ANALYSIS OF THE SPECTRA OF PLANAR ASYMMETRIC MOLECULES, WITH APPLICATION TO HYDROGEN TELLURIDE

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This is to certify that the

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ABSTRACT

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by N. Kent Moncur

The development of the vibration-rotation Hamiltonian for a planar asymmetric non-linear XYX molecule is outlined, and energy expressions are given by which energy levels and other quantities useful in an analysis of the spectra of such a molecule may be calculated. Since the upper vibrational states of some of the bands may interact through a Coriolis type resonance, a modified Hamiltonian is given which includes the necessary interaction terms for a description of these states.

A method is outlined by which the theoretical energy expressions can be used in an analysis of spectra, and is applied in the analysis of the absorption spectra of H_2Te near 2900 cm^{-1} and 4050 cm^{-1}.

Ground state combination differences from the infrared absorption bands $\nu_1+\nu_2$, $\nu_2+\nu_3$, $2\nu_1$, and $\nu_1+\nu_3$ are used in a least squares analysis to obtain ground state constants A, B, C, taus, and H_K for the molecular species $H_2{}^{130}Te$, $H_2{}^{128}Te$, $H_2{}^{126}Te$, $H_2{}^{125}Te$, and $H_2{}^{124}Te$. The upper states of the interacting bands $\nu_1+\nu_2$ and $\nu_2+\nu_3$ are simultaneously analyzed to obtain upper state constants

ν_o, A, B, C, taus, H_K, and the perturbation coefficients G_z and G_{xy}, for the species $H_2{}^{130}Te$, $H_2{}^{128}Te$, and $H_2{}^{126}Te$. The upper states of $2\nu_1$ and $\nu_1+\nu_3$ are treated in a similar manner for the species $H_2{}^{130}Te$, $H_2{}^{128}Te$, $H_2{}^{126}Te$, $H_2{}^{125}Te$, and $H_2{}^{124}Te$.

Using proper combinations of molecular constants from the different vibrational states analyzed, the equilibrium constants A_e, B_e, and C_e are obtained from which the equilibrium structure (r_e,θ) of H_2Te is calculated.

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By

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TO MY WIFE

ELAINE

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INTRODUCTION

The analysis of the infrared spectra of polyatomic molecules leads to precise information about their rotational and vibrational energy levels which in turn give information about inertial constants, centrifugal distortion constants, force constants, anharmonic constants, bond angles, bond lengths, and other data concerning their structure.

Since a polyatomic molecule is a many body problem, it is impossible to find exact expressions for the energy levels. A convenient approach to the problem is to treat the general theoretical expression for the Hamiltonian of polyatomic molecules by an expansion formulation in successive orders of approximation, and then apply it to the specific case involved, making simplifications whenever possible. The Born-Oppenheimer approximation is used to separate the electronic problem, which will not be considered here, from the vibration-rotation problem.

Molecules may be grouped into three general classes depending on their principal moments of inertia. Molecules, with all three principal moments of inertia equal ($I_a=I_b=I_c$), are called spherical top molecules and have

a spherical moment of inertia ellipsoid. Examples of these include CH_4, CCl_4, SiH_4. Molecules with two moments of inertia equal have an ellipsoid which is an ellipse of revolution and are called axially symmetric molecules. Examples of these are the prolate ($I_a<I_b=I_c$) molecules CH_3Cl and CH_3D, and oblate ($I_a=I_b<I_c$) molecules CD_3H and BF_3. These molecules generally have spectra with regular features. Asymmetric molecules have the most general moment of inertia ellipsoid with $I_a<I_b<I_c$. Examples of these are the non-planar molecules CH_2D_2, CH_2Cl_2, etc., and the planar molecules H_2CO, C_2H_4, H_2O, H_2S, H_2Se, and H_2Te. The spectra of asymmetric molecules are generally very irregular and identification of the absorption lines is one of the major problems in an analysis.

In the following, the development of the vibration-rotation Hamiltonian for a planar asymmetric non-linear XYX molecule will be outlined, and energy expressions will be given which may be used in an analysis of the vibration-rotation spectra. These expressions will be used in an analysis of the infrared absorption spectra of H_2Te.

CHAPTER I

THEORY OF THE ASYMMETRIC MOLECULE

A number of investigators have attacked the problem of finding the Hamiltonian of a semi-rigid, rotating, polyatomic molecule. A convenient formulation has been given by Darling and Dennison:[1]

$$H = \frac{1}{2}\sum_{\alpha}\sum_{\beta}\mu^{1/4}(P_\alpha - p_\alpha)\mu_{\alpha\beta}\mu^{-1/2}(P_\beta - p_\beta)\mu^{1/4} + \frac{1}{2}\sum_{k}\mu^{1/4}p_k\mu^{-1/2}p_k\mu^{1/4} + V \quad . \tag{1}$$

The subscripts α and β have the range x,y,z (the principal axes of inertia of the molecule), P_α and p_α are components of total and internal angular momentum respectively, and $\mu_{\alpha\beta}$ are the cofactors of a determinant which contains the moments of inertia. The p_k are the momenta conjugate to the normal coordinates q_k. In general, the eigenvalue problem using the Hamiltonian in the form of Eq. (1) is impossible to solve, so the usual procedure is to make an expansion in orders of magnitude,

$$H = H_o + H_1 + H_2 + \ldots \tag{2}$$

and apply perturbation theory to obtain the eigenvalues and eigenfunctions. Such an expansion is given by Gold-

smith, Amat and Nielsen.[2] The Hamiltonian is then cast into a more convenient form by applying a contact transformation:

$$H' = THT^{-1} = H'_o + \lambda H'_1 + \lambda^2 H'_2 + \ldots \tag{3}$$

$$T = e^{i\lambda S}, \quad T^{-1} = e^{-i\lambda S}$$

$$S = S_1 + S_2 + S_3 + \ldots ,$$

where S is a function of vibration and rotation operators. Substituting the expanded Hamiltonian of Eq. (2) into Eq. (3) and equating the coefficients of like powers of λ, one finds

$$H'_o = H_o \tag{4}$$

$$H'_1 = H_1 + i[S,H_o]$$

$$H'_2 = H_2 + \tfrac{i}{2}[S,(H_1+H'_1)] \quad .$$

S is then chosen such that all off diagonal H_1 terms are removed to H'_2 leaving H'_1 with only diagonal vibrational matrix elements, which simplifies the perturbation calculation. Herman and Shaffer[3] give a suitable S for transforming H.

For an asymmetric molecule the situation is somewhat simplified since S may be chosen such that $H'_1 = 0$. The energy is then obtained by the perturbation method of considering only the diagonal vibrational elements of $H' = H'_o + H'_2$. This approach is valid provided, no resonant denominators appear during the transformation,

and all off diagonal vibrational matrix elements of H_2' which have been ignored are small. These problems will arise later when the possibility of a Coriolis interaction is discussed. Some of the individual terms in the expanded Hamiltonian are considerably simplified for a non-linear XYX molecule and will be given in detail by Snyder[4] for both the untransformed and transformed Hamiltonian.

There are 3! ways the principal axes (a,b,c) of a molecule may be attached to a cartesian coordinate system (x,y,z). Since the molecules of interest here are near the oblate limit, where the angular momentum operator P_c becomes diagonal, the III^r system will be used, where a = x, b = y, c = z.

To 2^{nd} order of approximation, the transformed asymmetric top Hamiltonian as given by Chung and Parker[5] is

$$\begin{aligned} H' = {} & h_v + AP_a^2 + BP_b^2 + CP_c^2 + \tfrac{1}{4}\tau_{aaaa}P_a^4 + \tfrac{1}{4}\tau_{bbbb}P_b^4 \\ & + \tfrac{1}{4}\tau_{cccc}P_c^4 + \tfrac{1}{4}\tau_{bbcc}(P_b^2P_c^2 + P_c^2P_b^2) + \tfrac{1}{4}\tau_{aacc}(P_a^2P_c^2 + P_c^2P_a^2) \\ & + \tfrac{1}{4}\tau_{aabb}(P_a^2P_b^2 + P_b^2P_a^2) + \tfrac{1}{4}\tau_{bcbc}(P_bP_c + P_cP_b)^2 \\ & + \tfrac{1}{4}\tau_{acac}(P_aP_c + P_cP_a)^2 + \tfrac{1}{4}\tau_{abab}(P_aP_b + P_bP_a)^2. \end{aligned} \tag{5}$$

The P_a, P_b, and P_c are the components of angular momentum along the a, b, and c axes, and the taus are the centrifugal distortion constants.

Non-linear XYX Molecule

For a non-linear tri-atomic molecule in the ab plane

Dowling,[6] and Oka and Morino[7] have shown that the following relations exists between the taus:

$$\tau_{bcbc} = \tau_{acac} = 0 \tag{6}$$

$$\tau_{cccc} = (I_a^e/I_c^e)^4 \tau_{aaaa} + 2[I_a^e I_b^e/(I_c^e)^2]^2 \tau_{aabb} + (I_b^e/I_c^e)^4 \tau_{bbbb}$$

$$\tau_{bbcc} = (I_b^e/I_c^e)^2 \tau_{bbbb} + (I_a^e/I_c^e)^2 \tau_{aabb}$$

$$\tau_{aacc} = (I_a^e/I_c^e)^2 \tau_{aaaa} + (I_b^e/I_c^e)^2 \tau_{aabb}$$

where I_a^e, I_b^e, and I_c^e are the equilibrium moments of inertia. Using Eqs. (6) and the commutation relation

$$(P_a P_b + P_b P_a)^2 = 2(P_a^2 P_b^2 + P_b^2 P_a^2) + 5P_c^2 - 2P^2 \tag{7}$$

where $P = P_a^2 + P_b^2 + P_c^2$,

the Hamiltonian Eq. (5) simplifies to

$$H' = h_v + AP_a^2 + BP_b^2 + CP_c^2 + \tau_{aaaa} O_{aaaa} + \tau_{bbbb} O_{bbbb} + \tau_{aabb} O_{aabb} + \tau_{abab} O_{abab} , \tag{8}$$

where

$$O_{aaaa} = \tfrac{1}{4}[P_a^4 + r^2 P_c^4 + r(P_a^2 P_c^2 + P_c^2 P_a^2)] \tag{9}$$

$$O_{bbbb} = \tfrac{1}{4}[P_b^4 + s^2 P_c^4 + s(P_b^2 P_c^2 + P_c^2 P_b^2)]$$

$$O_{aabb} = \tfrac{1}{4}[2rsP_c^4 + (P_a^2 P_b^2 + P_b^2 P_a^2) + s(P_a^2 P_c^2 + P_c^2 P_a^2) + r(P_b^2 P_c^2 + P_c^2 P_b^2)]$$

$$O_{abab} = \tfrac{1}{4}[2(P_a^2 P_b^2 + P_b^2 P_a^2) - 2P^2 + 5P_c^2] \quad .$$

In the absence of any resonating states, the vibrationally dependent molecular constants A, B, and C of

Eq. (8) are defined as

$$A = A_e - \sum_i \alpha_i^A (v_i + \tfrac{1}{2}) \qquad (10)$$

$$B = B_e - \sum_i \alpha_i^B (v_i + \tfrac{1}{2})$$

$$C = C_e - \sum_i \alpha_i^C (v_i + \tfrac{1}{2}) \ .$$

A_e, B_e, and C_e are the equilibrium molecular constants and are inversely proportional to the equilibrium moments of inertia. Expressed in cm^{-1} they are defined as

$$A_e = h/8\pi^2 cI_a^e, \quad B_e = h/8\pi^2 cI_b^e, \quad C_e = h/8\pi^2 cI_c^e, \qquad (11)$$

where h is Planck's constant and c is the speed of light. Detailed expressions for the α_i will be given by Snyder.[4]

In Eq. (8), h_v is a pure vibrational term and is a constant within a vibrational state.

The r and s are defined by

$$r = C_e^2/A_e^2 \qquad (12)$$

$$s = C_e^2/B_e^2 \ .$$

Use of the planarity condition

$$I_c^e = I_a^e + I_b^e$$

gives

$$\frac{1}{C_e} = \frac{1}{A_e} + \frac{1}{B_e} ,$$

which can be used to express r and s in terms of only two of the equilibrium constants. Eliminating C_e from Eqs. (12) we have

$$r = B_e^2/(A_e+B_e)^2 \qquad (13)$$

$$s = A_e^2/(A_e+B_e)^2 \ .$$

In practice, when equilibrium constants are not available, ground state constants A and B are used in place of A_e and B_e to calculate r and s. We chose to eliminate C_e rather than A_e or B_e from the definition of r and s since for the type of molecules of interest, such as H_2S,[8] H_2Se,[9] etc., it happens that C_e differs from the ground state C more than A_e and B_e differ from the ground state A and B. Thus, calculations of r and s using A and B are closer to the actual values than those using C.

The Hamiltonian of Eq. (8) differs from that used by Hill and Edwards[10] in that the portion of the centrifugal distortion of the last term

$$\tau_{abab}\tfrac{1}{4}(-2P^2 + 5P_c^2) = -\tfrac{1}{2}\tau_{abab}P_a^2 - \tfrac{1}{2}\tau_{abab}P_b^2 + \tfrac{3}{4}\tau_{abab}P_c^2$$

was included by Hill in $AP_a^2 + BP_b^2 + CP_c^2$, thus, his definition of A, B, and C include $-\frac{1}{2}\tau_{abab}$, $-\frac{1}{2}\tau_{abab}$, and $+\frac{3}{4}\tau_{abab}$ respectively.

For a non-linear XYX molecule, Chung and Parker[11] have calculated the centrifugal distortion constants. In cm^{-1} they are

$$\tau_{aaaa} = -16A_e^3(\sin^2\gamma/\omega_1^2 + \cos^2\gamma/\omega_2^2) \qquad (14)$$

$$\tau_{bbbb} = -16B_e^3(\cos^2\gamma/\omega_1^2 + \sin^2\gamma/\omega_2^2)$$

$$\tau_{aabb} = -16(A_e B_e)^{3/2}(1/\omega_1^2 - 1/\omega_2^2)\sin\gamma\cos\gamma$$

$$\tau_{abab} = -16A_e B_e C_e/\omega_3^2 \quad .$$

The ω_i are the normal frequencies in cm^{-1}, and γ, a dimensionless quantity, is a function of the harmonic force constants.

Asymmetric Rotor Wave Functions

A perturbation treatment requires use of only the diagonal vibrational elements of the transformed Hamiltonian (except when vibrational resonances occur such as in a Coriolis interaction, then off diagonal elements must be considered), therefore, the rotational Hamiltonian is all that must be diagonalized. When forming the rotational matrix elements of the Hamiltonian it is convenient to use the combinations of the symmetric rotor wave functions suggested by Wilson[12] for a basis set. These combinations break each J submatrix, where J is the total angular momentum quantum number, into four smaller submatrices, designated E^+, E^-, O^+, and O^-. Thus, the size of the matrices that must be diagonalized is reduced. The basis set of wave functions used are

$$\Psi(J,K,\gamma) = \frac{1}{\sqrt{2}}[\psi(J,K) + (-1)^{\gamma}\psi(J,K)], \quad K \neq 0 \qquad (15)$$

$$\Psi(J,0,\gamma) = \psi(J,0) \quad K = 0,$$

where K is the projection of J along the axis which becomes unique in the nearest symmetric top limit of the

moment of inertia ellipsoid, so that $K \leq J$. The $\psi(J,K)$ are the symmetric rotor basis functions, and γ is an odd or even integer (except for $K = 0$ where only even γ exists). The symbols E^+, E^-, O^+, and O^- identifying the submatrices refer to the evenness (E,+) or oddness (O,-) of the (K,γ) values in the matrix. The matrix elements of the operators in the basis set $\Psi(J,K,\gamma)$ are given in Appendix I.

A convenient parameter κ, indicating the asymmetry of a molecule, has been defined by Ray,[13,14] where

$\kappa = \frac{2B-A-C}{A-C}$ and has the range $-1 \leq \kappa \leq 1$. $\kappa = -1$ for a prolate molecule (B=C), and $\kappa = +1$ for an oblate molecule (A=B).

The energy level of a given vibration-rotation state may be identified by the three vibration quantum numbers (v_1,v_2,v_3), the total angular momentum quantum number J, and both values of K to which the level corresponds in the prolate ($\kappa = -1$) and oblate ($\kappa = +1$) symmetric top limits. Thus, a rotational level for a particular vibrational state is designated by $J_{K_{-1}K_{+1}}$. In another method of labeling energy levels, the pseudo quantum number τ is used, where $\tau = K_{-1}-K_{+1}$. Thus, a level is labled as J_τ. In the III^r representation, $K_{-1}+K_{+1}$ is equal to J for levels with γ even and J+1 for those with γ odd. Fig. 1 gives an energy level diagram for J = 1, 2, and 3. The classification of the submatrices in terms of the parities of K_{-1} and K_{+1} is given in Table I.

Fig. 1. Energy Level Diagram

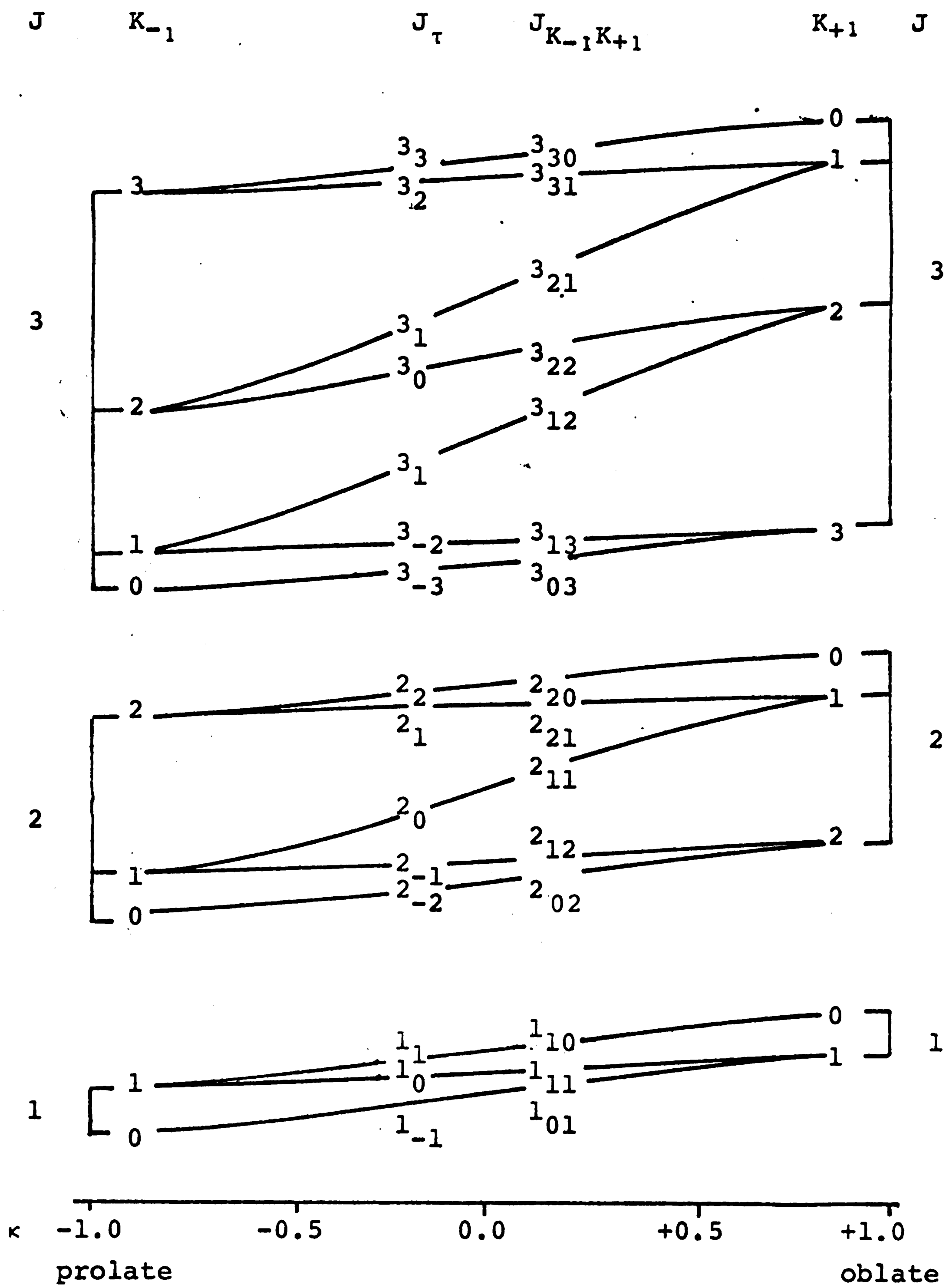


Table I. Classification of the Submatrices E^+, E^-, O^+, O^-

III^r Representation

Submatrix	γ	even J		odd J		Size of Submatrix	
		K_{-1}	K_{+1}	K_{-1}	K_{+1}	even J	odd J
E^+	e	e	e	o	e	J/2 +1	(J+1)/2
E^-	o	o	e	e	e	J/2	(J-1)/2
O^+	e	o	o	e	o	J/2	(J+1)/2
O^-	o	e	o	o	o	J/2	(J+1)/2

e = even

o = odd

The wave functions $A(J,\tau)$ which diagonalize the rotational matrix are linear combinations of the basis functions:

$$A(J,\tau) = \sum_K S_K^{J\tau} \Psi(J,K,\gamma) \ , \tag{16}$$

where the sum is over only those wave functions Ψ which form the same submatrix E^+, E^-, O^+, or O^-, i.e., even K even γ, even K odd γ, odd K even γ, or odd K odd γ.

Energy Expressions

The energy of a given vibration rotation state may be evaluated from

$$\begin{aligned} E(V,J,\tau) &= G(v_1,v_2,v_3) + W(A,B,C) \\ &= \langle v_1 v_2 v_3 | h_V | v_1 v_2 v_3 \rangle + A\langle P_a^2 \rangle + B\langle P_b^2 \rangle + C\langle P_c^2 \rangle \\ &\quad + \tau_{aaaa}\langle O_{aaaa} \rangle + \tau_{bbbb}\langle O_{bbbb} \rangle + \tau_{aabb}\langle O_{aabb} \rangle \\ &\quad + \tau_{abab}\langle O_{abab} \rangle \ , \end{aligned} \tag{17}$$

where

$$\begin{aligned} \langle v_1 v_2 v_3 | h_V | v_1 v_2 v_3 \rangle &= G(v_1,v_2,v_3) \\ &= G_o + \sum_i \omega_i (v_i + \tfrac{1}{2}) + \sum_{i \leq k} \sum X_{ik} (v_i + \tfrac{1}{2})(v_k + \tfrac{1}{2}) . \end{aligned} \tag{18}$$

$G(v_1,v_2,v_3)$ is the pure vibrational contribution to the energy.[15] The X_{ik} are the vibrational anharmonicity constants, and G_o is a constant term. $W(A,B,C)$ is the rotational energy where the average values of the rotational operators are taken in the representation $A(J,\tau)$ which diagonalize the rotational Hamiltonian. The cons-

tants A, B, and C are dependent on the vibrational state involved. Although the definition of the taus given in Eqs. (14) show them to be independent of the vibrational states, the empirical taus determined in an analysis may show a vibrational dependence because they may try to adjust for the effect of other centrifugal distortion terms from a higher order of the Hamiltonian expansion which have not been included here.

The difference between the ground and excited state energies involved in a transition is given by

$$\nu = G'(v_1',v_2',v_3') - G''(v_1'',v_2'',v_3'') + W'(A',B',C') - W''(A'',B'',C'') . \quad (19)$$

(G'-G") is the pure vibrational contribution which is called the band center or orgin, and is denoted by ν_o. (W'-W") is the difference between the excited and ground state rotational energy levels.

A second order vibrational resonance, which exists between states of the type (v_1,v_2,v_3) and (v_1-2,v_2,v_3+2), was first recognized by Darling and Dennison[1] in H_2O and later by Allen and Plyler[16] in H_2S. The vibrational energies of two such resonating states are given by

$$G_p = \tfrac{1}{2}[G_1(v_1,v_2,v_3) + G_2(v_1-2,v_2,v_3+2)] \pm \tfrac{1}{2}[(G_1-G_2)^2+\gamma^2 v_1(v_1-1)(v_3+1)(v_3+2)]^{1/2}, \quad (20)$$

where G_p represents the energy of a perturbed level, and

G_1 and G_2 that of the unperturbed levels as defined in Eq. (18). The interaction matrix element is represented by γ.

Higher Order Distortion Terms

When higher order terms in the rotational Hamiltonian are considered, many P^6 distortion terms appear. Pierce, DiCianni and Jackson[17] have suggested that for nearly symmetric rotors it may be a sufficiently good approximation to retain only those P^6 terms which do not vanish in the symmetric rotor limit. This results in the addition of the following four terms to the Hamiltonian:

$$H_J P^6 + H_{JK} P^4 P_c^2 + H_{KJ} P^2 P_c^4 + H_K P_c^6 \ . \qquad (21)$$

These H's derived from an analysis of the spectrum have only empirical significance.

Chung and Parker[5,18] have explicitly derived all the terms in the asymmetric rotor Hamiltonian that contribute to the energy in the fourth order of approximation. Using these results and the angular momentum commutation relations, Kneizys, Freedman, and Clough[19] reduced the number of rotational coefficients appearing in the Hamiltonian. When their results are examined, the same four terms that are in Eq. (21) are found among their P^6 terms, which lends more justification for their addition to the Hamiltonian.

Watson, in a recent work,[20] has shown that the ro-

tational Hamiltonian of an asymmetric molecule in general form may be transformed, by means of a unitary transformation, to a reduced Hamiltonian which has the same eigenvalues but fewer parameters. This procedure removes any possible indeterminacy which may exist in the coefficients. This reduced Hamiltonian, complete through the sextic terms, has been given in a form which is suitable for fitting to observed energies. For reasons that are not clear, our efforts to fit the observed ground state combination differences of H_2Te using Eq. (37) of Ref. (20) were not successful, since the constants would not converge to stable values. It may yet be possible to fit these combination differences with this equation by allowing only certain combinations of the constants to vary at one time in a fit, or by using a different form of the equation, however, this formulation of the Hamiltonian and energy expressions will not be considered further.

Selection Rules

In order that a transition from state n"→n' occur, the electric dipole matrix element

$$\int \psi^*_{n''} \mu \psi_{n'} dV \qquad (22)$$

must be non-zero. The selection rules for vibration-rotation transitions come from the vanishing or nonvanishing of this matrix element and have been given and discussed by Cross, Hainer and King,[14] Hill,[21] and many others. The

selection rules for J in the asymmetric rotor are the same as in the symmetric rotor, $\Delta J = -1, 0, +1$ corresponding to P, Q, and R branches respectively. The selection rules of the parity change of K_{-1} and K_{+1} are given in Table II.

If the change in the electric moment during a transition lies along the axis of least moment of inertia (a axis), the resulting band is called a type A band, and we see that the parity of K_{-1} does not change and that of K_{+1} does, i.e.; $\Delta K_{-1} = \pm 0, \pm 2, \pm 4, \ldots$ and $\Delta K_{+1} = \pm 1, \pm 3, \ldots$.

For a change in the electric moment along the greatest moment of inertia (c axis), a type C band results and the parity of K_{-1} does change while that of K_{+1} does not, $\Delta K_{-1} = \pm 1, \pm 3, \ldots$ and $\Delta K_{+1} = \pm 0, \pm 2, \pm 4, \ldots$.

For a change in the electric moment along the intermediate moment of inertia (b axis) a type B band results and the parity of both K_{-1} and K_{+1} change, $\Delta K_{-1} = \pm 1, \pm 3, \ldots$ and $\Delta K_{+1} = \pm 1, \pm 3, \ldots$.

The above selection rules are subject to the restrictions $K_{-1} + K_{+1} = J$ for even γ and $K_{-1} + K_{+1} = J+1$ for odd γ for both initial and final states. Transitions involving changes in K_{-1} and K_{+1} of 0 and ± 1 are all we normally need consider since changes greater than ± 1 generally involve transitions with intensities an order of magnitude weaker.[22] A type C band is not possible for a planar molecule in the ab plane since there can be no

Table II. Selection Rules by Parity Change of K_{-1} and K_{+1}

Band Type	Axis Parallel to Dipole Moment Change	Allowed Transitions K_{-1} K_{+1} $\leftrightarrow$ K_{-1} K_{+1}	The Parity Change is in
A	a	e e $\leftrightarrow$ e o o o $\leftrightarrow$ o e	K_{+1}
B	b	e e $\leftrightarrow$ o o e o $\leftrightarrow$ o e	K_{-1} and K_{+1}
C	c	e e $\leftrightarrow$ o e o o $\leftrightarrow$ e o	K_{-1}

out of plane vibrations. For a non-linear XYX molecule, any band which includes an odd multiple of ν_3 is a type A band, all others are type B bands.

We have found it convenient to use the familiar symmetric top notation for designating transitions. The terminology is ${}^{\Delta K}\Delta J_K(J)$ where J and K refer to the ground state quantum numbers, K being the K in the nearest symmetric top limit (K_{-1} for prolate and K_{+1} for oblate). Since the degeneracy in K is removed in an asymmetric molecule, there are two components to each transition, an even component which orginates from a symmetric energy level and an odd component orginating from an antisymmetric level. As usual the symbols P, Q, and R indicate changes in J and K of -1, 0, and +1 respectively. Thus, the possible transitions for A and B type bands include ${}^{R}R_K(J)$, ${}^{P}P_K(J)$, ${}^{R}Q_K(J)$, ${}^{P}Q_K(J)$, ${}^{R}P_K(J)$, and ${}^{P}R_K(J)$.

Intensities

The relative intensities of transitions within a band may be calculated with the expression

$$I \propto g|\mu(\kappa)|^2_{n'',n'} e^{(-W''hc/kT)} , \qquad (23)$$

where $e^{(-W''hc/kT)}$ is the Boltzman factor and $|\mu(\kappa)|^2_{n'',n'}$ the line strength. The line strength includes the factor (2J+1) which arises because of the (2J+1) fold degenercy of the total angular momentum in the absence of an external field. The g is the statistical weight factor of the

ground state level which arises when two of the nuclei in a molecule such as H_2Te are identical. For H_2Te the ratio of g for symmetric levels (ee, oo) and antisymmetric levels (eo, oe) is 1:3.

CHAPTER II

METHOD OF ANALYSIS

The rotational energy, including the four terms of Eq. (21) and written in a form which is convenient for the analysis of spectra, is

$$W = \alpha A + \beta B + \gamma C + \chi_1 \tau_{aaaa} + \chi_2 \tau_{bbbb} + \chi_3 \tau_{aabb} + \chi_4 \tau_{abab} + \chi_5 H_J + \chi_6 H_{JK} + \chi_7 H_{KJ} + \chi_8 H_K \,, \tag{24}$$

where

$$\begin{aligned} \alpha &= \langle P_a^2 \rangle \\ \beta &= \langle P_b^2 \rangle \\ \gamma &= \langle P_c^2 \rangle \\ \chi_1 &= \langle O_{aaaa} \rangle \\ \chi_2 &= \langle O_{bbbb} \rangle \\ \chi_3 &= \langle O_{aabb} \rangle \\ \chi_4 &= \langle O_{abab} \rangle \\ \chi_5 &= \langle P^6 \rangle = J^3 (J+1)^3 \\ \chi_6 &= \langle P^4 P_c^2 \rangle = J^2 (J+1)^2 \langle P_c^2 \rangle \\ \chi_7 &= \langle P^2 P_c^4 \rangle = J(J+1) \langle P_c^4 \rangle \\ \chi_8 &= \langle P_c^6 \rangle \quad . \end{aligned} \tag{25}$$

The average values of the operators are calculated from the eigenvectors of the diagonalized Hamiltonian.

The average value of any operator F may be expressed as

$$\langle J\tau|F|J\tau\rangle = \sum_K \sum_{K'} (S_K^{J\tau})^* S_{K'}^{J\tau} F_{KK'} \tag{26}$$

where

$$F_{KK'} = \int \Psi^*(J,K,\gamma) F \Psi(J,K',\gamma)\, dV$$

are the matrix elements of F in the original basis set. For simplification of the calculation it should be noted that since $F_{KK'} = F^*_{K'K}$ for a hermitian operator, then

$$\sum_K \sum_{K'} (S_K^{J\tau})^* S_{K'}^{J\tau} F_{KK'} = \sum_K |S_K^{J\tau}|^2 F_{KK} + \sum_{K<K'} \sum 2\mathrm{Re}[(S_K^{J\tau})^* S_{K'}^{J\tau} F_{KK'}]. \tag{27}$$

Re denotes the real part of the quantity enclosed with brackets.

