1345.9936	0.0006
(6)	16	5	11 -	16	4	12	1346.0696	0.001	1346.0694	0.0002
(6)	16	5	12 -	16	4	13	1346.0896	0.001	1346.0895	0.0001
(6)	15	5	10 -	15	4	11	1346.2734	0.000	1346.2734	0.0000
(6)	15	5	11 -	15	4	12	1346.2855	0.000	1346.2855	0.0000
(6)	14	5	9 -	14	4	10	1346.4577	0.000	1346.4575	0.0003
(6)	14	5	10 -	14	4	11	1346.4646	0.000	1346.4645	0.0000
(6)	13	5	8 -	13	4	9	1346.6247	0.000	1346.6233	0.0014
(6)	13	5	9 -	13	4	10	1346.6247	0.000	1346.6272	-0.0025
(6)	12	5	7 -	12	4	8	1346.7732	0.000	1346.7723	0.0009
(6)	12	5	8 -	12	4	9	1346.7732	0.000	1346.7744	-0.0012
(6)	11	5	6 -	11	4	7	1346.9062	0.000	1346.9057	0.0005
(6)	11	5	7 -	11	4	8	1346.9062	0.000	1346.9068	-0.0006
(6)	10	5	5 -	10	4	6	1347.0248	0.000	1347.0246	0.0002
(6)	10	5	6 -	10	4	7	1347.0248	0.000	1347.0251	-0.0003
(6)	9	5	4 -	9	4	5	1347.1299	0.000	1347.1300	-0.0001
(6)	9	5	5 -	9	4	6	1347.1299	0.000	1347.1302	-0.0003
(6)	8	5	3 -	8	4	4	1347.2226	0.000	1347.2227	-0.0001
(6)	8	5	4 -	8	4	5	1347.2226	0.000	1347.2227	-0.0002
(6)	7	5	2 -	7	4	3	1347.3031	0.000	1347.3033	-0.0002
(6)	7	5	3 -	7	4	4	1347.3031	0.000	1347.3033	-0.0002
(6)	6	5	1 -	6	4	2	1347.3722	0.000	1347.3725	-0.0003
(6)	6	5	2 -	6	4	3	1347.3722	0.000	1347.3725	-0.0003

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(6)	5	5	0 -	5	4	1	1347.4307	0.000	1347.4309	-0.0001
(6)	5	5	1 -	5	4	2	1347.4307	0.000	1347.4309	-0.0001
(6)	10	4	7 -	9	3	6	1347.4498	0.000	1347.4501	-0.0002
(6)	10	4	6 -	9	3	7	1347.4703	0.000	1347.4705	-0.0001
(6)	19	2	17 -	18	1	18	1348.7991	0.001	1348.7982	0.0008
(6)	19	3	16 -	18	2	17	1349.0298	0.001	1349.0292	0.0006
(6)	11	4	8 -	10	3	7	1349.7621	0.000	1349.7621	0.0000
(6)	11	4	7 -	10	3	8	1349.7999	0.000	1349.8000	0.0000
(6)	12	4	9 -	11	3	8	1352.0522	0.000	1352.0520	0.0002
(6)	12	4	8 -	11	3	9	1352.1184	0.000	1352.1183	0.0001
(6)	20	3	17 -	19	2	18	1352.1883	0.001	1352.1876	0.0007
(6)	13	4	10 -	12	3	9	1354.3157	0.000	1354.3156	0.0001
(6)	13	4	9 -	12	3	10	1354.4263	0.000	1354.4261	0.0002
(6)	20	2	18 -	19	1	19	1354.6220	0.001	1354.6210	0.0010
(6)	21	3	18 -	20	2	19	1355.4794	0.001	1355.4784	0.0010
(6)	14	4	11 -	13	3	10	1356.5478	0.000	1356.5475	0.0003
(6)	14	4	10 -	13	3	11	1356.7241	0.000	1356.7241	0.0000
(6)	15	4	12 -	14	3	11	1358.7418	0.000	1358.7416	0.0002
(6)	22	3	19 -	21	2	20	1358.9090	0.001	1358.9081	0.0009
(6)	15	4	11 -	14	3	12	1359.0142	0.000	1359.0139	0.0003
(6)	5	5	1 -	4	4	0	1359.5757	0.000	1359.5760	-0.0003
(6)	5	5	0 -	4	4	1	1359.5757	0.000	1359.5760	-0.0003
(6)	21	2	19 -	20	1	20	1360.6846	0.001	1360.6836	0.0010
(6)	16	4	13 -	15	3	12	1360.8909	0.000	1360.8905	0.0004
(6)	16	4	12 -	15	3	13	1361.2977	0.000	1361.2975	0.0001
(6)	6	5	2 -	5	4	1	1361.9478	0.000	1361.9478	-0.0001
(6)	6	5	1 -	5	4	2	1361.9478	0.000	1361.9478	-0.0001
(6)	17	4	14 -	16	3	13	1362.9863	0.001	1362.9858	0.0004
(6)	17	4	13 -	16	3	14	1363.5781	0.001	1363.5780	0.0002
(6)	7	5	3 -	6	4	2	1364.3092	0.000	1364.3094	-0.0002
(6)	7	5	2 -	6	4	3	1364.3092	0.000	1364.3094	-0.0002
(6)	18	4	15 -	17	3	14	1365.0186	0.001	1365.0182	0.0004
(6)	18	4	14 -	17	3	15	1365.8591	0.001	1365.8588	0.0002
(6)	8	5	4 -	7	4	3	1366.6603	0.000	1366.6603	0.0000
(6)	8	5	3 -	7	4	4	1366.6603	0.000	1366.6603	0.0000
(6)	22	2	20 -	21	1	21	1366.9775*	0.000	1366.9782	-0.0007
(6)	19	4	16 -	18	3	15	1366.9775	0.001	1366.9771	0.0004
(6)	25	6	19 -	25	5	20	1367.4330	0.001	1367.4326	0.0004
(6)	25	6	20 -	25	5	21	1367.6169	0.001	1367.6169	0.0000
(6)	24	6	18 -	24	5	19	1367.8490	0.001	1367.8490	0.0000
(6)	24	6	19 -	24	5	20	1367.9946	0.001	1367.9947	-0.0001
(6)	19	4	15 -	18	3	16	1368.1451	0.001	1368.1447	0.0004
(6)	23	6	17 -	23	5	18	1368.2368	0.001	1368.2370	-0.0002
(6)	23	6	18 -	23	5	19	1368.3518	0.001	1368.3519	-0.0001
(6)	22	6	16 -	22	5	17	1368.5982	0.001	1368.5985	-0.0004
(6)	22	6	17 -	22	5	18	1368.6886	0.001	1368.6889	-0.0003
(6)	20	4	17 -	19	3	16	1368.8520	0.001	1368.8517	0.0003
(6)	21	6	15 -	21	5	16	1368.9349	0.001	1368.9352	-0.0004
(6)	21	6	16 -	21	5	17	1368.9998*	0.000	1369.0063	-0.0065
(6)	9	5	5 -	8	4	4	1368.9998	0.000	1368.9999	-0.0001

UPPER STATE J	KA	KC	LOWER STATE J	KA	KC	OBSERVATION	PREC.	CALCULATION	RESID.
(6) 9	5	4	- 8	4	5	1368.9998	0.000	1369.0000	-0.0002
(6) 20	6	14	- 20	5	15	1369.2480	0.001	1369.2486	-0.0006
(6) 20	6	15	- 20	5	16	1369.3041	0.001	1369.3045	-0.0004
(6) 19	6	13	- 19	5	14	1369.5393	0.001	1369.5398	-0.0006
(6) 19	6	14	- 19	5	15	1369.5838	0.001	1369.5840	-0.0002
(6) 18	6	12	- 18	5	13	1369.8093	0.001	1369.8100	-0.0006
(6) 18	6	13	- 18	5	14	1369.8449	0.001	1369.8452	-0.0003
(6) 17	6	11	- 17	5	12	1370.0593	0.001	1370.0598	-0.0005
(6) 17	6	12	- 17	5	13	1370.0881	0.001	1370.0885	-0.0004
(6) 16	6	10	- 16	5	11	1370.2891	0.001	1370.2898	-0.0006
(6) 16	6	11	- 16	5	12	1370.3139	0.001	1370.3141	-0.0003
(6) 20	4	16	- 19	3	17	1370.4416	0.001	1370.4412	0.0004
(6) 15	6	9	- 15	5	10	1370.4990	0.001	1370.4994	-0.0004
(6) 15	6	10	- 15	5	11	1370.5215	0.001	1370.5219	-0.0003
(6) 21	4	18	- 20	3	17	1370.6309	0.001	1370.6306	0.0003
(6) 14	6	8	- 14	5	9	1370.6850	0.001	1370.6856	-0.0006
(6) 14	6	9	- 14	5	10	1370.7100	0.001	1370.7103	-0.0002
(6) 13	6	7	- 13	5	8	1370.8312	0.001	1370.8319	-0.0007
(6) 13	6	8	- 13	5	9	1370.8713	0.001	1370.8717	-0.0003
(6) 12	6	6	- 12	5	7	1371.1685	0.001	1371.1677	0.0008
(6) 12	6	7	- 12	5	8	1371.2106	0.001	1371.2097	0.0008
(6) 11	6	5	- 11	5	6	1371.2647	0.001	1371.2625	0.0021
(6) 11	6	6	- 11	5	7	1371.2647	0.001	1371.2660	-0.0013
(6) 10	5	6	- 9	4	5	1371.3277	0.000	1371.3278	-0.0001
(6) 10	5	5	- 9	4	6	1371.3277	0.000	1371.3280	-0.0003
(6) 10	6	4	- 10	5	5	1371.3833	0.001	1371.3828	0.0005
(6) 10	6	5	- 10	5	6	1371.3833	0.001	1371.3832	0.0001
(6) 9	6	3	- 9	5	4	1371.4987	0.001	1371.4983	0.0004
(6) 9	6	4	- 9	5	5	1371.4987	0.001	1371.4983	0.0004
(6) 8	6	2	- 8	5	3	1371.6040	0.001	1371.6034	0.0006
(6) 8	6	3	- 8	5	4	1371.6040	0.001	1371.6034	0.0006
(6) 7	6	1	- 7	5	2	1371.6975	0.001	1371.6968	0.0006
(6) 7	6	2	- 7	5	3	1371.6975	0.001	1371.6968	0.0006
(6) 6	6	0	- 6	5	1	1371.7790	0.001	1371.7783	0.0007
(6) 6	6	1	- 6	5	2	1371.7790	0.001	1371.7783	0.0007
(6) 22	4	19	- 21	3	18	1372.3027	0.001	1372.3024	0.0003
(6) 21	4	17	- 20	3	18	1372.7549	0.001	1372.7547	0.0002
(6) 11	5	7	- 10	4	6	1373.6436	0.000	1373.6433	0.0003
(6) 11	5	6	- 10	4	7	1373.6436	0.000	1373.6438	-0.0002
(6) 23	4	20	- 22	3	19	1373.8569	0.001	1373.8568	0.0001
(6) 22	4	18	- 21	3	19	1375.0866	0.000	1375.0931	-0.0064
(6) 24	4	21	- 23	3	20	1375.2843	0.001	1375.2845	-0.0002
(6) 12	5	8	- 11	4	7	1375.9460	0.000	1375.9454	0.0006
(6) 12	5	7	- 11	4	8	1375.9460	0.000	1375.9465	-0.0005
(6) 25	4	22	- 24	3	21	1376.5776	0.001	1376.5780	-0.0003
(6) 23	4	19	- 22	3	20	1377.4651	0.001	1377.4649	0.0001
(6) 26	4	23	- 25	3	22	1377.7315	0.001	1377.7322	-0.0006
(6) 13	5	9	- 12	4	8	1378.2344	0.000	1378.2334	0.0010
(6) 13	5	8	- 12	4	9	1378.2344	0.000	1378.2355	-0.0012
(6) 27	4	24	- 26	3	23	1378.7435	0.001	1378.7446	-0.0011

UPPER STATE J	KA	KC	LOWER STATE J	KA	KC	OBSERVATION	PREC.	CALCULATION	RESID.
(6) 28	4	25	- 27	3	24	1379.6139	0.001	1379.6155	-0.0016
(6) 24	4	20	- 23	3	21	1379.8802	0.001	1379.8802	0.0000
(6) 14	5	10	- 13	4	9	1380.5077	0.000	1380.5060	0.0017
(6) 14	5	9	- 13	4	10	1380.5077	0.000	1380.5101	-0.0024
(6) 25	4	21	- 24	3	22	1382.3497	0.001	1382.3500	-0.0003
(6) 15	5	11	- 14	4	10	1382.7624	0.000	1382.7622	0.0002
(6) 15	5	10	- 14	4	11	1382.7695	0.000	1382.7696	-0.0001
(6) 26	4	22	- 25	3	23	1384.8861	0.001	1384.8864	-0.0003
(6) 16	5	12	- 15	4	11	1385.0005	0.000	1385.0005	0.0001
(6) 16	5	11	- 15	4	12	1385.0134	0.000	1385.0132	0.0002
(6) 6	6	0	- 5	5	1	1386.3473	0.001	1386.3467	0.0006
(6) 6	6	1	- 5	5	0	1386.3473	0.001	1386.3467	0.0006
(6) 17	5	13	- 16	4	12	1387.2191	0.001	1387.2190	0.0001
(6) 17	5	12	- 16	4	13	1387.2406	0.001	1387.2404	0.0002
(6) 27	4	23	- 26	3	24	1387.5018	0.001	1387.5025	-0.0007
(6) 7	6	1	- 6	5	2	1388.6944	0.001	1388.6940	0.0004
(6) 7	6	2	- 6	5	1	1388.6944	0.001	1388.6940	0.0004
(6) 18	5	14	- 17	4	13	1389.4161	0.001	1389.4159	0.0002
(6) 18	5	13	- 17	4	14	1389.4505	0.001	1389.4504	0.0001
(6) 28	4	24	- 27	3	25	1390.2113	0.001	1390.2125	-0.0012
(6) 8	6	2	- 7	5	3	1391.0301	0.001	1391.0296	0.0005
(6) 8	6	3	- 7	5	2	1391.0301	0.001	1391.0296	0.0005
(6) 19	5	15	- 18	4	14	1391.5887	0.001	1391.5886	0.0002
(6) 19	5	14	- 18	4	15	1391.6431	0.001	1391.6429	0.0002
(6) 9	6	3	- 8	5	4	1393.3545	0.001	1393.3538	0.0007
(6) 9	6	4	- 8	5	3	1393.3545	0.001	1393.3538	0.0006
(6) 21	7	14	- 21	6	15	1393.3969	0.001	1393.3972	-0.0003
(6) 21	7	15	- 21	6	16	1393.3969	0.001	1393.3974	-0.0004
(6) 20	7	13	- 20	6	14	1393.7117	0.001	1393.7120	-0.0003
(6) 20	7	14	- 20	6	15	1393.7117	0.001	1393.7121	-0.0004
(6) 20	5	16	- 19	4	15	1393.7341	0.001	1393.7341	0.0001
(6) 20	5	15	- 19	4	16	1393.8179	0.001	1393.8177	0.0002
(6) 19	7	12	- 19	6	13	1394.0103	0.001	1394.0105	-0.0002
(6) 19	7	13	- 19	6	14	1394.0103	0.001	1394.0106	-0.0002
(6) 18	7	11	- 18	6	12	1394.2927	0.001	1394.2928	-0.0001
(6) 18	7	12	- 18	6	13	1394.2927	0.001	1394.2929	-0.0001
(6) 17	7	10	- 17	6	11	1394.5591	0.001	1394.5591	-0.0001
(6) 17	7	11	- 17	6	12	1394.5591	0.001	1394.5591	-0.0001
(6) 16	7	9	- 16	6	10	1394.8096	0.001	1394.8095	0.0000
(6) 16	7	10	- 16	6	11	1394.8096	0.001	1394.8096	0.0000
(6) 15	7	8	- 15	6	9	1395.0444	0.001	1395.0443	0.0002
(6) 15	7	9	- 15	6	10	1395.0444	0.001	1395.0443	0.0002
(6) 14	7	7	- 14	6	8	1395.2637	0.001	1395.2634	0.0003
(6) 14	7	8	- 14	6	9	1395.2637	0.001	1395.2634	0.0003
(6) 13	7	6	- 13	6	7	1395.4678	0.001	1395.4671	0.0006
(6) 13	7	7	- 13	6	8	1395.4678	0.001	1395.4671	0.0006
(6) 12	7	5	- 12	6	6	1395.6564	0.001	1395.6556	0.0008
(6) 12	7	6	- 12	6	7	1395.6564	0.001	1395.6556	0.0008
(6) 10	6	4	- 9	5	5	1395.6689	0.001	1395.6680	0.0009
(6) 10	6	5	- 9	5	4	1395.6689	0.001	1395.6684	0.0005

UPPER STATE J KA KC		LOWER STATE J KA KC		OBSERVATION	PREC.	CALCULATION	RESID.
(6)	11 7 4	- 11 6 5		1395.8298	0.001	1395.8289	0.0009
(6)	11 7 5	- 11 6 6		1395.8298	0.001	1395.8289	0.0009
(6)	21 5 17	- 20 4 16		1395.8484	0.001	1395.8485	-0.0001
(6)	21 5 16	- 20 4 17		1395.9744	0.001	1395.9747	-0.0003
(6)	10 7 3	- 10 6 4		1395.9883	0.001	1395.9873	0.0011
(6)	10 7 4	- 10 6 5		1395.9883	0.001	1395.9873	0.0011
(6)	9 7 2	- 9 6 3		1396.1320	0.001	1396.1308	0.0012
(6)	9 7 3	- 9 6 4		1396.1320	0.001	1396.1308	0.0012
(6)	8 7 1	- 8 6 2		1396.2609	0.001	1396.2596	0.0013
(6)	8 7 2	- 8 6 3		1396.2609	0.001	1396.2596	0.0013
(6)	7 7 0	- 7 6 1		1396.3752	0.001	1396.3737	0.0014
(6)	7 7 1	- 7 6 2		1396.3752	0.001	1396.3737	0.0014
(6)	22 5 18	- 21 4 17		1397.9260	0.001	1397.9263	-0.0004
(6)	11 6 5	- 10 5 6		1397.9801	0.001	1397.9779	0.0021
(6)	11 6 6	- 10 5 5		1397.9801	0.001	1397.9814	-0.0013
(6)	22 5 17	- 21 4 18		1398.1142	0.001	1398.1141	0.0001
(6)	23 5 19	- 22 4 18		1399.9550	0.001	1399.9561	-0.0011
(6)	23 5 18	- 22 4 19		1400.2366	0.001	1400.2367	-0.0001
(6)	12 6 6	- 11 5 7		1400.3145	0.001	1400.3138	0.0008
(6)	12 6 7	- 11 5 6		1400.3565	0.001	1400.3557	0.0008
(6)	24 5 20	- 23 4 19		1401.8552	0.001	1401.8590	-0.0038
(6)	24 5 19	- 23 4 20		1402.3430	0.001	1402.3435	-0.0005
(6)	13 6 7	- 12 5 8		1402.4082	0.001	1402.4090	-0.0008
(6)	13 6 8	- 12 5 7		1402.4482	0.001	1402.4488	-0.0006
(6)	14 6 8	- 13 5 9		1404.6940	0.001	1404.6944	-0.0004
(6)	14 6 9	- 13 5 8		1404.7186	0.001	1404.7190	-0.0003
(6)	15 6 9	- 14 5 10		1406.9399	0.001	1406.9405	-0.0006
(6)	15 6 10	- 14 5 9		1406.9624	0.001	1406.9627	-0.0003
(6)	16 6 10	- 15 5 11		1409.1634	0.001	1409.1639	-0.0005
(6)	16 6 11	- 15 5 10		1409.1874	0.001	1409.1877	-0.0003
(6)	17 6 11	- 16 5 12		1411.3674	0.001	1411.3678	-0.0004
(6)	17 6 12	- 16 5 11		1411.3952	0.001	1411.3954	-0.0002
(6)	7 7 1	- 6 6 0		1413.3639	0.001	1413.3623	0.0016
(6)	7 7 0	- 6 6 1		1413.3639	0.001	1413.3623	0.0016
(6)	18 6 12	- 17 5 13		1413.5523	0.001	1413.5527	-0.0004
(6)	18 6 13	- 17 5 12		1413.5856	0.001	1413.5859	-0.0003
(6)	8 7 2	- 7 6 1		1415.6767	0.001	1415.6753	0.0014
(6)	8 7 1	- 7 6 2		1415.6767	0.001	1415.6753	0.0014
(6)	19 6 13	- 18 5 14		1415.7179	0.001	1415.7183	-0.0004
(6)	19 6 14	- 18 5 13		1415.7586	0.001	1415.7590	-0.0004
(6)	24 8 16	- 24 7 17		1416.3505	0.001	1416.3484	0.0021
(6)	24 8 17	- 24 7 18		1416.3505	0.001	1416.3484	0.0021
(6)	23 8 15	- 23 7 16		1416.7721	0.001	1416.7709	0.0013
(6)	23 8 16	- 23 7 17		1416.7721	0.001	1416.7709	0.0013
(6)	22 8 14	- 22 7 15		1417.1774	0.001	1417.1768	0.0006
(6)	22 8 15	- 22 7 16		1417.1774	0.001	1417.1768	0.0006
(6)	21 8 13	- 21 7 14		1417.5663	0.001	1417.5661	0.0002
(6)	21 8 14	- 21 7 15		1417.5663	0.001	1417.5661	0.0002
(6)	20 6 14	- 19 5 15		1417.8637	0.001	1417.8641	-0.0005
(6)	20 6 15	- 19 5 14		1417.9139	0.001	1417.9142	-0.0003

UPPER STATE J KA KC		LOWER STATE J KA KC		OBSERVATION	PREC.	CALCULATION	RESID.
(6)	20 8 12	- 20 7 13		1417.9385	0.001	1417.9386	-0.0002
(6)	20 8 13	- 20 7 14		1417.9385	0.001	1417.9386	-0.0002
(6)	9 7 3	- 8 6 2		1417.9751	0.001	1417.9738	0.0013
(6)	9 7 2	- 8 6 3		1417.9751	0.001	1417.9738	0.0013
(6)	19 8 11	- 19 7 12		1418.2938	0.001	1418.2943	-0.0005
(6)	19 8 12	- 19 7 13		1418.2938	0.001	1418.2943	-0.0005
(6)	18 8 10	- 18 7 11		1418.6321	0.001	1418.6329	-0.0008
(6)	18 8 11	- 18 7 12		1418.6321	0.001	1418.6329	-0.0008
(6)	17 8 9	- 17 7 10		1418.9535	0.001	1418.9544	-0.0009
(6)	17 8 10	- 17 7 11		1418.9535	0.001	1418.9544	-0.0009
(6)	16 8 8	- 16 7 9		1419.2579	0.001	1419.2587	-0.0009
(6)	16 8 9	- 16 7 10		1419.2579	0.001	1419.2587	-0.0009
(6)	15 8 7	- 15 7 8		1419.5448	0.001	1419.5457	-0.0009
(6)	15 8 8	- 15 7 9		1419.5448	0.001	1419.5457	-0.0009
(6)	14 8 6	- 14 7 7		1419.8142	0.001	1419.8152	-0.0010
(6)	14 8 7	- 14 7 8		1419.8142	0.001	1419.8152	-0.0010
(6)	21 6 15	- 20 5 16		1419.9889	0.001	1419.9893	-0.0004
(6)	21 6 16	- 20 5 15		1420.0507	0.001	1420.0509	-0.0002
(6)	13 8 5	- 13 7 6		1420.0665	0.001	1420.0672	-0.0007
(6)	13 8 6	- 13 7 7		1420.0665	0.001	1420.0672	-0.0007
(6)	10 7 4	- 9 6 3		1420.2588	0.001	1420.2577	0.0011
(6)	10 7 3	- 9 6 4		1420.2588	0.001	1420.2577	0.0011
(6)	12 8 4	- 12 7 5		1420.3010	0.001	1420.3016	-0.0006
(6)	12 8 5	- 12 7 6		1420.3010	0.001	1420.3016	-0.0006
(6)	11 8 3	- 11 7 4		1420.5179	0.001	1420.5183	-0.0004
(6)	11 8 4	- 11 7 5		1420.5179	0.001	1420.5183	-0.0004
(6)	10 8 2	- 10 7 3		1420.7171	0.001	1420.7172	-0.0001
(6)	10 8 3	- 10 7 4		1420.7171	0.001	1420.7172	-0.0001
(6)	9 8 1	- 9 7 2		1420.8984	0.001	1420.8983	0.0001
(6)	9 8 2	- 9 7 3		1420.8984	0.001	1420.8983	0.0001
(6)	8 8 0	- 8 7 1		1421.0617	0.001	1421.0614	0.0003
(6)	8 8 1	- 8 7 2		1421.0617	0.001	1421.0614	0.0003
(6)	22 6 16	- 21 5 17		1422.0928	0.001	1422.0931	-0.0003
(6)	22 6 17	- 21 5 16		1422.1683	0.001	1422.1684	-0.0001
(6)	11 7 5	- 10 6 4		1422.5278	0.001	1422.5268	0.0010
(6)	11 7 4	- 10 6 5		1422.5278	0.001	1422.5268	0.0010
(6)	23 6 17	- 22 5 18		1424.1744	0.001	1424.1745	-0.0001
(6)	23 6 18	- 22 5 17		1424.2658	0.001	1424.2657	0.0000
(6)	12 7 6	- 11 6 5		1424.7817	0.001	1424.7810	0.0007
(6)	12 7 5	- 11 6 6		1424.7817	0.001	1424.7810	0.0007
(6)	24 6 18	- 23 5 19		1426.2329	0.001	1426.2324	0.0004
(6)	24 6 19	- 23 5 18		1426.3421	0.001	1426.3420	0.0001
(6)	13 7 7	- 12 6 6		1427.0210	0.001	1427.0203	0.0007
(6)	13 7 6	- 12 6 7		1427.0210	0.001	1427.0203	0.0007
(6)	25 6 19	- 24 5 20		1428.2678*	0.000	1428.2659	0.0019
(6)	25 6 20	- 24 5 19		1428.3961	0.001	1428.3959	0.0001
(6)	14 7 8	- 13 6 7		1429.2449	0.001	1429.2444	0.0005
(6)	14 7 7	- 13 6 8		1429.2449	0.001	1429.2444	0.0005
(6)	26 6 20	- 25 5 21		1430.2748	0.001	1430.2738	0.0010
(6)	26 6 21	- 25 5 20		1430.4264	0.001	1430.4262	0.0003

UPPER STATE J	KA	KC	LOWER STATE J	KA	KC	OBSERVATION	PREC.	CALCULATION	RESID.
(6) 15	7	9	- 14	6	8	1431.4537	0.001	1431.4533	0.0004
(6) 15	7	8	- 14	6	9	1431.4537	0.001	1431.4533	0.0004
(6) 27	6	21	- 26	5	22	1432.2964	0.001	1432.2548	0.0016
(6) 27	6	22	- 26	5	21	1432.4315	0.001	1432.4310	0.0005
(3) 28	1	28	- 29	1	29	1432.9586	0.001	1432.9584	0.0002
(3) 28	1	27	- 29	1	28	1433.2363	0.001	1433.2373	-0.0011
(3) 28	3	25	- 29	3	26	1433.6272	0.001	1433.6274	-0.0001
(6) 16	7	10	- 15	6	9	1433.6470	0.001	1433.6467	0.0003
(6) 16	7	9	- 15	6	10	1433.6470	0.001	1433.6467	0.0003
(3) 28	3	26	- 29	3	27	1434.1365	0.001	1434.1367	-0.0002
(3) 28	5	23	- 29	5	24	1435.2798*	0.000	1435.2853	-0.0055
(3) 27	1	27	- 28	1	28	1435.2798	0.001	1435.2792	0.0006
(3) 28	5	24	- 29	5	25	1435.2985	0.001	1435.2937	0.0047
(3) 27	1	26	- 28	1	27	1435.4375	0.001	1435.4385	-0.0009
(3) 27	2	26	- 28	2	27	1435.6291	0.001	1435.6277	0.0014
(3) 27	3	24	- 28	3	25	1435.7754	0.001	1435.7761	-0.0007
(6) 17	7	11	- 16	6	10	1435.8248	0.001	1435.8247	0.0001
(6) 17	7	10	- 16	6	11	1435.8248	0.001	1435.8247	0.0001
(3) 27	3	25	- 28	3	26	1436.2678	0.001	1436.2678	0.0000
(3) 27	5	22	- 28	5	23	1437.4359	0.001	1437.4361	-0.0002
(3) 27	5	23	- 28	5	24	1437.4487	0.001	1437.4430	0.0057
(3) 26	1	26	- 27	1	27	1437.5990	0.001	1437.5986	0.0005
(3) 26	1	25	- 27	1	26	1437.6362	0.001	1437.6367	-0.0005
(3) 26	2	25	- 27	2	26	1437.8532	0.001	1437.8520	0.0012
(3) 26	3	23	- 27	3	24	1437.9409	0.001	1437.9420	-0.0011
(6) 18	7	12	- 17	6	11	1437.9870	0.001	1437.9869	0.0001
(6) 18	7	11	- 17	6	12	1437.9870	0.001	1437.9869	0.0001
(3) 26	3	24	- 27	3	25	1438.4130	0.001	1438.4129	0.0001
(3) 26	5	21	- 27	5	22	1439.5926	0.001	1439.5952	-0.0027
(3) 26	5	22	- 27	5	23	1439.5926	0.001	1439.6008	-0.0082
(3) 25	2	23	- 26	2	24	1439.6782	0.001	1439.6736	0.0046
(3) 25	1	24	- 26	1	25	1439.8322	0.001	1439.8326	-0.0004
(3) 25	1	25	- 26	1	26	1439.9168	0.001	1439.9162	0.0005
(3) 25	2	24	- 26	2	25	1440.0809	0.001	1440.0805	0.0004
(3) 25	3	22	- 26	3	23	1440.1241	0.001	1440.1252	-0.0011
(6) 19	7	13	- 18	6	12	1440.1333	0.001	1440.1333	0.0000
(6) 19	7	12	- 18	6	13	1440.1333	0.001	1440.1333	0.0000
(6) 8	8	1	- 7	7	0	1440.4669	0.001	1440.4665	0.0005
(6) 8	8	0	- 7	7	1	1440.4669	0.001	1440.4665	0.0005
(3) 25	3	23	- 26	3	24	1440.5719	0.001	1440.5717	0.0002
(3) 25	4	21	- 26	4	22	1440.8063	0.001	1440.8079	-0.0016
(3) 25	5	20	- 26	5	21	1441.7640	0.001	1441.7629	0.0011
(3) 25	5	21	- 26	5	22	1441.7640	0.001	1441.7672	-0.0033
(3) 24	2	22	- 25	2	23	1441.8411	0.001	1441.8377	0.0034
(3) 24	1	23	- 25	1	24	1442.0268	0.001	1442.0269	-0.0001
(3) 24	1	24	- 25	1	25	1442.2328	0.001	1442.2322	0.0006
(6) 20	7	14	- 19	6	13	1442.2637	0.001	1442.2637	0.0000
(6) 20	7	13	- 19	6	14	1442.2637	0.001	1442.2638	0.0000
(3) 24	2	23	- 25	2	24	1442.3137	0.001	1442.3132	0.0005
(3) 24	3	21	- 25	3	22	1442.3242	0.001	1442.3254	-0.0012