The method of analysis involves calculating the average values of the operators starting from the best available values of the constants A, B, and C, from previous work or from an approximate symmetric top analysis. Hill and Edwards[10] have given a method of obtaining approximate values of the rotational constants (A+B) and C by using a rigid symmetric rotor approximation to the combination differences. Neglecting centrifugal distortion, the symmetric rotor approximation to the rotational energy is

$$W = [(A+B)/2]J(J+1) + [C-(A+B)/2]K^2 \ . \tag{28}$$

Using this expression, the ground state combination differences formed from the zero series (^RR and ^PP lines for

which K = J) are given by the simple expression

$$^{R}R_{J}(J) - {}^{P}P_{J+2}(J+2) = A'' + B'' + 4C''(J+1) \quad , \tag{29}$$

where the double prime indicates ground state. Thus, if a plot of the observed combination differences vrs (J+1) is made, (A"+B") and 4C" may be obtained from the intercept and slope of the straight line connecting these points. Although this may also be done with other series, the zero series is preferred because it usually contains the strongest lines on each side of the band center and has the lines least affected by the asymmetry and therefore the easiest to identify. In a similar manner the upper state combination differences formed from the zero series are given by

$$^{R}R_{J}(J) - {}^{P}P_{J}(J) = A' + B' + 4C'J \tag{30}$$

where the single prime indicates the upper state. A plot of the observed combination differences vrs. J gives (A'+B') as the intercept and 4C' as the slope of the straight line connecting the points.

The initial A, B, and C are used in a least squares fit of the assigned lines of the spectrum to get revised values of A, B, C, the taus and H'^{S}, and to help assign more lines. The process is repeated, this time calculating the average values of the operators using the revised A, B, C, taus, and H'^{S}, and including all newly assigned lines in the fit. This is continued until a stable set

of constants is obtained and all possible lines are assigned. It is usually necessary to refit more than once, since the average values of the operators change somewhat when small changes in the constants are made, and new lines are often assigned.

Line Fits

To fit the energy levels to the spectral lines, the best available constants are used to calculate the average values of the operators for each energy level of the ground and upper state, and to predict a spectrum using the expression

$$\nu_{calc} = \nu_o + W'(A',B',C') - W''(A'',B'',C'') \quad , \tag{31}$$

where the double prime indicates ground state and single prime upper state. The differences between the observed frequencies and the calculated frequencies are then fit to the expression

$$\begin{aligned} \nu_{obs} - \nu_{calc} = {} & \Delta\nu_o + \alpha'\Delta A' + \beta'\Delta B' + \gamma'\Delta C' \\ & + \sum_{i=1}^{4} \chi_i'\Delta\tau_i' + \sum_{i=5}^{8} \chi_i'\Delta H_i' - \alpha''\Delta A'' \\ & - \beta''\Delta B'' - \gamma''\Delta C'' - \sum_{i=1}^{4} \chi_i''\Delta\tau_i'' \\ & - \sum_{i=5}^{8} \chi_i''\Delta H_i'' \quad . \end{aligned} \tag{32}$$

The $\Delta\nu_o$, ΔA, ΔB, etc., obtained from the fit, are the changes in the initial constants ν_o, A, B, etc., i.e.: $\Delta\nu_o = \nu_o^* - \nu_o$ where ν_o^* is the revised constant. These

changes in the constants are made and the process repeated as explained above.

If, initially, only lines have been identified which are not greatly affected by the asymmetry, it may be desirable to use the combinations of the constants $\frac{A+B}{2}$ and $\frac{A-B}{2}$ instead of A and B. This was done by Hill *et al.*[10] and may be accomplished by replacing $\alpha\Delta A + \beta\Delta B$ in Eq. (32) by $\xi\Delta(\frac{A+B}{2}) + \eta\Delta(\frac{A-B}{2})$, where $\xi = \alpha+\beta$, and $\eta = \alpha-\beta$. The advantage of using these combinations of the constants is that $(\frac{A-B}{2})$, which determines the asymmetry, may be held constant in a fit until some lines which depend more on the asymmetry are identified.

Ground State Combination Difference Fits

In a similar manner, the ground state energy levels may be fit to the observed ground state combination differences. The average values of the operators for each ground state energy level are calculated and a set of combination differences calculated from the expression

$$\Delta\nu_{calc} = [W''(A'',B'',C'')]_1 - [W''(A'',B'',C'')]_2 , \qquad (33)$$

where this indicates level 1 - level 2. The difference between the observed and calculated combination differences are then fit to the expression

$$\Delta\nu_{obs}-\Delta\nu_{calc} = (\alpha''_1-\alpha''_2)\Delta A''+(\beta''_1-\beta''_2)\Delta B''+(\gamma''_1-\gamma''_2)\Delta C'' + \sum_{i=1}^{4}[(\chi''_i)_1-(\chi''_i)_2]\Delta\tau''_i + \sum_{i=5}^{8}[(\chi''_i)_1-(\chi''_i)_2]\Delta H''_i . \qquad (34)$$

Again, it may initially be desirable to write the above formula in terms of $\Delta(\frac{A+B}{2})$ and $\Delta(\frac{A-B}{2})$ instead of ΔA and ΔB.

It is generally advantageous to obtain the ground state constants from a fit with Eq. (34) as opposed to a line fit, since the upper state energy levels, which may be perturbed, are not involved, and the ground state combination differences from all bands may be fit simultaneously.

The upper state of a single band may also be analyzed by fitting its upper state combination differences in a similar manner. Since this method involves fitting differences in energy levels instead of the energy levels themselves and does not allow ν_o to be determined, we chose to analyze the upper state by fitting the spectrum to Eq. (32), holding the ground state constants fixed and varying ν_o and the upper state constants. In either case, the possibility of perturbations in the upper state may hamper the analysis.

Computer Programs

Several computer programs written in Fortran were used on Michigan State University's 3600 CDC computer. The main subroutines used to diagonalize the Hamiltonian and Perform least squares fits are respectively:

a. SUBROUTINE JHERMX

This subroutine, obtained from N. W. Naugle,[23] is

the adaption of the Threshold Jacobi Method for evaluating the eigenvalues and optionally, the eigenvectors of a hermitian matrix.

b. SUBROUTINE REGRESS

This subroutine is a stepwise multiple regression routine written by Efroymson,[24] and is used in all least square fits in this work. An explanation of the mathematical method including computer flow charts is given in Ref. (24).

The following gives the name and description of the computer programs used.

1. ENG-CALC

A, B, C, taus, and H's are input and the computer calculates and prints out ground state energy levels and the level identification J $K_{-1}K_{+1}$. Upper state rotational energy levels may be calculated by inputing upper state constants and inserting cards in the deck that calculate r and s with the ground state A and B, otherwise the program calculates r and s with the A and B that are input.

2. SPEC-CALC

Ground and upper state constants, and band center of the spectrum to be calculated are input. The computer calculates rotational energy levels for both ground and upper states and stores them in memory. Following the program is a deck of IBM cards which the computer reads. Each card contains the quantum numbers for an

allowed transition and the line strengths for this transition tabulated in steps of 0.1 in κ. The quantum numbers designate the location of the energy levels in memory and are output along with the frequency calculated with Eq. (31), and the intensity of the transition calculated with Eq.(23) and scaled such that the largest intensity is 10. The line strength is obtained by interpolating between the line strengths on the transition card.

3. CD-FIT

Ground state molecular constants are input along with all the observed ground state combination differences $\Delta\nu_{obs}$, and the quantum numbers $(J\ K_{-1}K_{+1})_1$-$(J\ K_{-1}K_{+1})_2$ that identify them. The quantities $(\Delta\nu_{obs}-\Delta\nu_{calc})$ are formed by the computer and fit by least squares to Eq. (34) to determine the revised constants. Any combination or all of the constants may be varied simultaneously.

Upper state combination differences may be fit in the same manner by inserting a card in the program which calculates r and s with the ground state A and B.

4. SPEC-FIT

Ground and upper state molecular constants and band center are input along with the observed frequencies of all the assigned transitions and the quantum numbers $(J'\ K'_{-1}K'_{+1}-\ J''\ K''_{-1}K''_{+1})$ that identify them. The quantities $(\nu_{obs}\ -\ \nu_{calc})$ are formed by the computer

and fit to Eq. (32) to determine the revised constants. Any or all of the ground and upper state constants may be simultaneously varied.

5. CD-CALC

All the frequencies, quantum numbers, and weights of the assigned transitions within a band are input. The computer forms and prints out all possible ground and/or upper state combination differences that can be obtained from the input transitions. When the same combination difference appears more than once within the same band, a weighted average is formed and printed out.

CHAPTER III

PERTURBATIONS IN EXCITED VIBRATIONAL STATES

Nielsen,[25] and Herman and Shaffer[3] have shown that in the event of an accidental degeneracy, some terms which have been transformed into H_2' from H_1 by S Eq. (4), may have resonance denominators and become very large. If this occurs, a modified function S* must be used in place of S so that terms with resonant denominators do not appear in the transformed Hamiltonian H_2'. The modified function S* is discussed and listed by Nielsen[25] and Herman and Shaffer.[3]

Coriolis Interaction

For a non-linear triatomic molecule such as H_2Te, where ω_1 is very nearly equal to ω_3, a Coriolis resonance does occur between states (v_1,v_2,v_3) and $(v_1\mp1,v_2,v_3\mp1)$, which leads to resonant denominator terms in H_2'. The modified function S* used in place of S in Eq.(4) now leaves the transformed Hamiltonian with H_1' non-zero and equal to

$$G_z(q_1p_3 - q_3p_1)P_z \quad , \tag{35}$$

and changes the molecular constant C [see Eq. (10)] to C* :

$$C^* = C_e - \sum_i \alpha_i^{C^*}(v_i+\tfrac{1}{2}) \tag{36}$$

where

$$\alpha_1^{C*} \neq \alpha_1^C$$

$$\alpha_2^{C*} = \alpha_2^C$$

$$\alpha_3^{C*} \neq \alpha_3^C \quad .$$

The explicit definitions of α_i and α_i^* will be given by Snyder.[4] The other terms in the transformed Hamiltonian are the same as before. In cm^{-1} G_z is

$$G_z = -\zeta_{13}(\omega_1+\omega_3)C_e/(\omega_1\omega_3)^{1/2} \quad , \tag{37}$$

where ζ_{13}, the Coriolis coupling coefficient for a non-linear XYX molecule is

$$\zeta_{13} = [(C_e/A_e)^{1/2}\cos\gamma - (C_e/B_e)^{1/2}\sin\gamma \,] \quad . \tag{38}$$

2nd Order Distortion Interaction

Upon examination of the transformed Hamiltonian, as suggested by Clough and Kneizys,[26] another interaction term

$$G_{xy}q_1q_3(P_xP_y - P_yP_x) \tag{39}$$

is found in H_2' which has non-zero vibrational matrix elements $\langle v_1,v_2,v_3|v_1\pm1,v_2,v_3\mp1\rangle$, connecting the same states as the Coriolis term, and is large enough that it cannot be ignored. This is a term which orginated in the untransformed H_2 Eq. (2). In cm^{-1} G_{xy} is

$$G_{xy} = -6(1/\omega_1\omega_3)^{1/2}A_eB_e[(C_e/A_e)^{1/2}\cos\gamma+(C_e/B_e)^{1/2}\sin\gamma] \quad . \tag{40}$$

The above two interaction terms also have the non-zero matrix elements $\langle v_1,v_2,v_3|v_1\pm1,v_2,v_3\pm1\rangle$, but as noted by Wilson,[12] since the energies of the interacting states must be reasonably close together for any effect to be observed, the interaction is seen only between the states (v_1,v_2,v_3) and $(v_1\pm1,v_2,v_3\mp1)$.

For H_2Te, some of the states that satisfy the requirements for these interactions to be observed are, ν_1 and ν_3, $\nu_1+\nu_2$ and $\nu_2+\nu_3$, $2\nu_1$ and $\nu_1+\nu_3$, $\nu_1+\nu_3$ and $2\nu_3$, $2\nu_1+\nu_2$ and $\nu_1+\nu_2+\nu_3$, $\nu_1+\nu_2+\nu_3$ and $\nu_2+2\nu_3$. Note that $\nu_1+\nu_3$ interacts with both $2\nu_1$ and $2\nu_3$, thus, an analysis of any of these states should include all three, even though one may be too weak to be observed. The same situation is true of the three bands $2\nu_1+\nu_2$, $\nu_1+\nu_2+\nu_3$, and $\nu_2+2\nu_3$.

The interaction terms which must be added to the Hamiltonian when analyzing these interacting bands is

$$H_I = G_z(q_1p_3-q_3p_1)P_z + G_{xy}q_1q_3(P_xP_y-P_yP_x) \quad . \tag{41}$$

The matrix elements of these operators are given in Appendix I.

Treatment of Two Interacting States

The two interacting states $\nu_1+\nu_2$ and $\nu_2+\nu_3$ will be considered in more detail. As mentioned earlier, each J block of the matrix elements of the Hamiltonian without the interaction terms may be factored into four submatrices

for each state, E_1^+, E_1^-, O_1^+, O_1^-, and E_3^+, E_3^-, O_3^+, O_3^-. The subscripts 1 and 3 refer to states $\nu_1+\nu_2$ and $\nu_2+\nu_3$ respectively. Similarly, each J block of the matrix elements of the Hamiltonian including the interaction terms may be factored into the four submatrices $(E_1^+ + E_3^-)$, $(E_3^+ + E_1^-)$, $(O_1^+ + O_3^-)$, and $(O_3^+ + O_1^-)$. The matrix elements of the interaction terms connect the submatrices of the states 1 and 3. The general form of $(E_1^+ + E_3^-)$ is shown in Fig. 2 and that of $(O_1^+ + O_3^-)$ in Fig. 3. The E_{KK}^i, are the matrix elements of the Hamiltonian in the basis set $\Psi(J,K,\gamma)$ for the vibrational state i, and E_{LL}^{ij}, are the matrix elements of the interaction terms of Eq. (41) connecting states i and j. The matrices $(E_3^+ + E_1^-)$ and $(O_3^+ + O_1^-)$ are obtained by interchanging the superscripts 1 and 3 on E_{KK}^j, and E_{LL}^{ij}, and the subscripts 1 and 3 on ψ_i.

The wave functions $A(V,J,\tau)$ which diagonalize the Hamiltonian with the interaction are now combinations of not only the rotational basis set $\Psi(J,K,\gamma)$, but also of the vibrational wave functions ψ_v of the two states involved. The basis set of wave functions is

$$\Phi_i = \psi_v \Psi(J,K,\gamma)$$

where v = 1 or 3. The $A(V,J,\tau)$ are linear combinations of the Φ_i:

$$A(V,J,\tau) = \sum_i S_i^{VJ\tau} \Phi_i \quad , \tag{42}$$

Fig. 2. Elements of the Submatrix $(E_1^+ + E_3^-)$

	Φ_1	Φ_2	Φ_3	Φ_4	.	.	Φ_L	Φ_{L+1}	Φ_{L+2}	Φ_{L+3}	.	.	Φ_N
$\Phi_1 = \psi_1\Psi(J,0,e)$	E^1_{00}	E^1_{02}	E^1_{04}	0	.	.	.	$E^{13}_{1,L+1}$	0	.	.	.	.
$\Phi_2 = \psi_1\Psi(J,2,e)$	E^1_{20}	E^1_{22}	E^1_{24}	E^1_{26}	0	.	.	$E^{13}_{2,L+1}$	$E^{13}_{2,L+2}$	0	.	.	.
$\Phi_3 = \psi_1\Psi(J,4,e)$	E^1_{40}	E^1_{42}	E^1_{44}	E^1_{46}	.	.	.	$E^{13}_{3,L+1}$	$E^{13}_{3,L+2}$	$E^{13}_{3,L+3}$	0	.	.
$\Phi_4 = \psi_1\Psi(J,6,e)$	0	E^1_{62}	E^1_{64}	E^1_{66}	.	.	.	0	$E^{13}_{4,L+2}$	$E^{13}_{4,L+3}$	.	.	.
.	.	0	.	.	.	.	.	.	0	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.	.	.	.
$\Phi_L = \psi_1\Psi(J,K,e)$	.	.	.	.	.	.	.	.	.	.	.	.	.
$\Phi_{L+1} = \psi_3\Psi(J,2,o)$	$E^{31}_{L+1,1}$	$E^{31}_{L+1,2}$	$E^{31}_{L+1,3}$	0	.	.	.	E^3_{22}	E^3_{24}	E^3_{26}	0	.	.
$\Phi_{L+2} = \psi_3\Psi(J,4,o)$	0	$E^{31}_{L+2,2}$	$E^{31}_{L+2,3}$	$E^{31}_{L+2,4}$	0	.	.	E^3_{42}	E^3_{44}	E^3_{46}	.	.	.
$\Phi_{L+3} = \psi_3\Psi(J,6,o)$	.	0	$E^{31}_{L+3,3}$	$E^{31}_{L+3,4}$	.	.	.	E^3_{62}	E^3_{64}	E^3_{66}	.	.	.
.	.	.	0	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.	.	.	.
$\Phi_N = \psi_3\Psi(J,K,o)$	.	.	.	.	.	.	.	.	.	.	.	.	.

Fig. 3. Elements of the Submatrix $(O_1^+ + O_3^-)$

	Φ_1	Φ_2	Φ_3	.	.	Φ_L	Φ_{L+1}	Φ_{L+2}	Φ_{L+3}	.	.	Φ_N
$\Phi_1 = \psi_1\Psi(J,1,e)$	E^1_{11}	E^1_{13}	E^1_{15}	0	.	.	$E^{13}_{1,L+1}$	$E^{13}_{1,L+2}$	0	.	.	.
$\Phi_2 = \psi_1\Psi(J,3,e)$	E^1_{31}	E^1_{33}	E^1_{35}	.	.	.	$E^{13}_{2,L+1}$	$E^{13}_{2,L+2}$	$E^{13}_{2,L+3}$	0	.	.
$\Phi_3 = \psi_1\Psi(J,5,e)$	E^1_{51}	E^1_{53}	E^1_{55}	.	.	.	0	$E^{13}_{3,L+2}$	$E^{13}_{3,L+3}$	.	.	.
.	0	.	.	.	.	.	.	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.	.	.
$\Phi_L = \psi_1\Psi(J,K,e)$	.	.	.	.	.	.	.	.	.	.	.	.
$\Phi_{L+1} = \psi_3\Psi(J,1,o)$	$E^{31}_{L+1,1}$	$E^{31}_{L+1,2}$	0	.	.	.	E^3_{11}	E^3_{13}	E^3_{15}	0	.	.
$\Phi_{L+2} = \psi_3\Psi(J,3,o)$	$E^{31}_{L+2,1}$	$E^{31}_{L+2,2}$	$E^{31}_{L+2,3}$	0	.	.	E^3_{31}	E^3_{33}	E^3_{35}	.	.	.
$\Phi_{L+3} = \psi_3\Psi(J,5,o)$	0	$E^{31}_{L+3,2}$	$E^{31}_{L+3,3}$	.	.	.	E^3_{51}	E^3_{53}	E^3_{55}	.	.	.
.	.	0	.	.	.	.	0	.	.	.	.	.
.	.	.	.	.	.	.	.	.	.	.	.	.
$\Phi_N = \psi_3\Psi(J,K,o)$	.	.	.	.	.	.	.	.	.	.	.	.

where the sum is over only those wave functions of the two interacting submatrices involved.

The energy of a given vibration-rotation state is the expectation value of the Hamiltonian in the representation $A(V,J,\tau)$:

$$E(V,J,\tau) = \langle VJ\tau|H|VJ\tau\rangle = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} H_{ij} \quad , \tag{43}$$

where

$$H_{ij} = \int \Phi_i^* H \Phi_j dV = \int \psi_v^* \Psi^*(J,K,\gamma) H \psi_{v'} \Psi(J',K',\gamma') dV \quad .$$

It is convenient to separate the sum in Eq. (43) into three parts:

$$\begin{aligned} E(V,J,\tau) = & \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} H_{ij}^1 \\ & + \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} H_{ij}^3 \\ & + \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} H_{ij}^{13} \quad , \end{aligned} \tag{44}$$

where H_{ij}^1 are the matrix elements of the Hamiltonian in state 1 ($\nu_1+\nu_2$), H_{ij}^3 are the matrix elements of the Hamiltonian in state 3 ($\nu_2+\nu_3$), and H_{ij}^{13} are the interaction matrix elements connecting states 1 and 3.

The Hamiltonian may be broken up into its various components such that Eq. (44) becomes

$$\begin{aligned} E(V,J,\tau) = & \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} [\nu_o^{(1)} + A^{(1)} (P_x^2)_{ij} + B^{(1)} (P_y^2)_{ij} \\ & + C^{*(1)} (P_z^2)_{ij} + \tau_{xxxx}^{(1)} (O_{xxxx})_{ij} + \tau_{yyyy}^{(1)} (O_{yyyy})_{ij} \\ & + \tau_{xxyy}^{(1)} (O_{xxyy})_{ij} + \tau_{xyxy}^{(1)} (O_{xyxy})_{ij}] \\ & + \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} [\nu_o^{(3)} + A^{(3)} (P_x^2)_{ij} + B^{(3)} (P_y^2)_{ij} \end{aligned} \tag{45}$$

$$+ C^{*(3)}(P_z^2)_{ij} + \tau^{(3)}_{xxxx}(O_{xxxx})_{ij} + \tau^{(3)}_{yyyy}(O_{yyyy})_{ij}$$

$$+ \tau^{(3)}_{xxyy}(O_{xxyy})_{ij} + \tau^{(3)}_{xyxy}(O_{xyxy})_{ij}]$$

$$+ \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau}[G_z(q_1p_3 - q_3p_1)_{ij}(P_z)_{ij}$$

$$+ G_{xy}(q_1q_3)_{ij}(P_xP_y - P_yP_x)_{ij}] \quad .$$

The three sums in both Eqs. (44) and (45) are not each summed over all i and j. The first is summed over only the i and j of state 1, the second over only the i and j of state 3, and the third over only the i and j which connect states 1 and 3.

To aid in the calculations, we can use the relation for any hermitian operator F,

$$\sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} F_{ij} = \sum_i |S_i^{VJ\tau}|^2 F_{ii} + 2\mathrm{Re}\sum_{i<j} \sum (S_i^{VJ\tau})^* S_j^{VJ\tau} F_{ij} \quad . \tag{46}$$

Consideration of higher order P^6 type distortion terms results in the addition of the four terms of Eq. (21) to both the first and second sums of Eq. (45).

The energy including these four terms may be expressed

$$E(VJ\tau) = \chi_o^{(1)}\nu_o^{(1)} + \alpha^{(1)}A^{(1)} + \beta^{(1)}B^{(1)} + \gamma^{(1)}C^{*(1)} \tag{47}$$

$$+ \chi_1^{(1)}\tau^{(1)}_{xxxx} + \chi_2^{(1)}\tau^{(1)}_{yyyy} + \chi_3^{(1)}\tau^{(1)}_{xxyy} + \chi_4^{(1)}\tau^{(1)}_{xyxy}$$

$$+ \chi_5^{(1)}H_J^{(1)} + \chi_6^{(1)}H_{JK}^{(1)} + \chi_7^{(1)}H_{KJ}^{(1)} + \chi_8^{(1)}H_K$$

$$+ \chi_o^{(3)}\nu_o^{(3)} + \alpha^{(3)}A^{(3)} + \beta^{(3)}B^{(3)} + \gamma^{(3)}C^{*(3)}$$

$$+ \chi_1^{(3)}\tau_{xxxx}^{(3)}+\chi_2^{(3)}\tau_{yyyy}^{(3)}+\chi_3^{(3)}\tau_{xxyy}^{(3)}+\chi_4^{(3)}\tau_{xyxy}^{(3)}$$

$$+ \chi_5^{(3)}H_J^{(3)}+\chi_6^{(3)}H_{JK}^{(3)}+\chi_7^{(3)}H_{KJ}^{(3)}+\chi_8^{(3)}H_K^{(3)}$$

$$+ \chi_9 G_z + \chi_{10} G_{xy} \quad .$$

The superscript 1 is for state $(\nu_1+\nu_2)$ and 3 for $(\nu_2+\nu_3)$. The α, β, γ, and χ_i represent the average values of the operators and are calculated with the expressions

$$\chi_o^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} \tag{48}$$

$$\alpha^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (P_x^2)_{ij}$$

$$\beta^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (P_y^2)_{ij}$$

$$\gamma^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (P_z^2)_{ij}$$

$$\chi_1^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (O_{xxxx})_{ij}$$

$$\chi_2^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (O_{yyyy})_{ij}$$

$$\chi_3^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (O_{xxyy})_{ij}$$

$$\chi_4^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (O_{xyxy})_{ij}$$

$$\chi_5^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} J^3 (J+1)^3$$

$$\chi_6^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (P_z^2)_{ij} J^2 (J+1)^2$$

$$\chi_7^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (P_z^4)_{ij} J(J+1)$$

$$\chi_8^{(n)} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (P_z^6)_{ij}$$

$$\chi_9 = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (q_1 p_3 - q_3 p_1)_{ij} (P_z)_{ij}$$

$$\chi_{10} = \sum_i \sum_j (S_i^{VJ\tau})^* S_j^{VJ\tau} (q_1 q_3)_{ij} (P_x P_y - P_y P_x)_{ij}$$

where n may be 1 or 3 and the sums of $\alpha^{(n)}$, $\beta^{(n)}$, $\gamma^{(n)}$, and $\chi_o^{(n)}$ through $\chi_8^{(n)}$ are over only those i and j of the state n, while the sums of χ_9 and χ_{10} are over only those i and j which connect states 1 and 3.

Computer Programs

Several more programs were written to aid in the analysis of the two interacting bands $\nu_1+\nu_2$ and $\nu_2+\nu_3$.

1. SPEC-FIT 1

Ground state constants, upper state constants and band center for both bands, perturbation constants G_z and G_{xy}, and all the frequencies of the assigned transitions with their quantum numbers are input. Using the constants that are input, the computer calculates a spectrum and the average values of all the operators for the upper state levels, and then fits the differences between the observed and calculated frequencies to Eq. (49) to obtain revised values of the upper state constants of both bands and G_z and G_{xy}.

$$\begin{aligned} \nu_{obs}-\nu_{calc} = \sum_n [&\chi_o^{(n)} \Delta\nu_o^{(n)} + \alpha^{(n)} \Delta A^{(n)} + \beta^{(n)} \Delta B^{(n)} \\ &+ \gamma^{(n)} \Delta C^{(n)} + \sum_{i=1}^{4} \chi_i^{(n)} \Delta\tau_i^{(n)} \\ &+ \sum_{i=1}^{8} \chi_i^{(n)} \Delta H_i^{(n)}] + \chi_9 \Delta G_z + \chi_{10} \Delta G_{xy} \end{aligned} \qquad (49)$$

In this equation n is equal to 1 and 3.

A listing of program SPEC-FIT 1 is in Appendix VI.

2. CORIOLIS

Ground state constants, upper state constants and band center for both bands are input along with the perturbation constants G_z and G_{xy}. The energies of all the upper state levels of both bands with and without the perturbation terms are calculated by the computer. The perturbed calculation, unperturbed calculation and their difference are printed out for each level. This calculation allows one to see the effect the perturbation has on the individual levels. Optionally, the matrix elements of the Hamiltonian before diagonalization and the eigenvectors of the diagonalized Hamiltonian may be printed out.

CHAPTER IV

THE INFRARED SPECTRA OF H_2Te

Previous spectroscopic work on hydrogen telluride has been quite limited. The far ultra-violet absorption spectra of H_2Te was reported on by Price, Teegan, and Walsh (1950).[27] The work of Rossmann and Straley[28] produced a prism spectrum of ν_2 near 860 cm^{-1} and a prism-grating spectrum of ν_1 and ν_3 which are overlapped near 2070 cm^{-1}. From these they determined approximate values for the molecular constants. In 1964 Hill, Edwards, Rossmann, Rao, and Nielsen[29] gave an analysis of a high-resolution ($\approx$0.1 cm^{-1}) spectrum of ν_2 from which they obtained values for both ground and upper state molecular constants.

This work will consider the combination bands $\nu_1+\nu_2$, $\nu_2+\nu_3$, $2\nu_1$, $\nu_1+\nu_3$, two bands near 4900 cm^{-1}, and a re-analysis of the fundamental ν_2.

Hydrogen telluride is an oblate planar asymmetric molecule and is the most nearly symmetric member of a series of asymmetric molecules which include H_2O, H_2S, and H_2Se. The geometry and normal modes of vibration of H_2Te are given in Figs. 4 and 5. As the figure shows, it is a non-linear triatomic molecule with a bond angle

Fig. 4. Geometry of H_2Te

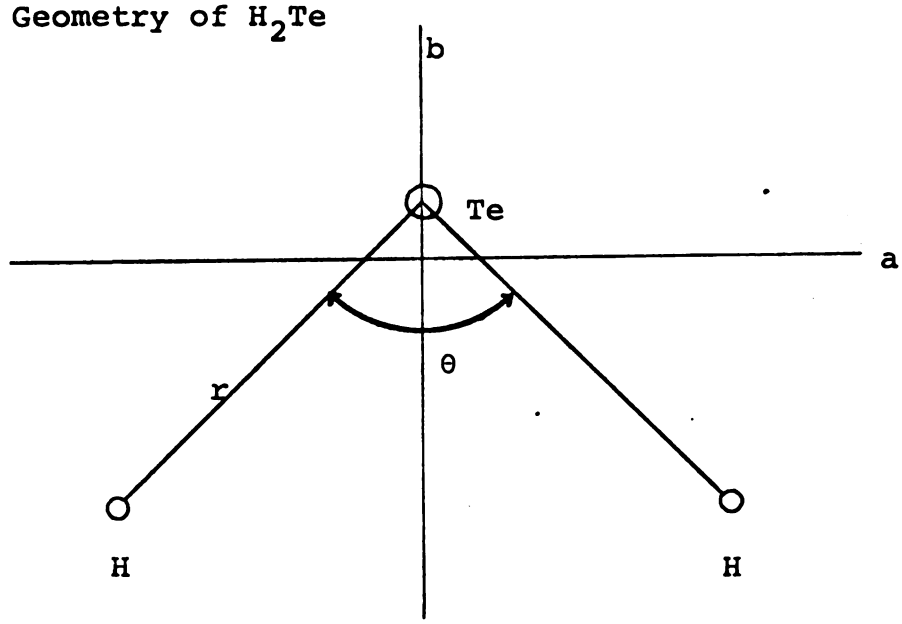
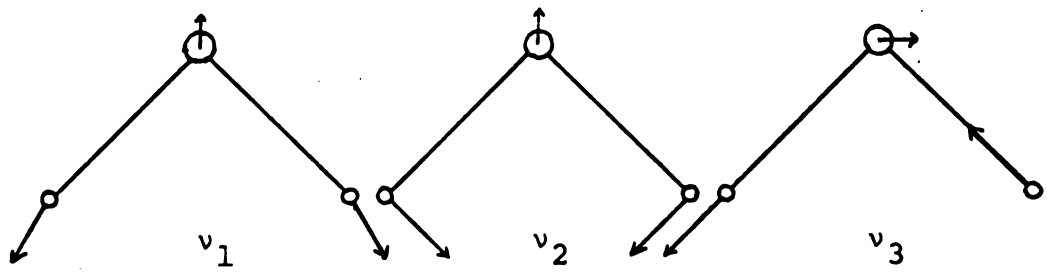


Fig. 5. Normal Modes of H_2Te



near 90°.