UPPER STATE J	KA	KC	LOWER STATE J	KA	KC	OBSERVATION	PREC.	CALCULATION	RESID.
(6) 9	8	2	- 8	7	1	1442.7291	0.001	1442.7288	0.0003
(6) 9	8	1	- 8	7	2	1442.7291	0.001	1442.7288	0.0003
(3) 24	3	22	- 25	3	23	1442.7436	0.001	1442.7436	0.0000
(3) 24	4	20	- 25	4	21	1443.0167	0.001	1443.0186	-0.0018
(3) 24	4	21	- 25	4	22	1443.0686	0.001	1443.0686	0.0000
(3) 24	5	19	- 25	5	20	1443.9402	0.001	1443.9393	0.0009
(3) 24	5	20	- 25	5	21	1443.9402	0.001	1443.9426	-0.0025
(3) 23	2	21	- 24	2	22	1444.0178	0.001	1444.0153	0.0025
(3) 23	1	22	- 24	1	23	1444.2209	0.001	1444.2210	-0.0001
(6) 21	7	15	- 20	6	14	1444.3779	0.001	1444.3781	-0.0002
(6) 21	7	14	- 20	6	15	1444.3779	0.001	1444.3781	-0.0002
(3) 23	3	20	- 24	3	21	1444.5471*	0.000	1444.5422	0.0048
(3) 23	2	22	- 24	2	23	1444.5471*	0.000	1444.5501	-0.0030
(3) 23	1	23	- 24	1	24	1444.5471*	0.000	1444.5465	0.0005
(3) 23	0	23	- 24	0	24	1444.5471*	0.000	1444.5469	0.0002
(3) 23	3	21	- 24	3	22	1444.9287	0.001	1444.9285	0.0001
(6) 10	8	3	- 9	7	2	1444.9729	0.001	1444.9731	-0.0002
(6) 10	8	2	- 9	7	3	1444.9729	0.001	1444.9731	-0.0002
(3) 24	6	18	- 25	6	19	1445.0778	0.001	1445.0749	0.0029
(3) 24	6	19	- 25	6	20	1445.0778	0.001	1445.0750	0.0028
(3) 23	4	19	- 24	4	20	1445.2358	0.001	1445.2374	-0.0016
(3) 23	4	20	- 24	4	21	1445.2789	0.001	1445.2793	-0.0004
(3) 23	5	18	- 24	5	19	1446.1253	0.001	1446.1246	0.0007
(3) 23	5	19	- 24	5	20	1446.1253	0.001	1446.1272	-0.0019
(3) 22	2	20	- 23	2	21	1446.2092	0.001	1446.2073	0.0019
(3) 22	1	21	- 23	1	22	1446.4163	0.001	1446.4163	0.0000
(6) 22	7	16	- 21	6	15	1446.4762	0.001	1446.4762	0.0000
(6) 22	7	15	- 21	6	16	1446.4762	0.001	1446.4763	0.0000
(3) 22	3	19	- 23	3	20	1446.7737	0.001	1446.7748	-0.0011
(3) 22	2	21	- 23	2	22	1446.7916	0.001	1446.7914	0.0002
(3) 22	0	22	- 23	0	23	1446.8330	0.001	1446.8338	-0.0008
(3) 22	1	22	- 23	1	23	1446.8596	0.001	1446.8591	0.0005
(3) 22	3	20	- 23	3	21	1447.1264	0.001	1447.1263	0.0001
(6) 11	8	4	- 10	7	3	1447.1993	0.001	1447.1995	-0.0002
(6) 11	8	3	- 10	7	4	1447.1993	0.001	1447.1995	-0.0002
(3) 23	6	17	- 24	6	18	1447.2217	0.001	1447.2192	0.0025
(3) 23	6	18	- 24	6	19	1447.2217	0.001	1447.2193	0.0024
(3) 22	4	18	- 23	4	19	1447.4629	0.001	1447.4644	-0.0015
(3) 22	4	19	- 23	4	20	1447.4983	0.001	1447.4988	-0.0006
(3) 22	5	17	- 23	5	18	1448.3193	0.001	1448.3191	0.0002
(3) 22	5	18	- 23	5	19	1448.3193	0.001	1448.3210	-0.0017
(3) 21	2	19	- 22	2	20	1448.4163	0.001	1448.4150	0.0014
(6) 23	7	17	- 22	6	16	1448.5576	0.001	1448.5580	-0.0004
(6) 23	7	16	- 22	6	17	1448.5576	0.001	1448.5581	-0.0005
(3) 21	1	20	- 22	1	21	1448.6145	0.001	1448.6146	-0.0001
(3) 21	3	18	- 22	3	19	1449.0211	0.001	1449.0220	-0.0009
(3) 21	2	20	- 22	2	21	1449.0374	0.001	1449.0373	0.0001
(3) 21	0	21	- 22	0	22	1449.1262	0.001	1449.1269	-0.0008
(3) 21	1	21	- 22	1	22	1449.1706	0.001	1449.1702	0.0005
(3) 21	3	19	- 22	3	20	1449.3368	0.001	1449.3368	0.0000

UPPER STATE			LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(3)	22	6	16 -	23	6	17	1449.3757	0.001	1449.3735	0.0022
(3)	22	6	17 -	23	6	18	1449.3757	0.001	1449.3736	0.0021
(6)	12	8	5 -	11	7	4	1449.4074	0.001	1449.4080	-0.0006
(6)	12	8	4 -	11	7	5	1449.4074	0.001	1449.4080	-0.0006
(3)	21	4	17 -	22	4	18	1449.6980	0.001	1449.6996	-0.0016
(3)	21	4	18 -	22	4	19	1449.7263	0.001	1449.7273	-0.0010
(3)	21	5	16 -	22	5	17	1450.5229	0.001	1450.5229	-0.0001
(3)	21	5	17 -	22	5	18	1450.5229	0.001	1450.5243	-0.0014
(6)	24	7	18 -	23	6	17	1450.6229	0.001	1450.6234	-0.0005
(6)	24	7	17 -	23	6	18	1450.6229	0.001	1450.6235	-0.0006
(3)	20	2	18 -	21	2	19	1450.6403	0.001	1450.6393	0.0010
(3)	20	1	19 -	21	1	20	1450.8177	0.001	1450.8178	-0.0001
(3)	20	3	17 -	21	3	18	1451.2820	0.001	1451.2827	-0.0007
(3)	20	2	19 -	21	2	20	1451.2820*	0.000	1451.2884	-0.0064
(3)	20	0	20 -	21	0	21	1451.4184	0.001	1451.4189	-0.0005
(3)	20	1	20 -	21	1	21	1451.4801	0.001	1451.4798	0.0004
(3)	21	6	15 -	22	6	16	1451.5400	0.001	1451.5381	0.0019
(3)	21	6	16 -	22	6	17	1451.5400	0.001	1451.5382	0.0019
(3)	20	3	18 -	21	3	19	1451.5598	0.001	1451.5599	-0.0001
(6)	13	8	6 -	12	7	5	1451.5982	0.001	1451.5988	-0.0006
(6)	13	8	5 -	12	7	6	1451.5982	0.001	1451.5988	-0.0006
(3)	20	4	16 -	21	4	17	1451.9418	0.001	1451.9431	-0.0013
(3)	20	4	17 -	21	4	18	1451.9640	0.001	1451.9649	-0.0009
(3)	20	5	15 -	21	5	16	1452.7361	0.001	1452.7362	-0.0001
(3)	20	5	16 -	21	5	17	1452.7361	0.001	1452.7372	-0.0011
(3)	19	2	17 -	20	2	18	1452.8318	0.001	1452.8811	0.0007
(3)	19	1	18 -	20	1	19	1453.0280	0.001	1453.0280	0.0001
(3)	19	2	18 -	20	2	19	1453.5449	0.001	1453.5451	-0.0002
(3)	19	3	16 -	20	3	17	1453.5550	0.001	1453.5557	-0.0007
(3)	19	0	19 -	20	0	20	1453.7073	0.001	1453.7078	-0.0005
(3)	20	6	14 -	21	6	15	1453.7152	0.001	1453.7133	0.0019
(3)	20	6	15 -	21	6	16	1453.7152	0.001	1453.7133	0.0019
(6)	14	8	6 -	13	7	7	1453.7709	0.001	1453.7718	-0.0009
(6)	14	8	7 -	13	7	6	1453.7709	0.001	1453.7718	-0.0009
(3)	19	1	19 -	20	1	20	1453.7885	0.001	1453.7881	0.0004
(3)	19	3	17 -	20	3	18	1453.7957	0.001	1453.7957	0.0000
(3)	19	4	15 -	20	4	16	1454.1937	0.001	1454.1950	-0.0012
(3)	19	4	16 -	20	4	17	1454.2109	0.001	1454.2118	-0.0009
(3)	19	5	14 -	20	5	15	1454.9589	0.001	1454.9591	-0.0001
(3)	19	5	15 -	20	5	16	1454.9589	0.001	1454.9597	-0.0008
(3)	18	2	16 -	19	2	17	1455.1416	0.001	1455.1411	0.0004
(3)	18	1	17 -	19	1	18	1455.2469	0.001	1455.2469	0.0000
(3)	18	2	17 -	19	2	18	1455.8077	0.001	1455.8078	-0.0001
(3)	18	3	15 -	19	3	16	1455.8393	0.001	1455.8398	-0.0006
(3)	19	6	13 -	20	6	14	1455.9008	0.001	1455.8992	0.0016
(3)	19	6	14 -	20	6	15	1455.9008	0.001	1455.8992	0.0016
(6)	15	8	8 -	14	7	7	1455.9263	0.001	1455.9273	-0.0009
(6)	15	8	7 -	14	7	8	1455.9263	0.001	1455.9273	-0.0009
(3)	18	0	18 -	19	0	19	1455.9924	0.001	1455.9928	-0.0003
(3)	18	3	16 -	19	3	17	1456.0442	0.001	1456.0441	0.0001

UPPER STATE			LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(3)	18	1	18 -	19	1	19	1456.0959	0.001	1456.0955	0.0004
(3)	18	4	14 -	19	4	15	1456.4541	0.001	1456.4552	-0.0011
(3)	18	4	15 -	19	4	16	1456.4670	0.001	1456.4679	-0.0009
(3)	19	7	12 -	20	7	13	1457.0723R	0.001	1457.0249	0.0475
(3)	19	7	13 -	20	7	14	1457.0723R	0.001	1457.0249	0.0475
(3)	18	5	13 -	19	5	14	1457.1915	0.001	1457.1917	-0.0002
(3)	18	5	14 -	19	5	15	1457.1915	0.001	1457.1921	-0.0006
(3)	17	2	15 -	18	2	16	1457.4199	0.001	1457.4199	0.0000
(3)	17	1	16 -	18	1	17	1457.4764	0.001	1457.4763	0.0001
(6)	16	8	9 -	15	7	8	1458.0644	0.001	1458.0651	-0.0007
(6)	16	8	8 -	15	7	9	1458.0644	0.001	1458.0651	-0.0007
(3)	17	2	16 -	18	2	17	1458.0769	0.001	1458.0770	-0.0001
(3)	18	6	12 -	19	6	13	1458.0974	0.001	1458.0960	0.0015
(3)	18	6	13 -	19	6	14	1458.0974	0.001	1458.0960	0.0014
(3)	17	3	14 -	18	3	15	1458.1337	0.001	1458.1342	-0.0004
(3)	17	0	17 -	18	0	18	1458.2678*	0.000	1458.2736	-0.0058
(3)	17	3	15 -	18	3	16	1458.3054	0.001	1458.3053	0.0001
(3)	17	1	17 -	18	1	18	1458.4025	0.001	1458.4022	0.0003
(3)	19	8	11 -	20	8	12	1458.6582R	0.001	1458.6792	-0.0210
(3)	19	8	12 -	20	8	13	1458.6582R	0.001	1458.6792	-0.0210
(3)	17	4	13 -	18	4	14	1458.7230	0.001	1458.7240	-0.0011
(3)	17	4	14 -	18	4	15	1458.7326	0.001	1458.7333	-0.0007
(3)	18	7	11 -	19	7	12	1459.2033	0.001	1459.2023	0.0011
(3)	18	7	12 -	19	7	13	1459.2033	0.001	1459.2023	0.0011
(3)	17	5	12 -	18	5	13	1459.4337	0.001	1459.4341	-0.0003
(3)	17	5	13 -	18	5	14	1459.4337	0.001	1459.4343	-0.0006
(3)	16	2	14 -	17	2	15	1459.7179*	0.000	1459.7176	0.0003
(3)	16	1	15 -	17	1	16	1459.7179*	0.000	1459.7178	0.0000
(6)	17	8	10 -	16	7	9	1460.1848	0.001	1460.1856	-0.0008
(6)	17	8	9 -	16	7	10	1460.1848	0.001	1460.1856	-0.0008
(3)	17	6	11 -	18	6	12	1460.3051	0.001	1460.3039	0.0012
(3)	17	6	12 -	18	6	13	1460.3051	0.001	1460.3039	0.0012
(3)	16	2	15 -	17	2	16	1460.3530	0.001	1460.3531	-0.0002
(3)	16	3	13 -	17	3	14	1460.4379	0.001	1460.4381	-0.0002
(3)	16	0	16 -	17	0	17	1460.5503	0.001	1460.5504	-0.0001
(3)	16	3	14 -	17	3	15	1460.5797	0.001	1460.5795	0.0002
(3)	16	1	16 -	17	1	17	1460.7088	0.001	1460.7086	0.0002
(3)	16	4	12 -	17	4	13	1461.0011	0.001	1461.0014	-0.0003
(3)	16	4	13 -	17	4	14	1461.0074	0.001	1461.0081	-0.0007
(3)	17	7	10 -	18	7	11	1461.3738	0.001	1461.3721	0.0017
(3)	17	7	11 -	18	7	12	1461.3738	0.001	1461.3721	0.0017
(3)	16	5	11 -	17	5	12	1461.6861	0.001	1461.6864	-0.0003
(3)	16	5	12 -	17	5	13	1461.6861	0.001	1461.6865	-0.0004
(3)	15	1	14 -	16	1	15	1461.9727	0.001	1461.9727	0.0000
(3)	15	2	13 -	16	2	14	1462.0341	0.001	1462.0340	0.0001
(6)	18	8	11 -	17	7	10	1462.2881	0.001	1462.2886	-0.0006
(6)	18	8	10 -	17	7	11	1462.2881	0.001	1462.2886	-0.0006
(3)	16	6	10 -	17	6	11	1462.5241	0.001	1462.5231	0.0010
(3)	16	6	11 -	17	6	12	1462.5241	0.001	1462.5231	0.0010
(3)	15	2	14 -	16	2	15	1462.6366	0.001	1462.6367	-0.0001