Preparation of H_2Te

The gas sample of hydrogen telluride was prepared by reacting powdered aluminum telluride with distilled water as discribed by Moser and Ertl.[30] The reaction is given by

$$Al_2Te_3 + 6H_2O \rightarrow 3H_2Te + 2Al(OH)_3 \quad . \tag{50}$$

A diagram of the apparatus used in the production of the gas is shown in Fig. 6. Small amounts of powdered aluminum telluride were allowed to fall on frozen distilled water in the reaction chamber. The reaction went slowly at first, but sped up when the heat of reaction began to melt the ice. The resulting gas was then passed through a drying tube and collected in the liquid nitrogen cold traps. The system was kept under a vacuum to draw the gas from the reaction chamber to the cold traps. Since any H_2Te that passed beyond the cold traps would contaminate the oil of the vacuum pump, a 5 gallon jar was evacuated and used as a vacuum in place of the pump. A bypass around the first cold trap was provided in the event the center tube plugged up. The most successful run produced a 58% yield of 23 grams of H_2Te from 45 grams of Al_2Te_3 and 80 grams H_2O. Care must be exercised when working with H_2Te since it is a very poisonous gas. It readily decomposes at room temperature or in the presence of H_2O, O_2 or ultraviolet light, so

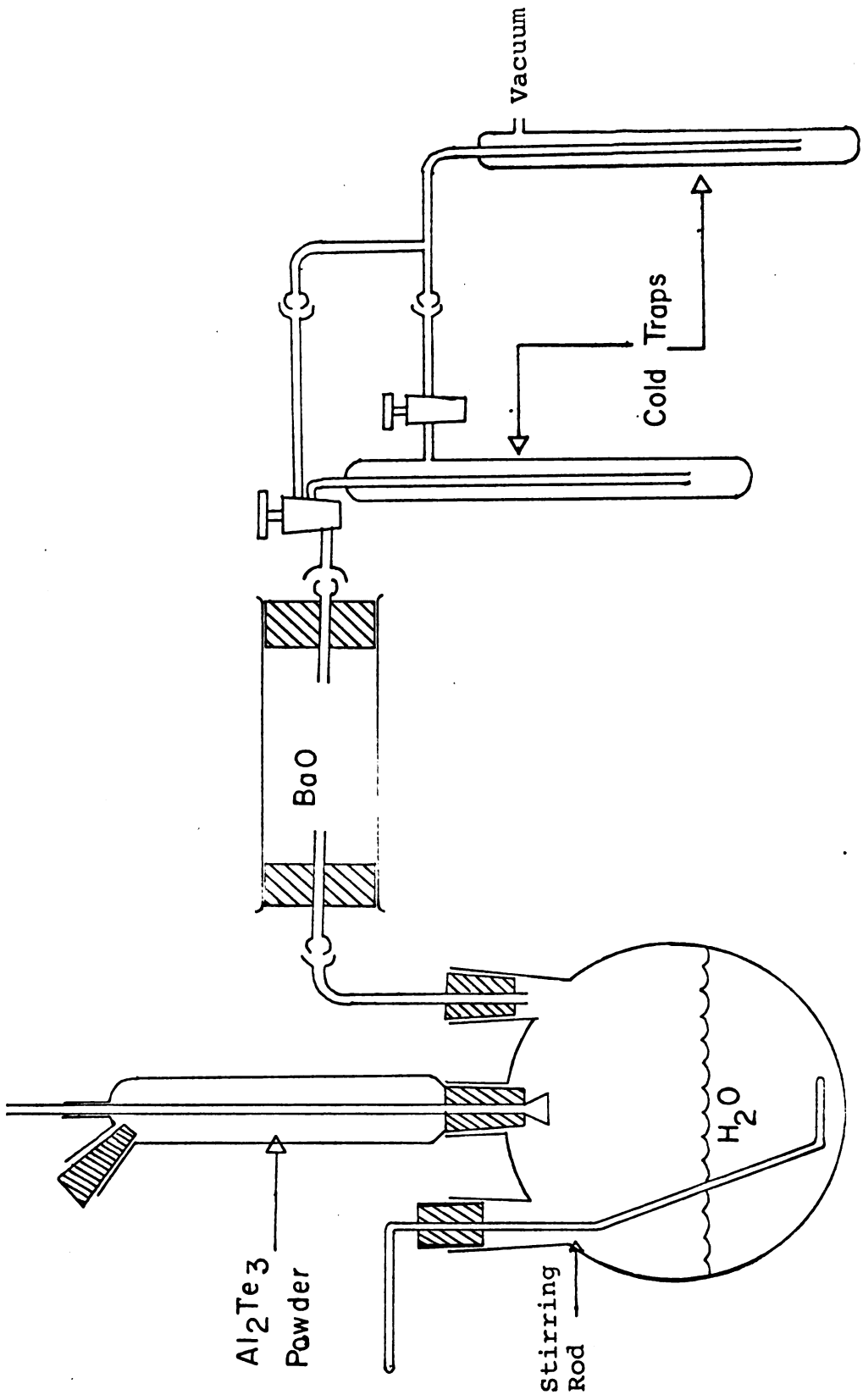


Fig 6. Apparatus for Production of H_2Te

the sample was kept as pure as possible and frozen at liquid nitrogen temperatures until used.

Experimental Conditions

The infrared absorption spectrum of H_2Te in the region 1.0 - 3.6μ was obtained with the Michigan State University high resolution infrared spectrometer. The spectrometer, which has been discussed in detail by Aubel[31] and Keck,[32] uses a Littrow-Pfund type nonochromator with 300 line/mm and 600 line/mm gratings mounted back to back on a turntable. In the 1-3 micron region the source used was a 300 watt zirconium arc and the detector a type N lead sulfide photoconductor cooled by liquid nitrogen. Beyond 3 μ a type P lead sulfide detector was used and the source was a zirconium arc box with a sapphire window which transmits radiation with wavelength greater than 3 microns. A small volume coolable multiple traverse cell of the J. U. White type[33,34] was used to hold the gas sample. All spectra were run with the cell maintained at -50° C by circulating methyl alcohol, cooled by heat exchange with dry ice and acetone, through the cooling coils of the cell.

The frequencies of the infrared lines were obtained by interpolating between fringes of constant frequency spacing which were recorded simultaneously with the infrared spectra.[35] These fringes were obtained from Edser-Butler bands produced by a Fabry-Perot etalon of ≈3 mm

spacing. The fringes were calibrated by recording both before and after the spectrum of interest, the absorption lines of molecules which have been accurately measured by Rank and co-workers.[36,37,38]

Infrared Absorption Bands of H_2Te

Strong absorption bands of H_2Te were found near 2900 cm^{-1} and 4050 cm^{-1}, with weaker bands near 4900 cm^{-1}. Slow speed slave recordings of these bands are shown in Figs. 7, 8, and 9.

Throughout the 2900 cm^{-1} region may be seen strong absorption lines of the (1-0) band of HCl which was used as a calibration gas before the H_2Te spectra and could not be entirely removed from the cell. Fortunately the HCl lines are widely spaced and seldom interfer with the H_2Te absorption lines.

The high resolution spectra were recorded on long charts with a resolution limit of 0.05 cm^{-1} at 2900 cm^{-1}, 0.04 cm^{-1} at 4050 cm^{-1}, and 0.06 cm^{-1} at 4900 cm^{-1}. Table III gives the experimental conditions under which the spectra were recorded.

The procedure by which measurments of the lines on the chart were actually made involves photographing the charts and making the measurments on the film by means of a Hydel semiautomatic digitized film reader connected to an IBM 526 card punch. This procedure is given in some detail by Barnett,[39] and in Ref. 35. To help minimize

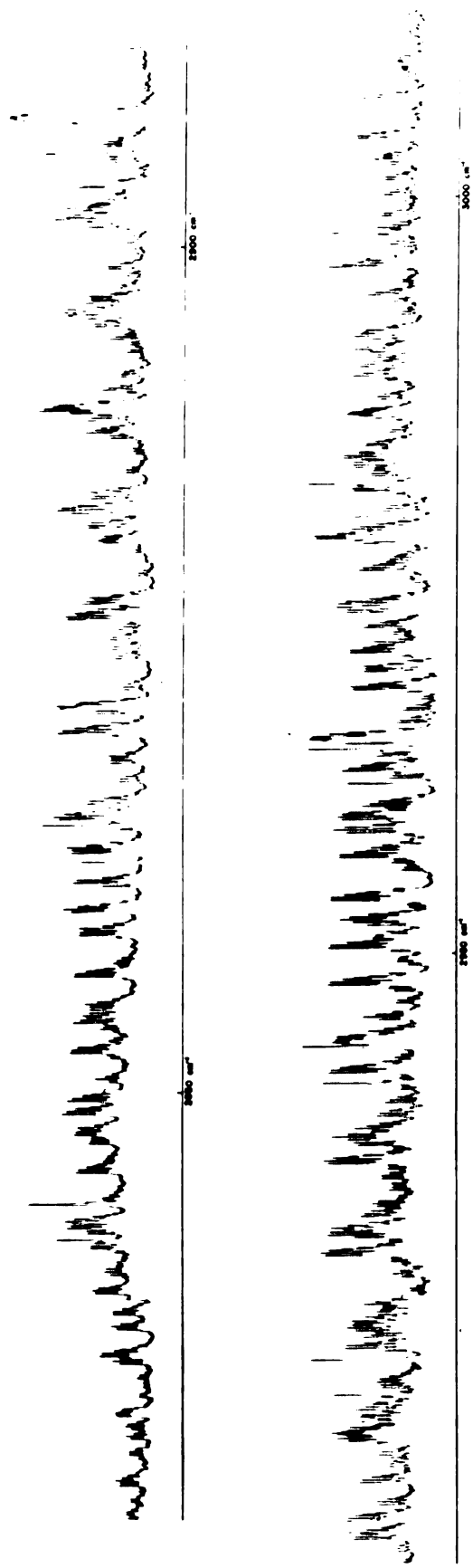
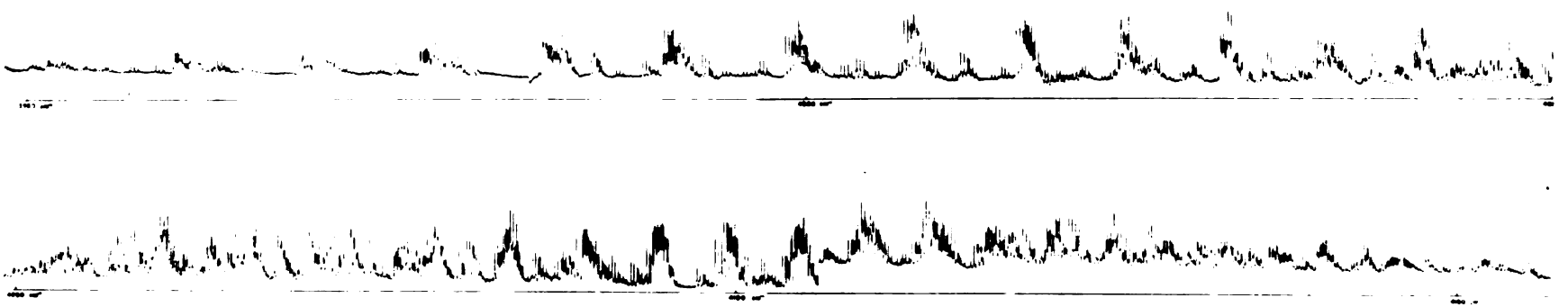


Fig. 7. Absorption Spectra of H_2Te near 2900 cm^{-1}

Fig. 8. Absorption Spectra of H_2Te near 4050 cm^{-1}



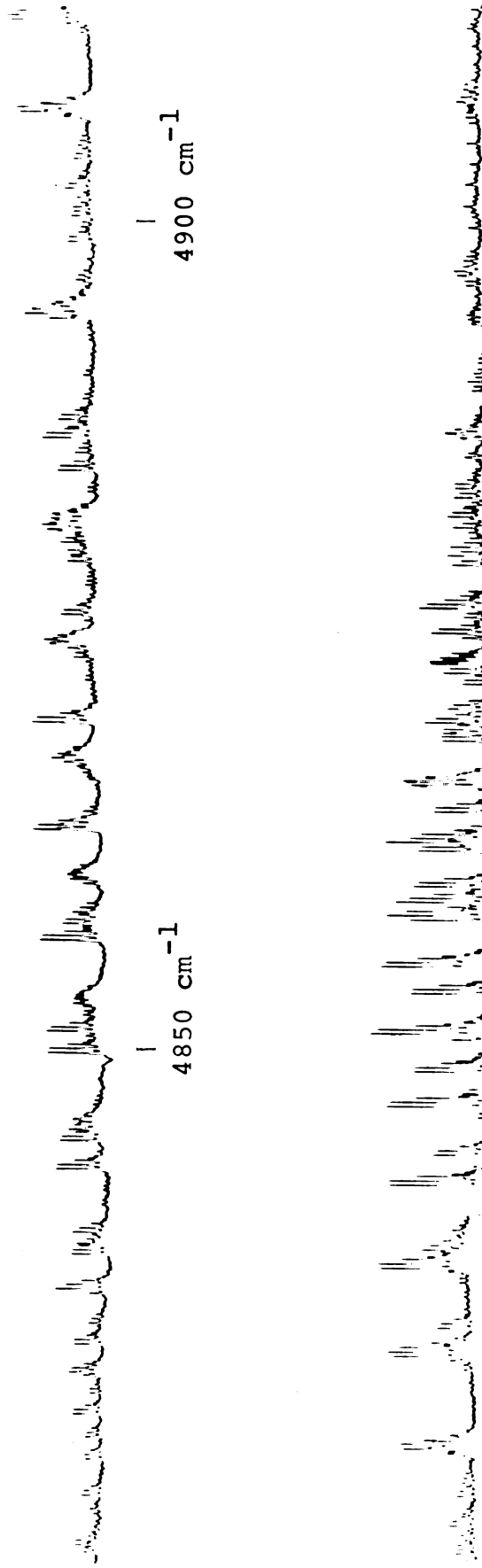


Fig. 9. Absorption Spectra of H_2Te near 4900 cm^{-1}

Table III. Experimental Conditions

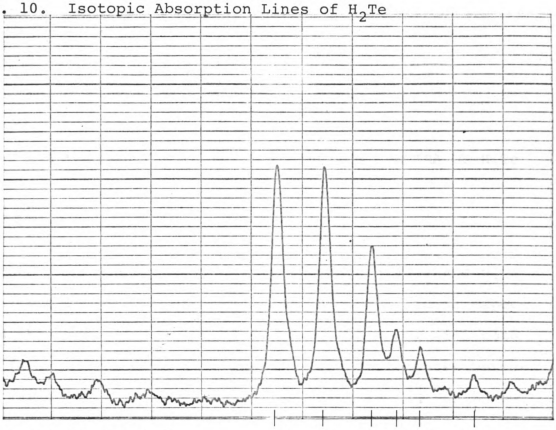
Region, cm^{-1}	2900		4050			4900	
Chart No.	6	7	3	5	9	4	8
Gas Pressure, mm	20	25	6	10-32	10-44	76	86
Gas Temperature	-50°C	-50°C	-50°C	-50°C	-50°C	-50°C	-50°C
Path Length in Cell, m	6.6	6.6	6.6	6.6	6.6	6.6	6.6
Source	Zirc. arc box		300 watt arc			300 watt arc	
Detector	PbS-P	PbS-P	PbS-N	PbS-N	PbS-N	PbS-N	PbS-N
Spectral Slitwidth, μ	20	21	14	14	15	16	16
Grating, lns/mm	300	300	300	300	300	300	300
Fringe Separation, cm^{-1}	0.26794	0.26795	0.32157	0.32157	0.32155	0.40194	0.40195
Resolution, cm^{-1}	0.05	0.05	0.04	0.04	0.04	0.06	0.06
Calibration Gases	HCl(1-0) HCN(0,0,1)		HCl(2-0) CO(2-0)			N_2O(2,0,1) HCN(1,0,1)	
Standard Deviation of Calibration Fit	0.0038	0.0036	0.0027	0.0024	0.0017	0.0028	0.0024

any experimental error, at least two recordings of the spectrum in each region were made (three in the 4050 cm^{-1} region). Each of these charts were individually measured and calibrated, and the frequencies obtained from charts of the same regions were averaged.

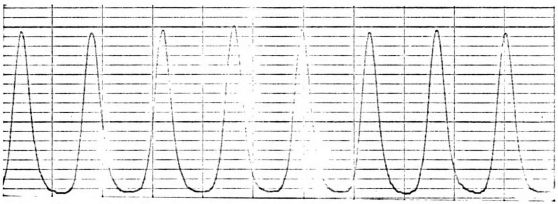
Isotopic Species of H_2Te

Tellurium in its natural state has the 6 isotopes ^{130}Te, ^{128}Te, ^{126}Te, ^{125}Te, ^{124}Te, and ^{122}Te occuring with percent abundance 34, 32, 19, 7, 5, and 2 respectively. The absorption lines of the 6 molecular species of H_2Te have been well resolved in all the bands recorded. A small region near 4980 cm^{-1} which clearly shows this isotope effect is reproduced in Fig. 10. Since $H_2{}^{130}Te$ had the strongest absorption lines, these were analyzed in detail first. It was then a relatively simple matter to analyze the other molecular species by working with the appropriate lines just to the right of the corresponding $H_2{}^{130}Te$ line. Unfortunately, many of these lines, especially those of the less abundent species, were blended or masked by other stronger transitions of another isotopic species, and could not be used in an analysis.

Fig. 10. Isotopic Absorption Lines of H_2Te



Tellurium Isotope	130	128	126	125	124	122
Percent Abundance	34	32	19	7	5	2



CHAPTER V

ANALYSIS OF THE INFRARED ABSORPTION SPECTRA OF H_2Te

The 2900 cm^{-1} Region

From Eq. (18) and the fact that ν_2 of H_2Te is at 860 cm^{-1} and a survey of the fundamentals ν_1 and ν_3 indicate they are overlapped near 2070 cm^{-1}, it is expected that the combination bands $\nu_1+\nu_2$ and $\nu_2+\nu_3$ will both be found in the 2900 cm^{-1} region. The differences between the sums of the fundamental frequencies and the observed band centers of the combination bands is due to the anharmonicities in the vibrations and any vibrational resonances that may exist in the band under consideration. Examination of the spectrum near 2900 cm^{-1} reveals several regularly spaced series of lines proceeding out in both directions from a group of strongly gathered lines near the center of the absorption region. The regularly spaced series were assigned as zero series ($^{R}R_{J}(J)$ and $^{P}P_{J}(J)$), first series ($^{R}R_{J-1}(J)$ and $^{P}P_{J-1}(J)$), second series ($^{R}R_{J-2}(J)$ and $^{P}P_{J-2}(J)$), etc. lines and the gathered lines assumed to be unresolved Q branch transitions of a type A band. Attempts to identify the gathered lines and the first few members of the series which are split because of the asymmetry, indicated that these

series and gathered lines were not those of an A band, but those of a type B band where the gathered lines were the $^{R}Q_{0}(J)$ transitions. After the band was assigned as a B band ($\nu_1+\nu_2$) with band center at 2911.42 cm^{-1}, most of the stronger and many of the weak lines in this region were identified and assigned to that band. After most of the transitions of the B band had been identified, several weaker series of unassigned lines were noted which eventually led to the identification of the type A band ($\nu_2+\nu_3$) with band center at 2915.97 cm^{-1}. This band was found to be much weaker than $\nu_1+\nu_2$ and many lines were masked, however, enough lines were identified to allow an analysis.

The ground state combination differences formed from the observed lines in these two bands were combined with those formed from the bands near 4050 cm^{-1} and used in a ground state analysis.

Although, as noted earlier, the upper states of $\nu_1+\nu_2$ and $\nu_2+\nu_3$ perturb each other, the initial analyses of both these upper states were made ignoring the interaction and the bands were fit separately to Eq. (32) holding the ground state constants obtained from the ground state analysis fixed and varying only the upper state constants. Even though the fits by this method were poor they allowed many assignments in both bands to be made. From Eqs. (37) and (40), initial estimates of

G_z and G_{xy} were made which were used along with the upper state constants from the single band fits as starting values to simultaneously fit the bands $\nu_1+\nu_2$ and $\nu_2+\nu_3$ to Eq. (49). The simultaneous analysis of the two bands including the the interaction terms gave a very good fit and helped to identify many more lines that were badly perturbed. One of the most notably affected series of lines were the lines of the $^{P}Q_1(J)$ series of $\nu_1+\nu_2$. Although these lines were strong and easily identified, they fit very poorly in the single band fit in which the interaction was ignored, the deviations being as large as 0.5 cm^{-1}. When these same lines were used in the perturbation analysis, they very well, with most deviations no larger than 0.01 cm^{-1}. The results of the simultaneous analysis of $\nu_1+\nu_2$ and $\nu_2+\nu_3$ are given in Tables IV, V, and VI. The ranges of the constants are for a simultaneous confidence interval of 95% which is about 6 times the standard error in these fits. The constants in the tables are given to six numbers past the decimal for $H_2{}^{130}Te$ so that future calculations will agree with those given in the appendicies. The significant integers may be determined from the simultaneous confidence intervals. All fits were made holding the ground state constants fixed at the values obtained from the ground state analysis. The assigned transitions of $\nu_1+\nu_2$ and $\nu_2+\nu_3$ for $H_2{}^{130}Te$ are listed in Appendix II, and Appendix V lists the calculated upper state energy levels for these two bands both with and

Table IV. Molecular Constants of $H_2{}^{130}Te$ for the States $\nu_1+\nu_2$ and $\nu_2+\nu_3$, (cm^{-1})

State	$\nu_1+\nu_2$	$\nu_2+\nu_3$
ν_o	2911.4157 ±0.0074	2915.9697 ±0.019
A	6.347845 ±0.0018	6.319069 ±0.0047
B	6.136936 ±0.0017	6.165087 ±0.0042
C^*	2.960471 ±0.00035	2.975441 ±0.0011
τ_{aaaa}	-0.003776 ±0.00013	-0.004229 ±0.00083
τ_{bbbb}	-0.003125 ±0.00008	-0.003736 ±0.00042
τ_{aabb}	+0.003113 ±0.00006	+0.003769 ±0.00070
τ_{abab}	-0.000953 ±0.00006	-0.000471 ±0.00028
H_K	-34×10^{-9} $\pm3\times10^{-9}$	-188×10^{-9} $\pm96\times10^{-9}$
κ	+0.876	+0.908
No. of pts.	199	47
G_z	+0.025882 ±0.033	
G_{xy}	-0.164134 ±0.0031	
Total No. of pts.	246	
Std. Dev.	0.007	

Table V. Molecular Constants of $H_2{}^{128}Te$ for the States $\nu_1+\nu_2$ and $\nu_2+\nu_3$.

State	$\nu_1+\nu_2$	$\nu_2+\nu_3$
ν_o	2911.583 ±0.010	2916.146 ±0.027
A	6.3488 ±0.0022	6.3176 ±0.0053
B	6.1369 ±0.0019	6.1659 ±0.0050
C^*	2.96089 ±0.00048	2.9755 ±0.0018
τ_{aaaa}	-0.00376 ±0.00015	-0.00376 ±0.00097
τ_{bbbb}	-0.00312 ±0.00009	-0.00356 ±0.00046
τ_{aabb}	+0.00311 ±0.00007	+0.00351 ±0.00090
τ_{abab}	-0.00096 ±0.00006	-0.00063 ±0.00036
H_K	-37×10^{-9} $\pm5\times10^{-9}$	-181×10^{-9} $\pm262\times10^{-9}$
κ	+0.875	+0.909
No. of pts.	167	35
G_z	+0.033 ±0.036	
G_{xy}	-0.1651 ±0.0034	
Total No. of pts.	202	
Std. Dev.	0.008	

Table VI. Molecular Constants of $H_2{}^{126}Te$ for the States $\nu_1+\nu_2$ and $\nu_2+\nu_3$.

State	$\nu_1+\nu_2$	$\nu_2+\nu_3$
ν_o	2911.752 ±0.008	2916.318 ±0.037
A	6.3506 ±0.0019	6.3216 ±0.0070
B	6.1378 ±0.0019	6.1662 ±0.0052
C^*	2.96171 ±0.00048	2.9762 ±0.0028
τ_{aaaa}	-0.00382 ±0.00014	-0.00417 ±0.00100
τ_{bbbb}	-0.00309 ±0.00007	-0.00353 ±0.00050
τ_{aabb}	+0.00311 ±0.00007	+0.00342 ±0.00160
τ_{abab}	-0.00099 ±0.00007	-0.00053 ±0.00081
H_K	-42×10^{-9} $\pm6\times10^{-9}$	-118×10^{-9} $\pm500\times10^{-9}$
κ	+0.874	+0.907
No. of pts.	139	20
G_z	+0.047 ±0.030	
G_{xy}	-0.1665 ±0.0029	
Total No. of pts.	159	
Std. Dev.	0.006	

without the interaction terms and the difference. This allows one to see how much each level is perturbed because of the interaction of the two bands. It can be seen for high J low K levels, the perturbation can contribute as much as several cm^{-1} to the energy.

The 4050 cm^{-1} Region

It is expected that the bands $2\nu_1$, $\nu_1+\nu_3$, and $2\nu_3$ will be near the 4050 cm^{-1} region. Darling and Dennison[1] have shown that a vibrational resonance can exist between states of the type (v_1,v_2,v_3) and $(v_1\pm2,v_2,v_3\mp2)$ which tends to push the two states apart. In analogy with H_2S, where the bands $2\nu_1$ and $\nu_1+\nu_3$ were separated by 2.24 cm^{-1} ($2\nu_3$ was not observed)[40], and H_2Se[21] where $2\nu_1$ and $\nu_1+\nu_3$ were separated by 2.04 cm^{-1}, the two bands of $H_2{}^{130}Te$, $2\nu_1$ at 4062.89 cm^{-1} and $\nu_1+\nu_3$ at 4063.37 cm^{-1}, were identified. The band $2\nu_3$ of H_2Te was not observed. The fact that the two bands were very close together and that the zero, first, second, etc. series within each band were nearly coincident, combined with the isotope effect to give the striking feature in this region of strong, badly overlapped series of lines proceeding out in both directions from the band center. Because of this, many lines were blended or masked and could not be used in the analysis. Between these large groups of lines were found weaker lines that were identified as the Q branches.

The ground state combination differences formed from the observed transitions listed in Appendix II. were combined with those formed from the bands near 2900 cm^{-1} and used in a ground state analysis.

As noted earlier, there is an interaction between the upper states of $2\nu_1$ and $\nu_1+\nu_3$, and also between $\nu_1+\nu_3$ and $2\nu_3$. Because of this, an analysis of the upper states of these bands should simultaneously include all three. Unfortunately, $2\nu_3$ of H_2Te was not observed and therefore could not be used in any such analysis. It was expected since $2\nu_1$ and $\nu_1+\nu_3$ were so close together ($\simeq 0.48$ cm^{-1}) and $2\nu_3$ was expected to be about 80 cm^{-1} away, the effect of the interaction between $2\nu_3$ and $\nu_1+\nu_3$ would be much smaller than that between $2\nu_1$ and $\nu_1+\nu_3$ and therefore the effect of $2\nu_3$ could be ignored and the two bands $2\nu_1$ and $\nu_1+\nu_3$ treated as two interacting bands.

The initial analysis of the upper states of $2\nu_1$ and $\nu_1+\nu_3$ ignored all interactions and each band was fit separately to Eq. (32), holding the ground state constants fixed and varying only the upper state constants. By this method many of the lines, such as the zero series and first members of the Q branches which were least affected by the interaction, were assigned and approximate values of the upper state constants were obtained. These constants were used as starting values along with the perturbation terms G_z and G_{xy} obtained from the analysis of the 2900 cm^{-1} region in a fit of the spectrum of $2\nu_1$ and

$\nu_1+\nu_3$ to Eq. (49). When the two bands were fit together with the interaction term included, many lines that were badly perturbed were identified in both bands. A few of the upper state energy levels were extremely sensitive to the values of the constants used, and a small change in the value of a constant resulted in a large change in the energy of that level. Any line that involved such a level was not included in the fit until near the end of the analysis when the constants used were almost the final ones. The results of the simultaneous analysis of $2\nu_1$ and $\nu_1+\nu_3$ are given in Tables VII , VIII , IX , X , and XI. The ranges of the constants are for a simultaneous confidence interval of 95% which for these fits is about 6 times the standard error. All fits were made with the ground state constants held fixed at the values obtained from the ground state analysis.

The definitions of G_z and G_{xy} (Eqs. (37) and (40)), show they are not vibrationally dependent, so one would expect to obtain the same values for these constants from the analysis of $\nu_1+\nu_2$ and $\nu_2+\nu_3$, and from the analysis of $2\nu_1$ and $\nu_1+\nu_3$. Different values of these constants were obtained from the bands in the two regions as can be seen from Tables IV and VII. One reason for this may be because the effect of the interaction of $2\nu_3$ with $\nu_1+\nu_3$ was ignored in the analysis of 4050 cm^{-1} region. Examination of the definition of G_{xy} in Eq. (37) shows that its theoretical value is relatively insensitive to the

Table VII. Molecular Constants of $H_2{}^{130}Te$ for the States $2\nu_1$ and $\nu_1+\nu_3$.

State	$2\nu_1$		$\nu_1+\nu_3$	
ν_o	4062.8902	±0.011	4063.3743	±0.012
A	6.068978	±0.0045	6.063802	±0.0047
B	5.940074	±0.0046	5.946441	±0.0046
C^*	2.956935	±0.00044	2.959565	±0.00052
τ_{aaaa}	-0.003281	±0.00017	-0.003351	±0.00028
τ_{bbbb}	-0.002679	±0.00018	-0.002805	±0.00014
τ_{aabb}	+0.002326	±0.00007	+0.002405	±0.00013
τ_{abab}	-0.000508	±0.000062	-0.000445	±0.00013
H_K	-31×10^{-9}	$\pm6\times10^{-9}$	-22×10^{-9}	$\pm6\times10^{-9}$
κ	+0.917		+0.924	
No. of pts.	214		187	
G_z	+0.011163	±0.0059		
G_{xy}	-0.229786	±0.0018		
Total No. of pts.	401			
Std. Dev.	0.011			

Table VIII. Molecular Constants of $H_2{}^{128}Te$ for the States $2\nu_1$ and $\nu_1+\nu_3$.

State	$2\nu_1$	$\nu_1+\nu_3$
ν_o	4063.109 ±0.012	4063.594 ±0.014
A	6.0695 ±0.0056	6.0636 ±0.0057
B	5.9413 ±0.0056	5.9478 ±0.0053
C^*	2.95761 ±0.00059	2.96078 ±0.00076
τ_{aaaa}	-0.00325 ±0.00022	-0.00312 ±0.00034
τ_{bbbb}	-0.00269 ±0.00021	-0.00282 ±0.00016
τ_{aabb}	+0.00229 ±0.00009	+0.00226 ±0.00016
τ_{abab}	-0.00048 ±0.00008	-0.00050 ±0.00015
H_K	-31×10^{-9} $\pm10\times10^{-9}$	-26×10^{-9} $\pm20\times10^{-9}$
κ	+0.918	+0.925
No. of pts.	179	144
G_z	+0.0134 ±0.0066	
G_{xy}	-0.2303 ±0.0022	
Total No. of pts.	323	
Std. Dev.	0.011	

Table IX. Molecular Constants of $H_2{}^{126}Te$ for the States $2\nu_1$ and $\nu_1+\nu_3$.

State	$2\nu_1$	$\nu_1+\nu_3$
ν_o	4063.340 ±0.016	4063.832 ±0.017
A	6.0685 ±0.0085	6.0630 ±0.0078
B	5.9448 ±0.0081	5.9503 ±0.0075
C^*	2.95846 ±0.00091	2.9599 ±0.0012
τ_{aaaa}	-0.00323 ±0.00034	-0.00308 ±0.00044
τ_{bbbb}	-0.00283 ±0.00033	-0.00279 ±0.00025
τ_{aabb}	+0.00235 ±0.00011	+0.00229 ±0.00022
τ_{abab}	-0.00050 ±0.00010	-0.00064 ±0.00021
H_K	-45×10^{-9} $\pm25\times10^{-9}$	-30×10^{-9} $\pm36\times10^{-9}$
κ	+0.920	+0.927
No. of pts.	134	113
G_z	+0.0166 ±0.0077	
G_{xy}	-0.2317 ±0.0028	
Total No. of pts.	247	
Std. Dev.	0.011	

Table X. Molecular Constants of $H_2{}^{125}Te$ for the States $2\nu_1$ and $\nu_1+\nu_3$.

State	$2\nu_1$	$\nu_1+\nu_3$
ν_o	4063.453 ±0.031	4063.948 ±0.011
A	6.065 ±0.010	6.060 ±0.010
B	5.950 ±0.010	5.955 ±0.010
C*	2.9592 ±0.0020	2.9596 ±0.0019
τ_{aaaa}	-0.00307 ±0.00052	-0.00305 ±0.00064
τ_{bbbb}	-0.00315 ±0.00058	-0.00296 ±0.00051
τ_{aabb}	+0.00252 ±0.00046	+0.00234 ±0.00029
τ_{abab}	-0.00068 ±0.00023	-0.00057 ±0.00023
H_K	-68×10^{-9} $\pm141\times10^{-9}$	-20×10^{-9} $\pm100\times10^{-9}$
κ	+0.925	+0.931
No. of pts.	30	57
G_z	+0.021 ±0.011	
G_{xy}	-0.2334 ±0.0040	
Total No. of pts.	87	
Std. Dev.	0.005	

Table XI. Molecular Constants of $H_2{}^{124}Te$ for the States $2\nu_1$ and $\nu_1+\nu_3$.

State	$2\nu_1$	$\nu_1+\nu_3$
ν_o	4063.588 ±0.019	4064.068 ±0.008
A	6.071 ±0.012	6.068 ±0.011
B	5.943 ±0.011	5.948 ±0.011
C^*	2.9582 ±0.0007	2.9605 ±0.0010
τ_{aaaa}	The distortion terms were held constant at the ground state values in this fit.	
τ_{bbbb}		
τ_{aabb}		
τ_{abab}		
H_K		
κ	0.919	0.924
No. of pts.	39	46
G_z	+0.0150 ±0.0085	
G_{xy}	-0.2305 ±0.0050	
Total No. of pts.	85	
Std. Dev.	0.006	

value of γ and therefore a fairly accurate estimate of its size can be made by substituting reasonable values of ω_1, ω_3, A_e, B_e, and C_e and most any value of γ in this equation. Doing this, we find theoretically, for a γ of 45°, $G_{xy} \simeq -0.11$. In all cases the experimental value obtained in the least squares fit was much larger than this by 50%-100%. The theoretical value of G_z is quite sensitive to the value of γ, so without knowing γ fairly accurately, a comparison between the theoretical value and experimental value cannot be made.

The 4900 cm^{-1} Region

Consideration of the sums of the fundamental vibration frequencies and the Darling-Dennison Resonance[1] between states of the type (v_1,v_2,v_3) and $(v_1 \mp 2, v_2, v_3 \mp 2)$ leads one to expect the bands $2\nu_1+\nu_2$ and $\nu_1+\nu_2+\nu_3$ to be overlapped in the 4900 cm^{-1} region. Examination of the absorption spectrum in this region revealed what appeared to be a single band with the zero, first, second, etc. series of the R and P branches distinct and well separated and a few Q branches between these series. Attempts to form ground state combination differences from these series which agreed with those combination differences formed from the bands in the other regions failed. However, it was possible by using ground state combination differences to identify a few ^RQ lines from the assigned ^RR lines and to identify a few ^PQ lines from the assigned ^PP lines.

It was concluded that the absorption lines observed were actually due to two bands separated less than 0.2 cm^{-1}, one band at 4891.7 cm^{-1} having strong transitions with $\Delta K=+1$, and very weak $\Delta K=-1$ transitions, and the other at 4891.9 cm^{-1} having strong $\Delta K=-1$ transitions and very weak $\Delta K=+1$ transitions.

As noted earlier, there is an interaction between the states $2\nu_1+\nu_2$ and $\nu_1+\nu_2+\nu_3$, and also between $\nu_1+\nu_2+\nu_3$ and $\nu_2+2\nu_3$. The two bands were assigned as $2\nu_1+\nu_2$ and $\nu_1+\nu_2+\nu_3$, and attempts made to analyze the two bands together, as was done in the 4050 cm^{-1} region, using the few identified lines were not successful, so the analysis was not carried further.

Ground State Analysis of H_2Te

As mentioned before, whenever possible it is generally better to analyze the ground state using ground state combination difference fits to Eq. (34) instead of line fits. An analysis by this method eliminates the upper state energy levels, which may be perturbed, and the ground state combination differences from all bands may be simultaneously used. The analysis of the ground state using combination differences may proceed before or at the same time the upper states are being analyzed, although final values of the ground state constants are not obtained until all possible assignments in all the bands have been made and combination differences formed from them. The

ground state combination differences are very useful in assigning new lines and verifying the assignments of others already identified. Thus, the analysis consists of a series of ground state combination difference fits and line fits, each time identifying more lines and forming more combination differences from these lines until as many assignments as possible are made. The ground state constants obtained by Hill et al.[29] were used for starting values. As many ground state combination differences as possible were formed from the four bands analyzed, and each was given a weight depending on the weights of the two lines used to form it. If the same combination difference was formed in more than one band, a weighted average was taken and given a weight equal to the sum of the separate weights. In this manner the ground state combination differences were formed and fit to Eq. (34). Tables XII, XIII, and XIV give the results of these fits. The ranges of the constants are for a simultaneous confidence limit of 95%, which is about 4 times the standard error in these fits. The observed and calculated ground state combination differences of $H_2{}^{130}Te$ are compared in Appendix III.

It was not necessary to include all four H terms to get a good fit, but if at least one of them was allowed to vary, the fit was improved. It was decided to include only H_K, although the choice was somewhat arbitrary as to which H term to use because, for our data mainly lines with K equal to or slightly less than J are observed,

Table XII. Ground State Molecular Constants of $H_2{}^{130}Te$

	$H_2{}^{130}Te$	Values quoted by Hill *et al.*[29]
A	6.247489 ±0.00049	6.2486
B	6.094834 ±0.00048	6.0970
C	3.035999 ±0.00024	3.0361 ±0.0014
τ_{aaaa}	-0.003139 ±0.000030	-0.0025 ±0.0014
τ_{bbbb}	-0.002791 ±0.000034	-0.0032 ±0.0010
τ_{aabb}	+0.002285 ±0.000046	+0.00219 ±0.00035
τ_{abab}	-0.000533 ±0.000025	-0.00055 ±0.00028
H_K	-20×10^{-9} $\pm12\times10^{-9}$	
κ	+0.905	+0.906
No. of pts.	218	118
Std. Dev.	0.006	0.028

Table XIII. Ground State Molecular Constants of $H_2{}^{128}Te$ and $H_2{}^{126}Te$

	$H_2{}^{128}Te$		$H_2{}^{126}Te$	
A	6.24899	±0.00053	6.25162	±0.00073
B	6.09460	±0.00051	6.09470	±0.00053
C	3.03642	±0.00025	3.03690	±0.00021
τ_{aaaa}	-0.003146	±0.000034	-0.003273	±0.000099
τ_{bbbb}	-0.002769	±0.000034	-0.002748	±0.000051
τ_{aabb}	+0.002268	±0.000047	+0.002312	±0.000054
τ_{abab}	-0.000531	±0.000026	-0.000555	±0.000026
H_K	-21×10^{-9}	$\pm12\times10^{-9}$	-23×10^{-9}	$\pm12\times10^{-9}$
κ	+0.904		+0.902	
No. of pts.	176		136	
Std. Dev.	0.006		0.005	

Table XIV. Ground State Molecular Constants of $H_2{}^{125}Te$ and $H_2{}^{124}Te$.

	$H_2{}^{125}Te$	$H_2{}^{124}Te$
A	6.2514 ±0.0018	6.2533 ±0.0021
B	6.0958 ±0.0020	6.0943 ±0.0018
C	3.03712 ±0.00059	3.03722 ±0.00014
τ_{aaaa}	-0.00315 ±0.00036	-0.00331 ±0.00031
τ_{bbbb}	-0.00288 ±0.00027	-0.00271 ±0.00025
τ_{aabb}	+0.00236 ±0.00021	+0.00228 ±0.00014
τ_{abab}	-0.00059 ±0.00012	-0.00054 ±0.00009
H_K	-41×10^{-9} $\pm42\times10^{-9}$	-24×10^{-9} $\pm32\times10^{-9}$
κ	+0.903	+0.901
No. of pts.	49	44
Std. Dev.	0.005	0.004

giving a high correlation between the quantum coefficients of the H's and therefore, the effect on the energy levels of any of the H's is about the same.

Reanalysis of ν_2

Because of limited computer programs available at that time, the analysis of ν_2 by Hill et al.[29] used only transitions involving $J \leq 12$ even though quite a number of lines were identified with $J > 12$. For this reason it was decided to reanalyze the upper state of ν_2 including all the identified transitions. The ground state constants obtained from the analyses of the other regions were used and were not varied. The spectra had a resolution limit $\simeq 0.10$ cm^{-1} and the various isotopes were not resolved on this record. ν_2 is a type B band and fortunately the upper state is not perturbed so the spectrum was fit to Eq. (32). The results are given in Table XV.

Vibrational Analysis

The band center of a particular state may be written as a function of the normal frequencies ω_i and anharmonic constants X_{ik}. From Eq. (18), in the absence of a vibrational resonance,

$$\nu_o(v_1,v_2,v_3) = G(v_1,v_2,v_3) - G(0,0,0) \qquad (51)$$

$$= \sum_i v_i\omega_i + \sum_i \sum_k X_{ik}[v_iv_k + \tfrac{1}{2}(v_i+v_k)] \quad .$$

Expanding these sums for the bands that are available

Table XV. Molecular Constants of H_2Te for the State ν_2.

	Values obtained from this analysis		Values quoted by Hill et at.29	
ν_o	860.765	±0.022	860.79	±0.01
A	6.4296	±0.0050	6.4306	
B	6.2259	±0.0048	6.2258	
C	3.00555	±0.00052	3.0064	±0.0017
τ_{aaaa}	-0.00379	±0.00056	-0.0034	±0.0016
τ_{bbbb}	-0.00318	±0.00040	-0.0029	±0.0013
τ_{aabb}	+0.00314	±0.00016	+0.00257	±0.00046
τ_{abab}	-0.00095	±0.00014	-0.00088	±0.00036
H_K	-46×10^{-9}	$\pm10\times10^{-9}$		
κ	+0.880		+0.880	
No of pts.	170		96	
Std. Dev.	0.026		0.029	

we have

$$\nu_o(0,1,0) = \omega_2 + 2X_{22} + \tfrac{1}{2}X_{12} + \tfrac{1}{2}X_{23} \qquad (52)$$

$$\nu_o(1,1,0) = \omega_1 + 2X_{11} + \omega_2 + 2X_{22} + 2X_{12} + \tfrac{1}{2}X_{13} + \tfrac{1}{2}X_{23}$$

$$\nu_o(0,1,1) = \omega_2 + 2X_{22} + \omega_3 + 2X_{33} + \tfrac{1}{2}X_{12} + \tfrac{1}{2}X_{13} + 2X_{23}$$

$$\nu_o(1,0,1) = \omega_1 + 2X_{11} + \omega_3 + 2X_{33} + \tfrac{1}{2}X_{12} + 2X_{13} + \tfrac{1}{2}X_{23} ,$$

and from Eq. (20) we have for $2\nu_1$,

$$\nu_o(2,0,0) = \tfrac{1}{2}[(2\omega_1+6X_{11}+X_{12}+X_{13})+(2\omega_3+6X_{33}+X_{13}+X_{23})]$$
$$- \tfrac{1}{2}[4\gamma^2+\{(2\omega_1+6X_{11}+X_{12}+X_{13})-(2\omega_3+6X_{33}+X_{13}+X_{23})\}^2]^{1/2}.$$

Unfortunately the above band centers that have been observed are not enough to solve for the constants ω_i and X_{ik}, but if additional data is sometime obtained, it may be possible to solve for some of these constants individually or at least more useful combinations of them. This additional data could come from a positive identification and analysis of the bands near 4900 cm^{-1}, and from an analysis of the fundamentals ν_1 and ν_3 which have been observed overlapped near 2070 cm^{-1}. Besides yielding valuable information for a vibrational analysis, ν_1 and ν_3 perturb each other through the interaction term Eq. (41) and they could be simultaneously analyzed as two interacting bands in the same manner as $\nu_1+\nu_2$ and $\nu_2+\nu_3$.

CHAPTER VI

STRUCTURE CALCULATIONS

It can be seen from the definition of A, B, and C in Eq. (10) that by the analysis of the proper set of bands one can solve for the α's and consequently the equilibrium constants A_e, B_e, and C_e. With the equilibrium constants available, the equilibrium structure may easily be calculated. The constants obtained from the analysis of the ground state and the bands ν_2, $\nu_1+\nu_2$, $\nu_2+\nu_3$ and $\nu_1+\nu_3$ are sufficient to allow a least squares analysis determination of the α_i^A, and α_i^B. In principle the α_i^C cannot be determined from these bands since the analysis of the upper states of the bands $\nu_1+\nu_2$, $\nu_2+\nu_3$, and $\nu_1+\nu_3$ yields C^* instead of C because of the Coriolis interaction. However, since the Coriolis perturbation coefficient G_z determined in the fits is so small, it may well be possible that $C^* \simeq C$ for the states analyzed, then the α_i^C may be determined and C_e calculated. A test of the validity of this would be a comparison of the calculated quantities C_e and $A_eB_e/(A_e+B_e)$ which, because of the planarity condition $I_c^e = I_a^e + I_b^e$, should be equal.

From Eq. (10) we can determine the relations,

$$A_e = A(0,0,0) + \tfrac{1}{2}\sum \alpha_i^A \qquad (53)$$

and

$$A(0,0,0)-A(v_1,v_2,v_3) = \alpha_1^A v_1 + \alpha_2^A v_2 + \alpha_3^A v_3 \ , \qquad (54)$$

with similar relations for B and C. The constants from the ground state and the four bands mentioned were used in a least squares fit to Eq. (54) to determine the α_i^A, and similarly, α_i^B and α_i^C assuming $C^* = C$. The results of this fit are given in Table XVI along with the equilibrium constants A_e, B_e, C_e calculated with Eq. (53) and the equilibrium moments of inertia calculated from A_e, B_e, and C_e through Eq. (11). The ranges given for the α_i determined in the fit are the standard errors. The equilibrium structural parameters r_e and θ [see Fig. 4.] listed in Table XVI were calculated using the equations,

$$r_e = [(1/2m)\{I_b^e + [(2m/M) + 1\,]I_a^e\}]^{1/2} \qquad (55)$$

$$\tan(\tfrac{\theta}{2}) = [I_b^e/\{I_a^e[(2m/M) + 1]\}]^{1/2}$$

where m and M stand for the masses of the hydrogen and tellurium atoms respectively. In these calculations, the constants from the 130 isotope of H_2Te were used, except for the constants from ν_2 where the isotopes were not resolved. This is valid since the α_i are approximately equal for each isotope i.e.; ${}^{i}\alpha_j^A \simeq {}^{130}\alpha_j^A$, ${}^{i}\alpha_j^B \simeq {}^{130}\alpha_j^B$, ${}^{i}\alpha_j^C \simeq {}^{130}\alpha_j^C$ where i is equal to 128, 126, 125, 124, and 122.

Examination of the equilibrium constants obtained shows that C_e and $A_eB_e/(A_e+B_e)$ differ by only 0.001 cm^{-1} which tends to suggest the validity of the assumption $C^* \simeq C$.

Table XVI Equilibrium Structure of H_2Te

α_1^A	$+0.0787 \pm 0.002$ cm^{-1}	α_1^B	$+0.0885 \pm 0.0004$ cm^{-1}
α_2^A	-0.1793 ± 0.002	α_2^B	-0.1306 ± 0.0003
α_3^A	$+0.1064 \pm 0.003$	α_3^B	$+0.0602 \pm 0.0004$
Std. Dev.	0.002	Std. Dev.	0.0004
A_e	6.2504 cm^{-1}	B_e	6.1038 cm^{-1}
I_a^e	4.4783×10^{-40} g cm^2	I_b^e	4.5858×10^{-40} g cm^2

Assuming $C = C^*$

α_1^C	$+0.0454 \pm 0.0004$ cm^{-1}
α_2^C	$+0.0302 \pm 0.0003$
α_3^C	$+0.0308 \pm 0.0004$
Std. Dev.	0.0004
C_e	3.0892 cm^{-1}
I_c^e	9.0608×10^{-40} g cm^2

$(r_e)_{H\text{-}Te} = 1.646$ Å

$\theta = 90° 38'$

CHAPTER VII

CONCLUSION

The development of the vibration-rotation Hamiltonian for a planar asymmetric non-linear XYX molecule has been outlined and energy expressions by which energy levels and other quantities, useful in an analysis of the spectra of such a molecule, may be calculated have been given. Since the upper vibrational states of some of the bands may interact through a Coriolis type resonance, a modified Hamiltonian was given which included the necessary interaction terms for a description of these states.

High resolution ($\simeq 0.05$ cm^{-1}) calibrated recordings of the vibration-rotation absorption spectra of H_2Te were obtained near 2900 cm^{-1}, 4050 cm^{-1}, and 4900 cm^{-1}. The frequencies of all individual absorption lines in these regions were measured from these recordings.

A method was outlined by which the theoretical energy expressions could be used to analyze spectra, and was applied in the analysis of H_2Te. Computer programs were written which would calculate energy levels, line frequencies, perform least squares fits of ground state combination differences or line frequencies and make a simultaneous least squares fit of the upper states of two bands

which perturb each other through a Coriolis like interaction.

The results of the ground state analysis yielded the ground state constants A, B, and C, centrifugal distortion constants (taus and H_K) for the molecular species $H_2{}^{130}Te$, $H_2{}^{128}Te$, $H_2{}^{126}Te$, $H_2{}^{125}Te$, and $H_2{}^{124}Te$. From the upper state analysis came the molecular constants, centrifugal distortion constants, and band centers for the bands ν_2, $\nu_1+\nu_2$, $\nu_2+\nu_3$, $2\nu_1$, and $\nu_1+\nu_3$, and the perturbation coefficients G_z and G_{xy} of the interacting states. The upper states of the species $H_2{}^{130}Te$, $H_2{}^{128}Te$, $H_2{}^{126}Te$, $H_2{}^{125}Te$, and $H_2{}^{124}Te$ were all analyzed in the bands $2\nu_1$ and $\nu_1+\nu_3$, while the analysis of the upper states of $\nu_1+\nu_2$ and $\nu_2+\nu_3$ included the species $H_2{}^{130}Te$, $H_2{}^{128}Te$, and $H_2{}^{126}Te$.

Finally, by a proper combination of molecular constants from the different vibrational states, the equilibrium constants A_e, B_e, and C_e were obtained, from which the equilibrium structure (r_e and θ) of H_2Te was calculated.

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APPENDIX I

NONVANISHING MATRIX ELEMENTS OF THE HAMILTONIAN OPERATORS

The nonvanishing matrix elements of the Hamiltonian operators in the symmetric top basis $\psi(J,K)$ are given below.

$f = J(J+1)$

$$\langle K|P_x|K\pm1\rangle = \pm\frac{i}{2}[f-K(K\pm1)]^{1/2}$$

$$\langle K|P_y|K\pm1\rangle = \frac{1}{2}[f-K(K\pm1)]^{1/2}$$

$$\langle K|P_z|K\rangle = K$$

$$\langle K|P_x^2|K\rangle = \frac{1}{2}(f-K^2)$$

$$\langle K|P_x^2|K\pm2\rangle = -\frac{1}{4}[f-K(K\pm1)]^{1/2}[f-(K\pm1)(K\pm2)]^{1/2}$$

$$\langle K|P_y^2|K\rangle = \langle K|P_x^2|K\rangle$$

$$\langle K|P_y^2|K\pm2\rangle = -\langle K|P_x^2|K\pm2\rangle$$

$$\langle K|P_z^2|K\rangle = K^2$$

$$\langle K|P_x^4|K\rangle = \frac{1}{8}[3f^2-2f-6fK^2+5K^2+3K^4]$$

$$\langle K|P_x^4|K\pm2\rangle = -\frac{1}{8}[2f-K^2-(K\pm2)^2]\{[f-K(K\pm1)][f-(K\pm1)(K\pm2)]\}^{1/2}$$

$$\langle K|P_x^4|K\pm4\rangle = \frac{1}{16}\{[f-K(K\pm1)][f-(K\pm1)(K\pm2)][f-(K\pm2)(K\pm3)][f-(K\pm3)(K\pm4)]\}^{1/2}$$

$$\langle K|P_y^4|K\rangle = \langle K|P_x^4|K\rangle$$

$$\langle K|P_y^4|K\pm 2\rangle = -\langle K|P_x^4|K\pm 2\rangle$$

$$\langle K|P_y^4|K\pm 4\rangle = \langle K|P_x^4|K\pm 4\rangle$$

$$\langle K|P_z^4|K\rangle = K^4$$

$$\langle K|P_x^2P_z^2+P_z^2P_x^2|K\rangle = K^2(f-K^2)$$

$$\langle K|P_x^2P_z^2+P_z^2P_x^2|K\pm 2\rangle = -\tfrac{1}{4}[K^2+(K\pm 2)^2]\{[f-K(K\pm 1)][f-(K\pm 1)(K\pm 2)]\}^{1/2}$$

$$\langle K|P_y^2P_z^2+P_z^2P_y^2|K\rangle = \langle K|P_x^2P_z^2+P_z^2P_x^2|K\rangle$$

$$\langle K|P_y^2P_z^2+P_z^2P_y^2|K\pm 2\rangle = -\langle K|P_x^2P_z^2+P_z^2P_x^2|K\pm 2\rangle$$

$$\langle K|P_x^2P_y^2+P_y^2P_x^2|K\rangle = \tfrac{1}{4}[f^2+2f+2fK^2-5K^2+K^4]$$

$$\langle K|P_x^2P_y^2+P_y^2P_x^2|K\pm 4\rangle = -\tfrac{1}{8}\{[f-K(K\pm 1)][f-(K\pm 1)(K\pm 2)][f-(K\pm 2)(K\pm 3)][f-(K\pm 3)(K\pm 4)]\}^{1/2}$$

$$\langle K|P_xP_y+P_yP_x|K\pm 2\rangle = \pm\tfrac{i}{2}[f-K(K\pm 1)]^{1/2}[f-(K\pm 1)(K\pm 2)]^{1/2}$$

The non-zero matrix elements of the Hamiltonian operators in the basis set $\Psi(J,K,\gamma)$ are given below.

$K \neq 1$, $K \neq 0$,

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K})|P_x^2|\tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K})\rangle = \tfrac{1}{2}(f-K^2)$$

$K = 1$,

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1})|P_x^2|\tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1})\rangle = \tfrac{1}{2}(f-K^2) \mp \tfrac{1}{4}f$$

$K \neq 0$,

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K})|P_x^2|\tfrac{1}{\sqrt{2}}(\psi_{K+2} \pm \psi_{-K-2})\rangle = -\tfrac{1}{4}\{[f-K(K+1)][f-(K+1)(K+2)]\}^{1/2}$$

$K = 0,$

$$\langle \psi_o | P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_2+\psi_{-2}) \rangle = \sqrt{2}[f(f-2)]^{1/2}$$

$K \neq 1,\ K \neq 0,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_y^2 | \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) \rangle = \tfrac{1}{2}(f-K^2)$$

$K = 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) | P_y^2 | \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) \rangle = \tfrac{1}{2}(f-K^2) \pm \tfrac{1}{4}f$$

$K \neq 0,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_K) | P_y^2 | \tfrac{1}{\sqrt{2}}(\psi_{K+2} \pm \psi_{-K-2}) \rangle = -\langle P_x^2 \rangle$$

$K = 0,$

$$\langle \psi_0 | P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_2+\psi_{-2}) \rangle = -\langle P_x^2 \rangle$$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K} | P_z^2 | \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) \rangle = K^2$$

$K \neq 0,\ K \neq 1,\ K \neq 2,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x^4 | \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) \rangle = \tfrac{1}{8}[3f^2-2f-6fK^2+5K^2+3K^4]$$

$K = 0,$

$$\langle \psi_0 | P_x^4 | \psi_0 \rangle = \tfrac{1}{8}[3f^2-2f]$$

$K = 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) | P_x^4 | \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) \rangle = \tfrac{1}{8}[(3f^2-8f+8) \mp 2f(f-1)]$$

$K = 2,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_2 \pm \psi_{-2}) | P_x^4 | \tfrac{1}{\sqrt{2}}(\psi_2 \pm \psi_{-2}) \rangle = \tfrac{1}{8}[3f^2-26f+68] \pm \tfrac{1}{16}f(f-2)$$

$K \neq 0,\ K \neq 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x^4 | \tfrac{1}{\sqrt{2}}(\psi_{K+2} \pm \psi_{-K-2}) \rangle =$$
$$-\tfrac{1}{8}[2f-K^2-(K+2)^2]\{[f-K(K+1)][f-(K+1)(K+2)]\}^{1/2}$$

$K = 0,$

$$\langle \psi_0 | P_x^4 | \tfrac{1}{\sqrt{2}}(\psi_2+\psi_{-2}) \rangle = {}_2\tfrac{-1}{\sqrt{2}}(f-2)\,[f(f-2)]^{1/2}$$

$K = 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) | P_x^4 | \tfrac{1}{\sqrt{2}}(\psi_3 \pm \psi_{-3}) \rangle = -\tfrac{1}{8}\{(f-2)(f-6)\}^{1/2}[(2f-10) \mp \tfrac{1}{2}f]$$

$K \neq 0,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x^4 | \tfrac{1}{\sqrt{2}}(\psi_{K+4} \pm \psi_{-K-4}) \rangle = (1/16)\{[f-K(K+1)][f - (K+1)(K+2)][f-(K+2)(K+3)][f-(K+3)(K+4)]\}^{1/2}$$

$K = 0,$

$$\langle \psi_0 | P_x^4 | \tfrac{1}{\sqrt{2}}(\psi_4+\psi_{-4}) \rangle = {}_8\tfrac{1}{\sqrt{2}}\{f(f-2)(f-6)(f-12)\}^{1/2}$$

$K \neq 0,\ K \neq 1,\ K \neq 2,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_y^4 | \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) \rangle = \langle P_x^4 \rangle$$

$K = 0,$

$$\langle \psi_0 | P_y^4 | \psi_0 \rangle = \langle \psi_o | P_x^4 | \psi_0 \rangle$$

$K = 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) | P_y^4 | \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) \rangle = \tfrac{1}{8}[3f^2-8f+8 \pm 2f(f-1)]$$

$K = 2,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_2 \pm \psi_{-2}) | P_y^4 | \tfrac{1}{\sqrt{2}}(\psi_2 \pm \psi_{-2}) \rangle = \langle P_x^4 \rangle$$

$K \neq 0,\ K \neq 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_y^4 | \tfrac{1}{\sqrt{2}}(\psi_{K+2} \pm \psi_{-K-2}) \rangle = -\langle P_x^4 \rangle$$

$K = 0,$

$$\langle \psi_0 | P_y^4 | \tfrac{1}{\sqrt{2}}(\psi_2+\psi_{-2}) \rangle = -\langle P_x^4 \rangle$$

$K = 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) | P_y^4 | \tfrac{1}{\sqrt{2}}(\psi_3 \pm \psi_{-3}) \rangle = \tfrac{1}{8}\{(f-2)(f-6)\}^{1/2}[(2f-10) \pm \tfrac{1}{2}f]$$

$K \neq 0,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_y^4 | \tfrac{1}{\sqrt{2}}(\psi_{K+4} \pm \psi_{-K-4}) \rangle = \langle \quad P_x^4 \quad \rangle$$

$K = 0,$

$$\langle \psi_0 | P_y^4 | \tfrac{1}{\sqrt{2}}(\psi_4 + \psi_{-4}) \rangle = \langle \quad P_x^4 \quad \rangle$$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_z^4 | \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) \rangle = K^4$$

$K \neq 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x^2 P_z^2 + P_z^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) \rangle = K^2(f-K^2)$$

$K = 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) | P_x^2 P_z^2 + P_z^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) \rangle = (f-1) \mp \tfrac{1}{2}f$$

$K \neq 0,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x^2 P_z^2 + P_z^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_{K+2} \pm \psi_{-K-2}) \rangle = -\tfrac{1}{4}[K^2 + (K+2)^2]\{ [f-K(K+1)][f-(K+1)(K+2)] \}^{1/2}$$

$K = 0,$

$$\langle \psi_0 | P_x^2 P_z^2 + P_z^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_2 + \psi_{-2}) \rangle = -\sqrt{2}[f(f-2)]^{1/2}$$

$K \neq 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_y^2 P_z^2 + P_z^2 P_y^2 | \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) \rangle = K^2(f-K^2)$$

$K = 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) | P_y^2 P_z^2 + P_z^2 P_y^2 | \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) \rangle = (f-1) \pm \tfrac{1}{2}f$$

$K \neq 0,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_y^2 P_z^2 + P_z^2 P_y^2 | \tfrac{1}{\sqrt{2}}(\psi_{K+2} \pm \psi_{-K-2}) \rangle = - \langle \quad | P_x^2 P_z^2 + P_z^2 P_x^2 | \quad \rangle$$

$K = 0,$

$$\langle \psi_0 | P_y^2 P_z^2 + P_z^2 P_y^2 | \tfrac{1}{\sqrt{2}}(\psi_2 + \psi_{-2}) \rangle = - \langle \quad | P_x^2 P_z^2 + P_z^2 P_x^2 | \quad \rangle$$

$K \neq 0, \; K \neq 2,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x^2 P_y^2 + P_y^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) \rangle = \tfrac{1}{4}[f^2 + 2f - 2fK^2 - 5K^2 + K^4]$$

$K = 0,$

$$\langle \psi_0 | P_x^2 P_y^2 + P_y^2 P_x^2 | \psi_0 \rangle = \tfrac{1}{4}[f^2 + 2f]$$

$K = 2,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_2 \pm \psi_{-2}) | P_x^2 P_y^2 + P_y^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_2 \pm \psi_{-2}) \rangle = \tfrac{1}{4}(f^2 - 6f - 4) \mp \tfrac{1}{8} f(f-2)$$

$K \neq 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x^2 P_y^2 + P_y^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_{K+2} \pm \psi_{-K-2}) \rangle = 0$$

$K = 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) | P_x^2 P_y^2 + P_y^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_3 \pm \psi_{-3}) \rangle = \mp \tfrac{1}{8} f \{ (f-2)(f-6) \}^{1/2}$$

$K \neq 0,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x^2 P_y^2 + P_y^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_{K+4} \pm \psi_{-K-4}) \rangle = -\tfrac{1}{8} \{ [f - K(K+1)[[f-(K+1)(K+2)][f-(K+2)(K+3)][f-(K+3)(K+4)] \}^{1/2}$$

$K = 0,$

$$\langle \psi_0 | P_x^2 P_y^2 + P_y^2 P_x^2 | \tfrac{1}{\sqrt{2}}(\psi_4 + \psi_{-4}) \rangle = \frac{-1}{4\sqrt{2}} \{ f(f-2)(f-6)(f-12) \}^{1/2}$$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_z | \tfrac{1}{\sqrt{2}}(\psi_K \mp \psi_{-K}) \rangle = K$$

$K = 1,$

$$\langle \tfrac{1}{\sqrt{2}}(\psi_1 \pm \psi_{-1}) | P_x P_y + P_y P_x | \tfrac{1}{\sqrt{2}}(\psi_1 \mp \psi_{-1}) \rangle = \pm \tfrac{i}{2} f$$

$K \neq 0$,

$$\langle \frac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x P_y + P_y P_x | \frac{1}{\sqrt{2}}(\psi_{K+2} \mp \psi_{-K-2}) \rangle = + \frac{i}{2}[f-K(K+1)]^{1/2}[f-(K+1)(K+2)]^{1/2}$$

$K = 0$,

$$\langle \psi_0 | P_x P_y + P_y P_x | \frac{1}{\sqrt{2}}(\psi_2 - \psi_{-2}) \rangle = +\frac{i}{\sqrt{2}}[f(f-2)]^{1/2}$$

$K > 2$,

$$\langle \frac{1}{\sqrt{2}}(\psi_K \pm \psi_{-K}) | P_x P_y + P_y P_x | \frac{1}{\sqrt{2}}(\psi_{K-2} \mp \psi_{-K+2}) \rangle = -\frac{i}{2}[f-K(K-1)]^{1/2}[f-(K-1)(K-2)]^{1/2}$$

APPENDIX II

ASSIGNED LINES AND OBSERVED FREQUENCIES OF $H_2{}^{130}Te$ FOR THE STATES $\nu_1+\nu_2$, $\nu_2+\nu_3$, $2\nu_1$, AND $\nu_1+\nu_3$

The observed frequencies of $H_2{}^{130}Te$ are compared with the calculated frequencies, where the ground state rotational energy levels are calculated with Eq. (24) and the upper state energy levels with Eq. (47).