UPPER STATE				LOWER STATE				OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(3)	15	3	12	-	16	3	13	1462.7517	0.001	1462.7516	0.0000
(3)	17	8	9	-	18	8	10	1462.7877	0.001	1462.7967	-0.0090
(3)	17	8	10	-	18	8	11	1462.7877	0.001	1462.7967	-0.0090
(3)	15	0	15	-	16	0	16	1462.8236	0.001	1462.8238	-0.0001
(3)	15	3	13	-	16	3	14	1462.8682	0.001	1462.8678	0.0003
(3)	15	1	15	-	16	1	16	1463.0151	0.001	1463.0150	0.0001
(3)	15	4	11	-	16	4	12	1463.2885	0.001	1463.2874	0.0010
(3)	15	4	12	-	16	4	13	1463.2885	0.001	1463.2920	-0.0036
(3)	16	7	9	-	17	7	10	1463.5494	0.001	1463.5475	0.0019
(3)	16	7	10	-	17	7	11	1463.5494	0.001	1463.5475	0.0019
(3)	15	5	10	-	16	5	11	1463.9485	0.001	1463.9486	-0.0001
(3)	15	5	11	-	16	5	12	1463.9485	0.001	1463.9488	-0.0003
(3)	14	1	13	-	15	1	14	1464.2418	0.000	1464.2419	-0.0001
(6)	19	8	12	-	18	7	11	1464.3688*	0.000	1464.3744	-0.0056
(6)	19	8	11	-	18	7	12	1464.3688*	0.000	1464.3744	-0.0056
(3)	14	2	12	-	15	2	13	1464.3688*	0.000	1464.3684	0.0004
(3)	15	6	9	-	16	6	10	1464.7545	0.001	1464.7537	0.0008
(3)	15	6	10	-	16	6	11	1464.7545	0.001	1464.7537	0.0008
(3)	16	8	8	-	17	8	9	1464.8720	0.001	1464.8776	-0.0056
(3)	16	8	9	-	17	8	10	1464.8720	0.001	1464.8776	-0.0056
(3)	14	2	13	-	15	2	14	1464.9280	0.000	1464.9282	-0.0002
(3)	14	3	11	-	15	3	12	1465.0762	0.000	1465.0761	0.0001
(3)	14	0	14	-	15	0	15	1465.0947	0.000	1465.0948	-0.0001
(3)	14	3	12	-	15	3	13	1465.1744	0.000	1465.1739	0.0005
(3)	14	1	14	-	15	1	15	1465.3219	0.000	1465.3219	0.0000
(3)	14	4	10	-	15	4	11	1465.5830	0.000	1465.5821	0.0009
(3)	14	4	11	-	15	4	12	1465.5830	0.000	1465.5852	-0.0022
(3)	15	7	8	-	16	7	9	1465.7347	0.001	1465.7328	0.0019
(3)	15	7	9	-	16	7	10	1465.7347	0.001	1465.7328	0.0019
(3)	14	5	9	-	15	5	10	1466.2209	0.001	1466.2210	-0.0001
(3)	14	5	10	-	15	5	11	1466.2209	0.001	1466.2210	-0.0001
(6)	20	8	13	-	19	7	12	1466.4430	0.001	1466.4431	-0.0001
(6)	20	8	12	-	19	7	13	1466.4430	0.001	1466.4431	-0.0001
(3)	13	1	12	-	14	1	13	1466.5262	0.000	1466.5263	-0.0001
(3)	13	2	11	-	14	2	12	1466.7198	0.000	1466.7197	0.0000
(3)	15	8	7	-	16	8	8	1466.9710	0.001	1466.9742	-0.0032
(3)	15	8	8	-	16	8	9	1466.9710	0.001	1466.9742	-0.0032
(3)	14	6	8	-	15	6	9	1466.9965	0.001	1466.9959	0.0007
(3)	14	6	9	-	15	6	10	1466.9965	0.001	1466.9959	0.0007
(3)	13	2	12	-	14	2	13	1467.2279	0.000	1467.2279	0.0000
(3)	13	0	13	-	14	0	14	1467.3650	0.000	1467.3651	-0.0001
(3)	13	3	10	-	14	3	11	1467.4198	0.000	1467.4194	0.0005
(3)	13	3	11	-	14	3	12	1467.5152	0.000	1467.5145	0.0007
(3)	13	1	13	-	14	1	14	1467.6297	0.000	1467.6298	0.0000
(3)	13	4	9	-	14	4	10	1467.8863	0.000	1467.8856	0.0007
(3)	13	4	10	-	14	4	11	1467.8863	0.000	1467.8876	-0.0013
(3)	14	7	7	-	15	7	8	1467.9318	0.001	1467.9301	0.0016
(3)	14	7	8	-	15	7	9	1467.9318	0.001	1467.9301	0.0016
(6)	21	8	14	-	20	7	13	1468.4955	0.001	1468.4947	0.0008
(6)	21	8	13	-	20	7	14	1468.4955	0.001	1468.4947	0.0008

UPPER STATE				LOWER STATE				OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC				
(3)	13	5	8	-	14	5	9	1468.5034	0.001	1468.5034	0.0000
(3)	13	5	9	-	14	5	10	1468.5034	0.001	1468.5035	-0.0001
(3)	12	1	11	-	13	1	12	1468.8265	0.000	1468.8266	-0.0001
(3)	12	2	10	-	13	2	11	1469.0860	0.000	1469.0862	-0.0001
(3)	13	6	7	-	14	6	8	1469.2502	0.001	1469.2498	0.0004
(3)	13	6	8	-	14	6	9	1469.2502	0.001	1469.2498	0.0004
(3)	12	2	11	-	13	2	12	1469.5362	0.000	1469.5362	0.0000
(3)	12	3	9	-	13	3	10	1469.5774	0.000	1469.5780	-0.0006
(3)	12	0	12	-	13	0	13	1469.6368	0.000	1469.6367	0.0001
(3)	12	3	10	-	13	3	11	1469.6598	0.000	1469.6606	-0.0008
(3)	12	1	12	-	13	1	13	1469.9390	0.000	1469.9390	0.0000
(3)	13	7	6	-	14	7	7	1470.1416	0.001	1470.1405	0.0011
(3)	13	7	7	-	14	7	8	1470.1416	0.001	1470.1405	0.0011
(3)	12	4	8	-	13	4	9	1470.1982	0.000	1470.1978	0.0004
(3)	12	4	9	-	13	4	10	1470.1982	0.000	1470.1990	-0.0008
(6)	22	8	15	-	21	7	14	1470.5304	0.001	1470.5293	0.0010
(6)	22	8	14	-	21	7	15	1470.5304	0.001	1470.5293	0.0010
(3)	12	5	7	-	13	5	8	1470.7960	0.001	1470.7960	0.0000
(3)	12	5	8	-	13	5	9	1470.7960	0.001	1470.7960	0.0000
(3)	11	1	10	-	12	1	11	1471.1430	0.000	1471.1438	-0.0002
(3)	13	8	5	-	14	8	6	1471.2170	0.001	1471.2176	-0.0006
(3)	13	8	6	-	14	8	7	1471.2170	0.001	1471.2176	-0.0006
(3)	11	2	9	-	12	2	10	1471.4655	0.000	1471.4655	-0.0001
(3)	12	6	6	-	13	6	7	1471.5157	0.001	1471.5155	0.0002
(3)	12	6	7	-	13	6	8	1471.5157	0.001	1471.5155	0.0002
(3)	11	2	10	-	12	2	11	1471.8536	0.000	1471.8534	0.0002
(3)	11	0	11	-	12	0	12	1471.9120	0.000	1471.9120	0.0000
(3)	11	3	8	-	12	3	9	1472.0105	0.000	1472.0107	-0.0002
(3)	11	3	9	-	12	3	10	1472.0427	0.000	1472.0429	-0.0002
(3)	11	1	11	-	12	1	12	1472.2501	0.000	1472.2502	-0.0001
(3)	12	7	5	-	13	7	6	1472.3653	0.001	1472.3646	0.0007
(3)	12	7	6	-	13	7	7	1472.3653	0.001	1472.3646	0.0007
(3)	11	4	7	-	12	4	8	1472.5191	0.000	1472.5188	0.0003
(3)	11	4	8	-	12	4	9	1472.5191	0.000	1472.5195	-0.0005
(3)	11	5	6	-	12	5	7	1473.0986	0.001	1473.0988	-0.0002
(3)	11	5	7	-	12	5	8	1473.0986	0.001	1473.0988	-0.0002
(3)	12	8	4	-	13	8	5	1473.3655	0.001	1473.3658	-0.0003
(3)	12	8	5	-	13	8	6	1473.3655	0.001	1473.3658	-0.0003
(3)	10	1	9	-	11	1	10	1473.4764	0.000	1473.4764	0.0000
(3)	11	6	5	-	12	6	6	1473.7931	0.001	1473.7931	-0.0001
(3)	11	6	6	-	12	6	7	1473.7931	0.001	1473.7931	-0.0001
(3)	10	2	8	-	11	2	9	1473.8556	0.000	1473.8554	0.0001
(3)	10	2	9	-	11	2	10	1474.1800	0.000	1474.1799	0.0001
(3)	10	0	10	-	11	0	11	1474.1938	0.000	1474.1938	0.0000
(3)	10	3	7	-	11	3	8	1474.3750	0.000	1474.3752	-0.0002
(3)	10	3	8	-	11	3	9	1474.3951	0.000	1474.3952	-0.0001
(3)	10	1	10	-	11	1	11	1474.5637	0.000	1474.5636	0.0001
(3)	11	7	4	-	12	7	5	1474.6035	0.001	1474.6030	0.0006
(3)	11	7	5	-	12	7	6	1474.6035	0.001	1474.6030	0.0006
(3)	10	4	6	-	11	4	7	1474.8489	0.000	1474.8487	0.0002

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(3)	10	4	7 -	11	4	8	1474.8489	0.000	1474.8491	-0.0002
(3)	10	5	5 -	11	5	6	1475.4117	0.001	1475.4119	-0.0002
(3)	10	5	6 -	11	5	7	1475.4117	0.001	1475.4119	-0.0002
(3)	11	8	3 -	12	8	4	1475.5321	0.001	1475.5324	-0.0003
(3)	11	8	4 -	12	8	5	1475.5321	0.001	1475.5324	-0.0003
(3)	9	1	8 -	10	1	9	1475.8263	0.000	1475.8265	-0.0002
(3)	10	6	4 -	11	6	5	1476.0826	0.001	1476.0829	-0.0002
(3)	10	6	5 -	11	6	6	1476.0826	0.001	1476.0829	-0.0002
(3)	9	2	7 -	10	2	8	1476.2534	0.000	1476.2534	0.0001
(3)	9	0	9 -	10	0	10	1476.4846	0.000	1476.4846	0.0000
(3)	9	2	8 -	10	2	9	1476.5160	0.000	1476.5158	0.0001
(3)	9	3	6 -	10	3	7	1476.7351	0.000	1476.7350	0.0000
(3)	9	3	7 -	10	3	8	1476.7479	0.000	1476.7478	0.0000
(3)	10	7	3 -	11	7	4	1476.8557	0.001	1476.8559	-0.0003
(3)	10	7	4 -	11	7	5	1476.8557	0.001	1476.8559	-0.0003
(3)	9	1	9 -	10	1	10	1476.8799	0.000	1476.8799	0.0001
(3)	9	4	5 -	10	4	6	1477.1874	0.000	1477.1873	0.0000
(3)	9	4	6 -	10	4	7	1477.1874	0.000	1477.1876	-0.0002
(3)	10	8	2 -	11	8	3	1477.7177	0.001	1477.7181	-0.0004
(3)	10	8	3 -	11	8	4	1477.7177	0.001	1477.7181	-0.0004
(3)	9	5	4 -	10	5	5	1477.7350	0.001	1477.7352	-0.0002
(3)	9	5	5 -	10	5	6	1477.7350	0.001	1477.7352	-0.0002
(3)	8	1	7 -	9	1	8	1478.1934	0.000	1478.1934	0.0001
(3)	9	6	3 -	10	6	4	1478.3842	0.001	1478.3847	-0.0005
(3)	9	6	4 -	10	6	5	1478.3842	0.001	1478.3847	-0.0005
(3)	8	2	6 -	9	2	7	1478.6571	0.000	1478.6571	0.0000
(3)	8	0	8 -	9	0	9	1478.7870	0.000	1478.7871	-0.0001
(3)	8	2	7 -	9	2	8	1478.8615	0.000	1478.8614	0.0001
(3)	8	3	5 -	9	3	6	1479.0989	0.000	1479.0985	0.0004
(3)	8	3	6 -	9	3	7	1479.1063	0.000	1479.1064	0.0000
(3)	9	7	3 -	10	7	4	1479.1231	0.001	1479.1238	-0.0008
(3)	9	7	2 -	10	7	3	1479.1231	0.001	1479.1238	-0.0008
(3)	8	1	8 -	9	1	9	1479.1989	0.000	1479.1992	-0.0003
(3)	8	4	4 -	9	4	5	1479.5350	0.000	1479.5349	0.0001
(3)	8	4	5 -	9	4	6	1479.5350	0.000	1479.5350	0.0000
(3)	9	8	1 -	10	8	2	1479.9228	0.001	1479.9236	-0.0008
(3)	9	8	2 -	10	8	3	1479.9228	0.001	1479.9236	-0.0008
(3)	8	5	3 -	9	5	4	1480.0687	0.001	1480.0688	-0.0001
(3)	8	5	4 -	9	5	5	1480.0687	0.001	1480.0688	-0.0001
(3)	7	1	6 -	8	1	7	1480.5771	0.000	1480.5772	-0.0001
(3)	8	6	2 -	9	6	3	1480.6980	0.001	1480.6988	-0.0009
(3)	8	6	3 -	9	6	4	1480.6980	0.001	1480.6988	-0.0009
(3)	7	2	5 -	8	2	6	1481.0648	0.000	1481.0646	0.0001
(3)	7	0	7 -	8	0	8	1481.1031	0.000	1481.1032	-0.0001
(3)	7	2	6 -	8	2	7	1481.2166	0.000	1481.2166	0.0000
(3)	8	7	1 -	9	7	2	1481.4056	0.001	1481.4069	-0.0013
(3)	8	7	2 -	9	7	3	1481.4056	0.001	1481.4069	-0.0013
(3)	7	3	4 -	8	3	5	1481.4696	0.000	1481.4678	0.0018
(3)	7	3	5 -	8	3	6	1481.4696	0.000	1481.4723	-0.0026
(3)	7	1	7 -	8	1	8	1481.5219	0.000	1481.5219	-0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(3)	7	4	3 -	8	4	4	1481.8915	0.000	1481.8913	0.0002
(3)	7	4	4 -	8	4	5	1481.8915	0.000	1481.8914	0.0002
(3)	7	5	2 -	8	5	3	1482.4126	0.001	1482.4128	-0.0002
(3)	7	5	3 -	8	5	4	1482.4126	0.001	1482.4128	-0.0002
(3)	6	1	5 -	7	1	6	1482.9778	0.000	1482.9778	0.0000
(3)	7	6	1 -	8	6	2	1483.0242	0.001	1483.0252	-0.0010
(3)	7	6	2 -	8	6	3	1483.0242	0.001	1483.0252	-0.0010
(3)	6	0	6 -	7	0	7	1483.4342	0.000	1483.4343	-0.0001
(3)	6	2	4 -	7	2	5	1483.4747	0.000	1483.4746	0.0001
(3)	6	2	5 -	7	2	6	1483.5817	0.000	1483.5816	0.0001
(3)	7	7	0 -	8	7	1	1483.7036	0.001	1483.7054	-0.0018
(3)	7	7	1 -	8	7	2	1483.7036	0.001	1483.7054	-0.0018
(3)	6	3	3 -	7	3	4	1483.8462*	0.000	1483.8436	0.0027
(3)	6	1	6 -	7	1	7	1483.8462*	0.000	1483.8483	-0.0021
(3)	6	3	4 -	7	3	5	1483.8462*	0.000	1483.8459	0.0003
(3)	6	4	2 -	7	4	3	1484.2568	0.000	1484.2566	0.0002
(3)	6	4	3 -	7	4	4	1484.2568	0.000	1484.2566	0.0002
(3)	6	5	1 -	7	5	2	1484.7668	0.001	1484.7671	-0.0003
(3)	6	5	2 -	7	5	3	1484.7668	0.001	1484.7671	-0.0003
(3)	6	6	0 -	7	6	1	1485.3628	0.001	1485.3640	-0.0012
(3)	6	6	1 -	7	6	2	1485.3628	0.001	1485.3640	-0.0012
(3)	5	1	4 -	6	1	5	1485.3951	0.000	1485.3951	0.0000
(3)	5	0	5 -	6	0	6	1485.7811	0.000	1485.7814	-0.0003
(3)	5	2	3 -	6	2	4	1485.8862	0.000	1485.8861	0.0001
(3)	5	2	4 -	6	2	5	1485.9566	0.000	1485.9564	0.0002
(3)	5	1	5 -	6	1	6	1486.1784	0.000	1486.1785	0.0000
(3)	5	3	2 -	6	3	3	1486.2272	0.000	1486.2264	0.0009
(3)	5	3	3 -	6	3	4	1486.2272	0.000	1486.2274	-0.0002
(3)	5	4	1 -	6	4	2	1486.6312	0.000	1486.6308	0.0004
(3)	5	4	2 -	6	4	3	1486.6312	0.000	1486.6308	0.0004
(3)	5	5	0 -	6	5	1	1487.1317	0.001	1487.1319	-0.0002
(3)	5	5	1 -	6	5	2	1487.1317	0.001	1487.1319	-0.0002
(3)	4	1	3 -	5	1	4	1487.8285	0.000	1487.8288	-0.0003
(3)	4	0	4 -	5	0	5	1488.1445	0.000	1488.1446	-0.0001
(3)	4	2	2 -	5	2	3	1488.2990	0.000	1488.2988	0.0001
(3)	4	2	3 -	5	2	4	1488.3410	0.000	1488.3409	0.0001
(3)	4	1	4 -	5	1	5	1488.5124	0.000	1488.5124	0.0000
(3)	4	3	1 -	5	3	2	1488.6171	0.000	1488.6164	0.0007
(3)	4	3	2 -	5	3	3	1488.6171	0.000	1488.6168	0.0003
(3)	4	4	0 -	5	4	1	1489.0144	0.000	1489.0140	0.0004
(3)	4	4	1 -	5	4	2	1489.0144	0.000	1489.0140	0.0004
(3)	11	1	11 -	11	1	10	1489.7231	0.000	1489.7229	0.0002
(3)	3	1	2 -	4	1	3	1490.2787	0.000	1490.2787	0.0000
(3)	3	0	3 -	4	0	4	1490.5236	0.000	1490.5237	-0.0001
(3)	3	2	1 -	4	2	2	1490.7133	0.000	1490.7130	0.0003
(3)	3	2	2 -	4	2	3	1490.7352	0.000	1490.7350	0.0002
(3)	3	1	3 -	4	1	4	1490.8501	0.000	1490.8501	0.0000
(3)	3	3	0 -	4	3	1	1491.0144	0.000	1491.0138	0.0006
(3)	3	3	1 -	4	3	2	1491.0144	0.000	1491.0140	0.0004
(3)	10	1	10 -	10	1	9	1491.4627	0.000	1491.4629	-0.0001

UPPER STATE			LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(3)	2	1	1 -	3	1	2	1492.7442	0.000	1492.7444	-0.0001
(3)	2	0	2 -	3	0	3	1492.9175	0.000	1492.9177	-0.0002
(3)	9	1	9 -	9	1	8	1493.0509	0.000	1493.0511	-0.0002
(3)	2	2	0 -	3	2	1	1493.1296	0.000	1493.1293	0.0003
(3)	2	2	1 -	3	2	2	1493.1387	0.000	1493.1384	0.0002
(3)	2	1	2 -	3	1	3	1493.1910	0.000	1493.1912	-0.0002
(3)	8	1	8 -	8	1	7	1494.4843	0.000	1494.4845	-0.0002
(3)	1	1	0 -	2	1	1	1495.2254	0.000	1495.2255	-0.0001
(3)	1	0	1 -	2	0	2	1495.3252	0.000	1495.3254	-0.0003
(3)	1	1	1 -	2	1	2	1495.5355	0.000	1495.5355	0.0000
(3)	7	1	7 -	7	1	6	1495.7605	0.000	1495.7608	-0.0003
(3)	6	1	6 -	6	1	5	1496.8786	0.000	1496.8785	0.0001
(3)	0	0	0 -	1	0	1	1497.7450	0.000	1497.7451	-0.0001
(3)	5	1	5 -	5	1	4	1497.8368	0.000	1497.8369	-0.0001
(3)	4	1	4 -	4	1	3	1498.6355	0.000	1498.6356	-0.0001
(3)	3	1	3 -	3	1	2	1499.2742	0.000	1499.2743	-0.0001
(3)	2	1	2 -	2	1	1	1499.7531	0.000	1499.7532	-0.0001
(3)	1	1	1 -	1	1	0	1500.0722	0.000	1500.0723	-0.0002
(3)	1	1	0 -	1	1	1	1500.4065	0.000	1500.4067	-0.0002
(3)	3	3	1 -	3	3	0	1500.7339	0.000	1500.7334	0.0005
(3)	3	3	0 -	3	3	1	1500.7339	0.000	1500.7334	0.0005
(3)	2	1	1 -	2	1	2	1500.7557	0.000	1500.7561	-0.0005
(3)	4	3	2 -	4	3	1	1500.7679	0.000	1500.7676	0.0004
(3)	4	3	1 -	4	3	2	1500.7679	0.000	1500.7679	0.0000
(3)	5	3	3 -	5	3	2	1500.8112	0.000	1500.8102	0.0010
(3)	5	3	2 -	5	3	3	1500.8112	0.000	1500.8116	-0.0004
(3)	6	3	4 -	6	3	3	1500.8632	0.000	1500.8611	0.0021
(3)	6	3	3 -	6	3	4	1500.8632	0.000	1500.8651	-0.0019
(3)	7	3	5 -	7	3	4	1500.9196	0.000	1500.9193	0.0003
(3)	7	3	4 -	7	3	5	1500.9297	0.000	1500.9294	0.0003
(3)	8	3	6 -	8	3	5	1500.9837	0.000	1500.9836	0.0001
(3)	8	3	5 -	8	3	6	1501.0060	0.000	1501.0059	0.0002
(3)	9	3	7 -	9	3	6	1501.0519	0.000	1501.0517	0.0002
(3)	9	3	6 -	9	3	7	1501.0961	0.000	1501.0961	0.0000
(3)	10	3	8 -	10	3	7	1501.1194	0.000	1501.1194	0.0000
(3)	4	4	1 -	4	4	0	1501.1594	0.000	1501.1591	0.0003
(3)	4	4	0 -	4	4	1	1501.1594	0.000	1501.1591	0.0003
(3)	11	3	9 -	11	3	8	1501.1767	0.000	1501.1772	-0.0006
(3)	12	3	10 -	12	3	9	1501.1892	0.000	1501.1900	-0.0008
(3)	10	3	7 -	10	3	8	1501.2062*	0.000	1501.2013	0.0049
(3)	5	4	2 -	5	4	1	1501.2062*	0.000	1501.2062	0.0000
(3)	5	4	1 -	5	4	2	1501.2062*	0.000	1501.2062	0.0000
(3)	6	4	3 -	6	4	2	1501.2630	0.000	1501.2627	0.0003
(3)	6	4	2 -	6	4	3	1501.2630	0.000	1501.2627	0.0002
(3)	3	1	2 -	3	1	3	1901.2799	0.000	1501.2800	-0.0001
(3)	11	3	8 -	11	3	9	1501.3168	0.000	1501.3174	-0.0006
(3)	7	4	4 -	7	4	3	1501.3292	0.000	1501.3289	0.0003
(3)	7	4	3 -	7	4	4	1501.3292	0.000	1501.3289	0.0003
(3)	12	3	9 -	12	3	10	1501.3859	0.000	1501.3863	-0.0004
(3)	8	4	5 -	8	4	4	1501.4049	0.000	1501.4047	0.0002