ASSIGNED LINES OF $H_2{}^{130}Te$ FOR $\nu_1+\nu_2$

I	K-	K+		J	K-	K+	OBS	OBS-CALC	WT
1	1	1	-	0	0	0	2920.733	0.011	0.00
2	0	2	-	1	1	1	2926.437	-0.002	1.00
2	1	2	-	1	0	1	2926.610	0.006	1.00
3	0	3	-	2	1	2	2932.283	0.009	0.40
4	1	4	-	3	0	3	2937.893	0.007	0.40
5	0	5	-	4	1	4	2943.338	-0.001	1.00
6	1	6	-	5	0	5	2948.640	-0.001	1.00
7	0	7	-	6	1	6	2953.793	-0.000	0.40
8	1	8	-	7	0	7	2958.798	0.002	1.00
9	0	9	-	8	1	8	2963.646	-0.004	1.00
10	1	10	-	9	0	9	2968.353	-0.003	1.00
11	0	11	-	10	1	10	2972.907	-0.007	0.40
12	1	12	-	11	0	11	2977.306	-0.018	0.40
13	0	13	-	12	1	12	2981.571	-0.013	1.00
14	1	14	-	13	0	13	2985.681	-0.013	0.40
15	0	15	-	14	1	14	2989.640	-0.012	0.40
16	1	16	-	15	0	15	2993.450	-0.003	0.40
17	0	17	-	16	1	16	2997.119	0.027	0.40
1	0	0	-	1	0	1	2902.251	-0.035	0.00
1	0	1	-	2	1	2	2896.018	-0.008	0.01
2	1	2	-	3	0	3	2889.924	0.007	0.40
3	0	3	-	4	1	4	2883.534	-0.002	1.00
4	1	4	-	5	0	5	2877.018	0.004	0.01
5	0	5	-	6	1	6	2870.350	0.005	0.40
6	1	6	-	7	0	7	2863.539	0.006	0.40
7	0	7	-	8	1	8	2856.585	0.007	1.00
8	1	8	-	9	0	9	2849.490	0.006	1.00
9	0	9	-	10	1	10	2842.252	-0.001	0.40
10	1	10	-	11	0	11	2834.878	-0.009	0.01
11	0	11	-	12	1	12	2827.378	-0.011	0.40
12	1	12	-	13	0	13	2819.740	-0.021	0.40
13	0	13	-	14	1	14	2811.970	-0.036	0.00
2	2	1	-	1	1	0	2933.545	0.007	1.00
3	1	2	-	2	2	1	2938.981	-0.000	0.40
4	2	3	-	3	1	2	2945.175	0.002	0.40
5	1	4	-	4	2	3	2950.865	-0.003	1.00
6	2	5	-	5	1	4	2956.456	0.006	1.00
7	1	6	-	6	2	5	2961.882	0.003	1.00
8	2	7	-	7	1	6	2967.168	0.010	1.00
9	1	8	-	8	2	7	2972.301	0.011	1.00
10	2	9	-	9	1	8	2977.306	0.032	0.00
11	1	10	-	10	2	9	2982.121	0.008	1.00
12	2	11	-	11	1	10	2986.813	0.007	1.00
13	1	12	-	12	2	11	2991.349	-0.006	0.00
15	1	14	-	14	2	13	3000.028	0.011	0.01
1	1	0	-	2	2	1	2889.780	-0.010	0.40
2	2	1	-	3	1	2	2884.439	-0.003	1.00

3	1	2	=	4	2	3	2877.962	=0.005	0.40
3	2	2	=	4	1	3	2878.029	=0.006	0.01
4	2	3	=	5	1	4	2871.785	0.004	0.00
5	1	4	=	6	2	5	2865.424	0.018	0.00
6	2	5	=	7	1	6	2858.893	0.003	0.40
7	1	6	=	8	2	7	2852.238	0.007	0.40
8	2	7	=	9	1	8	2845.439	0.006	1.00
9	1	8	=	10	2	9	2838.508	0.010	0.70
10	2	9	=	11	1	10	2831.441	0.010	0.01
11	1	10	=	12	2	11	2824.238	0.005	0.01
12	2	11	=	13	1	12	2816.916	0.008	0.00
3	3	1	=	2	2	0	2946.540	0.001	0.40
4	3	2	=	3	2	1	2952.585	0.007	1.00
5	2	3	=	4	3	2	2957.989	0.008	1.00
6	3	4	=	5	2	3	2963.919	=0.011	0.01
7	2	5	=	6	3	4	2969.410	0.004	1.00
8	3	6	=	7	2	5	2975.148	0.003	1.00
9	2	7	=	8	3	6	2980.538	0.007	1.00
10	3	8	=	9	2	7	2985.773	0.003	0.40
11	2	9	=	10	3	8	2990.872	0.009	1.00
13	2	11	=	12	3	10	3000.619	0.003	0.70
14	3	12	=	13	2	11	3005.276	=0.002	0.01
15	2	13	=	14	3	12	3009.777	=0.020	0.01
3	3	1	=	4	2	2	2872.919	=0.002	1.00
3	2	1	=	4	3	2	2871.502	=0.005	0.40
4	2	2	=	5	3	3	2866.126	=0.009	0.00
4	3	2	=	5	2	3	2866.337	=0.005	0.01
5	2	3	=	6	3	4	2860.180	0.015	0.00
6	3	4	=	7	2	5	2853.954	=0.006	0.70
7	2	5	=	8	3	6	2847.595	0.002	0.40
8	3	6	=	9	2	7	2841.093	0.006	0.40
9	2	7	=	10	3	8	2834.450	0.008	0.40
10	3	8	=	11	2	9	2827.689	0.026	0.00
11	2	9	=	12	3	10	2820.759	0.006	0.01
12	3	10	=	13	2	11	2813.726	0.009	0.00
4	4	1	=	3	3	0	2959.433	=0.006	1.00
5	3	2	=	4	4	1	2963.844	=0.029	0.00
5	4	2	=	4	3	1	2965.809	=0.001	1.00
6	3	3	=	5	4	2	2970.826	=0.009	0.40
6	4	3	=	5	3	2	2971.303	=0.000	0.40
7	3	4	=	6	4	3	2976.970	=0.001	0.40
7	4	4	=	6	3	3	2977.033	=0.003	0.01
8	4	5	=	7	3	4	2982.785	=0.002	0.40
9	3	6	=	8	4	5	2988.404	=0.002	0.40
10	4	7	=	9	3	6	2993.882	0.002	0.40
11	3	8	=	10	4	7	2999.204	0.001	1.00
12	4	9	=	11	3	8	3004.418	0.038	0.00
13	3	10	=	12	4	9	3009.454	0.042	0.00
3	3	0	=	4	4	1	2865.448	=0.009	0.00
4	3	1	=	5	4	2	2859.287	=0.003	0.40
4	4	1	=	5	3	2	2861.666	0.003	1.00
5	4	2	=	6	3	3	2854.850	=0.005	0.00
5	3	2	=	6	4	3	2854.361	=0.004	0.40
6	4	3	=	7	3	4	2848.758	=0.004	1.00

7	3	4	8	4	5	2842.652	-0.008	0.01
9	4	5	9	3	6	2836.450	-0.001	0.40
9	3	6	10	4	7	2830.099	0.006	0.01
10	4	7	11	3	8	2823.596	-0.001	0.01
5	5	1	4	4	0	2972.665	-0.019	0.00
6	4	2	5	5	1	2976.090	-0.003	0.40
6	5	2	5	4	1	2979.156	-0.006	1.00
7	5	3	6	4	2	2984.556	0.001	0.40
7	4	3	6	5	2	2983.594	-0.006	0.40
8	5	4	7	4	3	2990.173	-0.004	0.40
10	5	6	9	4	5	3001.426	-0.008	1.00
11	4	7	10	5	6	3007.160	-0.007	0.40
12	5	8	11	4	7	3012.545	-0.005	0.70
13	4	9	12	5	8	3017.776	-0.008	0.40
14	5	10	13	4	9	3022.864	-0.007	0.00
4	4	0	5	5	1	2853.578	0.008	0.00
5	5	1	6	4	2	2850.582	0.000	0.01
5	4	1	6	5	2	2847.098	-0.004	0.40
6	5	2	7	4	3	2843.580	-0.008	0.00
7	4	3	8	5	4	2837.310	-0.009	0.01
8	5	4	9	4	5	2831.520	-0.008	0.01
9	4	5	10	5	6	2825.445	-0.004	0.01
10	5	6	11	4	7	2819.237	-0.001	0.00
6	6	1	5	5	0	2985.501	-0.003	0.40
7	5	2	6	6	1	2988.083	0.006	0.00
8	6	3	7	5	2	2997.932	-0.001	0.40
9	5	4	8	6	3	3003.021	0.046	0.00
10	6	5	9	5	4	3009.094	0.001	0.40
11	5	6	10	6	5	3014.761	-0.014	0.00
5	5	0	6	6	1	2841.952	0.000	1.00
6	6	1	7	5	2	2839.571	-0.004	0.40
7	5	2	8	6	3	2830.812	-0.005	0.00
8	6	3	9	5	4	2826.431	0.001	0.01
7	7	1	6	6	0	3002.645	-0.016	1.00
8	7	2	7	6	1	3005.946	0.011	0.40
9	6	3	8	7	2	3008.480	0.014	1.00
6	6	0	7	7	1	2830.659	-0.003	0.01
7	6	1	8	7	2	2822.840	-0.006	0.00
8	8	1	7	7	0	3016.538	-0.020	1.00
9	9	1	8	8	0	3030.616	-0.025	0.01
10	10	1	9	9	0	3044.831	-0.049	0.01
1	0	1	1	1	0	2909.173	0.005	0.01
1	1	0	1	0	1	2914.770	-0.000	1.00
2	2	0	2	1	1	2915.209	-0.012	0.40
3	3	0	3	2	1	2915.936	0.001	1.00
4	4	0	4	3	1	2916.951	-0.000	1.00
5	5	0	5	4	1	2918.308	-0.001	1.00
6	6	0	6	5	1	2920.028	-0.007	0.00
2	1	2	2	2	1	2901.624	0.001	1.00
3	1	2	3	2	1	2902.674	-0.002	0.40
4	2	2	4	3	1	2903.413	-0.003	0.40
5	3	2	5	4	1	2904.222	-0.007	0.40
6	4	2	6	5	1	2905.040	-0.001	1.00
6	5	2	6	6	1	2902.825	0.021	0.00

7	5	2	=	7	6	1	2905.770	=0.004	1.00
9	7	2	=	9	8	1	2906.765	0.002	0.40
3	2	1	=	2	1	2	2921.389	=0.008	0.40
3	2	1	=	3	1	2	2920.883	0.001	0.40
4	4	1	=	4	3	2	2922.846	=0.001	0.40
5	4	1	=	5	3	2	2921.317	=0.015	0.01
5	5	1	=	5	4	2	2923.601	=0.009	0.40
6	5	1	=	6	4	2	2921.739	=0.022	0.01
6	6	1	=	6	5	2	2924.184	=0.005	1.00
7	6	1	=	7	5	2	2922.386	=0.011	0.40
3	0	3	=	3	1	2	2895.319	=0.001	0.40
4	2	3	=	4	3	2	2895.800	0.003	0.40
5	2	3	=	5	3	2	2896.797	0.001	0.40
6	4	3	=	6	5	2	2897.077	0.003	0.01
6	3	3	=	6	4	2	2897.803	=0.004	0.00
7	4	3	=	7	5	2	2898.977	=0.009	1.00
8	5	3	=	8	6	2	2900.276	=0.019	0.00
8	6	3	=	8	7	2	2898.395	0.012	1.00
3	1	2	=	3	0	3	2927.281	0.006	0.40
4	3	2	=	4	2	3	2927.860	=0.009	1.00
4	2	2	=	4	1	3	2927.488	0.002	0.40
5	4	2	=	5	3	3	2928.520	=0.008	0.00
5	3	2	=	5	2	3	2928.110	=0.006	0.40
6	5	2	=	6	4	3	2929.292	=0.006	0.40
6	4	2	=	6	3	3	2928.520	0.001	0.00
7	5	2	=	7	4	3	2928.854	=0.007	0.01
7	6	2	=	7	5	3	2930.134	=0.007	0.40
8	7	2	=	8	6	3	2930.990	0.013	0.40
4	1	4	=	4	2	3	2888.576	=0.002	1.00
5	1	4	=	5	2	3	2889.337	=0.004	1.00
7	3	4	=	7	4	3	2891.272	0.010	0.70
7	4	4	=	7	5	3	2891.127	0.001	0.40
8	5	4	=	8	6	3	2892.133	0.000	0.40
9	5	4	=	9	6	3	2893.698	=0.014	0.01
9	6	4	=	9	7	3	2893.164	0.001	0.01
4	2	3	=	4	1	4	2933.387	=0.002	1.00
5	2	3	=	5	1	4	2933.967	0.002	0.40
6	4	3	=	6	3	4	2934.665	=0.008	0.01
7	4	3	=	7	3	4	2935.280	=0.008	0.00
8	6	3	=	8	5	4	2936.266	=0.000	0.40
9	6	3	=	9	5	4	2936.518	0.005	0.40
5	0	5	=	5	1	4	2881.733	0.002	0.40
6	2	5	=	6	3	4	2882.647	=0.004	0.40
7	2	5	=	7	3	4	2883.701	0.006	0.00
8	4	5	=	8	5	4	2884.842	0.024	0.00
9	4	5	=	9	5	4	2886.084	=0.005	0.01
10	6	5	=	10	7	4	2887.260	=0.005	0.01
5	1	4	=	5	0	5	2939.314	0.010	0.40
6	3	4	=	6	2	5	2940.000	0.005	0.01
7	3	4	=	7	2	5	2940.746	=0.005	0.40
8	5	4	=	8	4	5	2941.561	=0.014	0.20
9	5	4	=	9	4	5	2942.358	=0.012	0.01
6	1	6	=	6	2	5	2874.742	=0.001	0.40
7	1	6	=	7	2	5	2875.857	0.014	0.20

7	5	2	=	7	6	1	2905,770	=0,004	1,00
9	7	2	=	9	8	1	2906,765	0,002	0,40
2	2	1	=	2	1	2	2921,389	=0,008	0,40
3	2	1	=	3	1	2	2920,883	0,001	0,40
4	4	1	=	4	3	2	2922,846	=0,001	0,40
5	4	1	=	5	3	2	2921,317	=0,015	0,01
5	5	1	=	5	4	2	2923,601	=0,009	0,40
6	5	1	=	6	4	2	2921,739	=0,022	0,01
6	6	1	=	6	5	2	2924,184	=0,005	1,00
7	6	1	=	7	5	2	2922,386	=0,011	0,40
3	0	3	=	3	1	2	2895,319	=0,001	0,40
4	2	3	=	4	3	2	2895,800	0,003	0,40
5	2	3	=	5	3	2	2896,797	0,001	0,40
6	4	3	=	6	5	2	2897,077	0,003	0,01
6	3	3	=	6	4	2	2897,803	=0,004	0,00
7	4	3	=	7	5	2	2898,977	=0,009	1,00
8	5	3	=	8	6	2	2900,276	=0,019	0,00
8	6	3	=	8	7	2	2898,395	0,012	1,00
3	1	2	=	3	0	3	2927,281	0,006	0,40
4	3	2	=	4	2	3	2927,860	=0,009	1,00
4	2	2	=	4	1	3	2927,688	0,002	0,40
5	4	2	=	5	3	3	2928,520	=0,008	0,00
5	3	2	=	5	2	3	2928,110	=0,006	0,40
6	5	2	=	6	4	3	2929,292	=0,006	0,40
6	4	2	=	6	3	3	2928,520	0,001	0,00
7	5	2	=	7	4	3	2928,854	=0,007	0,01
7	6	2	=	7	5	3	2930,134	=0,007	0,40
8	7	2	=	8	6	3	2930,990	0,013	0,40
4	1	4	=	4	2	3	2888,576	=0,002	1,00
5	1	4	=	5	2	3	2889,337	=0,004	1,00
7	3	4	=	7	4	3	2891,272	0,010	0,70
7	4	4	=	7	5	3	2891,127	0,001	0,40
8	5	4	=	8	6	3	2892,133	0,000	0,40
9	5	4	=	9	6	3	2893,698	=0,014	0,01
9	6	4	=	9	7	3	2893,164	0,001	0,01
4	2	3	=	4	1	4	2933,387	=0,002	1,00
5	2	3	=	5	1	4	2933,967	0,002	0,40
6	4	3	=	6	3	4	2934,665	=0,008	0,01
7	4	3	=	7	3	4	2935,280	=0,008	0,00
8	6	3	=	8	5	4	2936,266	=0,000	0,40
9	6	3	=	9	5	4	2936,518	0,005	0,40
5	0	5	=	5	1	4	2881,733	0,002	0,40
6	2	5	=	6	3	4	2882,647	=0,004	0,40
7	2	5	=	7	3	4	2883,701	0,006	0,00
8	4	5	=	8	5	4	2884,842	0,024	0,00
9	4	5	=	9	5	4	2886,084	=0,005	0,01
10	6	5	=	10	7	4	2887,260	=0,005	0,01
5	1	4	=	5	0	5	2939,314	0,010	0,40
6	3	4	=	6	2	5	2940,000	0,005	0,01
7	3	4	=	7	2	5	2940,746	=0,005	0,40
8	5	4	=	8	4	5	2941,561	=0,014	0,20
9	5	4	=	9	4	5	2942,358	=0,012	0,01
6	1	6	=	6	2	5	2874,742	=0,001	0,40
7	1	6	=	7	2	5	2875,857	0,014	0,20

9	3	6	=	9	4	5	2878.362	0.003	0.01
10	5	6	=	10	6	5	2879.726	0.001	0.01
11	5	6	=	11	6	5	2881.146	-0.025	0.00
6	2	5	=	6	1	6	2945.096	0.032	0.00
7	2	5	=	7	1	6	2945.849	0.004	0.20
9	4	5	=	9	3	6	2947.556	-0.003	0.40
7	0	7	=	7	1	6	2867.616	-0.003	0.40
8	2	7	=	8	3	6	2868.923	0.016	0.00
7	1	6	=	7	0	7	2950.674	0.006	0.40
8	2	7	=	8	1	8	2956.127	0.009	0.40
9	2	7	=	9	1	8	2957.066	0.009	0.40
9	0	9	=	9	1	8	2852.965	-0.000	0.01
9	1	8	=	9	0	9	2961.416	0.001	0.00
10	2	9	=	10	1	10	2966.571	0.009	0.40
3	3	0	=	2	2	1	2952.239	-0.002	1.00
4	4	0	=	3	3	1	2965.012	-0.003	1.00
5	5	0	=	4	4	1	2977.949	-0.004	0.40
6	6	0	=	5	5	1	2991.059	-0.028	0.00
7	7	0	=	6	6	1	3004.418	-0.015	0.00
8	8	0	=	7	7	1	3017.975	-0.017	0.40
9	9	0	=	8	8	1	3031.749	-0.010	0.40
10	10	0	=	9	9	1	3045.715	-0.020	0.01
11	11	0	=	10	10	1	3059.896	-0.044	1.00
3	2	1	=	2	1	2	2957.836	-0.001	0.01
5	5	1	=	4	2	2	2985.379	0.004	0.01
5	4	1	=	4	3	2	2982.493	-0.023	0.00
6	6	1	=	5	3	2	2998.404	-0.015	1.00
6	5	1	=	5	4	2	2994.762	-0.027	0.01
7	6	1	=	6	5	2	3006.990	-0.021	1.00
6	6	1	=	7	7	0	2825.681	0.008	0.00
8	7	2	=	7	4	3	3029.032	0.010	0.01
5	2	3	=	4	1	4	2995.582	0.010	0.40
7	4	3	=	6	3	4	3021.186	-0.013	0.40
6	3	4	=	5	0	5	3013.899	0.006	0.01
7	3	4	=	6	2	5	3026.775	-0.012	0.00

ASSIGNED LINES OF $H_2{}^{130}Te$ FOR $\nu_2+\nu_3$

J	K-	K+		J	K-	K+	OBS	OBS-CALC	WT
2	1	2	-	1	1	1	2931.070	0.007	0.01
2	0	2	-	1	0	1	2931.174	-0.035	0.00
3	1	3	-	2	1	2	2936.970	0.003	0.40
4	0	4	-	3	0	3	2942.725	0.039	0.00
5	1	5	-	4	1	4	2948.278	0.001	1.00
8	0	8	-	7	0	7	2964.275	-0.034	0.01
9	1	9	-	8	1	8	2969.379	-0.013	0.40
10	0	10	-	9	0	9	2974.329	-0.002	0.40
0	0	0	-	1	0	1	2906.840	0.000	0.01
1	1	1	-	2	1	2	2900.782	-0.000	0.01
2	0	2	-	3	0	3	2894.515	-0.007	0.40
3	1	3	-	4	1	4	2888.227	-0.002	1.00
4	0	4	-	5	0	5	2881.813	-0.001	0.40
5	1	5	-	6	1	6	2875.281	-0.003	0.40
6	0	6	-	7	0	7	2868.634	-0.004	0.40
8	0	8	-	9	0	9	2855.000	0.003	0.40
9	1	9	-	10	1	10	2847.995	0.001	0.40
10	0	10	-	11	0	11	2840.864	0.003	0.01
11	1	11	-	12	1	12	2833.628	0.043	0.01
2	1	1	-	1	1	0	2937.582	-0.003	0.40
4	1	3	-	3	1	2	2949.867	0.002	0.40
5	2	4	-	4	2	3	2955.683	0.006	0.40
6	1	5	-	5	1	4	2961.416	0.015	0.00
7	2	6	-	6	2	5	2967.000	-0.001	0.40
11	2	10	-	10	2	9	2988.083	-0.053	0.01
2	1	1	-	3	1	2	2888.486	-0.003	0.01
3	2	2	-	4	2	3	2882.647	0.017	0.00
4	1	3	-	5	1	4	2876.478	0.004	0.40
5	2	4	-	6	2	5	2870.221	0.006	0.01
6	1	5	-	7	1	6	2863.852	0.012	0.00
7	2	6	-	8	2	7	2857.352	-0.001	0.40
8	1	7	-	9	1	8	2850.746	-0.007	0.40
9	2	8	-	10	2	9	2844.004	-0.037	0.01
10	1	9	-	11	1	10	2837.192	-0.019	0.00
4	2	2	-	3	2	1	2957.066	0.020	0.00
5	3	3	-	4	3	2	2962.704	0.003	0.00
7	3	5	-	6	3	4	2974.574	0.001	0.01
8	2	6	-	7	2	5	2980.283	-0.006	0.40
5	3	3	-	6	3	4	2864.883	-0.003	0.40
6	2	4	-	7	2	5	2858.786	0.009	0.40
8	2	6	-	9	2	7	2846.229	-0.002	0.00
9	3	7	-	10	3	8	2839.750	-0.042	0.00
4	3	1	-	3	3	0	2962.831	0.007	0.01
6	5	1	-	5	5	0	2989.019	-0.004	1.00
1	1	1	-	1	1	0	2912.920	-0.003	0.40
2	2	1	-	2	2	0	2913.354	-0.016	0.01
3	3	1	-	3	3	0	2914.041	0.002	0.40

1	1	0	-	1	1	1	2919,163	-0,008	0,00
2	2	0	-	2	2	1	2919,311	0,003	0,40
4	4	0	-	4	4	1	2919,859	-0,002	0,40
2	0	2	-	2	2	1	2906,257	0,029	0,00
3	2	2	-	3	2	1	2907,340	0,002	0,01
5	4	2	-	5	4	1	2909,133	-0,056	0,00
6	5	2	-	6	5	1	2910,273	-0,102	0,00
7	6	2	-	7	6	1	2911,542	-0,193	0,00
2	1	1	-	2	1	2	2925,444	0,000	0,40
3	1	3	-	3	1	2	2900,010	-0,003	0,00
4	1	3	-	4	3	2	2900,456	-0,034	0,00
5	3	3	-	5	3	2	2901,527	0,010	0,01
3	2	2	-	3	0	3	2931,929	-0,008	0,40
4	0	4	-	4	2	3	2893,346	-0,033	0,00
5	2	4	-	5	2	3	2894,179	0,029	0,00
5	3	3	-	5	1	4	2938,679	-0,007	0,40
5	1	5	-	5	1	4	2886,676	0,006	0,00
6	1	5	-	6	3	4	2887,591	-0,010	0,00
2	2	0	-	1	0	1	2944,286	-0,002	0,40
4	4	0	-	3	2	1	2970,339	0,000	1,00
4	3	1	-	5	5	0	2851,937	0,004	0,40

ASSIGNED LINES OF $H_2{}^{130}Te$ FOR $2\nu_1$

J	K-	K+		J	K-	K+	OBS	OBS-CALC	WT
1	1	1	-	0	0	0	4071,860	-0,003	-0,00
2	0	2	-	1	1	1	4077,426	-0,002	0,70
2	1	2	-	1	0	1	4077,561	-0,007	0,01
3	0	3	-	2	1	2	4082,997	0,003	1,00
4	1	4	-	3	0	3	4088,337	-0,001	0,40
5	0	5	-	4	1	4	4093,514	-0,000	1,00
6	1	6	-	5	0	5	4098,528	-0,002	1,00
7	0	7	-	6	1	6	4103,380	-0,004	0,40
8	1	8	-	7	0	7	4108,072	-0,003	1,00
9	0	9	-	8	1	8	4112,602	-0,000	0,70
10	1	10	-	9	0	9	4116,962	-0,002	1,00
11	0	11	-	10	1	10	4121,160	0,001	0,40
0	0	0	-	1	1	1	4053,606	-0,002	0,01
1	1	1	-	2	0	2	4047,397	0,005	0,00
1	0	1	-	2	1	2	4047,256	0,001	1,00
2	1	2	-	3	0	3	4040,882	0,001	1,00
3	0	3	-	4	1	4	4034,249	-0,006	1,00
4	1	4	-	5	0	5	4027,471	0,005	0,40
5	0	5	-	6	1	6	4020,524	0,003	0,70
6	1	6	-	7	0	7	4013,425	0,003	0,01
7	0	7	-	8	1	8	4006,174	0,005	1,00
8	1	8	-	9	0	9	3998,763	0,000	1,00
9	0	9	-	10	1	10	3991,194	-0,010	1,00
10	1	10	-	11	0	11	3983,494	-0,001	0,40
11	0	11	-	12	1	12	3975,633	-0,001	1,00
12	1	12	-	13	0	13	3967,624	0,002	1,00
13	0	13	-	14	1	14	3959,460	0,001	0,20
14	1	14	-	15	0	15	3951,153	0,009	0,50
15	0	15	-	16	1	16	3942,695	0,018	0,40
2	2	1	-	1	1	0	4083,295	-0,001	1,00
3	1	2	-	2	2	1	4088,562	0,002	0,00
3	2	2	-	2	1	1	4088,966	0,006	0,01
4	1	3	-	3	2	2	4093,914	0,007	0,20
4	2	3	-	3	1	2	4093,969	0,009	1,00
5	1	4	-	4	2	3	4098,926	0,007	1,00
6	2	5	-	5	1	4	4103,748	0,002	1,00
7	1	6	-	6	2	5	4108,410	0,001	1,00
8	2	7	-	7	1	6	4112,907	-0,002	0,70
9	1	8	-	8	2	7	4117,246	0,001	0,40
10	2	9	-	9	1	8	4121,402	-0,015	0,01
11	1	10	-	10	2	9	4125,425	0,001	0,01
12	2	11	-	11	1	10	4129,295	0,033	0,00
13	1	12	-	12	2	11	4132,948	0,018	0,00
1	1	0	-	2	2	1	4040,782	-0,006	0,40
2	2	1	-	3	1	2	4034,249	0,049	0,00
2	1	1	-	3	2	2	4033,933	-0,006	0,01
3	1	2	-	4	2	3	4027,343	-0,003	0,40

4	2	3	-	5	1	4	4020,560	-0,009	0,40
5	1	4	-	6	2	5	4013,445	-0,012	0,00
6	2	5	-	7	1	6	4006,174	-0,011	1,00
7	1	6	-	8	2	7	3998,763	0,002	1,00
8	2	7	-	9	1	8	3991,194	0,011	1,00
9	1	8	-	10	2	9	3983,457	0,003	1,00
10	2	9	-	11	1	10	3975,577	0,003	1,00
11	1	10	-	12	2	11	3967,544	0,000	1,00
12	2	11	-	13	1	12	3959,365	0,001	1,00
13	1	12	-	14	2	13	3951,031	-0,004	0,50
14	2	13	-	15	1	14	3942,549	-0,007	0,01
15	1	14	-	16	2	15	3933,924	-0,003	1,00
4	2	2	-	3	3	1	4099,144	-0,028	0,00
4	3	2	-	3	2	1	4099,942	-0,004	0,40
5	2	3	-	4	3	2	4104,391	0,002	0,40
6	3	4	-	5	2	3	4109,104	-0,004	0,70
7	2	5	-	6	3	4	4113,551	-0,015	0,00
8	3	6	-	7	2	5	4117,882	0,011	0,40
9	2	7	-	8	3	6	4122,031	0,020	0,01
10	3	8	-	9	2	7	4125,986	0,000	0,20
11	2	9	-	10	3	8	4129,784	-0,012	0,01
12	3	10	-	11	2	9	4133,429	-0,010	0,00
13	2	11	-	12	3	10	4136,907	-0,007	0,00
14	3	12	-	13	2	11	4140,222	0,004	0,01
2	2	0	-	3	3	1	4027,616	0,006	0,00
3	2	1	-	4	3	2	4020,112	-0,005	1,00
4	3	2	-	5	2	3	4013,708	-0,003	0,00
5	2	3	-	6	3	4	4006,576	0,002	0,01
6	3	4	-	7	2	5	3999,142	0,004	0,40
7	2	5	-	8	3	6	3991,524	-0,030	1,00
8	3	6	-	9	2	7	3983,829	0,015	0,40
9	2	7	-	10	3	8	3975,936	0,015	0,70
10	3	8	-	11	2	9	3967,884	0,006	0,40
11	2	9	-	12	3	10	3959,684	-0,002	1,00
12	3	10	-	13	2	11	3951,355	0,011	0,70
13	2	11	-	14	3	12	3942,857	0,002	0,20
14	3	12	-	15	2	13	3934,211	-0,006	0,40
15	2	13	-	16	3	14	3925,423	-0,009	0,40
5	3	2	-	4	4	1	4109,823	-0,006	0,40
5	4	2	-	4	3	1	4110,445	0,008	0,40
6	4	3	-	5	3	2	4114,742	-0,008	0,40
7	3	4	-	6	4	3	4118,829	-0,003	0,01
8	4	5	-	7	3	4	4122,902	-0,064	0,00
9	3	6	-	8	4	5	4126,856	-0,045	0,00
10	4	7	-	9	3	6	4130,677	0,003	0,40
11	3	8	-	10	4	7	4134,263	-0,018	0,00
3	3	0	-	4	4	1	4014,142	-0,003	0,40
4	4	1	-	5	3	2	4009,772	-0,003	1,00
4	3	1	-	5	4	2	4005,825	0,003	1,00
6	4	3	-	7	3	4	3992,195	-0,013	0,00
7	3	4	-	8	4	5	3984,516	-0,005	0,40
8	4	5	-	9	3	6	3976,560	-0,070	0,00
9	3	6	-	10	4	7	3968,610	0,023	0,01
10	4	7	-	11	3	8	3960,414	0,023	0,00

11	3	8	-	12	4	9	3952,057	0,012	0,01
12	4	9	-	13	3	10	3943,561	0,012	0,50
13	3	10	-	14	4	11	3934,911	0,005	0,20
14	4	11	-	15	3	12	3926,114	-0,002	0,40
15	3	12	-	16	4	13	3917,174	-0,006	0,40
6	5	2	-	5	4	1	4120,359	-0,004	0,00
7	4	3	-	6	5	2	4123,872	-0,013	0,00
8	5	4	-	7	4	3	4128,213	-0,013	0,00
9	4	5	-	8	5	4	4131,942	0,043	0,01
10	5	6	-	9	4	5	4135,540	0,057	0,01
4	4	0	-	5	5	1	4000,488	0,001	0,40
5	4	1	-	6	5	2	3991,090	0,004	1,00
6	5	2	-	7	4	3	3984,730	-0,059	0,00
7	4	3	-	8	5	4	3977,603	-0,001	0,40
8	5	4	-	9	4	5	3969,581	0,004	0,00
10	5	6	-	11	4	7	3953,153	0,065	0,40
11	4	7	-	12	5	8	3944,611	0,011	0,00
12	5	8	-	13	4	9	3935,984	0,023	0,00
13	4	9	-	14	5	10	3927,192	0,019	0,40
14	5	10	-	15	4	11	3918,244	0,006	0,01
6	6	1	-	5	5	0	4130,556	-0,055	0,00
7	5	2	-	6	6	1	4129,086	-0,014	0,00
8	6	3	-	7	5	2	4133,944	-0,002	0,01
8	7	2	-	7	6	1	4138,366	-0,001	0,01
10	7	4	-	9	6	3	4145,616	0,004	0,00
8	8	1	-	7	7	0	4152,873	0,042	0,00
9	7	2	-	8	8	1	4146,764	0,014	0,40
10	8	3	-	9	7	2	4151,273	-0,000	0,40
10	9	2	-	9	8	1	4153,796	0,011	0,40
11	8	3	-	10	9	2	4156,329	-0,034	0,00
5	5	0	-	6	6	1	3986,752	0,010	0,01
6	6	1	-	7	5	2	3984,677	-0,005	0,00
7	5	2	-	8	6	3	3971,832	-0,007	0,01
8	6	3	-	9	5	4	3962,440	-0,002	0,01
9	5	4	-	10	6	5	3954,344	-0,041	0,01
6	6	0	-	7	7	1	3973,015	0,010	0,01
8	8	1	-	9	7	2	3960,354	-0,024	0,00
10	8	3	-	11	7	4	3931,139	-0,016	0,40
8	8	0	-	9	9	1	3945,854	0,018	0,00
1	0	1	-	1	1	0	4059,399	0,003	0,40
2	1	1	-	2	2	0	4058,381	-0,035	0,00
3	2	1	-	3	3	0	4056,891	-0,017	0,01
1	1	0	-	1	0	1	4065,763	-0,006	0,00
2	2	0	-	2	1	1	4065,309	0,027	0,00
3	3	0	-	3	2	1	4064,628	0,005	0,40
4	4	0	-	4	3	1	4063,871	0,003	0,01
5	5	0	-	5	4	1	4063,102	0,003	1,00
6	6	0	-	6	5	1	4062,375	-0,003	1,00
7	7	0	-	7	6	1	4061,730	-0,005	0,40
8	8	0	-	8	7	1	4061,176	0,006	0,40
9	9	0	-	9	8	1	4060,674	0,011	0,40
10	10	0	-	10	9	1	4060,196	0,015	0,00
11	11	0	-	11	10	1	4059,685	-0,006	0,00
2	0	2	-	2	1	1	4053,048	-0,008	0,00

2	1	2	-	2	2	1	4052,584	-0,004	0,40
3	1	2	-	3	2	1	4052,255	0,000	0,40
3	2	2	-	3	3	1	4051,288	-0,001	0,40
4	2	2	-	4	3	1	4051,117	0,009	0,01
4	3	2	-	4	4	1	4049,470	0,002	1,00
5	3	2	-	5	4	1	4050,181	-0,004	0,00
6	5	2	-	6	6	1	4044,016	0,011	0,40
6	4	2	-	6	5	1	4048,608	-0,006	0,40
7	5	2	-	7	6	1	4046,780	-0,017	0,40
8	7	2	-	8	8	1	4035,964	-0,019	0,00
2	1	1	-	2	0	2	4070,954	-0,010	0,00
2	2	1	-	2	1	2	4071,182	0,027	0,00
3	2	1	-	3	1	2	4069,508	0,016	0,00
3	3	1	-	3	2	2	4071,592	-0,005	0,40
4	4	1	-	4	3	2	4070,954	-0,005	0,40
5	4	1	-	5	3	2	4065,309	-0,007	0,01
5	5	1	-	5	4	2	4070,189	-0,001	1,00
6	5	1	-	6	4	2	4062,762	0,010	0,40
6	6	1	-	6	5	2	4069,295	-0,001	1,00
7	6	1	-	7	5	2	4059,964	-0,012	-0,00
7	7	1	-	7	6	2	4068,288	-0,001	1,00
8	8	1	-	8	7	2	4067,197	0,014	1,00
3	0	3	-	3	1	2	4046,034	-0,005	0,40
3	1	3	-	3	2	2	4045,990	0,010	0,01
4	1	3	-	4	2	2	4044,769	0,003	0,00
4	2	3	-	4	3	2	4044,585	-0,000	1,00
5	2	3	-	5	3	2	4043,211	0,006	0,40
5	3	3	-	5	4	2	4042,786	0,006	0,70
6	4	3	-	6	5	2	4040,523	0,003	0,40
3	2	2	-	3	1	3	4076,804	0,008	0,01
3	1	2	-	3	0	3	4076,851	-0,003	0,40
4	3	2	-	4	2	3	4075,240	0,002	1,00
5	4	2	-	5	3	3	4073,158	0,002	0,01
6	5	2	-	6	4	3	4070,501	0,002	0,01
4	1	4	-	4	2	3	4039,026	-0,004	0,70
5	1	4	-	5	2	3	4037,388	-0,004	1,00
6	3	4	-	6	4	3	4035,360	0,002	0,70
7	3	4	-	7	4	3	4033,124	0,001	0,01
4	2	3	-	4	1	4	4082,181	0,005	1,00
5	2	3	-	5	1	4	4080,369	-0,004	0,40
6	4	3	-	6	3	4	4078,129	0,010	0,40
7	4	3	-	7	3	4	4075,576	0,003	-0,00
8	6	3	-	8	5	4	4072,285	0,006	-0,00
5	0	5	-	5	1	4	4031,902	-0,005	0,70
6	2	5	-	6	3	4	4029,949	0,002	1,00
7	2	5	-	7	3	4	4027,687	0,031	0,00
8	4	5	-	8	5	4	4024,932	-0,065	0,01
5	1	4	-	5	0	5	4087,358	0,004	1,00
6	3	4	-	6	2	5	4085,173	-0,000	1,00
7	3	4	-	7	2	5	4082,604	-0,008	0,40
8	5	4	-	8	4	5	4079,604	-0,020	0,00
6	1	6	-	6	2	5	4024,626	-0,006	1,00
7	1	6	-	7	2	5	4022,378	0,005	0,01
8	3	6	-	8	4	5	4019,796	0,016	0,40