UPPER STATE			LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(3)	8	4	4 -	8	4	5	1501.4049	0.000	1501.4049	0.0000
(3)	9	4	6 -	9	4	5	1501.4906	0.000	1501.4903	0.0003
(3)	9	4	5 -	9	4	6	1501.4906	0.000	1501.4908	-0.0002
(3)	10	4	7 -	10	4	6	1501.5861	0.000	1501.5856	0.0006
(3)	10	4	6 -	10	4	7	1501.5861	0.000	1501.5867	-0.0006
(3)	11	4	8 -	11	4	7	1501.6929	0.000	1501.6906	0.0023
(3)	11	4	7 -	11	4	8	1501.6929	0.000	1501.6930	-0.0001
(3)	5	5	1 -	5	5	0	1501.6999	0.001	1501.7003	-0.0004
(3)	5	5	0 -	5	5	1	1501.6999	0.001	1501.7003	-0.0004
(3)	6	5	2 -	6	5	1	1501.7642	0.001	1501.7643	-0.0001
(3)	6	5	1 -	6	5	2	1501.7642	0.001	1501.7643	-0.0001
(3)	12	4	9 -	12	4	8	1501.8066	0.000	1501.8052	0.0014
(3)	12	4	8 -	12	4	9	1501.8066	0.000	1501.8100	-0.0035
(3)	7	5	3 -	7	5	2	1501.8389	0.001	1501.8390	-0.0001
(3)	7	5	2 -	7	5	3	1501.8389	0.001	1501.8390	-0.0001
(3)	8	5	4 -	8	5	3	1501.9244	0.001	1501.9243	0.0001
(3)	8	5	3 -	8	5	4	1501.9244	0.001	1501.9243	0.0001
(3)	13	4	10 -	13	4	9	1501.9244*	0.000	1501.9291	-0.0047
(3)	13	4	9 -	13	4	10	1501.9379	0.000	1501.9382	-0.0004
(3)	4	1	3 -	4	1	4	1501.9786	0.000	1501.9778	0.0008
(3)	9	5	5 -	9	5	4	1502.0202	0.001	1502.0204	-0.0002
(3)	9	5	4 -	9	5	5	1502.0202	0.001	1502.0204	-0.0002
(3)	14	4	11 -	14	4	10	1502.0616	0.000	1502.0619	-0.0004
(3)	14	4	10 -	14	4	11	1502.0779	0.000	1502.0783	-0.0004
(3)	10	5	6 -	10	5	5	1502.1271	0.001	1502.1273	-0.0002
(3)	10	5	5 -	10	5	6	1502.1271	0.001	1502.1273	-0.0002
(3)	15	4	12 -	15	4	11	1502.2054*	0.000	1502.2030	0.0023
(3)	15	4	11 -	15	4	12	1502.2309	0.000	1502.2313	-0.0004
(3)	11	5	7 -	11	5	6	1502.2448	0.001	1502.2448	0.0000
(3)	11	5	6 -	11	5	7	1502.2448	0.001	1502.2448	-0.0001
(3)	6	6	1 -	6	6	0	1502.3516	0.001	1502.3526	-0.0010
(3)	6	6	0 -	6	6	1	1502.3516	0.001	1502.3526	-0.0010
(3)	12	5	8 -	12	5	7	1502.3731	0.001	1502.3731	0.0000
(3)	12	5	7 -	12	5	8	1502.3731	0.001	1502.3732	-0.0001
(3)	7	6	2 -	7	6	1	1502.4402	0.001	1502.4410	-0.0008
(3)	7	6	1 -	7	6	2	1502.4402	0.001	1502.4410	-0.0008
(3)	13	5	9 -	13	5	8	1502.5121	0.001	1502.5121	0.0000
(3)	13	5	8 -	13	5	9	1502.5121	0.001	1502.5123	-0.0001
(3)	8	6	3 -	8	6	2	1502.5413	0.001	1502.5418	-0.0006
(3)	8	6	2 -	8	6	3	1502.5413	0.001	1502.5418	-0.0006
(3)	1	0	1 -	0	0	0	1502.6117	0.000	1502.6118	-0.0001
(3)	9	6	4 -	9	6	3	1502.6549	0.001	1502.6551	-0.0002
(3)	9	6	3 -	9	6	4	1502.6549	0.001	1502.6551	-0.0002
(3)	14	5	10 -	14	5	9	1502.6619	0.001	1502.6619	0.0000
(3)	14	5	9 -	14	5	10	1502.6619	0.001	1502.6621	-0.0003
(3)	10	6	5 -	10	6	4	1502.7805	0.001	1502.7807	-0.0002
(3)	10	6	4 -	10	6	5	1502.7805	0.001	1502.7807	-0.0002
(3)	15	5	11 -	15	5	10	1502.8225	0.001	1502.8223	0.0001
(3)	15	5	10 -	15	5	11	1502.8225	0.001	1502.8228	-0.0004
(3)	5	1	4 -	5	1	5	1502.8488	0.000	1502.8489	-0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC	J	KA	KC				
(3)	11	6	6	11	6	5	1502.9186	0.001	1502.9186	0.0001
(3)	11	6	5	11	6	6	1502.9186	0.001	1502.9186	0.0001
(3)	16	5	12	16	5	11	1502.9936	0.001	1502.9934	0.0002
(3)	16	5	11	16	5	12	1502.9936	0.001	1502.9944	-0.0007
(3)	12	6	7	12	6	6	1503.0689	0.001	1503.0686	0.0003
(3)	12	6	6	12	6	7	1503.0689	0.001	1503.0686	0.0003
(3)	7	7	1	7	7	0	1503.1085	0.001	1503.1104	-0.0019
(3)	7	7	0	7	7	1	1503.1085	0.001	1503.1104	-0.0019
(3)	17	5	13	17	5	12	1503.1756	0.001	1503.1751	0.0005
(3)	17	5	12	17	5	13	1503.1756	0.001	1503.1768	-0.0012
(3)	8	7	2	8	7	1	1503.2359	0.001	1503.2374	-0.0015
(3)	8	7	1	8	7	2	1503.2359	0.001	1503.2374	-0.0015
(3)	13	6	8	13	6	7	1503.2359*	0.000	1503.2308	0.0052
(3)	13	6	7	13	6	8	1503.2359*	0.000	1503.2308	0.0052
(3)	18	5	14	18	5	13	1503.3680	0.001	1503.3671	0.0009
(3)	18	5	13	18	5	14	1503.3680	0.001	1503.3701	-0.0021
(3)	9	7	3	9	7	2	1503.3789	0.001	1503.3797	-0.0008
(3)	9	7	2	9	7	3	1503.3789	0.001	1503.3797	-0.0008
(3)	14	6	9	14	6	8	1503.4058	0.001	1503.4049	0.0009
(3)	14	6	8	14	6	9	1503.4058	0.001	1503.4049	0.0009
(3)	10	7	4	10	7	3	1503.5369	0.001	1503.5371	-0.0002
(3)	10	7	3	10	7	4	1503.5369	0.001	1503.5371	-0.0002
(3)	19	5	15	19	5	14	1503.5708	0.001	1503.5695	0.0013
(3)	19	5	14	19	5	15	1503.5708	0.001	1503.5746	-0.0038
(3)	15	6	10	15	6	9	1503.5919	0.001	1503.5909	0.0010
(3)	15	6	9	15	6	10	1503.5919	0.001	1503.5909	0.0010
(3)	11	7	5	11	7	4	1503.7096	0.001	1503.7094	0.0002
(3)	11	7	4	11	7	5	1503.7096	0.001	1503.7094	0.0002
(3)	16	6	11	16	6	10	1503.7899*	0.000	1503.7886	0.0013
(3)	16	6	10	16	6	11	1503.7899*	0.000	1503.7886	0.0013
(3)	20	5	15	20	5	16	1503.7899*	0.000	1503.7903	-0.0004
(3)	12	7	6	12	7	5	1503.8967	0.001	1503.8962	0.0005
(3)	12	7	5	12	7	6	1503.8967	0.001	1503.8962	0.0005
(3)	6	1	5	6	1	6	1503.8967*	0.000	1503.8922	0.0045
(3)	8	8	1	8	8	0	1503.9655	0.001	1503.9665	-0.0010
(3)	8	8	0	8	8	1	1503.9655	0.001	1503.9665	-0.0010
(3)	17	6	12	17	6	11	1504.0000	0.001	1503.9979	0.0021
(3)	17	6	11	17	6	12	1504.0000	0.001	1503.9980	0.0021
(3)	21	5	17	21	5	16	1504.0000	0.001	1504.0038	-0.0037
(3)	13	7	7	13	7	6	1504.0983	0.001	1504.0971	0.0012
(3)	13	7	6	13	7	7	1504.0983	0.001	1504.0971	0.0012
(3)	9	8	2	9	8	1	1504.1637	0.001	1504.1643	-0.0006
(3)	9	8	1	9	8	2	1504.1637	0.001	1504.1643	-0.0006
(3)	18	6	13	18	6	12	1504.2194	0.001	1504.2187	0.0007
(3)	18	6	12	18	6	13	1504.2194	0.001	1504.2188	0.0007
(3)	14	7	8	14	7	7	1504.3135	0.001	1504.3117	0.0018
(3)	14	7	7	14	7	8	1504.3135	0.001	1504.3117	0.0018
(3)	10	8	3	10	8	2	1504.3820	0.001	1504.3822	-0.0002
(3)	10	8	2	10	8	3	1504.3820	0.001	1504.3822	-0.0002
(3)	19	6	14	19	6	13	1504.4522	0.001	1504.4508	0.0014
(3)	19	6	13	19	6	14	1504.4522	0.001	1504.4509	0.0013
(3)	15	7	9	15	7	8	1504.5413	0.001	1504.5392	0.0020
(3)	15	7	8	15	7	9	1504.5413	0.001	1504.5392	0.0020
(3)	11	8	4	11	8	3	1504.6194	0.001	1504.6196	-0.0001
(3)	11	8	3	11	8	4	1504.6194	0.001	1504.6196	-0.0001
(3)	16	7	10	16	7	9	1504.7807	0.001	1504.7786	0.0021
(3)	16	7	9	16	7	10	1504.7807	0.001	1504.7786	0.0021
(3)	12	8	5	12	8	4	1504.8759	0.001	1504.8759	0.0000
(3)	12	8	4	12	8	5	1504.8759	0.001	1504.8759	0.0000
(3)	9	9	1	9	9	0	1504.9160	0.001	1504.9120	0.0041
(3)	9	9	0	9	9	1	1504.9160	0.001	1504.9120	0.0041
(3)	2	1	2	1	1	1	1504.9344	0.000	1504.9344	0.0000
(3)	17	7	11	17	7	10	1505.0298	0.001	1505.0278	0.0020
(3)	17	7	10	17	7	11	1505.0298	0.001	1505.0278	0.0020
(3)	2	0	2	1	0	1	1505.0535	0.000	1505.0536	-0.0001
(3)	7	1	6	7	1	7	1505.1063	0.000	1505.1062	0.0001
(3)	13	8	6	13	8	5	1505.1499	0.001	1505.1504	-0.0005
(3)	13	8	5	13	8	6	1505.1499	0.001	1505.1504	-0.0005
(3)	10	9	2	10	9	1	1505.2825	0.001	1505.2792	0.0033
(3)	10	9	1	10	9	2	1505.2825	0.001	1505.2792	0.0033
(3)	18	7	12	18	7	11	1505.2825*	0.000	1505.2824	0.0001
(3)	18	7	11	18	7	12	1505.2825*	0.000	1505.2824	0.0001
(3)	2	1	1	1	1	0	1505.2929	0.000	1505.2929	0.0000
(3)	14	8	7	14	8	6	1505.4411	0.001	1505.4425	-0.0014
(3)	14	8	6	14	8	7	1505.4411	0.001	1505.4425	-0.0014
(3)	19	7	13	19	7	12	1505.5283	0.001	1505.5293	-0.0010
(3)	19	7	12	19	7	13	1505.5283	0.001	1505.5293	-0.0010
(3)	11	9	3	11	9	2	1505.6750	0.001	1505.6732	0.0018
(3)	11	9	2	11	9	3	1505.6750	0.001	1505.6732	0.0018
(3)	15	8	8	15	8	7	1505.7488	0.001	1505.7515	-0.0028
(3)	15	8	7	15	8	8	1505.7488	0.001	1505.7515	-0.0028
(3)	16	8	9	16	8	8	1506.0712	0.001	1506.0767	-0.0055
(3)	16	8	8	16	8	9	1506.0712	0.001	1506.0767	-0.0055
(3)	12	9	4	12	9	3	1506.0929	0.001	1506.0920	0.0009
(3)	12	9	3	12	9	4	1506.0929	0.001	1506.0920	0.0009
(3)	8	1	7	8	1	8	1506.4889	0.000	1506.4887	0.0002
(3)	13	9	4	13	9	5	1506.5336	0.001	1506.5335	0.0001
(3)	13	9	5	13	9	4	1506.5336	0.001	1506.5335	0.0001
(3)	14	9	6	14	9	5	1506.9955	0.001	1506.9958	-0.0003
(3)	14	9	5	14	9	6	1506.9955	0.001	1506.9958	-0.0003
(3)	3	1	3	2	1	2	1507.2860	0.000	1507.2861	-0.0001
(3)	15	9	7	15	9	6	1507.4765	0.001	1507.4770	-0.0006
(3)	15	9	6	15	9	7	1507.4765	0.001	1507.4770	-0.0006
(3)	3	0	3	2	0	2	1507.4967	0.000	1507.4970	-0.0003
(3)	3	2	2	2	2	1	1507.7374	0.000	1507.7372	0.0002
(3)	3	2	1	2	2	0	1507.7486	0.000	1507.7484	0.0002
(3)	3	1	2	2	1	1	1507.8419	0.000	1507.8420	-0.0001
(3)	16	9	8	16	9	7	1507.9741	0.001	1507.9754	-0.0013
(3)	16	9	7	16	9	8	1507.9741	0.001	1507.9754	-0.0013
(3)	9	1	8	9	1	9	1508.0368	0.000	1508.0368	0.0000

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(3)	17	9	9	-	17	9	8	1508.4889	0.001	1508.4892	-0.0003
(3)	17	9	8	-	17	9	9	1508.4889	0.001	1508.4892	-0.0003
(3)	18	9	10	-	18	9	9	1509.0171	0.001	1509.0169	0.0002
(3)	18	9	9	-	18	9	10	1509.0171	0.001	1509.0169	0.0002
(3)	19	9	11	-	19	9	10	1509.5581	0.001	1509.5568	0.0012
(3)	19	9	10	-	19	9	11	1509.5581	0.001	1509.5568	0.0012
(3)	4	1	4	-	3	1	3	1509.6368	0.000	1509.6369	-0.0001
(3)	10	1	9	-	10	1	10	1509.7469	0.000	1509.7466	0.0003
(3)	4	0	4	-	3	0	3	1509.9383	0.000	1509.9384	-0.0001
(3)	4	2	3	-	3	2	2	1510.1958	0.000	1510.1955	0.0003
(3)	4	2	2	-	3	2	1	1510.2246	0.000	1510.2244	0.0002
(3)	4	1	3	-	3	1	2	1510.4020	0.000	1510.4021	0.0000
(3)	4	3	2	-	3	3	1	1510.4875	0.000	1510.4871	0.0004
(3)	4	3	1	-	3	3	0	1510.4875	0.000	1510.4873	0.0002
(3)	11	1	10	-	11	1	11	1511.6135	0.000	1511.6133	0.0002
(3)	5	1	5	-	4	1	4	1511.9860	0.000	1511.9860	0.0000
(3)	5	0	5	-	4	0	4	1512.3740	0.000	1512.3741	-0.0001
(3)	5	2	4	-	4	2	3	1512.6594	0.000	1512.6593	0.0001
(3)	5	2	3	-	4	2	2	1512.7189	0.000	1512.7187	0.0002
(3)	5	3	3	-	4	3	2	1512.9624	0.000	1512.9618	0.0006
(3)	5	3	2	-	4	3	1	1512.9624	0.000	1512.9623	0.0000
(3)	5	1	4	-	4	1	3	1512.9719	0.000	1512.9721	-0.0001
(3)	5	4	2	-	4	4	1	1513.3516	0.000	1513.3513	0.0003
(3)	5	4	1	-	4	4	0	1513.3516	0.000	1513.3513	0.0003
(3)	6	1	6	-	5	1	5	1514.3323	0.000	1514.3324	-0.0001
(3)	6	0	6	-	5	0	5	1514.8001	0.000	1514.8002	-0.0001
(3)	6	2	5	-	5	2	4	1515.1280	0.000	1515.1279	0.0001
(3)	6	2	4	-	5	2	3	1515.2345	0.000	1515.2344	0.0001
(3)	6	3	4	-	5	3	3	1515.4475	0.000	1515.4463	0.0012
(3)	6	3	3	-	5	3	2	1515.4475	0.000	1515.4479	-0.0004
(3)	6	1	5	-	5	1	4	1515.5506	0.000	1515.5507	0.0000
(3)	6	4	3	-	5	4	2	1515.8384	0.000	1515.8380	0.0003
(3)	6	4	2	-	5	4	1	1515.8384	0.000	1515.8380	0.0003
(3)	6	5	2	-	5	5	1	1516.3325	0.001	1516.3327	-0.0002
(3)	6	5	1	-	5	5	0	1516.3325	0.001	1516.3327	-0.0002
(3)	7	1	7	-	6	1	6	1516.6751	0.000	1516.6752	-0.0001
(3)	7	0	7	-	6	0	6	1517.2127	0.000	1517.2129	-0.0002
(3)	7	2	6	-	6	2	5	1517.6004	0.000	1517.6004	0.0000
(3)	7	2	5	-	6	2	4	1517.7745	0.000	1517.7744	0.0002
(3)	7	3	5	-	6	3	4	1517.9426	0.000	1517.9408	0.0018
(3)	7	3	4	-	6	3	3	1517.9426	0.000	1517.9446	-0.0019
(3)	7	1	6	-	6	1	5	1518.1362	0.000	1518.1364	-0.0002
(3)	7	4	4	-	6	4	3	1518.3353	0.000	1518.3350	0.0003
(3)	7	4	3	-	6	4	2	1518.3353	0.000	1518.3350	0.0003
(3)	7	5	3	-	6	5	2	1518.8360	0.001	1518.8361	-0.0001
(3)	7	5	2	-	6	5	1	1518.8360	0.001	1518.8361	-0.0001
(3)	8	1	8	-	7	1	7	1519.0135	0.000	1519.0135	0.0001
(3)	7	6	2	-	6	6	1	1519.4289	0.001	1519.4296	-0.0007
(3)	7	6	1	-	6	6	0	1519.4289	0.001	1519.4296	-0.0007
(3)	8	0	8	-	7	0	7	1519.6083	0.000	1519.6083	0.0000