9	3	6	-	9	4	5	4016,884	0,030	0,00
6	2	5	-	6	1	6	4092,364	0,004	1,00
7	2	5	-	7	1	6	4089,775	-0,030	1,00
8	4	5	-	8	3	6	4086,787	-0,077	1,00
7	0	7	-	7	1	6	4017,206	-0,003	0,01
9	2	7	-	9	3	6	4011,789	0,012	0,01
10	4	7	-	10	5	6	4008,580	0,016	0,00
7	1	6	-	7	0	7	4097,204	0,006	1,00
8	3	6	-	8	2	7	4094,268	0,009	0,40
9	3	6	-	9	2	7	4090,961	0,027	1,00
8	1	8	-	8	2	7	4009,635	-0,002	0,01
8	2	7	-	8	1	8	4101,870	0,002	1,00
9	1	8	-	9	0	9	4106,379	0,008	0,40
10	3	8	-	10	2	9	4102,635	-0,005	0,40
10	2	9	-	10	1	10	4110,682	-0,023	0,01
11	2	9	-	11	1	10	4106,562	-0,006	0,20
12	4	9	-	12	3	10	4102,038	-0,002	0,01
1	1	1	-	2	2	0	4034,816	-0,027	0,01
2	2	1	-	3	3	0	4021,612	-0,004	0,40
4	4	1	-	5	5	0	3996,864	0,004	0,40
6	6	1	-	7	7	0	3970,788	0,008	0,01
3	3	0	-	2	2	1	4100,928	-0,001	1,00
4	4	0	-	3	3	1	4111,934	0,002	0,40
5	5	0	-	4	4	1	4122,752	0,009	0,40
6	6	0	-	5	5	1	4133,429	-0,001	0,01
7	7	0	-	6	6	1	4144,037	-0,001	0,00
8	8	0	-	7	7	1	4154,592	-0,004	0,40
9	9	0	-	8	8	1	4165,143	0,015	0,40
2	1	2	-	3	2	1	4016,284	0,002	0,40
3	1	2	-	4	4	1	4001,776	-0,001	0,01
4	3	2	-	5	4	1	3989,830	0,006	1,00
5	3	2	-	6	6	1	3973,825	-0,003	1,00
6	4	2	-	7	7	1	3959,243	0,002	1,00
6	5	2	-	7	6	1	3961,714	0,012	1,00
7	5	2	-	8	8	1	3944,417	0,004	1,00
7	6	2	-	8	7	1	3946,889	0,008	1,00
8	6	2	-	9	9	1	3929,363	-0,002	0,40
8	7	2	-	9	8	1	3931,519	0,001	1,00
9	7	2	-	10	10	1	3914,125	-0,006	1,00
9	8	2	-	10	9	1	3915,581	-0,010	0,01
10	9	2	-	11	10	1	3899,063	-0,009	1,00
11	9	2	-	12	12	1	3883,262	0,010	0,01
3	0	3	-	4	3	2	3996,658	-0,006	0,00
6	4	3	-	7	5	2	3955,916	0,010	1,00
7	4	3	-	8	7	2	3939,733	0,012	0,01
8	6	3	-	9	7	2	3927,568	-0,023	0,01
9	6	3	-	10	9	2	3909,046	-0,013	0,40
4	1	4	-	5	2	3	3977,510	0,007	0,01
5	1	4	-	6	4	3	3963,649	0,008	0,00
6	3	4	-	7	4	3	3949,656	0,008	0,40
7	3	4	-	8	6	3	3935,116	0,037	0,00
8	5	4	-	9	6	3	3920,892	-0,027	0,40
10	7	4	-	11	8	3	3891,653	0,079	0,00
5	0	5	-	6	3	4	3958,116	0,008	1,00

7	2	5	-	8	5	4	3929,670	-0,016	0,00
8	4	5	-	9	5	4	3915,093	-0,067	0,00
7	1	6	-	8	4	5	3924,297	0,015	0,01
8	3	6	-	9	4	5	3909,753	0,020	0,00
9	3	6	-	10	6	5	3894,988	0,043	0,00
3	2	1	-	2	1	2	4106,448	0,001	0,40
4	4	1	-	3	1	2	4120,359	0,025	0,00
5	4	1	-	4	3	2	4126,473	-0,027	0,00
6	6	1	-	5	3	2	4143,522	-0,004	0,40
7	6	1	-	6	5	2	4144,593	0,003	0,01
8	8	1	-	7	5	2	4166,735	0,002	0,01
6	5	2	-	5	2	3	4144,256	0,007	0,01
6	4	3	-	5	1	4	4151,937	0,019	0,40
7	4	3	-	6	3	4	4161,474	-0,010	0,40
8	6	3	-	7	3	4	4170,246	-0,002	0,00
6	3	4	-	5	0	5	4159,086	0,015	0,00
7	3	4	-	6	2	5	4168,638	-0,010	0,01

ASSIGNED LINES OF $H_2{}^{130}Te$ FOR $\nu_1+\nu_3$

J	K-	K+		J	K-	K+	OBS	OBS-CALC	WT
1	0	1	-	0	0	0	4072,285	-0,046	0,00
2	1	2	-	1	1	1	4077,909	-0,005	0,01
2	0	2	-	1	0	1	4078,083	0,002	0,40
3	1	3	-	2	1	2	4083,521	0,010	1,00
4	0	4	-	3	0	3	4088,886	0,005	0,40
5	1	5	-	4	1	4	4094,093	0,004	0,40
6	0	6	-	5	0	5	4099,144	0,002	0,40
7	1	7	-	6	1	6	4104,039	0,001	1,00
8	0	8	-	7	0	7	4108,780	0,002	1,00
9	1	9	-	8	1	8	4113,362	0,003	0,40
10	0	10	-	9	0	9	4117,779	-0,002	1,00
11	1	11	-	10	1	10	4122,031	-0,011	0,20
12	0	12	-	11	0	11	4126,141	-0,000	0,70
13	1	13	-	12	1	12	4130,082	0,005	0,70
14	0	14	-	13	0	13	4133,876	0,030	0,00
15	1	15	-	14	1	14	4137,464	0,016	0,70
0	0	0	-	1	0	1	4054,242	-0,002	0,40
1	1	1	-	2	1	2	4047,950	-0,011	0,01
1	0	1	-	2	0	2	4047,851	-0,009	0,00
2	0	2	-	3	0	3	4041,384	-0,010	0,40
3	1	3	-	4	1	4	4034,770	-0,002	0,40
4	0	4	-	5	0	5	4028,009	-0,000	0,01
5	1	5	-	6	1	6	4021,087	-0,009	0,40
6	0	6	-	7	0	7	4014,025	-0,009	0,00
7	1	7	-	8	1	8	4006,830	0,007	0,00
8	0	8	-	9	0	9	3999,471	0,005	0,01
9	1	9	-	10	1	10	3991,965	0,004	0,00
10	0	10	-	11	0	11	3984,314	0,003	0,01
11	1	11	-	12	1	12	3976,500	-0,017	0,00
3	2	2	-	2	2	1	4089,012	0,002	0,40
3	1	2	-	2	1	1	4089,538	0,004	0,40
4	1	3	-	3	1	2	4094,492	0,004	1,00
5	2	4	-	4	2	3	4099,474	0,008	0,70
6	1	5	-	5	1	4	4104,329	0,002	1,00
7	2	6	-	6	2	5	4109,017	-0,010	0,40
8	1	7	-	7	1	6	4113,574	0,004	0,01
9	2	8	-	8	2	7	4117,955	-0,000	1,00
10	1	9	-	9	1	8	4122,177	-0,004	0,20
11	2	10	-	10	2	9	4126,233	-0,013	0,70
12	1	11	-	11	1	10	4130,150	0,000	0,70
13	2	12	-	12	2	11	4133,876	-0,014	0,00
14	1	13	-	13	1	12	4137,399	-0,067	0,00
15	2	14	-	14	2	13	4140,832	-0,043	0,40
1	1	0	-	2	1	1	4041,727	-0,003	0,01
2	1	1	-	3	1	2	4035,152	0,001	0,40
3	2	2	-	4	2	3	4028,009	0,013	0,00
4	1	3	-	5	1	4	4021,087	-0,009	0,40
5	2	4	-	6	2	5	4014,007	0,002	0,00

6	1	5	- 7	1	6	4006,781	0,015	0,00
7	2	6	- 8	2	7	3999,364	-0,015	0,01
8	1	7	- 9	1	8	3991,853	0,008	0,70
9	2	8	- 10	2	9	3984,159	-0,005	0,40
3	2	1	- 2	2	0	4094,137	-0,005	0,40
4	2	2	- 3	2	1	4100,691	-0,003	0,01
5	3	3	- 4	3	2	4104,905	0,011	0,01
6	2	4	- 5	2	3	4109,653	-0,011	0,01
7	3	5	- 6	3	4	4114,150	-0,002	1,00
8	2	6	- 7	2	5	4118,493	-0,002	0,40
9	3	7	- 8	3	6	4122,648	-0,030	0,00
10	2	8	- 9	2	7	4126,695	-0,005	0,00
11	3	9	- 10	3	8	4130,556	-0,006	1,00
12	2	10	- 11	2	9	4134,263	0,000	0,01
13	3	11	- 12	3	10	4137,783	-0,017	0,01
14	2	12	- 13	2	11	4141,162	-0,012	0,40
15	3	13	- 14	3	12	4144,361	-0,021	0,01
2	2	0	- 3	2	1	4029,000	-0,005	0,70
3	3	1	- 4	3	2	4022,448	0,004	0,40
4	2	2	- 5	2	3	4014,454	-0,005	0,01
5	3	3	- 6	3	4	4007,083	0,005	0,00
6	2	4	- 7	2	5	3999,684	-0,010	0,40
7	3	5	- 8	3	6	3992,132	-0,008	0,01
8	2	6	- 9	2	7	3984,441	0,003	0,01
4	3	1	- 3	3	0	4104,462	0,002	0,40
5	4	2	- 4	4	1	4109,104	0,005	0,01
5	3	2	- 4	3	1	4111,567	0,003	0,40
6	4	3	- 5	4	2	4114,862	-0,009	0,00
6	3	3	- 5	3	2	4115,337	-0,000	1,00
7	4	4	- 6	4	3	4119,375	-0,003	0,01
8	3	5	- 7	3	4	4123,574	0,017	0,00
9	4	6	- 8	4	5	4127,530	0,002	1,00
10	3	7	- 9	3	6	4131,346	0,002	0,70
11	4	8	- 10	4	7	4135,006	0,009	0,20
12	3	9	- 11	3	8	4138,490	0,002	0,70
13	4	10	- 12	4	9	4141,809	-0,007	0,40
14	3	11	- 13	3	10	4144,975	-0,004	0,01
3	3	0	- 4	3	1	4016,126	-0,001	0,40
5	4	2	- 6	4	3	3999,585	-0,006	0,01
6	3	3	- 7	3	4	3992,792	-0,004	0,01
7	4	4	- 8	4	5	3985,067	0,000	0,40
8	3	5	- 9	3	6	3977,218	-0,003	0,40
10	3	7	- 11	3	8	3961,072	0,011	0,00
11	4	8	- 12	4	9	3952,773	0,013	0,01
5	4	1	- 4	4	0	4114,271	0,001	0,01
6	4	2	- 5	4	1	4122,177	0,040	0,00
7	5	3	- 6	5	2	4124,284	-0,019	0,01
8	4	4	- 7	4	3	4128,811	-0,003	0,40
9	5	5	- 8	5	4	4132,479	-0,009	0,01
10	4	6	- 9	4	5	4136,124	0,010	0,70
11	5	7	- 10	5	6	4139,562	0,010	0,70
12	4	8	- 11	4	7	4142,850	0,020	0,20
13	5	9	- 12	5	8	4145,954	0,012	0,40
14	4	10	- 13	4	9	4148,915	0,027	0,01

15	5	11	-	14	5	10	4151,685	0,016	0,40
4	4	0	-	5	4	1	4003,174	-0,002	0,40
6	4	2	-	7	4	3	3986,571	0,008	1,00
6	5	1	-	5	5	0	4123,574	-0,012	0,00
7	6	2	-	6	6	1	4126,708	0,028	0,00
8	5	3	-	7	5	2	4134,777	-0,017	0,00
9	6	4	-	8	6	3	4137,399	0,008	0,00
10	5	5	-	9	5	4	4141,042	0,010	0,00
5	5	0	-	6	5	1	3990,204	-0,028	0,01
6	5	1	-	7	5	2	3977,649	-0,008	0,00
7	6	2	-	8	6	3	3969,405	-0,014	0,00
8	5	3	-	9	5	4	3963,280	-0,011	0,40
9	6	4	-	10	6	5	3954,882	0,005	0,00
10	5	5	-	11	5	6	3946,518	-0,011	0,01
11	6	6	-	12	6	7	3937,973	0,023	0,01
7	6	1	-	6	6	0	4132,422	-0,009	0,00
8	6	2	-	7	6	1	4142,355	0,050	0,01
9	7	3	-	8	7	2	4140,879	0,069	0,00
10	6	4	-	9	6	3	4146,325	-0,015	0,40
6	6	0	-	7	6	1	3977,370	0,006	0,40
8	7	1	-	7	7	0	4140,832	-0,005	0,00
1	1	1	-	1	1	0	4060,100	-0,003	1,00
2	2	1	-	2	2	0	4059,734	-0,003	0,00
3	3	1	-	3	3	0	4059,236	0,001	1,00
4	4	1	-	4	4	0	4058,589	0,000	0,40
5	5	1	-	5	5	0	4057,805	0,005	1,00
6	6	1	-	6	6	0	4056,891	0,012	0,01
7	7	1	-	7	7	0	4055,870	0,022	1,00
8	8	1	-	8	8	0	4054,703	-0,036	0,40
9	9	1	-	9	9	0	4053,549	-0,052	0,40
11	11	1	-	11	11	0	4051,557	0,063	0,00
1	1	0	-	1	1	1	4066,105	0,003	0,40
2	2	0	-	2	2	1	4065,309	-0,001	0,01
3	3	0	-	3	3	1	4064,188	-0,003	1,00
4	4	0	-	4	4	1	4062,817	-0,003	0,40
5	5	0	-	5	5	1	4061,281	-0,003	0,40
6	6	0	-	6	6	1	4059,685	0,018	0,00
7	7	0	-	7	7	1	4058,033	-0,000	0,00
8	8	0	-	8	8	1	4056,456	0,022	0,01
2	0	2	-	2	2	1	4053,099	-0,001	0,40
3	2	2	-	3	2	1	4052,706	0,002	1,00
3	1	2	-	3	3	1	4051,859	-0,003	0,40
4	3	2	-	4	3	1	4051,550	-0,006	0,00
4	2	2	-	4	4	1	4050,181	-0,035	0,01
5	4	2	-	5	4	1	4049,470	0,015	0,01
6	4	2	-	6	6	1	4045,792	0,013	0,01
2	1	1	-	2	1	2	4072,096	-0,010	0,40
3	3	1	-	3	1	2	4071,820	0,001	0,00
4	3	1	-	4	3	2	4067,663	-0,006	0,00
5	5	1	-	5	3	2	4070,676	-0,038	0,00
3	1	3	-	3	1	2	4046,552	-0,005	0,40
4	1	3	-	4	3	2	4045,110	-0,002	0,40
4	2	3	-	4	2	2	4045,280	-0,002	0,40
5	3	3	-	5	3	2	4043,712	0,003	0,40

5	2	3	-	5	4	2	4043,326	0,000	0,40
6	3	3	-	6	5	2	4041,101	-0,007	0,00
7	5	3	-	7	5	2	4039,689	-0,000	0,01
3	2	2	-	3	0	3	4077,308	0,005	1,00
3	1	2	-	3	1	3	4077,371	0,001	0,01
4	2	2	-	4	2	3	4075,986	0,000	0,01
5	4	2	-	5	2	3	4073,342	0,001	0,40
6	4	2	-	6	4	3	4072,285	0,012	0,00
7	6	2	-	7	4	3	4067,436	-0,028	0,00
4	0	4	-	4	2	3	4039,575	0,002	1,00
5	2	4	-	5	2	3	4037,936	-0,003	0,40
6	2	4	-	6	4	3	4035,917	0,003	0,40
7	4	4	-	7	4	3	4033,671	0,002	0,40
4	1	3	-	4	1	4	4082,703	-0,001	0,40
5	3	3	-	5	1	4	4080,881	0,003	0,40
6	3	3	-	6	3	4	4078,692	-0,014	0,01
5	1	5	-	5	1	4	4032,479	-0,003	1,00
6	1	5	-	6	3	4	4030,524	-0,003	1,00
8	3	5	-	8	5	4	4025,586	-0,002	0,40
10	5	5	-	10	7	4	4019,191	-0,013	0,01
5	2	4	-	5	0	5	4087,906	0,004	0,01
6	2	4	-	6	2	5	4085,739	0,006	0,01
7	4	4	-	7	2	5	4083,166	0,008	0,00
6	0	6	-	6	2	5	4025,241	-0,003	0,70
7	2	6	-	7	2	5	4023,000	0,008	0,40
8	2	6	-	8	4	5	4020,410	0,006	0,40
9	4	6	-	9	4	5	4017,486	0,005	0,20
6	1	5	-	6	1	6	4092,944	0,003	0,40
7	3	5	-	7	1	6	4090,370	-0,021	0,01
8	3	5	-	8	3	6	4087,446	-0,009	0,01
7	1	7	-	7	1	6	4017,862	-0,002	0,40
8	1	7	-	8	3	6	4015,322	0,003	0,40
9	3	7	-	9	3	6	4012,449	0,005	0,70
10	3	7	-	10	5	6	4009,243	0,009	0,70
11	5	7	-	11	5	6	4005,695	0,005	0,01
7	2	6	-	7	0	7	4097,818	0,001	0,01
9	4	6	-	9	2	7	4091,553	-0,009	0,01
8	0	8	-	8	2	7	4010,339	-0,001	0,40
10	2	8	-	10	4	7	4004,362	0,009	0,20
8	1	7	-	8	1	8	4102,534	0,004	0,01
9	1	9	-	9	1	8	4002,658	-0,016	0,00
10	0	10	-	10	2	9	3994,858	-0,006	0,40
2	1	1	-	3	3	0	4022,532	-0,035	0,00
3	2	1	-	4	4	0	4007,834	0,001	0,40
4	3	1	-	5	5	0	3993,569	-0,001	1,00
5	4	1	-	6	6	0	3978,864	0,001	0,40
6	5	1	-	7	7	0	3963,756	0,001	0,40
7	6	1	-	8	8	0	3948,306	0,005	0,01
8	7	1	-	9	9	0	3932,571	0,000	1,00
9	8	1	-	10	10	0	3916,639	-0,009	0,01
10	9	1	-	11	11	0	3900,603	-0,013	0,40
2	2	0	-	1	0	1	4090,290	-0,001	0,40
4	4	0	-	3	2	1	4113,306	0,008	0,01
5	5	0	-	4	3	1	4124,668	0,002	0,01

6	6	0	-	5	4	1	4136,016	-0,008	0,40
7	7	0	-	6	5	1	4147,421	0,015	0,00
8	8	0	-	7	6	1	4158,832	0,014	0,01
2	0	2	-	3	2	1	4016,792	-0,003	-0,00
3	2	2	-	4	4	1	4002,221	-0,005	0,40
4	2	2	-	5	4	1	3990,569	-0,003	0,01
5	4	2	-	6	6	1	3973,099	0,001	0,00
7	6	2	-	8	8	1	3941,984	-0,009	0,40
9	8	2	-	10	10	1	3908,697	-0,078	0,00
3	1	3	-	4	3	2	3997,164	-0,017	0,40
4	1	3	-	5	3	2	3983,931	0,003	0,00
5	3	3	-	6	5	2	3969,483	0,004	0,01
6	3	3	-	7	5	2	3956,489	-0,005	0,40
6	4	3	-	7	6	2	3955,038	0,006	0,01
7	5	3	-	8	7	2	3940,147	0,008	1,00
8	5	3	-	9	7	2	3928,521	0,082	0,00
4	0	4	-	5	2	3	3978,033	-0,013	-0,00
6	2	4	-	7	4	3	3950,210	0,006	0,40
7	4	4	-	8	6	3	3935,630	0,006	0,01
8	4	4	-	9	6	3	3921,493	-0,014	1,00
9	6	4	-	10	8	3	3905,768	-0,001	0,40
5	1	5	-	6	3	4	3958,687	0,005	0,00
6	1	5	-	7	3	4	3944,609	-0,008	0,00
7	3	5	-	8	5	4	3930,280	0,008	0,01
8	3	5	-	9	5	4	3915,746	-0,006	0,01
9	5	5	-	10	7	4	3900,766	-0,058	0,00
10	5	5	-	11	7	4	3886,009	-0,054	-0,00
6	0	6	-	7	2	5	3939,208	-0,001	0,01
7	2	6	-	8	4	5	3924,908	0,008	0,40
8	2	6	-	9	4	5	3910,366	0,009	0,40
9	4	6	-	10	6	5	3895,584	0,011	0,01
10	4	6	-	11	6	5	3880,674	0,073	0,00
7	1	7	-	8	3	6	3919,614	0,002	0,00
8	1	7	-	9	3	6	3905,094	0,009	0,01
9	3	7	-	10	5	6	3890,345	0,011	0,00
8	0	8	-	9	2	7	3899,902	0,007	0,00

APPENDIX III

GROUND STATE COMBINATION DIFFERENCES FOR $H_2{}^{130}Te$

J	K-	K+		J	K-	K+	OBS	OBS-CALC	WT
2	2	1	-	1	0	1	24,984	0,003	2,41
2	1	2	-	1	1	0	12,147	0,006	1,59
2	1	1	-	1	1	1	24,378	0,007	0,02
3	3	1	-	2	1	1	37,679	0,007	0,42
3	3	1	-	3	1	3	25,514	0,006	0,04
3	3	0	-	1	1	0	61,683	0,003	0,57
3	3	0	-	2	1	2	49,557	0,019	0,02
3	2	1	-	2	2	1	36,303	-0,003	2,96
3	2	1	-	3	0	3	24,601	0,002	2,39
3	2	1	-	1	0	1	61,290	0,004	0,53
3	1	2	-	2	1	2	36,959	0,004	2,55
3	1	2	-	1	1	0	49,106	0,010	1,02
3	1	3	-	2	1	1	12,165	0,001	0,03
3	0	3	-	1	0	1	36,691	0,004	0,99
3	0	3	-	2	2	1	11,704	-0,003	2,51
4	4	1	-	3	2	1	50,481	0,003	2,16
4	4	0	-	2	2	0	86,303	-0,006	0,40
4	4	1	-	2	2	1	86,788	0,004	0,97
4	4	1	-	4	2	3	25,770	0,000	1,03
4	4	1	-	3	0	3	75,087	0,010	0,59
4	3	1	-	3	3	1	48,061	-0,003	1,59
4	3	1	-	4	1	3	24,275	0,006	0,40
4	3	2	-	3	1	2	49,382	0,007	2,77
4	3	2	-	4	1	4	37,595	0,004	2,94
4	3	2	-	2	1	2	86,346	0,016	1,16
4	3	2	-	3	3	0	36,787	-0,004	1,16
4	2	2	-	2	2	0	73,621	0,003	0,57
4	2	3	-	3	0	3	49,313	0,006	2,45
4	2	3	-	2	2	1	61,019	0,005	0,40
4	2	3	-	3	2	1	24,715	0,007	2,38
4	1	4	-	2	1	2	48,748	0,009	2,71
4	1	4	-	3	1	2	11,787	0,003	3,68
5	5	0	-	5	3	2	12,906	-0,009	1,14
5	5	0	-	3	3	0	110,893	0,002	0,59
5	5	1	-	4	3	1	63,385	0,003	0,04
5	5	0	-	4	3	2	74,090	-0,009	0,40
5	5	1	-	3	3	1	111,446	0,001	0,40
5	4	1	-	4	4	1	59,643	-0,001	2,56
5	4	1	-	5	2	3	23,887	0,000	0,43
5	4	2	-	4	2	2	61,778	0,013	0,02
5	4	1	-	3	2	1	110,113	-0,009	0,60
5	4	1	-	4	2	3	85,410	-0,004	1,01
5	3	2	-	4	3	2	61,184	-0,000	2,13
5	3	2	-	3	3	0	97,967	-0,009	1,00
5	3	2	-	5	1	4	37,173	0,004	1,62
5	3	2	-	4	1	4	98,785	0,009	0,40
5	3	3	-	4	3	1	37,287	0,005	0,02

5	2	3	-	4	2	3	61,534	0,007	2,56
5	2	3	-	3	2	1	86,244	0,008	0,03
5	2	3	-	5	0	5	49,973	0,010	1,62
5	2	3	-	4	4	1	35,744	-0,013	0,03
5	2	3	-	3	0	3	110,827	-0,008	0,02
5	1	4	-	4	1	4	61,614	0,007	3,33
5	1	4	-	4	3	2	24,023	0,007	1,96
5	1	4	-	3	1	2	73,402	0,011	1,54
5	0	5	-	3	0	3	60,867	-0,005	0,44
5	0	5	-	4	2	3	11,560	-0,004	2,14
6	6	1	-	5	4	1	76,356	-0,001	1,02
6	6	1	-	4	4	1	135,998	-0,003	1,16
6	6	0	-	4	4	0	135,407	0,000	0,02
6	6	1	-	6	4	3	26,485	-0,008	0,02
6	6	1	-	5	2	3	100,240	-0,004	0,02
6	5	1	-	5	5	1	71,051	-0,001	0,61
6	5	2	-	5	3	2	74,222	-0,008	2,05
6	5	2	-	6	3	4	37,599	0,000	0,81
6	5	2	-	5	5	0	61,317	0,002	0,57
6	5	1	-	4	3	1	134,464	0,031	0,01
6	5	2	-	4	3	2	135,422	0,008	0,01
6	5	2	-	5	1	4	111,413	0,015	0,42
6	4	2	-	5	4	2	73,020	-0,008	0,03
6	4	2	-	4	2	2	134,797	0,004	0,01
6	4	3	-	5	4	1	49,863	-0,001	0,98
6	4	3	-	5	2	3	73,746	-0,005	1,15
6	4	3	-	6	2	5	49,813	-0,003	0,85
6	4	3	-	4	4	1	109,519	0,011	0,01
6	3	4	-	5	1	4	73,800	0,000	4,21
6	3	4	-	5	3	2	36,618	-0,013	0,48
6	3	4	-	6	1	6	62,414	0,001	2,39
6	3	4	-	4	1	4	135,398	-0,009	1,00
6	3	4	-	4	3	2	97,815	-0,000	0,02
6	2	5	-	5	0	5	73,901	0,003	2,09
6	2	5	-	5	2	3	23,931	-0,004	0,84
6	2	5	-	4	2	3	85,462	0,000	0,02
6	1	6	-	4	1	4	72,994	0,001	2,36
6	1	6	-	5	1	4	11,384	-0,002	3,24
7	7	0	-	6	5	2	98,507	-0,009	0,02
7	7	0	-	5	3	2	172,734	-0,012	0,02
7	7	1	-	6	5	1	89,365	-0,008	0,59
7	7	1	-	5	5	1	160,414	-0,011	0,01
7	6	1	-	7	4	3	23,085	-0,002	0,04
7	6	1	-	5	4	1	158,646	-0,014	0,40
7	6	1	-	6	6	1	82,302	-0,001	0,57
7	6	1	-	6	4	3	108,787	-0,009	0,02
7	6	1	-	5	2	3	182,542	-0,005	0,02
7	5	2	-	6	5	2	84,610	-0,004	2,29
7	5	2	-	5	5	0	145,930	0,001	0,40
7	5	2	-	5	3	2	158,836	-0,008	1,71
7	5	2	-	6	3	4	122,211	-0,002	1,16
7	5	3	-	6	3	3	85,906	-0,004	0,02
7	5	2	-	7	3	4	36,303	0,001	0,02
7	5	2	-	5	1	4	196,021	0,009	0,57

7	4	3	-	6	4	3	85,703	-0.006	1.45
7	4	3	-	7	2	5	49,478	-0.012	1.33
7	4	3	-	5	2	3	159,448	-0.012	0.53
7	4	3	-	6	6	1	59,221	0.005	0.02
7	4	3	-	6	2	5	135,517	-0.008	0.60
7	3	4	-	6	3	4	85,905	-0.006	0.03
7	3	4	-	5	3	2	122,545	0.003	0.59
7	3	4	-	6	5	2	48,319	0.007	0.02
7	2	5	-	6	2	5	86,026	-0.009	1.40
7	2	5	-	5	2	3	109,962	-0.008	0.55
7	2	5	-	5	0	5	159,940	0.007	0.04
7	2	5	-	6	4	3	36,224	0.004	1.33
7	2	5	-	7	0	7	74,818	-0.007	0.31
7	1	6	-	6	1	6	86,184	0.009	1.99
7	1	6	-	5	1	4	97,570	0.009	1.57
7	1	6	-	6	3	4	23,768	0.007	1.75
7	0	7	-	5	0	5	85,101	-0.007	0.59
7	0	7	-	6	2	5	11,206	-0.005	2.01
8	8	1	-	7	6	1	102,363	-0.021	0.58
8	8	1	-	8	6	3	27,415	-0.012	0.02
8	7	2	-	7	5	2	99,537	-0.013	0.61
8	7	2	-	8	5	4	37,871	-0.012	0.59
8	7	2	-	6	5	2	184,137	-0.027	0.02
8	7	1	-	7	7	1	93,416	-0.010	0.40
8	7	2	-	6	3	4	221,741	-0.022	0.02
8	6	3	-	7	4	3	98,040	-0.004	0.44
8	6	3	-	7	6	1	74,956	-0.001	0.42
8	6	3	-	8	4	5	49,429	-0.014	0.29
8	6	3	-	6	4	3	183,745	-0.009	0.01
8	5	4	-	6	5	2	146,284	0.003	0.02
8	5	4	-	7	5	2	61,666	-0.001	0.42
8	5	4	-	6	3	4	183,871	-0.009	0.44
8	5	4	-	8	3	6	61,856	-0.011	0.05
8	5	4	-	7	1	6	160,090	-0.029	0.01
8	4	5	-	6	4	3	134,313	0.002	0.06
8	4	5	-	7	4	3	48,608	0.006	0.71
8	4	5	-	7	2	5	98,087	-0.004	1.63
8	4	5	-	6	2	5	184,110	-0.017	0.44
8	4	5	-	8	2	7	74,471	-0.008	0.44
8	4	5	-	7	0	7	172,909	-0.007	0.04
8	3	6	-	7	1	6	98,252	0.000	1.30
8	3	6	-	6	3	4	122,015	0.002	0.59
8	3	6	-	8	1	8	87,212	0.001	0.02
8	2	7	-	6	2	5	109,646	-0.002	1.99
8	2	7	-	7	2	5	23,617	0.004	0.71
8	2	7	-	7	0	7	98,440	0.003	2.00
8	1	8	-	6	1	6	97,207	-0.008	1.14
8	1	8	-	7	1	6	11,036	-0.004	1.99
9	8	1	-	7	6	1	206,847	-0.002	0.02
9	8	1	-	8	8	1	104,469	0.004	0.40
9	7	2	-	7	5	2	206,376	0.021	0.01
9	7	2	-	9	5	4	34,872	0.020	0.01
9	6	3	-	9	4	5	48,660	0.002	0.01
9	6	3	-	7	4	3	207,318	0.011	0.57