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(3)	8	2	7	-	7	2	6	1520.0761	0.000	1520.0759	0.0002
(3)	8	2	6	-	7	2	5	1520.3415	0.000	1520.3414	0.0001
(3)	8	3	6	-	7	3	5	1520.4458	0.000	1520.4453	0.0005
(3)	8	3	5	-	7	3	4	1520.4530	0.000	1520.4529	0.0001
(3)	8	1	7	-	7	1	6	1520.7273	0.000	1520.7275	-0.0002
(3)	8	4	5	-	7	4	4	1520.8426	0.000	1520.8423	0.0002
(3)	8	4	4	-	7	4	3	1520.8426	0.000	1520.8424	0.0002
(3)	9	1	9	-	8	1	8	1521.3474*	0.000	1521.3464	0.0010
(3)	8	5	4	-	7	5	3	1521.3474*	0.000	1521.3505	-0.0031
(3)	8	5	3	-	7	5	2	1521.3474*	0.000	1521.3505	-0.0031
(3)	8	6	3	-	7	6	2	1521.9571	0.001	1521.9576	-0.0005
(3)	8	6	2	-	7	6	1	1521.9571	0.001	1521.9576	-0.0005
(3)	9	0	9	-	8	0	8	1521.9833	0.000	1521.9834	-0.0001
(3)	9	2	8	-	8	2	7	1522.5538	0.000	1522.5536	0.0002
(3)	8	7	2	-	7	7	1	1522.6413	0.001	1522.6425	-0.0012
(3)	8	7	1	-	7	7	0	1522.6413	0.001	1522.6425	-0.0012
(3)	9	2	7	-	8	2	6	1522.9376	0.000	1522.9374	0.0002
(3)	9	3	7	-	8	3	6	1522.9592	0.000	1522.9590	0.0002
(3)	9	3	6	-	8	3	5	1522.9735	0.000	1522.9734	0.0002
(3)	9	1	8	-	8	1	7	1523.3220	0.000	1523.3220	0.0000
(3)	9	4	6	-	8	4	5	1523.3605	0.000	1523.3603	0.0002
(3)	9	4	5	-	8	4	4	1523.3605	0.000	1523.3605	0.0000
(3)	10	1	10	-	9	1	9	1523.6732	0.000	1523.6732	0.0000
(3)	9	5	5	-	8	5	4	1523.8758	0.001	1523.8760	-0.0001
(3)	9	5	4	-	8	5	3	1523.8758	0.001	1523.8760	-0.0001
(3)	10	0	10	-	9	0	9	1524.3360	0.000	1524.3359	0.0001
(3)	9	6	4	-	8	6	3	1524.4978	0.001	1524.4981	-0.0003
(3)	9	6	3	-	8	6	2	1524.4978	0.001	1524.4981	-0.0003
(3)	10	2	9	-	9	2	8	1525.0326	0.000	1525.0325	0.0001
(3)	9	7	3	-	8	7	2	1525.2095	0.001	1525.2102	-0.0007
(3)	9	7	2	-	8	7	1	1525.2095	0.001	1525.2102	-0.0007
(3)	10	3	8	-	9	3	7	1525.4803	0.000	1525.4804	-0.0001
(3)	10	3	7	-	9	3	6	1525.5007*	0.000	1525.5052	-0.0045
(3)	10	2	8	-	9	2	7	1525.5637	0.000	1525.5637	0.0001
(3)	10	4	7	-	9	4	6	1525.8892	0.000	1525.8890	0.0003
(3)	10	4	6	-	9	4	5	1525.8892	0.000	1525.8894	-0.0002
(3)	10	1	9	-	9	1	8	1525.9177	0.000	1525.9179	-0.0001
(3)	11	1	11	-	10	1	10	1525.9931	0.000	1525.9931	0.0000
(3)	10	5	6	-	9	5	5	1526.4124	0.001	1526.4125	-0.0001
(3)	10	5	5	-	9	5	4	1526.4124	0.001	1526.4125	-0.0001
(3)	11	0	11	-	10	0	10	1526.6645	0.000	1526.6644	0.0000
(3)	10	6	5	-	9	6	4	1527.0509	0.001	1527.0511	-0.0002
(3)	10	6	4	-	9	6	3	1527.0509	0.001	1527.0511	-0.0002
(3)	11	2	10	-	10	2	9	1527.5115	0.000	1527.5115	0.0000
(3)	10	7	4	-	9	7	3	1527.7928	0.001	1527.7930	-0.0002
(3)	10	7	3	-	9	7	2	1527.7928	0.001	1527.7930	-0.0002
(3)	11	3	9	-	10	3	8	1528.0031	0.000	1528.0033	-0.0001
(3)	11	3	8	-	10	3	7	1528.0412	0.000	1528.0415	-0.0003
(3)	11	2	9	-	10	2	8	1528.2203	0.000	1528.2201	0.0001
(3)	12	1	12	-	11	1	11	1528.3057	0.000	1528.3055	0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(3)	11	4	8	-	10	4	7	1528.4290	0.000	1528.4286	0.0004
(3)	11	4	7	-	10	4	6	1528.4290	0.000	1528.4295	-0.0005
(3)	11	1	10	-	10	1	9	1528.5124	0.000	1528.5125	-0.0001
(3)	11	5	7	-	10	5	6	1528.9602	0.001	1528.9602	0.0000
(3)	11	5	6	-	10	5	5	1528.9602	0.001	1528.9602	0.0000
(3)	12	0	12	-	11	0	11	1528.9691	0.000	1528.9690	0.0001
(3)	11	6	6	-	10	6	5	1529.6165	0.001	1529.6164	0.0001
(3)	11	6	5	-	10	6	4	1529.6165	0.001	1529.6164	0.0001
(3)	12	2	11	-	11	2	10	1529.9896	0.000	1529.9897	0.0000
(3)	11	7	5	-	10	7	4	1530.3910	0.001	1530.3906	0.0005
(3)	11	7	4	-	10	7	3	1530.3910	0.001	1530.3906	0.0005
(3)	12	3	10	-	11	3	9	1530.4960	0.000	1530.4967	-0.0007
(3)	12	3	9	-	11	3	8	1530.5198	0.000	1530.5206	-0.0008
(3)	13	1	13	-	12	1	12	1530.6102	0.000	1530.6100	0.0002
(3)	12	2	10	-	11	2	9	1530.9055	0.000	1530.9055	0.0000
(3)	12	4	9	-	11	4	8	1530.9800	0.000	1530.9794	0.0006
(3)	12	4	8	-	11	4	7	1530.9800	0.000	1530.9811	-0.0010
(3)	12	1	11	-	11	1	10	1531.1031	0.000	1531.1032	0.0000
(3)	13	0	13	-	12	0	12	1531.2510	0.000	1531.2509	0.0001
(3)	12	5	8	-	11	5	7	1531.5189	0.001	1531.5191	-0.0002
(3)	12	5	7	-	11	5	6	1531.5189	0.001	1531.5191	-0.0003
(3)	12	6	7	-	11	6	6	1532.1944	0.001	1532.1941	0.0003
(3)	12	6	6	-	11	6	5	1532.1944	0.001	1532.1941	0.0003
(3)	13	2	12	-	12	2	11	1532.4659	0.000	1532.4659	0.0000
(3)	14	1	14	-	13	1	13	1532.9064	0.000	1532.9062	0.0003
(3)	12	7	6	-	11	7	5	1533.0036	0.001	1533.0026	0.0010
(3)	12	7	5	-	11	7	4	1533.0036	0.001	1533.0026	0.0010
(3)	13	3	11	-	12	3	10	1533.2271	0.000	1533.2262	0.0009
(3)	13	3	10	-	12	3	9	1533.2870	0.000	1533.2867	0.0003
(3)	14	0	14	-	13	0	13	1533.5121	0.000	1533.5122	-0.0001
(3)	13	4	10	-	12	4	9	1533.5424	0.000	1533.5414	0.0011
(3)	13	4	9	-	12	4	8	1533.5424	0.000	1533.5444	-0.0020
(3)	13	2	11	-	12	2	10	1533.6171	0.000	1533.6171	0.0000
(3)	13	1	12	-	12	1	11	1533.6867	0.000	1533.6869	-0.0002
(3)	13	5	9	-	12	5	8	1534.0893	0.001	1534.0893	0.0000
(3)	13	5	8	-	12	5	7	1534.0893	0.001	1534.0893	0.0000
(3)	13	6	8	-	12	6	7	1534.7844	0.001	1534.7839	0.0005
(3)	13	6	7	-	12	6	6	1534.7844	0.001	1534.7839	0.0005
(3)	14	2	13	-	13	2	12	1534.9391	0.000	1534.9392	-0.0001
(3)	15	1	15	-	14	1	14	1535.1937	0.000	1535.1937	0.0000
(3)	13	7	7	-	12	7	6	1535.6302	0.001	1535.6287	0.0015
(3)	13	7	6	-	12	7	5	1535.6302	0.001	1535.6287	0.0015
(3)	15	0	15	-	14	0	14	1535.7596*	0.000	1535.7558	0.0038
(3)	14	3	12	-	13	3	11	1535.7596*	0.000	1535.7601	-0.0006
(3)	14	3	11	-	13	3	10	1535.8833	0.000	1535.8831	0.0003
(3)	14	4	11	-	13	4	10	1536.1154	0.000	1536.1146	0.0008
(3)	14	4	10	-	13	4	9	1536.1154	0.000	1536.1199	-0.0044
(3)	14	1	13	-	13	1	12	1536.2601	0.000	1536.2602	-0.0002
(3)	14	2	12	-	13	2	11	1536.3514	0.000	1536.3513	0.0001
(3)	14	5	10	-	13	5	9	1536.6707	0.001	1536.6707	0.0000

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(3)	14	5	9	-	13	5	8	1536.6707	0.001	1536.6708	-0.0001
(3)	14	6	9	-	13	6	8	1537.3867	0.001	1537.3859	0.0008
(3)	14	6	8	-	13	6	7	1537.3867	0.001	1537.3859	0.0008
(3)	15	2	14	-	14	2	13	1537.4086	0.000	1537.4086	0.0000
(3)	16	1	16	-	15	1	15	1537.4726	0.000	1537.4725	0.0001
(3)	16	0	16	-	15	0	15	1537.9845	0.000	1537.9848	-0.0002
(3)	14	7	8	-	13	7	7	1538.2702	0.001	1538.2683	0.0018
(3)	14	7	7	-	13	7	6	1538.2702	0.001	1538.2683	0.0018
(3)	15	3	13	-	14	3	12	1538.3268	0.000	1538.3267	0.0002
(3)	15	3	12	-	14	3	11	1538.5150	0.000	1538.5152	-0.0002
(3)	15	4	12	-	14	4	11	1538.6987	0.001	1538.6993	-0.0005
(3)	15	4	11	-	14	4	10	1538.7074	0.000	1538.7080	-0.0006
(3)	15	1	14	-	14	1	13	1538.8197	0.000	1538.8198	-0.0001
(3)	15	2	13	-	14	2	12	1539.1038	0.000	1539.1037	0.0001
(3)	15	5	11	-	14	5	10	1539.2635	0.001	1539.2635	0.0000
(3)	15	5	10	-	14	5	9	1539.2635	0.001	1539.2637	-0.0002
(3)	17	1	17	-	16	1	16	1539.7428	0.001	1539.7426	0.0002
(3)	16	2	15	-	15	2	14	1539.8729	0.000	1539.8729	0.0000
(3)	15	6	10	-	14	6	9	1540.0010	0.001	1539.9999	0.0011
(3)	15	6	9	-	14	6	8	1540.0010	0.001	1539.9999	0.0011
(3)	17	0	17	-	16	0	16	1540.2020	0.001	1540.2022	-0.0002
(3)	16	3	14	-	15	3	13	1540.9078	0.000	1540.9078	0.0000
(3)	15	7	9	-	14	7	8	1540.9230	0.001	1540.9208	0.0022
(3)	15	7	8	-	14	7	7	1540.9230	0.001	1540.9208	0.0022
(3)	16	3	13	-	15	3	12	1541.1769	0.000	1541.1772	-0.0003
(3)	16	4	13	-	15	4	12	1541.2946	0.000	1541.2952	-0.0006
(3)	16	4	12	-	15	4	11	1541.3086	0.000	1541.3092	-0.0006
(3)	16	1	15	-	15	1	14	1541.3620	0.000	1541.3618	0.0001
(3)	16	2	14	-	15	2	13	1541.8681*	0.000	1541.8693	-0.0012
(3)	16	5	12	-	15	5	11	1541.8681*	0.000	1541.8676	0.0005
(3)	16	5	11	-	15	5	10	1541.8681*	0.000	1541.8679	0.0001
(3)	18	1	18	-	17	1	17	1542.0041	0.001	1542.0039	0.0002
(3)	17	2	16	-	16	2	15	1542.3313	0.001	1542.3313	0.0000
(3)	18	0	18	-	17	0	17	1542.4107	0.001	1542.4109	-0.0002
(3)	16	6	11	-	15	6	10	1542.6270	0.001	1542.6258	0.0012
(3)	16	6	10	-	15	6	9	1542.6270	0.001	1542.6258	0.0012
(3)	17	3	15	-	16	3	14	1543.4988	0.001	1543.4987	0.0001
(3)	16	7	10	-	15	7	9	1543.5872	0.001	1543.5850	0.0022
(3)	16	7	9	-	15	7	8	1543.5872	0.001	1543.5850	0.0022
(3)	17	3	14	-	16	3	13	1543.8690	0.001	1543.8694	-0.0005
(3)	17	1	16	-	16	1	15	1543.8826	0.001	1543.8827	-0.0001
(3)	17	4	14	-	16	4	13	1543.9017	0.001	1543.9024	-0.0007
(3)	17	4	13	-	16	4	12	1543.9233	0.001	1543.9242	-0.0009
(3)	19	1	19	-	18	1	18	1544.2569	0.001	1544.2566	0.0003
(3)	17	5	13	-	16	5	12	1544.4832	0.001	1544.4831	0.0001
(3)	17	5	12	-	16	5	11	1544.4832	0.001	1544.4837	-0.0005
(3)	19	0	19	-	18	0	18	1544.6125	0.001	1544.6130	-0.0005
(3)	17	2	15	-	16	2	14	1544.6436	0.001	1544.6432	0.0004
(3)	18	2	17	-	17	2	16	1544.7826	0.001	1544.7828	-0.0001
(3)	17	6	12	-	16	6	11	1545.2649	0.001	1545.2635	0.0014

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(3)	17	6	11	-	16	6	10	1545.2649	0.001	1545.2635	0.0014
(3)	18	3	16	-	17	3	15	1546.0974	0.001	1546.0973	0.0002
(3)	17	7	11	-	16	7	10	1546.2610	0.001	1546.2590	0.0021
(3)	17	7	10	-	16	7	9	1546.2610	0.001	1546.2590	0.0021
(3)	18	1	17	-	17	1	16	1546.3789	0.001	1546.3790	-0.0001
(3)	20	1	20	-	19	1	19	1546.5014	0.001	1546.5010	0.0004
(3)	18	4	15	-	17	4	14	1546.5198	0.001	1546.5206	-0.0008
(3)	18	4	14	-	17	4	13	1546.5526	0.001	1546.5537	-0.0010
(3)	18	3	15	-	17	3	14	1546.5928	0.001	1546.5933	-0.0005
(3)	20	0	20	-	19	0	19	1546.8100	0.001	1546.8107	-0.0007
(3)	18	5	14	-	17	5	13	1547.1101	0.001	1547.1099	0.0003
(3)	18	5	13	-	17	5	12	1547.1101	0.001	1547.1109	-0.0008
(3)	19	2	18	-	18	2	17	1547.2266	0.001	1547.2266	0.0000
(3)	18	2	16	-	17	2	15	1547.4213	0.001	1547.4208	0.0005
(3)	18	6	13	-	17	6	12	1547.9145	0.001	1547.9128	0.0017
(3)	18	6	12	-	17	6	11	1547.9145	0.001	1547.9128	0.0017
(3)	19	3	17	-	18	3	16	1548.7020	0.001	1548.7018	0.0002
(3)	21	1	21	-	20	1	20	1548.7377	0.001	1548.7372	0.0006
(3)	19	1	18	-	18	1	17	1548.8476	0.001	1548.8477	0.0000
(3)	18	7	12	-	17	7	11	1548.9395	0.001	1548.9381	0.0014
(3)	18	7	11	-	17	7	10	1548.9395	0.001	1548.9381	0.0014
(3)	21	0	21	-	20	0	20	1549.0050	0.001	1549.0056	-0.0006
(3)	19	4	16	-	18	4	15	1549.1487	0.001	1549.1495	-0.0008
(3)	19	4	15	-	18	4	14	1549.1973	0.001	1549.1985	-0.0011
(3)	19	3	16	-	18	3	15	1549.3494	0.001	1549.3500	-0.0006
(3)	20	2	19	-	19	2	18	1549.6619	0.001	1549.6619	0.0000
(3)	19	5	15	-	18	5	14	1549.7486	0.001	1549.7480	0.0006
(3)	19	5	14	-	18	5	13	1549.7486	0.001	1549.7496	-0.0011
(3)	19	2	17	-	18	2	16	1550.1984	0.001	1550.1976	0.0009
(3)	19	6	14	-	18	6	13	1550.5753	0.001	1550.5736	0.0017
(3)	19	6	13	-	18	6	12	1550.5753	0.001	1550.5737	0.0017
(3)	22	1	22	-	21	1	21	1550.9660	0.001	1550.9655	0.0005
(3)	22	0	22	-	21	0	21	1551.1996	0.001	1551.2004	-0.0009
(3)	20	1	19	-	19	1	18	1551.2862	0.001	1551.2862	-0.0001
(3)	20	3	18	-	19	3	17	1551.3113	0.001	1551.3111	0.0002
(3)	19	7	13	-	18	7	12	1551.6089	0.001	1551.6094	-0.0006
(3)	19	7	12	-	18	7	11	1551.6089	0.001	1551.6094	-0.0006
(3)	20	4	17	-	19	4	16	1551.7879	0.001	1551.7887	-0.0008
(3)	20	4	16	-	19	4	15	1551.8584	0.001	1551.8596	-0.0012
(3)	21	2	20	-	20	2	19	1552.0885	0.001	1552.0883	0.0002
(3)	20	3	17	-	19	3	16	1552.1394	0.001	1552.1402	-0.0008
(3)	20	5	16	-	19	5	15	1552.3982	0.001	1552.3973	0.0009
(3)	20	5	15	-	19	5	14	1552.3982	0.001	1552.4000	-0.0019
(3)	20	2	18	-	19	2	17	1552.9705	0.001	1552.9694	0.0011
(3)	23	1	23	-	22	1	22	1553.1870	0.001	1553.1864	0.0006
(3)	20	6	15	-	19	6	14	1553.2476	0.001	1553.2458	0.0018
(3)	20	6	14	-	19	6	13	1553.2476	0.001	1553.2458	0.0018
(3)	23	0	23	-	22	0	22	1553.4018	0.001	1553.4026	-0.0007
(3)	21	1	20	-	20	1	19	1553.6933	0.001	1553.6933	0.0000
(3)	21	3	19	-	20	3	18	1553.9240	0.001	1553.9239	0.0001

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(3)	21	4	18	-	20	4	17	1554.4370	0.001	1554.4377	-0.0007
(3)	22	2	21	-	21	2	20	1554.5052	0.001	1554.5051	0.0002
(3)	21	4	17	-	20	4	16	1554.5367	0.001	1554.5382	-0.0014
(3)	21	3	18	-	20	3	17	1554.9629	0.001	1554.9638	-0.0009
(3)	21	5	17	-	20	5	16	1555.0591	0.001	1555.0579	0.0012
(3)	21	5	16	-	20	5	15	1555.0591	0.001	1555.0621	-0.0031
(3)	24	1	24	-	23	1	23	1555.4007	0.001	1555.4000	0.0006
(3)	21	2	19	-	20	2	18	1555.7340	0.001	1555.7327	0.0014
(3)	21	6	16	-	20	6	15	1555.9314	0.001	1555.9291	0.0023
(3)	21	6	15	-	20	6	14	1555.9314	0.001	1555.9292	0.0022
(3)	22	1	21	-	21	1	20	1556.0685	0.001	1556.0685	0.0000
(3)	22	3	20	-	21	3	19	1556.5389	0.001	1556.5389	0.0000
(3)	23	2	22	-	22	2	21	1556.9121	0.001	1556.9120	0.0001
(3)	22	4	19	-	21	4	18	1557.0951	0.001	1557.0956	-0.0005
(3)	22	4	18	-	21	4	17	1557.2348	0.001	1557.2355	-0.0007
(3)	25	1	25	-	24	1	24	1557.6092*	0.000	1557.6069	0.0023
(3)	22	5	18	-	21	5	17	1557.7294	0.001	1557.7294	-0.0001
(3)	22	5	17	-	21	5	16	1557.7356	0.001	1557.7360	-0.0004
(3)	22	3	19	-	21	3	18	1557.8184	0.001	1557.8193	-0.0009
(3)	23	1	22	-	22	1	21	1558.4127	0.001	1558.4127	-0.0001
(3)	22	2	20	-	21	2	19	1558.4856	0.001	1558.4836	0.0020
(3)	22	6	17	-	21	6	16	1558.6261	0.001	1558.6234	0.0027
(3)	22	6	16	-	21	6	15	1558.6261	0.001	1558.6236	0.0025
(3)	23	3	21	-	22	3	20	1559.1555	0.001	1559.1553	0.0002
(3)	24	2	23	-	23	2	22	1559.3092	0.001	1559.3089	0.0003
(3)	23	4	20	-	22	4	19	1559.7614	0.001	1559.7616	-0.0002
(3)	26	1	26	-	25	1	25	1559.8078	0.001	1559.8072	0.0006
(3)	23	4	19	-	22	4	18	1559.9516	0.001	1559.9531	-0.0015
(3)	23	5	19	-	22	5	18	1560.4114	0.001	1560.4119	-0.0005
(3)	23	5	18	-	22	5	17	1560.4211	0.001	1560.4219	-0.0008
(3)	23	3	20	-	22	3	19	1560.7032	0.001	1560.7042	-0.0010
(3)	24	1	23	-	23	1	22	1560.7281	0.001	1560.7281	0.0000
(3)	23	2	21	-	22	2	20	1561.2215	0.001	1561.2188	0.0027
(3)	25	2	24	-	24	2	23	1561.6964	0.001	1561.6958	0.0007
(3)	24	3	22	-	23	3	21	1561.7722	0.001	1561.7719	0.0003
(3)	27	1	27	-	26	1	26	1562.0020	0.001	1562.0014	0.0006
(3)	24	4	21	-	23	4	20	1562.4349	0.001	1562.4347	0.0002
(3)	24	4	20	-	23	4	19	1562.6910	0.001	1562.6925	-0.0015
(3)	25	1	24	-	24	1	23	1563.0174	0.001	1563.0176	-0.0002
(3)	24	5	20	-	23	5	19	1563.1045	0.001	1563.1051	-0.0006
(3)	24	5	19	-	23	5	18	1563.1196	0.001	1563.1198	-0.0002
(3)	24	3	21	-	23	3	20	1563.6135	0.001	1563.6145	-0.0010
(3)	24	2	22	-	23	2	21	1563.9386	0.001	1563.9349	0.0038
(3)	28	1	28	-	27	1	27	1564.1903	0.001	1564.1899	0.0004
(3)	25	3	23	-	24	3	22	1564.3884	0.001	1564.3881	0.0003
(3)	26	1	25	-	25	1	24	1565.2848	0.001	1565.2851	-0.0003
(3)	25	5	21	-	24	5	20	1565.8076	0.001	1565.8086	-0.0010
(3)	25	5	20	-	24	5	19	1565.8299	0.001	1565.8301	-0.0002
(3)	29	1	29	-	28	1	28	1566.3733	0.001	1566.3730	0.0003
(3)	25	3	22	-	24	3	21	1566.5445	0.001	1566.5454	-0.0009

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(3)	25	2	23	-	24	2	22	1566.6330	0.001	1566.6284	0.0046
(3)	26	3	24	-	25	3	23	1567.0034	0.001	1567.0031	0.0003
(3)	27	1	26	-	26	1	25	1567.5342	0.001	1567.5348	-0.0006
(3)	26	5	22	-	25	5	21	1568.5125	0.001	1568.5222	-0.0097
(3)	26	5	21	-	25	5	20	1568.5521*	0.000	1568.5530	-0.0008
(3)	26	3	23	-	25	3	22	1569.4905	0.001	1569.4911	-0.0006
(3)	27	3	25	-	26	3	24	1569.6167	0.001	1569.6165	0.0002
(3)	28	1	27	-	27	1	26	1569.7704	0.001	1569.7709	-0.0005
(3)	29	1	28	-	28	1	27	1571.9960	0.001	1571.9971	-0.0011
(3)	28	3	26	-	27	3	25	1572.2283	0.001	1572.2283	0.0000
(3)	27	3	24	-	26	3	23	1572.4452	0.001	1572.4455	-0.0003
(3)	29	3	27	-	28	3	26	1574.8382	0.001	1574.8385	-0.0003
(3)	28	3	25	-	27	3	24	1575.4024	0.001	1575.4025	-0.0001
(3)	29	3	26	-	28	3	25	1578.3564	0.001	1578.3558	0.0005
(4)	1	0	1	-	0	0	0	72492.5600	0.100	72492.3125	0.2475
(4)	2	0	2	-	1	0	1	144916.7000	0.200	144916.4772	0.2228
(4)	2	1	2	-	1	1	1	140752.6300	0.200	140752.5853	0.0447
(4)	2	1	1	-	1	1	0	149224.5000	0.200	149224.4234	0.0766
(4)	3	0	3	-	2	0	2	217204.5900	0.300	217204.4775	0.1125
(4)	3	1	3	-	2	1	2	211081.2800	0.300	211081.1375	0.1425
(4)	3	1	2	-	2	1	1	223788.2500	0.300	223787.9891	0.2609
(4)	3	2	2	-	2	2	1	217491.4700	0.300	217491.3780	0.0920
(4)	3	2	1	-	2	2	0	217764.3700	0.300	217764.2967	0.0733
(4)	4	0	4	-	3	0	3	289288.7600	0.400	289288.8797	-0.1197
(4)	4	1	4	-	3	1	3	281353.5500	0.400	281353.4300	0.1200
(4)	4	1	3	-	3	1	2	298292.1500	0.400	298292.1982	-0.0482
(4)	4	2	3	-	3	2	2	289915.8200	0.400	289915.9688	-0.1488
(4)	4	2	2	-	3	2	1	290597.4900	0.400	290597.4421	0.0479
(4)	2	1	1	-	2	1	2	12707.8300	0.100	12707.7947	0.0353
(4)	3	1	2	-	3	1	3	25414.5600	0.100	25414.6462	-0.0862
(4)	4	1	3	-	4	1	4	42353.5200	0.400	42353.4145	0.1055
(4)	5	1	4	-	5	1	5	63516.6000	0.100	63516.6284	-0.0284
(4)	2	2	0	-	2	2	1	68.2672	0.020	68.2652	0.0020
(4)	7	2	5	-	7	2	6	8519.3000	0.200	8519.0123	0.2877
(4)	8	2	6	-	8	2	7	14114.7800	0.200	14114.5826	0.1974
(4)	9	2	7	-	9	2	8	21999.9000	0.200	21999.6578	0.2422
(4)	10	2	8	-	10	2	9	32644.7400	0.200	32644.7558	-0.0158
(4)	4	3	1	-	4	3	2	4.3300	0.020	4.3273	0.0027
(4)	5	3	2	-	5	3	3	17.3084	0.020	17.3040	0.0044
(4)	6	3	3	-	6	3	4	51.8938	0.020	51.8809	0.0129
(4)	4	4	1	-	4	4	0	0.1660	0.020	0.1569	0.0091
(4)	5	4	2	-	5	4	1	1.3925	0.020	1.3886	0.0039
(4)	6	4	3	-	6	4	2	6.7855	0.020	6.7772	0.0083
(4)	7	4	4	-	7	4	3	24.0663	0.020	24.0404	0.0259
(4)	8	4	5	-	8	4	4	69.0985	0.020	69.0309	0.0676
(6)	1	0	1	-	0	0	0	72727.2500	0.100	72727.3676	-0.1176
(6)	2	0	2	-	1	0	1	145389.8600	0.200	145390.0104	-0.1504
(6)	2	1	2	-	1	1	1	140463.4500	0.200	140463.6753	-0.2253
(6)	2	1	1	-	1	1	0	150400.8400	0.200	150401.0448	-0.2048
(6)	3	0	3	-	2	0	2	217922.7600	0.300	217923.2505	-0.4905

UPPER STATE				LOWER STATE			OBSERVATION	PREC.	CALCULATION	RESID.
	J	KA	KC		J	KA	KC					
(6)	3	1	3	-	2	1	2	210657.4100	0.300	210657.7523	-0.3423
(6)	3	1	2	-	2	1	1	225562.0200	0.300	225562.3637	-0.3437
(6)	3	2	2	-	2	2	1	218056.1900	0.300	218056.2075	-0.0175
(6)	3	2	1	-	2	2	0	218314.3900	0.300	218314.4369	-0.0469
(6)	4	0	4	-	3	0	3	290262.2100	0.400	290262.7296	-0.5196
(6)	4	1	4	-	3	1	3	280806.7700	0.400	280807.3385	-0.5685
(6)	4	1	3	-	3	1	2	300675.3300	0.400	300675.7104	-0.3804
(6)	2	1	1	-	2	1	2	14906.2900	0.200	14906.2177	0.0723
(6)	3	1	2	-	3	1	3	29811.2000	0.200	29810.8291	0.3709
(6)	4	1	3	-	4	1	4	49679.1600	0.200	49679.2009	-0.0409
(6)	2	2	0	-	2	2	1	64.5718	0.020	64.5717	0.0001
(6)	7	2	5	-	7	2	6	8061.7600	0.200	8061.7520	0.0080
(6)	8	2	6	-	8	2	7	13350.9000	0.200	13350.9618	-0.0618
(6)	9	2	7	-	9	2	8	20794.2300	0.200	20794.2962	-0.0662
(6)	10	2	8	-	10	2	9	30825.1400	0.200	30825.4910	-0.3510
(6)	3	3	0	-	3	3	1	0.5270	0.020	0.5259	0.0011
(6)	4	3	1	-	4	3	2	3.6850	0.020	3.6813	0.0037
(6)	5	3	2	-	5	3	3	14.7318	0.020	14.7245	0.0073
(6)	6	3	3	-	6	3	4	44.1840	0.020	44.1637	0.0203
(6)	7	4	3	-	7	4	4	0.5945	0.020	0.5916	0.0029
(6)	8	4	4	-	8	4	5	1.7006	0.020	1.7752	-0.0746
(6)	9	4	5	-	9	4	6	4.6174	0.020	4.6161	0.0013
(6)	10	4	6	-	10	4	7	10.7710	0.020	10.7706	0.0004
(6)	11	4	7	-	11	4	8	23.0743	0.020	23.0755	-0.0012
(3)	1	0	1	-	0	0	0	73062.6300	0.100	73062.2769	0.3531
(3)	3	1	3	-	2	1	2	211341.3900	0.300	211341.2962	0.0938
(3)	3	1	2	-	2	1	1	226916.9400	0.300	226916.6916	0.2484
(3)	4	1	4	-	3	1	3	281687.9900	0.400	281687.8863	0.1037
(3)	2	1	1	-	2	1	2	15578.4000	0.200	15578.6562	-0.2562
(3)	3	1	2	-	3	1	3	31154.4400	0.200	31154.0516	0.3884
(3)	7	2	5	-	7	2	6	10171.5300	0.200	10171.1223	0.4077
(3)	8	2	6	-	8	2	7	16842.5800	0.200	16842.5865	-0.0065
(3)	9	2	7	-	9	2	8	26232.4000	0.200	26232.7870	-0.3870
(3)	3	3	0	-	3	3	1	0.8020	0.020	0.7980	0.0040
(3)	4	3	1	-	4	3	2	5.5828	0.020	5.5834	-0.0006
(3)	5	3	2	-	5	3	3	22.3130	0.020	22.3180	-0.0050
(3)	6	3	3	-	6	3	4	66.8725	0.020	66.8874	-0.0149
(3)	7	4	3	-	7	4	4	1.0615	0.020	1.0614	0.0001