9	5	4	-	7	5	2	171,502	-0,002	0,03
9	5	4	-	8	7	2	71,962	0,009	0,59
9	5	4	-	8	5	4	109,838	0,002	0,04
9	5	4	-	9	3	6	61,472	0,002	0,04
9	5	4	-	8	3	6	171,700	-0,004	0,01
9	4	5	-	8	4	5	110,044	-0,003	0,77
9	4	5	-	7	4	3	158,653	0,004	0,02
9	4	5	-	8	6	3	60,613	0,008	0,02
9	4	5	-	7	2	5	208,127	-0,011	0,40
9	4	5	-	9	2	7	74,071	-0,010	0,04
9	3	6	-	7	3	4	146,335	-0,001	0,40
9	3	6	-	7	1	6	208,480	-0,006	0,01
9	3	6	-	9	1	8	86,759	-0,001	0,02
9	3	6	-	8	3	6	110,231	-0,003	0,05
9	3	6	-	8	5	4	48,368	0,001	0,40
9	3	6	-	8	1	8	197,440	-0,005	0,01
9	2	7	-	7	2	5	134,054	-0,004	0,99
9	2	7	-	8	4	5	35,968	0,001	0,44
9	2	7	-	8	2	7	110,439	-0,006	0,40
9	1	8	-	8	1	8	110,680	-0,005	1,61
9	1	8	-	7	1	6	121,722	-0,004	1,84
9	1	8	-	8	3	6	23,471	-0,003	1,08
9	0	9	-	7	0	7	109,308	-0,004	2,04
9	0	9	-	8	2	7	10,867	-0,008	0,44
10	10	1	-	8	8	1	232,639	0,020	0,57
10	7	4	-	9	5	4	121,834	0,006	0,02
10	6	5	-	9	4	5	121,901	-0,008	0,04
10	6	5	-	8	4	5	231,946	-0,010	0,02
10	6	5	-	9	2	7	195,969	-0,020	0,01
10	5	6	-	9	5	4	60,639	-0,001	0,01
10	5	6	-	9	3	6	122,103	-0,007	0,72
10	4	7	-	8	4	5	158,305	-0,008	0,02
10	4	7	-	9	4	5	48,263	-0,003	0,01
10	4	7	-	9	2	7	122,351	0,004	0,02
10	3	8	-	8	3	6	146,088	-0,001	0,59
10	3	8	-	9	1	8	122,616	0,001	0,40
10	3	8	-	9	3	6	35,853	-0,002	0,02
10	2	9	-	8	2	7	133,793	0,002	1,96
10	2	9	-	9	0	9	122,922	0,005	1,14
10	2	9	-	9	2	7	23,351	0,005	0,27
10	1	10	-	8	1	8	121,398	0,000	1,79
10	1	10	-	9	1	8	10,715	0,003	0,03
11	10	1	-	9	8	1	254,733	0,021	0,57
11	7	4	-	9	7	2	220,134	0,016	0,40
11	5	6	-	10	5	6	133,867	0,004	0,02
11	5	6	-	10	7	4	72,673	-0,002	0,01
11	4	7	-	9	4	5	182,387	-0,009	0,02
11	3	8	-	9	3	6	170,286	0,003	0,02
11	2	9	-	9	2	7	158,102	-0,006	0,27
11	2	9	-	10	2	9	134,751	-0,010	0,40
11	1	10	-	10	1	10	135,117	-0,014	0,04
11	1	10	-	9	1	8	145,825	-0,018	0,02
11	1	10	-	10	3	8	23,222	-0,006	0,02
11	0	11	-	9	0	9	133,468	-0,001	0,63

11	0	11	-	10	2	9	10,544	-0,009	0,02
12	3	10	-	10	3	8	170,106	-0,004	0,04
12	4	9	-	10	4	7	182,233	-0,004	0,02
12	3	10	-	11	1	10	146,878	-0,004	0,33
12	2	11	-	10	2	9	157,882	0,002	0,04
12	1	12	-	10	1	10	145,528	0,003	0,97
13	3	10	-	12	3	10	158,477	-0,014	0,02
13	0	13	-	11	0	11	157,566	0,004	0,40
15	2	13	-	13	2	11	206,011	0,010	0,02

APPENDIX IV

CALCULATED GROUND STATE ENERGY LEVELS

GROUND STATE CONSTANTS

A = 6.2474800000
B = 6.0948340000
C = 3.0359990000

TAAAA = -0.0031390000
TBBBB = -0.0027910000
TAABB = 0.0022850000
TAAAB = -0.0009330000
HJ = -0.0000000000000
HJK = -0.0000000000000
HKJ = -0.0000000000000
HK = -0.0000000020000

KAPPA = 0.90403

J	K-	K+	ENG
1	1	0	12.3420
1	0	1	9.1299
1	1	1	9.2825
2	2	0	37.0200
2	0	2	24.4715
2	1	2	24.4834
2	1	1	33.6538
2	2	1	34.1104
3	3	0	74.0218
3	1	2	61.4379
3	2	2	61.4968
3	2	1	70.4160
3	0	3	45.8170

APPENDIX IV

CALCULATED GROUND STATE ENERGY LEVELS

GROUND STATE CONSTANTS

A = 6.247480000
B = 6.094834000
C = 3.035999000

TAAA = -0.003139000
TBBB = -0.002791000
TAAB = 0.002285000
TAAB = -0.000533000
HJ = -0.000000000000
HJK = -0.000000000000
HKJ = -0.000000000000
HK = -0.000000020000

KAPPA = 0.90403

J	K-	K+	ENG
1	1	0	12.3420
1	0	1	9.1299
1	1	1	9.2825
2	2	0	37.0200
2	0	2	24.4715
2	1	2	24.4834
2	1	1	33.6538
2	2	1	34.1104
3	3	0	74.0218
3	1	2	61.4379
3	2	2	61.4968
3	2	1	70.4160
3	0	3	45.8170

3	3	1	71.3255
3	1	3	45.8177
4	4	0	123.3285
4	2	2	110.6378
4	0	4	73.2219
4	3	2	110.8133
4	1	4	73.2220
4	3	1	119.3891
4	1	3	95.1197
4	4	1	120.8942
4	2	3	95.1245
5	5	0	184.9126
5	3	2	171.9977
5	1	4	134.8291
5	4	2	172.4027
5	2	4	134.8296
5	4	1	180.5382
5	2	3	156.6516
5	0	5	106.6889
5	5	1	182.7706
5	3	3	156.6710
5	1	5	106.6889
6	6	0	258.7354
6	4	2	245.4309
6	2	4	208.6260
6	0	6	146.2152
6	5	2	246.2274
6	3	4	208.6286
6	1	6	146.2152
6	5	1	253.8226
6	3	3	230.3444
6	1	5	180.5865
6	6	1	256.8955
6	4	3	230.4021
6	2	5	180.5865

7	7	0	344.7436
7	5	2	330.8415
7	3	4	294.5394
7	1	6	232.3898
7	6	2	332.2417
7	4	4	294.5487
7	2	6	232.3898
7	6	1	339.1984
7	4	3	316.1115
7	2	5	266.6219
7	0	7	191.7971
7	7	1	343.1953
7	5	3	316.2543
7	3	5	266.6222
7	1	7	191.7971
8	8	0	442.8654
8	6	2	428.1297
8	4	4	392.4808
8	2	6	330.6413
8	0	8	243.4303
8	7	2	430.3918
8	5	4	392.5086
8	3	6	330.6414
8	1	8	243.4303
8	7	1	436.6210
8	5	3	413.8457
8	3	5	364.7120
8	1	7	290.2346
8	8	1	441.5825
8	6	3	414.1559
8	4	5	364.7132
8	2	7	290.2346
9	9	0	553.0095
9	7	2	537.1966
9	5	4	502.3450
9	3	6	440.8753
9	1	8	354.1154
9	8	2	540.6155
9	6	4	502.4169
9	4	6	440.8755
9	2	8	354.1154

9	8	1	546.0478
9	6	3	523.4181
9	4	5	474.7604
9	2	7	400.6797
9	0	9	301.1093
9	9	1	551.9555
9	7	3	524.0267
9	5	5	474.7646
9	3	7	400.6797
9	1	9	301.1093
10	10	0	675.0459
10	8	2	657.9465
10	6	4	624.0068
10	4	6	562.9845
10	2	8	476.7308
10	0	10	364.8279
10	9	2	662.8421
10	7	4	624.1728
10	5	6	562.9853
10	3	8	476.7308
10	1	10	364.8279
10	9	1	667.4400
10	7	3	644.6777
10	5	5	596.6563
10	3	7	523.0265
10	1	9	424.0260
10	10	1	674.2011
10	8	3	645.7777
10	6	5	596.6690
10	4	7	523.0265
10	2	9	424.0260
11	11	0	808.9104
11	9	2	790.2889
11	7	4	757.3145
11	5	6	696.8479
11	3	8	611.1586
11	1	10	499.9589
11	10	2	796.9925
11	8	4	757.6674
11	6	6	696.8507
11	4	8	611.1586
11	2	10	499.9589
11	10	1	800.7600
11	8	3	777.4567
11	6	5	730.2730

11	4	7	657.1559
11	2	9	558.7873
11	0	11	434.5787
11	11	1	808.1964
11	9	3	779.3087
11	7	5	730.3967
11	5	7	657.1560
11	3	9	558.7873
11	1	11	434.5787
12	12	0	954.4110
12	10	2	934.1387
12	8	4	902.0899
12	6	6	842.3298
12	4	8	757.2679
12	2	10	646.8408
12	0	12	510.3531
12	11	2	942.9795
12	9	4	902.7847
12	7	6	842.3384
12	5	8	757.2679
12	3	10	646.8408
12	1	12	510.3531
12	11	1	945.9458
12	9	3	921.5811
12	7	5	875.4645
12	5	7	802.9357
12	3	9	705.2634
12	1	11	581.9058
12	12	1	953.8144
12	10	3	924.5052
12	8	5	875.5457
12	6	7	802.9362
12	4	9	705.2434
12	2	11	581.9058
13	13	0	1111.4369
13	11	2	1089.4145
13	9	4	1058.1206
13	7	6	999.2779
13	5	8	914.9143
13	3	10	805.3318
13	1	12	669.8571
13	12	2	1100.7085
13	10	4	1059.4030
13	8	6	999.3012
13	6	8	914.9144
13	4	10	805.3318
13	2	12	669.8571

13	12	1	1103.0015
13	10	3	1076.8864
13	8	5	1032.0616
13	6	7	960.2190
13	4	9	863.3115
13	2	11	740.8820
13	0	13	592.1410
13	13	1	1110.9302
13	11	3	1051.2329
13	9	5	1032.2425
13	7	7	960.2207
13	5	9	863.3115
13	3	11	740.8820
13	1	13	592.1410
14	14	0	1279.8686
14	12	2	1256.0314
14	10	4	1225.1637
14	8	6	1167.5199
14	6	8	1083.9390
14	4	10	975.2766
14	2	12	840.9001
14	0	14	679.9310
14	13	2	1270.0793
14	11	4	1227.3954
14	9	6	1167.5779
14	7	8	1093.9394
14	5	10	975.2766
14	3	12	840.9001
14	1	14	679.9310
14	13	1	1271.7902
14	11	3	1243.2339
14	9	5	1199.8656
14	7	7	1128.8435
14	5	9	1032.7747
14	3	11	911.3531
14	1	13	763.8017
14	14	1	1279.4308
14	12	3	1249.3301
14	10	5	1200.2420
14	8	7	1128.8487
14	6	9	1032.7747
14	4	11	911.3531
14	2	13	763.8017
15	15	0	1459.6107
15	13	2	1433.8839
15	11	4	1402.9587
15	9	6	1346.8589
15	7	8	1264.1675

15	5	10	1156.5059
15	3	12	1023.3158
15	1	14	863.7271
15	14	2	1450.9882
15	12	4	1406.6307
15	10	6	1346.9940
15	8	8	1264.1691
15	6	10	1156.5059
15	4	12	1023.3158
15	2	14	863.7271
15	14	1	1452.2328
15	12	3	1420.5232
15	10	5	1378.6411
15	8	7	1308.6292
15	6	9	1213.4817
15	4	11	1093.1516
15	2	13	946.8832
15	0	15	773.7097
15	15	1	1459.2273
15	13	3	1428.5988
15	11	5	1379.3787
15	9	7	1308.6435
15	7	9	1213.4818
15	5	11	1093.1516
15	3	13	946.8832
15	1	15	773.7097
16	16	0	1650.6042
16	14	2	1622.8194
16	12	4	1591.2524
16	10	6	1537.0467
16	8	8	1455.4084
16	6	10	1348.8355
16	4	12	1216.9239
16	2	14	1058.8177
16	0	16	873.4420
16	15	2	1643.3303
16	13	4	1596.9729
16	11	6	1537.3424
16	9	8	1455.4131
16	7	10	1348.8355
16	5	12	1216.9239
16	3	14	1058.8177
16	1	16	873.4420
16	15	1	1644.2156
16	13	3	1608.6982
16	11	5	1548.1096
16	9	7	1499.3752
16	7	9	1405.2454
16	5	11	1256.0954

16	3	13	1141.2068
16	1	15	949.6190
16	16	1	1650.2472
16	14	3	1618.7963
16	12	5	1569.4759
16	10	7	1499.4119
16	8	9	1405.2458
16	6	11	1286.0954
16	4	13	1141.2068
16	2	15	969.6190
17	17	0	1852.8334
17	15	2	1822.6154
17	13	4	1789.8310
17	11	6	1737.8734
17	9	8	1657.4505
17	7	10	1552.0652
17	5	12	1421.5294
17	3	14	1265.0114
17	1	16	1081.4611
17	16	2	1847.0031
17	14	4	1798.2818
17	12	6	1738.4856
17	10	8	1657.4637
17	8	10	1552.0653
17	6	12	1421.5294
17	4	14	1265.0114
17	2	16	1081.4611
17	16	1	1847.6196
17	14	3	1807.7465
17	12	5	1767.9494
17	10	7	1700.8559
17	8	9	1607.8615
17	6	11	1489.9971
17	4	13	1346.5794
17	2	15	1176.6882
17	0	17	979.1705
17	17	1	1852.5412
17	15	3	1819.6362
17	13	5	1770.3439
17	11	7	1700.9436
17	9	9	1607.8628
17	7	11	1489.9871
17	5	13	1346.5794
17	3	15	1176.6882
17	1	17	979.1705
18	18	0	2066.3186
18	16	2	2032.9850
18	14	4	1998.5424
18	12	6	1948.9556

18	10	8	1870.0598
18	8	10	1765.9773
18	6	12	1636.9216
18	4	14	1482.1023
18	2	16	1300.4776
18	0	18	1090.8156
18	17	2	2061.9083
18	15	4	2010.4128
18	13	6	1950.1588
18	11	8	1870.0944
18	9	10	1765.9777
18	7	12	1636.9216
18	5	14	1482.1023
18	3	16	1300.4776
18	1	18	1090.8156
18	17	1	2062.3283
18	15	3	2017.6865
18	13	5	1977.8140
18	11	7	1912.8130
18	9	9	1821.1070
18	7	11	1704.6130
18	5	13	1562.7928
18	3	15	1394.7134
18	1	17	1199.2352
18	18	1	2066.0738
18	16	3	2030.8035
18	14	5	1981.7735
18	12	7	1913.0113
18	10	9	1821.1106
18	8	11	1704.6130
18	6	13	1562.7928
18	4	15	1394.7134
18	2	17	1199.2352
19	19	0	2221.0886
19	17	2	2253.6256
19	15	4	2217.2956
19	13	6	2169.9268
19	11	8	2092.9736
19	9	10	1990.3348
19	7	12	1862.8728
19	5	14	1709.8687
19	3	16	1530.2943
19	1	18	1322.9206
19	18	2	2247.9538
19	16	4	2233.2163
19	14	6	2172.1739
19	12	8	2093.0594
19	10	10	1990.3362
19	8	12	1862.8729
19	6	14	1709.8687
19	4	16	1530.2943

19	2	18	1322.9206
19	18	1	2268.2330
19	16	3	2238.5329
19	14	5	2197.3788
19	12	7	2134.9460
19	10	9	2044.7364
19	8	11	1929.7414
19	6	13	1789.6227
19	4	15	1623.4752
19	2	17	1430.1663
19	0	19	1208.3751
19	19	1	2290.8946
19	17	3	2252.0282
19	15	5	2203.5241
19	13	7	2135.3709
19	11	9	2044.7467
19	9	11	1929.7415
19	7	13	1789.6227
19	5	15	1623.4752
19	3	17	1430.1665
19	1	19	1208.3751
20	20	0	2527.1442
20	18	2	2484.2997
20	16	4	2446.0290
20	14	6	2400.3434
20	12	8	2325.8923
20	10	10	2224.8789
20	8	12	2099.1372
20	6	14	1948.0726
20	4	16	1770.6788
20	2	18	1565.7328
20	0	20	1331.8238
20	19	2	2525.0535
20	17	4	2466.5515
20	15	6	2404.3232
20	13	8	2326.0936
20	11	10	2224.8832
20	9	12	2099.1373
20	7	14	1948.0726
20	5	16	1770.6788
20	3	18	1565.7328
20	1	20	1331.8238
20	19	1	2525.2339
20	17	3	2470.2538
20	15	5	2426.4093
20	13	7	2366.8971
20	11	9	2278.4793
20	9	11	2165.1211
20	7	13	2026.8274
20	5	15	1862.7387
20	3	17	1671.7338

20	1	19	1452.4939
20	20	1	2527.0908
20	18	3	2483.1907
20	16	5	2435.3923
20	14	7	2367.7426
20	12	9	2278.5967
20	10	11	2165.1215
20	8	13	2026.8274
20	6	15	1862.7387
20	4	17	1671.7338
20	2	19	1452.4939

APPENDIX V

CALCULATED UPPER STATE ENERGY LEVELS FOR THE STATES $\nu_1+\nu_2$, $\nu_2+\nu_3$, $2\nu_1$, and $\nu_1+\nu_3$ of $H_2{}^{130}Te$

The output from PROGRAM CORIOLIS is given. The upper state energy levels are calculated with Eq. (47) both with and without the perturbation terms G_z and G_{xy}. The perturbed calculation, unperturbed calculation and their difference are printed out for each level.

GROUND STATE CONSTANTS

```
A =     6.2474890000
B =     6.0948340000
C =     3.0359990000

TAAAA =      -0.0031390000
TBBBB =      -0.0027910000
TAABB =       0.0022850000
TABAB =      -0.0005330000
HJ    =      -0.0000000000000
HJK   =      -0.0000000000000
HKJ   =      -0.0000000000000
HK    =      -0.0000000020000
```

UPPER STATE CONSTANTS

```
A =     6.3478450000          ν1+ν2
B =     6.1369360000
C =     2.9604710000

TAAAA =      -0.0037760000
TBBBB =      -0.0031250000
TAABB =       0.0031130000
TABAB =      -0.0009530000
HJ    =      -0.0000000000000
HJK   =      -0.0000000000000
HKJ   =      -0.0000000000000
HK    =      -0.0000000034000

BAND CENTER =      2911.415700

KAPPA =      0.8755

A =     6.3190690000          ν2+ν3
B =     6.1650870000
C =     2.9754410000

TAAAA =      -0.0042290000
TBBBB =      -0.0037360000
TAABB =       0.0037690000
TABAB =      -0.0004170000
HJ    =      -0.0000000000000
HJK   =      -0.0000000000000
HKJ   =      -0.0000000000000
HK    =      -0.0000000188000

BAND CENTER =      2915.969700

KAPPA =      0.9079

GZ    =       -0.000000
GXY   =       -0.000000

GZ    =        0.025882
GXY   =       -0.164134
```

$\nu_1+\nu_2$						$\nu_2+\nu_3$					
J	K-	K+	P ENG	UP ENG	P-UP	J	K-	K+	P ENG	UP ENG	P-UP
1	1	0	2923.900	2923.900	0.000						
						1	1	0	2928.454	2928.454	0.000
1	0	1	2920.510	2920.512	-0.002						
						1	1	1	2925.265	2925.263	0.002
						1	0	1	2925.110	2925.109	0.001
1	1	1	2920.722	2920.723	-0.001						
2	2	0	2948.875	2948.866	0.009						
2	0	2	2935.721	2935.722	-0.001						
						2	1	2	2940.345	2940.354	-0.009
						2	2	0	2953.418	2953.414	0.005
						2	0	2	2940.339	2940.338	0.000
2	1	2	2935.734	2935.739	-0.005						
2	1	1	2945.248	2945.262	-0.014						
						2	2	1	2950.390	2950.375	0.014
						2	1	1	2949.927	2949.915	0.012
2	2	1	2945.880	2945.892	-0.012						
3	3	0	2986.351	2986.305	0.047						
3	1	2	2973.092	2973.093	-0.002						
						3	2	2	2977.754	2977.799	-0.045
						3	3	0	2990.856	2990.833	0.023
						3	1	2	2977.721	2977.721	0.000
3	2	2	2973.155	2973.178	-0.023						
3	2	1	2982.320	2982.363	-0.043						
3	0	3	2956.758	2956.762	-0.004						
						3	3	1	2988.061	2988.010	0.051
						3	1	3	2961.451	2961.454	-0.004
						3	2	1	2987.161	2987.096	0.065
						3	0	3	2961.450	2961.453	-0.003
3	3	1	2983.559	2983.616	-0.057						
3	1	3	2956.758	2956.763	-0.005						

4	4	0	3036,340	3036,203	0,137
4	2	2	3022,806	3022,806	-0,000
4	0	4	2983,703	2983,709	-0,007
4	3	2	3022,994	3023,057	-0,064
4	1	4	2983,703	2983,709	-0,007
4	3	1	3031,693	3031,784	-0,092
4	1	3	3006,605	3006,619	-0,014
4	4	1	3033,661	3033,854	-0,194
4	2	3	3006,611	3006,627	-0,017
5	5	0	3098,847	3098,537	0,311
5	3	2	3084,767	3084,766	0,001
5	1	4	3045,993	3046,012	-0,019
5	4	2	3085,199	3085,342	-0,143
5	2	4	3045,993	3046,013	-0,019
5	4	1	3093,330	3093,492	-0,163
5	2	3	3068,794	3068,821	-0,027
5	0	5	3016,561	3016,569	-0,009
5	5	1	3096,013	3096,553	-0,540
5	3	3	3068,815	3068,852	-0,037
5	1	5	3016,561	3016,569	-0,009
6	6	0	3173,858	3173,266	0,592
6	4	2	3158,863	3158,869	-0,006
6	2	4	3120,580	3120,616	-0,036
6	0	6	3055,330	3055,341	-0,011

4	3	2	3027,564	3027,691	-0.127
4	1	4	2988,503	2988,506	-0.003
4	4	0	3040.755	3040.686	0.069
4	2	2	3027.462	3027.457	0.005
4	0	4	2988.503	2988.506	-0.003
4	4	1	3038.254	3038.128	0.126
4	2	3	3011.307	3011.327	-0.020
4	3	1	3036.846	3036.619	0.226
4	1	3	3011,303	3011.320	-0.016
5	4	2	3089.727	3090.001	-0.274
5	2	4	3050,802	3050.821	-0.019
5	5	0	3103.095	3102,936	0.159
5	3	2	3089,481	3089.460	0.021
5	1	4	3050.801	3050.820	-0.018
5	5	1	3100,927	3100.673	0.254
5	3	3	3073,515	3073,567	-0.052
5	1	5	3021.499	3021,502	-0.003
5	4	1	3099.072	3098.445	0.627
5	2	3	3073.501	3073,539	-0.037
5	0	5	3021.499	3021.502	-0.003

6	5	2	3159,700	3159,997	-0,288
6	3	4	3120,582	3120,620	-0,038
6	1	6	3055,330	3055,341	-0,011
6	5	1	3167,192	3167,446	-0,254
6	3	3	3143,238	3143,281	-0,044
6	1	5	3091,279	3091,303	-0,023
6	6	1	3170,416	3171,641	-1,225
6	4	3	3143,301	3143,374	-0,073
6	2	5	3091,280	3091,303	-0,023
7	7	0	3261,329	3260,328	1,001
7	5	2	3244,973	3245,004	-0,031
7	3	4	3207,373	3207,432	-0,059
7	1	6	3142,465	3142,493	-0,028
7	6	2	3246,395	3246,941	-0,546
7	4	4	3207,381	3207,447	-0,066
7	2	6	3142,465	3142,493	-0,028
7	6	1	3253,238	3253,605	-0,366
7	4	3	3229,828	3229,890	-0,063
7	2	5	3178,235	3178,278	-0,043
7	0	7	3100,008	3100,022	-0,014

6	5	2	3164,197	3164,689	-0.492
6	3	4	3125.402	3125.446	-0.044
6	1	6	3060.435	3060.438	-0.002
6	6	0	3177.847	3177.532	0.315
6	4	2	3163,690	3163,625	0.066
6	2	4	3125,399	3125,441	-0.042
6	0	6	3060.435	3060.438	-0.002
6	6	1	3176,022	3175,571	0.451
6	4	3	3148.002	3148.113	-0.110
6	2	5	3096.230	3096,250	-0.020
6	5	1	3173,936	3172,529	1.407
6	3	3	3147,961	3148,028	-0.067
6	1	5	3096.230	3096.249	-0.020
7	6	2	3250.934	3251,711	-0.778
7	4	4	3212.216	3212.301	-0.085
7	2	6	3147.587	3147,608	-0.021
7	7	0	3264,967	3264,406	0.561
7	5	2	3250,010	3249,837	0.174
7	3	4	3212,207	3212,282	-0.075
7	1	6	3147,587	3147,608	-0,021
7	7	1	3263,469	3262,734	0.735
7	5	3	3234.687	3234,891	-0.204
7	3	5	3183,202	3183,246	-0.044
7	1	7	3105,307	3105,309	-0.002
7	6	1	3256.792	3258,823	-2.031
7	4	3	3234,580	3234,680	-0.101
7	2	5	3183,201	3183,245	-0.044

						7	0	7	3105.307	3105.309	-0.002
7	7	1	3241.396	3259.029	2.367						
7	5	3	3229.986	3230.119	-0.133						
7	3	5	3178.235	3178.278	-0.043						
7	1	7	3100.008	3100.022	-0.014						
8	8	0	3361.188	3359.629	1.559						
8	6	2	3342.985	3343.066	-0.081						
8	4	4	3306.266	3306.352	-0.087						
8	2	6	3241.766	3241.816	-0.049						
8	0	8	3150.593	3150.610	-0.016						
						8	7	2	3349.882	3351.013	-1.131
						8	5	4	3311.144	3311.290	-0.147
						8	3	6	3246.911	3246.957	-0.046
						8	1	8	3156.106	3156.107	-0.001
						8	8	0	3364.395	3363.470	0.925
						8	6	2	3348.394	3347.978	0.416
						8	4	4	3311.117	3311.234	-0.116
						8	2	6	3246.910	3246.957	-0.046
						8	0	8	3156.106	3156.107	-0.001
8	7	2	3345.133	3346.137	-1.004						
8	5	4	3306.288	3306.397	-0.108						
8	3	6	3241.766	3241.816	-0.049						
8	1	8	3150.593	3150.610	-0.016						
8	7	1	3351.419	3351.927	-0.508						
8	5	3	3328.425	3328.513	-0.088						
8	3	5	3277.325	3277.394	-0.069						
8	1	7	3199.548	3199.580	-0.032						
						8	8	1	3363.191	3362.057	1.134
						8	6	3	3333.481	3333.817	-0.336
						8	4	5	3282.314	3282.393	-0.079
						8	2	7	3204.869	3204.891	-0.022
						8	7	1	3355.154	3357.287	-2.133
						8	5	3	3333.233	3333.362	-0.129
						8	3	5	3282.313	3282.391	-0.078
						8	1	7	3204.869	3204.891	-0.022
8	8	1	3361.302	3358.608	2.694						
8	6	3	3328.775	3329.004	-0.229						
8	4	5	3277.326	3277.396	-0.070						
8	2	7	3199.548	3199.580	-0.032						
9	9	0	3473.342	3471.049	2.292						
9	7	2	3452.811	3452.957	-0.146						
9	5	4	3417.130	3417.248	-0.118						
9	3	6	3353.119	3353.196	-0.077						
9	1	8	3262.524	3262.561	-0.037						
						9	8	2	3460.960	3462.534	-1.573
						9	6	4	3422.071	3422.309	-0.239
						9	4	6	3358.291	3358.371	-0.081
						9	2	8	3268.067	3268.090	-0.023
						9	9	0	3476.060	3474.617	1.443

9	7	2	3458.848	3457,931	0.917
9	5	4	3422.000	3422,162	-0.163
9	3	6	3358.291	3358.371	-0.080
9	1	8	3268,067	3268.090	-0.023

9	8	2	3455,693	3457,501	-1,808
9	6	4	3417,190	3417,361	-0,172
9	4	6	3353,119	3353,196	-0,077
9	2	8	3262,524	3262,561	-0,037

9	8	1	3461,670	3462,374	-0,705
9	6	3	3438,858	3438,987	-0,130
9	4	5	3388,434	3388,536	-0,102
9	2	7	3311,173	3311,228	-0,056
9	0	9	3207,080	3207,100	-0,019

9	9	1	3475.109	3473,426	1.682
9	7	3	3444,301	3444,796	-0.495
9	5	5	3393.451	3393,578	-0.127
9	3	7	3316,523	3316,571	-0.049
9	1	9	3212.822	3212,823	-0.001

9	8	1	3465.502	3467,888	-2.385
9	6	3	3443.780	3443.909	-0.129
9	4	5	3393,446	3393,569	-0.123
9	2	7	3316.523	3316,571	-0.049
9	0	9	3212,822	3212,823	-0.001

9	9	1	3473,506	3470,252	3,254
9	7	3	3439,552	3439,940	-0,387
9	5	5	3388,438	3388,543	-0,106
9	3	7	3311,173	3311,228	-0,056
9	1	9	3207,080	3207,100	-0,019

10	10	0	3597,691	3594,442	3,249
10	8	2	3574,382	3574,586	-0,205
10	6	4	3539,814	3539,964	-0,150
10	4	6	3476,394	3476,506	-0,112
10	2	8	3386,450	3386,513	-0,062
10	0	10	3269,465	3269,487	-0,022

10	9	2	3584.053	3586,204	-2,151
10	7	4	3544,872	3545,243	-0.370
10	5	6	3481.599	3481,723	-0.125
10	3	8	3392.030	3392,082	-0.052
10	1	10	3275,440	3275,440	0.000

10	10	0	3599.891	3597,729	2.162
10	8	2	3581.369	3579,582	1.787
10	6	4	3544.699	3544,902	-0.203
10	4	6	3481.597	3481,721	-0.124
10	2	8	3392.030	3392.082	-0.052
10	0	10	3275,440	3275,440	0.000

10	9	2	3577,842	3580,946	-3,105
10	7	4	3539,954	3540,223	-0,269
10	5	6	3476,394	3476,507	-0,113
10	3	8	3386,450	3386,513	-0,062
10	1	10	3269,465	3269,487	-0,022

10	9	1	3583,898	3584,910	-1,012

10	7	3	3560.922	3561.132	-0.211
10	5	5	3511.427	3511.570	-0.144
10	3	7	3434.755	3434.840	-0.085
10	1	9	3331.389	3331.431	-0.042

10	10	1	3599.149	3596.718	2.431
10	8	3	3567.077	3567.716	-0.639
10	6	5	3516.481	3516.672	-0.191
10	4	7	3440.140	3440.223	-0.083
10	2	9	3337.170	3337.194	-0.025

10	9	1	3587.799	3590.605	-2.806
10	7	3	3566.085	3566.129	-0.043
10	5	5	3516.466	3516.643	-0.178
10	3	7	3440.140	3440.223	-0.083
10	1	9	3337.170	3337.194	-0.025

10	10	1	3597.890	3593.817	4.072
10	8	3	3562.168	3562.825	-0.657
10	6	5	3511.438	3511.592	-0.154
10	4	7	3434.755	3434.840	-0.085
10	2	9	3331.389	3331.431	-0.042

11	11	0	3734.141	3729.644	4.496
11	9	2	3707.643	3707.874	-0.231
11	7	4	3674.131	3674.313	-0.182
11	5	6	3611.444	3611.600	-0.156
11	3	8	3522.230	3522.324	-0.094
11	1	10	3406.139	3406.185	-0.047

11	10	2	3719.008	3721.949	-2.942
11	8	4	3679.415	3679.967	-0.552
11	6	6	3616.687	3616.867	-0.181
11	4	8	3527.854	3527.941	-0.087
11	2	10	3412.162	3412.188	-0.026

11	11	0	3735.825	3732.684	3.141
11	9	2	3715.814	3712.827	2.987
11	7	4	3679.028	3679.247	-0.218
11	5	6	3616.682	3616.858	-0.176
11	3	8	3527.854	3527.941	-0.087
11	1	10	3412.162	3412.188	-0.026

11	10	2	3711.472	3716.374	-4.901
11	8	4	3674.435	3674.856	-0.420
11	6	6	3611.446	3611.605	-0.159
11	4	8	3522.230	3522.324	-0.094
11	2	10	3406.139	3406.185	-0.047

11	10	1	3717.966	3719.487	-1.521
11	8	3	3694.403	3694.757	-0.354
11	6	5	3646.148	3646.343	-0.195
11	4	7	3570.152	3570.274	-0.122
11	2	9	3467.594	3467.663	-0.069
11	0	11	3337.742	3337.767	-0.025

11	11	1	3735.254	3731.816	3.438
11	9	3	3701.740	3702.441	-0.700
11	7	5	3651.257	3651.530	-0.273
11	5	7	3575.577	3575.703	-0.126
11	3	9	3473.421	3473.476	-0.054
11	1	11	3343.938	3343.937	0.001

11	10	1	3721,970	3725,424	-3,453
11	8	3	3700,075	3699,814	0,261
11	6	5	3651,213	3651,453	-0,240
11	4	7	3575,577	3575,703	-0,126
11	2	9	3473,421	3473,476	-0,054
11	0	11	3343,938	3343,937	0,001

11	11	1	3734,353	3729,149	5,205
11	9	3	3696,391	3697,546	-1,155
11	7	5	3646,180	3646,401	-0,221
11	5	7	3570,152	3570,274	-0,122
11	3	9	3467,594	3467,663	-0,069
11	1	11	3337,742	3337,767	-0,025

12	12	0	3882,611	3876,484	6,127
12	10	2	3852,556	3852,746	-0,190
12	8	4	3819,854	3820,073	-0,219
12	6	6	3758,107	3758,317	-0,211
12	4	8	3669,706	3669,838	-0,132
12	2	10	3554,599	3554,675	-0,076
12	0	12	3411,902	3411,930	-0,028

12	11	2	3865,641	3869,691	-4,050
12	9	4	3825,566	3826,353	-0,787
12	7	6	3763,391	3763,640	-0,249
12	5	8	3675,378	3675,509	-0,130
12	3	10	3560,680	3560,738	-0,057
12	1	12	3418,289	3418,287	0,002

12	12	0	3883,817	3879,377	4,440
12	10	2	3856,595	3857,560	-0,965
12	8	4	3824,766	3824,942	-0,176
12	6	6	3763,375	3763,612	-0,237
12	4	8	3675,378	3675,508	-0,130
12	2	10	3560,680	3560,738	-0,057
12	0	12	3418,289	3418,287	0,002

12	11	2	3861,912	3863,672	-1,760
12	9	4	3820,464	3821,126	-0,662
12	7	6	3758,112	3758,332	-0,220
12	5	8	3669,706	3669,838	-0,132
12	3	10	3554,599	3554,675	-0,076
12	1	12	3411,902	3411,930	-0,028

12	11	1	3863,683	3866,038	-2,355
12	9	3	3839,111	3839,679	-0,568
12	7	5	3792,419	3792,676	-0,257
12	5	7	3717,203	3717,371	-0,168
12	3	9	3615,539	3615,641	-0,103
12	1	11	3486,765	3486,817	-0,052

12	12	1	3883,385	3878,621	4,764
12	10	3	3848,211	3848,802	-0,591
12	8	5	3797,615	3797,989	-0,375
12	6	7	3722,671	3722,850	-0,179
12	4	9	3621,420	3621,511	-0,091
12	2	11	3493,022	3493,049	-0,027

12	11	1	3867,898	3872,325	-4,427
12	9	3	3845,806	3844,764	1,042

					12	7	5	3797,503	3797,805	-0,302
					12	5	7	3722,670	3722,848	-0,178
					12	3	9	3621,420	3621,511	-0,091
					12	1	11	3493,022	3493,049	-0,027
12	12	1	3882,820	3876,083	6,736					
12	10	3	3841,859	3843,974	-2,115					
12	8	5	3792,500	3792,815	-0,315					
12	6	7	3717,204	3717,372	-0,168					
12	4	9	3615,539	3615,641	-0,103					
12	2	11	3486,765	3486,817	-0,052					
13	13	0	4043,041	4034,791	8,250					
13	11	2	4009,089	4009,129	-0,040					
13	9	4	3976,714	3976,987	-0,273					
13	7	6	3916,195	3916,474	-0,278					
13	5	8	3828,705	3828,885	-0,180					
13	3	10	3714,675	3714,787	-0,112					
13	1	12	3573,261	3573,318	-0,057					
					13	12	2	4023,744	4029,350	-5,606
					13	10	4	3983,198	3984,268	-1,070
					13	8	6	3921,528	3921,859	-0,331
					13	6	8	3834,427	3834,608	-0,181
					13	4	10	3720,823	3720,918	-0,095
					13	2	12	3579,722	3579,750	-0,028
					13	13	0	4043,839	4037,736	6,103
					13	11	2	4013,242	4013,670	-0,428
					13	9	4	3981,675	3981,689	-0,014
					13	7	6	3921,485	3921,784	-0,299
					13	5	8	3834,427	3834,607	-0,181
					13	3	10	3720,823	3720,918	-0,095
					13	1	12	3579,722	3579,750	-0,028
13	12	2	4019,377	4022,719	-3,342					
13	10	4	3977,828	3978,893	-1,065					
13	8	6	3916,210	3916,512	-0,302					
13	6	8	3828,705	3828,885	-0,180					
13	4	10	3714,675	3714,787	-0,112					
13	2	12	3573,261	3573,318	-0,057					
13	12	1	4020,822	4024,468	-3,645					
13	10	3	3994,890	3995,745	-0,854					
13	8	5	3950,027	3950,361	-0,334					
13	6	7	3875,732	3875,957	-0,225					
13	4	9	3775,052	3775,195	-0,143					
13	2	11	3647,457	3647,540	-0,083					
13	0	13	3491,937	3491,969	-0,031					
					13	13	1	4043,520	4037,072	6,448
					13	11	3	4006,377	4006,583	-0,207
					13	9	5	3955,380	3955,873	-0,493
					13	7	7	3881,241	3881,481	-0,239
					13	5	9	3780,991	3781,126	-0,135
					13	3	11	3653,785	3653,846	-0,060
					13	1	13	3498,455	3498,452	0,003
					13	12	1	4025,414	4031,272	-5,858
					13	10	3	4003,365	4000,815	2,550
					13	8	5	3955,114	3955,466	-0,352

						13	6	7	3881.238	3881.474	-0.237
						13	4	9	3780.991	3781.126	-0.135
						13	2	11	3653,785	3653.846	-0.060
						13	0	13	3498,455	3498.452	0.003
13	13	1	4043,231	4034,459	8,772						
13	11	3	3998,205	4001.954	-3,749						
13	9	5	3950,216	3950.666	-0,449						
13	7	7	3875,733	3875,961	-0,227						
13	5	9	3775,052	3775.195	-0,143						
13	3	11	3647,457	3647,540	-0,083						
13	1	13	3491,937	3491,969	-0,031						
14	14	0	4215,389	4204,409	10,980						
14	12	2	4177,210	4176,934	0,276						
14	10	4	4144,418	4144,774	-0,356						
14	8	6	4085,502	4085,861	-0,359						
14	6	8	3999,035	3999,274	-0,239						
14	4	10	3886,182	3886.336	-0,154						
14	2	12	3746,160	3746,250	-0,091						
14	0	14	3577,835	3577,870	-0,035						
						14	13	2	4193,088	4200,849	-7,760
						14	11	4	4152,178	4153,575	-1,397
						14	9	6	4090.896	4091,324	-0,428
						14	7	8	4004,802	4005,040	-0,238
						14	5	10	3892,399	3892,539	-0,140
						14	3	12	3752,708	3752,771	-0,063
						14	1	14	3584,391	3584,386	0,005
						14	14	0	4215.869	4207,744	8,124
						14	12	2	4181.434	4181,016	0,418
						14	10	4	4149,566	4149,159	0.406
						14	8	6	4090,784	4091,136	-0,352
						14	6	8	4004,801	4005,038	-0,237
						14	4	10	3892,399	3892,539	-0,140
						14	2	12	3752,708	3752,771	-0,063
						14	0	14	3584,391	3584,386	0,005
14	13	2	4187,960	4193,387	-5,427						
14	11	4	4146,214	4148,013	-1,799						
14	9	6	4085,540	4085,956	-0,417						
14	7	8	3999,035	3999,274	-0,239						
14	5	10	3886,182	3886,336	-0,154						
14	3	12	3746,160	3746,250	-0.091						
14	1	14	3577,835	3577,870	-0,035						
14	13	1	4189,150	4194,649	-5,499						
14	11	3	4161,617	4162,839	-1,221						
14	9	5	4118,713	4119,151	-0,438						
14	7	7	4045,540	4045,838	-0.298						
14	5	9	3945,945	3946,137	-0,192						
14	3	11	3819,632	3819,752	-0,121						
14	1	13	3665,616	3665,678	-0,062						
						14	14	1	4215,640	4207,164	8,476
						14	12	3	4176,100	4175,511	0,589
						14	10	5	4124,372	4124,986	-0,613
						14	8	7	4051,086	4051,393	-0,307
						14	6	9	3951,942	3952,127	-0,185
						14	4	11	3826,040	3826,140	-0,100
						14	2	13	3672,225	3672,254	-0,029

						14	13	1	4194.304	4202.203	-7.899
						14	11	3	4172.640	4167.867	4.773
						14	9	5	4123.783	4124.147	-0.364
						14	7	7	4051.074	4051.374	-0.300
						14	5	9	3951.942	3952.127	-0.185
						14	3	11	3826.040	3826.140	-0.100
						14	1	13	3672.225	3672.254	-0.029
14	14	1	4215.549	4204.125	11.423						
14	12	3	4165.305	4171.298	-5.993						
14	10	5	4119.128	4119.776	-0.648						
14	8	7	4045.545	4045.848	-0.303						
14	6	9	3945.945	3946.137	-0.192						
14	4	11	3819.632	3819.752	-0.121						
14	2	13	3665.616	3665.678	-0.062						
15	15	0	4399.621	4385.213	14.408						
15	13	2	4356.870	4356.023	0.847						
15	11	4	4322.691	4323.156	-0.465						
15	9	6	4265.784	4266.239	-0.455						
15	7	8	4180.484	4180.797	-0.313						
15	5	10	4068.917	4069.122	-0.205						
15	3	12	3930.399	3930.530	-0.130						
15	1	14	3763.819	3763.887	-0.068						
						15	14	2	4373.454	4384.119	-10.665
						15	12	4	4332.350	4334.138	-1.788
						15	10	6	4271.277	4271.820	-0.543
						15	8	8	4186.284	4186.585	-0.300
						15	6	10	4075.200	4075.390	-0.190
						15	4	12	3937.042	3937.147	-0.104
						15	2	14	3770.485	3770.514	-0.029
						15	15	0	4399.879	4389.449	10.429
						15	13	2	4361.147	4359.398	1.748
						15	11	4	4328.445	4327.040	1.405
						15	9	6	4271.007	4271.383	-0.376
						15	7	8	4186.280	4186.577	-0.297
						15	5	10	4075.200	4075.390	-0.190
						15	3	12	3937.042	3937.147	-0.104
						15	1	14	3770.485	3770.514	-0.029
15	14	2	4367.491	4375.541	-8.050						
15	12	4	4325.095	4328.332	-3.237						
15	10	6	4265.878	4266.459	-0.581						
15	8	8	4180.485	4180.800	-0.315						
15	6	10	4068.917	4069.122	-0.205						
15	4	12	3930.399	3930.530	-0.130						
15	2	14	3763.819	3763.887	-0.068						
15	14	1	4368.483	4376.435	-7.952						
15	12	3	4339.172	4340.890	-1.718						
15	10	5	4298.157	4298.753	-0.596						
15	8	7	4226.408	4226.798	-0.390						
15	6	9	4128.012	4128.265	-0.253						
15	4	11	4003.090	4003.255	-0.165						
15	2	13	3850.697	3850.796	-0.098						
15	0	15	3669.583	3669.622	-0.039						
						15	15	1	4399.721	4388.956	10.764
						15	13	3	4357.219	4355.260	1.959

15	11	5	4304,419	4305.108	-0,689
15	9	7	4231.982	4232.359	-0.378
15	7	9	4134.059	4134,299	-0.241
15	5	11	4009,579	4009,725	-0,145
15	3	13	3857,411	3857,477	-0.066
15	1	15	3676,040	3676,032	0.007

15	14	1	4399.746	4385.042	14,704
15	12	3	4343,188	4345.897	-2.709
15	10	5	4303.213	4303,496	-0.283
15	8	7	4231,947	4232.308	-0.361
15	6	9	4134,058	4134,299	-0,240
15	4	11	4009,579	4009.725	-0.145
15	2	13	3857,411	3857,477	-0,066
15	0	15	3676.040	3676.032	0.007

15	15	1	4374,336	43a4,965	-10,629
15	13	3	4353,412	4351,767	1.645
15	11	5	4298,991	4299,956	-0,965
15	9	7	4226,421	4226,824	-0,404
15	7	9	4128,012	4128,265	-0,253
15	5	11	4003,090	4003,255	-0,165
15	3	13	3850,697	3850.796	-0,098
15	1	15	3669,583	3669,622	-0,039

GROUND STATE CONSTANTS

A =	6.2474890000
B =	6.0948340000
C =	3.0359990000
TAAAA =	-0.003139000
TBBBB =	-0.002791000
TAABB =	0.002285000
TABAB =	-0.000533000
HJ =	-0.000000000000
HJK =	-0.000000000000
HKJ =	-0.000000000000
HK =	-0.000000020000

UPPER STATE CONSTANTS $2\nu_1$

A =	6.0689780000
B =	5.9400740000
C =	2.9569350000
TAAAA =	-0.003281000
TBBBB =	-0.002679000
TAABB =	0.002326000
TABAB =	-0.000508000
HJ =	-0.000000000000
HJK =	-0.000000000000
HKJ =	-0.000000000000
HK =	-0.000000031000
BAND CENTER =	4062.890200
KAPPA =	0.9172

$\nu_1+\nu_3$

A =	6.0638020000
B =	5.9464410000
C =	2.9595650000
TAAAA =	-0.003351000
TBBBB =	-0.002805000
TAABB =	0.002405000
TABAB =	-0.000445000
HJ =	-0.000000000000
HJK =	-0.000000000000
HKJ =	-0.000000000000
HK =	-0.000000022000
BAND CENTER =	4063.374300
KAPPA =	0.9244
GZ =	-0.000000
GXY =	-0.000000
GZ =	0.011163
GXY =	-0.229786

$2\nu_1$						$\nu_1+\nu_3$					
J	K-	K+	P ENG	UP ENG	P-UP	J	K-	K+	P ENG	UP ENG	P-UP
1	1	0	4074,899	4074,899	0,000						
						1	1	0	4075,384	4075,384	0,000
1	0	1	4071,738	4071,786	-0,048						
						1	1	1	4072,445	4072,397	0,048
						1	0	1	4072,331	4072,279	0,052
1	1	1	4071,863	4071,915	-0,052						
2	2	0	4098,936	4098,909	0,027						
2	0	2	4086,710	4086,714	-0,004						
						2	1	2	4087,197	4087,220	-0,023
						2	2	0	4099,421	4099,396	0,025
						2	0	2	4087,211	4087,210	0,001
2	1	2	4086,698	4086,724	-0,026						
2	1	1	4095,436	4095,668	-0,233						
						2	2	1	4096,757	4096,525	0,233
						2	1	1	4096,589	4096,175	0,414
2	2	1	4095,638	4096,052	-0,414						
3	3	0	4135,039	4134,905	0,134						
3	1	2	4122,671	4122,686	-0,015						
						3	2	2	4123,120	4123,238	-0,118
						3	3	0	4135,516	4135,392	0,124
						3	1	2	4123,188	4123,187	0,000
3	2	2	4122,614	4122,738	-0,124						
3	2	1	4130,930	4131,467	-0,537						
3	0	3	4107,477	4107,497	-0,020						
						3	3	1	4133,257	4132,688	0,570
						3	1	3	4107,994	4108,007	-0,013
						3	2	1	4131,162	4131,993	-0,831
						3	0	3	4107,995	4108,007	-0,011
3	3	1	4133,094	4132,230	0,864						
3	1	3	4107,476	4107,498	-0,021						

4	4	0	4183,257	4182,864	0,393
4	2	2	4170,497	4170,567	-0,070
4	0	4	4134,155	4134,182	-0,028
4	3	2	4170,362	4170,722	-0,360
4	1	4	4134,155	4134,182	-0,028
4	3	1	4178,225	4179,156	-0,931
4	1	3	4155,403	4155,471	-0,067
4	4	1	4181,772	4180,412	1,361
4	2	3	4155,398	4155,475	-0,076
5	5	0	4243,637	4242,753	0,885
5	3	2	4230,723	4230,288	0,435
5	1	4	4194,043	4194,128	-0,085
5	4	2	4229,827	4230,645	-0,818
5	2	4	4194,043	4194,128	-0,086
5	4	1	4237,314	4238,699	-1,385
5	2	3	4215,202	4215,344	-0,142
5	0	5	4166,736	4166,772	-0,035
5	5	1	4242,592	4240,550	2,042
5	3	3	4215,183	4215,360	-0,178
5	1	5	4166,736	4166,772	-0,035
6	6	0	4316,200	4314,525	1,675
6	4	2	4302,436	4301,767	0,670
6	2	4	4265,763	4265,933	-0,170
6	0	6	4205,219	4205,263	-0,044

4	3	2	4170.945	4171,228	-0.283
4	1	4	4134.698	4134,711	-0,013
4	4	0	4183,714	4183,348	0.366
4	2	2	4171,110	4171,076	0,035
4	0	4	4134,698	4134,711	-0,013
4	4	1	4181,917	4180,850	1,067
4	2	3	4155,920	4155,990	-0,070
4	3	1	4178,482	4179,706	-1,224
4	1	3	4155,926	4155,986	-0,060
5	4	2	4229,993	4231,157	-1,164
5	2	4	4194,591	4194,663	-0,072
5	5	0	4244,055	4243,227	0,827
5	3	2	4230,953	4230,806	0,147
5	1	4	4194,592	4194,662	-0,071
5	5	1	4242,712	4240,962	1,750
5	3	3	4215,707	4215,881	-0,174
5	1	5	4167,311	4167,324	-0,013
5	4	1	4237,599	4239,277	-1,678
5	2	3	4215,729	4215,866	-0,137
5	0	5	4167,311	4167,324	-0,013

						6	5	2	4301,034	4302,988	-1,954
						6	3	4	4266,313	4266,476	-0,163
						6	1	6	4205,831	4205,844	-0,014
						6	6	0	4316,562	4314,982	1,580
						6	4	2	4302,675	4302,297	0,378
						6	2	4	4266,316	4266,474	-0,158
						6	0	6	4205,831	4205,844	-0,014
6	5	2	4300,901	4302,468	-1,567						
6	3	4	4265,760	4265,935	-0,175						
6	1	6	4205,219	4205,263	-0,044						
6	5	1	4308,183	4310,054	-1,871						
6	3	3	4286,803	4287,053	-0,249						
6	1	5	4238,575	4238,676	-0,100						
						6	6	1	4315,615	4312,962	2,653
						6	4	3	4287,274	4287,627	-0,353
						6	2	5	4239,156	4239,235	-0,079
						6	5	1	4308,499	4310,660	-2,162
						6	3	3	4287,335	4287,582	-0,247
						6	1	5	4239,156	4239,235	-0,079
6	6	1	4315,523	4312,583	2,940						
6	4	3	4286,747	4287,100	-0,353						
6	2	5	4238,575	4238,676	-0,100						
7	7	0	4400,933	4398,122	2,811						
7	5	2	4385,995	4384,912	1,083						
7	3	4	4349,234	4349,526	-0,292						
7	1	6	4288,995	4289,112	-0,117						
						7	6	2	4383,575	4386,674	-3,099
						7	4	4	4349,780	4350,081	-0,300
						7	2	6	4289,614	4289,700	-0,087
						7	7	0	4401,228	4398,552	2,677
						7	5	2	4386,215	4385,455	0,760
						7	3	4	4349,791	4350,072	-0,281
						7	1	6	4289,614	4289,700	-0,087
7	6	2	4383,502	4386,144	-2,642						
7	4	4	4349,224	4349,534	-0,310						
7	2	6	4288,995	4289,112	-0,117						
7	6	1	4390,817	4393,175	-2,357						
7	4	3	4370,113	4370,513	-0,401						
7	2	5	4322,195	4322,387	-0,192						
7	0	7	4249,599	4249,651	-0,052						
						7	7	1	4400,591	4396,773	3.819
						7	5	3	4370,531	4371,161	-0,630
						7	3	5	4322,781	4322,953	-0,172
						7	1	7	4250,254	4250,267	-0,014
						7	6	1	4391,166	4393,808	-2,642
						7	4	3	4370,666	4371,051	-0,384
						7	2	5	4322,781	4322,952	-0,171

				7 0 7	4250,254 4250,267 -0,014
7 7 1	4400,531	4396,434	4,097		
7 5 3	4369,990	4370,630	-0,640		
7 3 5	4322,195	4322,388	-0,193		
7 1 7	4249,599	4249,651	-0,052		
8 8 0	4497,791	4493,468	4,324		
8 6 2	4481,320	4479,626	1,694		
8 4 4	4444,367	4444,821	-0,454		
8 2 6	4384,493	4384,709	-0,215		
8 0 8	4299,872	4299,933	-0,061		
				8 7 2	4477,572 4482,161 -4,588
				8 5 4	4444,895 4445,396 -0,500
				8 3 6	4385,117 4385,302 -0,185
				8 1 8	4300,575 4300,589 -0,014
				8 8 0	4498,017 4493,859 4,158
				8 6 2	4481,504 4480,180 1,324
				8 4 4	4444,925 4445,370 -0,445
				8 2 6	4385,117 4385,302 -0,185
				8 0 8	4300,575 4300,589 -0,014
8 7 2	4477,566	4481,620	-4,054		
8 5 4	4444,337	4444,845	-0,508		
8 3 6	4384,493	4384,709	-0,215		
8 1 8	4299,872	4299,933	-0,061		
8 7 1	4485,197	4488,011	-2,813		
8 5 3	4464,982	4465,627	-0,645		
8 3 5	4417,507	4417,825	-0,319		
8 1 7	4345,299	4345,432	-0,134		
				8 8 1	4497,604 4492,305 5,299
				8 6 3	4465,415 4466,410 -0,994
				8 4 5	4418,096 4418,396 -0,300
				8 2 7	4345,960 4346,055 -0,095
				8 7 1	4485,580 4488,669 -3,089
				8 5 3	4465,636 4466,172 -0,536
				8 3 5	4418,097 4418,394 -0,298
				8 1 7	4345,960 4346,055 -0,095
8 8 1	4497,575	4492,014	5,561		
8 6 3	4464,787	4465,876	-1,089		
8 4 5	4417,506	4417,826	-0,321		
8 2 7	4345,299	4345,432	-0,134		
9 9 0	4606,711	4600,468	6,242		
9 7 2	4588,332	4585,808	2,524		
9 5 4	4551,054	4551,714	-0,661		
9 3 6	4491,614	4491,959	-0,345		
9 1 8	4407,480	4407,631	-0,151		
				9 8 2	4582,976 4589,385 -6,409
				9 6 4	4551,546 4552,330 -0,783
				9 4 6	4492,242 4492,556 -0,314
				9 2 8	4408,190 4408,293 -0,103
				9 9 0	4606,869 4600,812 6,058

						9	7	2	4588,461	4586,366	2,095
						9	5	4	4551,618	4552,264	-0,646
						9	3	6	4492,242	4492,556	-0,314
						9	1	8	4408,190	4408,293	-0,103
9	8	2	4583,031	4588,831	-5,800						
9	6	4	4550,984	4551,778	-0,793						
9	4	6	4491,614	4491,960	-0,346						
9	2	8	4407,480	4407,631	-0,151						
9	8	1	4591,296	4594,512	-3,216						
9	6	3	4571,902	4572,272	-0,371						
9	4	5	4524,408	4524,894	-0,486						
9	2	7	4452,652	4452,892	-0,239						
9	0	9	4356,032	4356,102	-0,069						
						9	9	1	4606,610	4599,458	7,153
						9	7	3	4571,201	4573,287	-2,086
						9	5	5	4524,996	4525,468	-0,472
						9	3	7	4453,319	4453,519	-0,200
						9	1	9	4356,789	4356,803	-0,014
						9	8	1	4591,714	4595,190	-3,477
						9	6	3	4572,152	4572,825	-0,673
						9	4	5	4525,000	4525,465	-0,464
						9	2	7	4453,319	4453,519	-0,200
						9	0	9	4356,789	4356,803	-0,014
9	9	1	4606,609	4599,220	7,389						
9	7	3	4570,997	4572,757	-1,760						
9	5	5	4524,404	4524,898	-0,494						
9	3	7	4452,652	4452,892	-0,239						
9	1	9	4356,032	4356,102	-0,069						
10	10	0	4727,621	4719,016	8,605						
10	8	2	4706,945	4703,355	3,590						
10	6	4	4669,167	4670,086	-0,919						
10	4	6	4610,245	4610,758	-0,514						
10	2	8	4526,666	4526,930	-0,264						
10	0	10	4418,073	4418,151	-0,078						
						10	9	2	4699,732	4708,278	-8,546
						10	7	4	4669,617	4670,782	-1,165
						10	5	6	4610,873	4611,353	-0,480
						10	3	8	4527,380	4527,595	-0,215
						10	1	10	4418,890	4418,904	-0,014
						10	10	0	4727,721	4719,305	8,415
						10	8	2	4706,999	4703,903	3,096
						10	6	4	4669,758	4670,629	-0,872
						10	4	6	4610,874	4611,353	-0,478
						10	2	8	4527,380	4527,595	-0,215
						10	0	10	4418,890	4418,904	-0,014
10	9	2	4699,832	4707,706	-7,873						
10	7	4	4669,030	4670,232	-1,201						
10	5	6	4610,244	4610,759	-0,515						
10	3	8	4526,666	4526,930	-0,264						
10	1	10	4418,073	4418,151	-0,078						
10	9	1	4709,072	4712,630	-3,558						

10	7	3	4689,882	4690,311	-0,429
10	5	5	4642,784	4643,486	-0,702
10	3	7	4571,550	4571,925	-0,375
10	1	9	4475,533	4475,701	-0,168

10	10	1	4727,561	4718,120	9,441
10	8	3	4688,627	4691,695	-3,068
10	6	5	4643,366	4644,063	-0,697
10	4	7	4572,219	4572,552	-0,333
10	2	9	4476,296	4476,408	-0,111

10	9	1	4709,526	4713,323	-3,797
10	7	3	4690,112	4690,867	-0,755
10	5	5	4643,377	4644,053	-0,675
10	3	7	4572,219	4572,552	-0,333
10	1	9	4476,296	4476,408	-0,111

10	10	1	4727,584	4717,939	9,645
10	8	3	4688,470	4691,177	-2,707
10	6	5	4642,773	4643,496	-0,724
10	4	7	4571,550	4571,925	-0,375
10	2	9	4475,533	4475,701	-0,168

11	11	0	4860,451	4848,993	11,458
11	9	2	4837,067	4832,162	4,905
11	7	4	4798,522	4799,793	-1,271
11	5	6	4740,260	4740,986	-0,726
11	3	8	4657,308	4657,715	-0,407
11	1	10	4549,449	4549,634	-0,185

11	10	2	4827,771	4838,760	-10,989
11	8	4	4799,019	4800,641	-1,622
11	6	6	4740,886	4741,575	-0,688
11	4	8	4658,024	4658,377	-0,354
11	2	10	4550,272	4550,392	-0,120

11	11	0	4860,502	4849,227	11,275
11	9	2	4837,029	4832,682	4,347
11	7	4	4799,230	4800,319	-1,089
11	5	6	4740,889	4741,572	-0,683
11	3	8	4658,024	4658,377	-0,354
11	1	10	4550,272	4550,392	-0,120

11	10	2	4827,894	4838,165	-10,271
11	8	4	4798,316	4800,099	-1,783
11	6	6	4740,257	4740,989	-0,732
11	4	8	4657,308	4657,715	-0,407
11	2	10	4549,449	4549,634	-0,185

11	10	1	4838,465	4842,317	-3,851
11	8	3	4819,205	4819,586	-0,381
11	6	5	4772,504	4773,476	-0,972
11	4	7	4701,868	4702,414	-0,546
11	2	9	4606,526	4606,816	-0,290
11	0	11	4485,987	4486,073	-0,086

11	11	1	4860,405	4848,179	12,226
11	9	3	4817,148	4821,519	-4,370
11	7	5	4773,074	4774,059	-0,985
11	5	7	4702,538	4703,036	-0,498
11	3	9	4607,293	4607,524	-0,231
11	1	11	4486,870	4486,884	-0,014

						11	10	1	4838,959	4843,021	-4,062
						11	8	3	4819,400	4820,140	-0,739
						11	6	5	4773,100	4774,032	-0,932
						11	4	7	4702,538	4703,036	-0,498
						11	2	9	4607,293	4607,524	-0,231
						11	0	11	4486,870	4486,884	-0,014
11	11	1	4860,446	4848,053	12,394						
11	9	3	4817,098	4821,027	-3,969						
11	7	5	4772,478	4773,503	-1,025						
11	5	7	4701,868	4702,414	-0,546						
11	3	9	4606,526	4606,816	-0,290						
11	1	11	4485,987	4486,073	-0,086						
12	12	0	5005,132	4990,277	14,854						
12	10	2	4978,604	4972,123	6,481						
12	8	4	4939,694	4940,663	-0,969						
12	6	6	4881,518	4882,509	-0,990						
12	4	8	4799,272	4799,855	-0,582						
12	2	10	4692,226	4692,542	-0,315						
12	0	12	4559,763	4559,857	-0,094						
						12	11	2	4967,009	4980,749	-13,740
						12	9	4	4938,875	4941,790	-2,915
						12	7	6	4882,140	4883,085	-0,945
						12	5	8	4799,986	4800,507	-0,522
						12	3	10	4693,050	4693,298	-0,248
						12	1	12	4560,720	4560,735	-0,015
						12	12	0	5005,146	4990,463	14,683
						12	10	2	4978,460	4972,587	5,873
						12	8	4	4939,922	4941,158	-1,236
						12	6	6	4882,148	4883,077	-0,929
						12	4	8	4799,986	4800,507	-0,522
						12	2	10	4693,050	4693,298	-0,248
						12	0	12	4560,720	4560,735	-0,015
12	11	2	4967,120	4980,121	-13,001						
12	9	4	4938,652	4941,261	-2,609						
12	7	6	4881,511	4882,516	-1,006						
12	5	8	4799,272	4799,855	-0,582						
12	3	10	4692,226	4692,542	-0,315						
12	1	12	4559,763	4559,857	-0,094						
12	11	1	4979,399	4983,524	-4,125						
12	9	3	4959,712	4959,930	-0,218						
12	7	5	4913,423	4914,723	-1,299						
12	5	7	4843,470	4844,229	-0,759						
12	3	9	4748,881	4749,320	-0,439						
12	1	11	4629,221	4629,423	-0,202						
						12	12	1	5005,088	4989,524	15,564
						12	10	3	4956,655	4962,622	-5,968
						12	8	5	4913,974	4915,323	-1,348
						12	6	7	4844,137	4844,837	-0,700
						12	4	9	4749,646	4750,022	-0,376
						12	2	11	4630,108	4630,238	-0,129
						12	11	1	4979,935	4984,240	-4,305
						12	9	3	4959,881	4960,470	-0,589

								12	7	5	4914.028	4915.258	-1.230
								12	5	7	4844.137	4844.837	-0.699
								12	3	9	4749.646	4750.022	-0.376
								12	1	11	4630.108	4630.238	-0.129
12	12	1	5005.140	4989.444	15.696								
12	10	3	4956.627	4962.178	-5.551								
12	8	5	4913.370	4914.786	-1.417								
12	6	7	4843.469	4844.229	-0.760								
12	4	9	4748.881	4749.320	-0.439								
12	2	11	4629.221	4629.423	-0.202								
13	13	0	5161.597	5142.758	18.840								
13	11	2	5131.466	5123.122	8.344								
13	9	4	5091.519	5092.498	-0.979								
13	7	6	5033.866	5035.176	-1.309								
13	5	8	4952.410	4953.207	-0.797								
13	3	10	4846.259	4846.732	-0.473								
13	1	12	4714.836	4715.055	-0.219								
								13	12	2	5117.340	5134.155	-16.814
								13	10	4	5090.027	5094.103	-4.076
								13	8	6	5034.480	5035.737	-1.257
								13	6	8	4953.118	4953.840	-0.722
								13	4	10	4847.079	4847.478	-0.399
								13	2	12	4715.796	4715.934	-0.138
								13	13	0	5161.586	5142.914	18.672
								13	11	2	5131.213	5123.496	7.717
								13	9	4	5091.721	5092.938	-1.217
								13	7	6	5034.499	5035.714	-1.215
								13	5	8	4953.118	4953.840	-0.722
								13	3	10	4847.079	4847.478	-0.399
								13	1	12	4715.796	4715.934	-0.138
13	12	2	5117.396	5133.484	-16.088								
13	10	4	5089.824	5093.595	-3.772								
13	8	6	5033.847	5035.196	-1.349								
13	6	8	4952.410	4953.207	-0.797								
13	4	10	4846.259	4846.732	-0.473								
13	2	12	4714.836	4715.055	-0.219								
13	12	1	5131.785	5136.193	-4.408								
13	10	3	5111.226	5111.178	0.047								
13	8	5	5065.375	5067.064	-1.689								
13	6	7	4996.203	4997.223	-1.020								
13	4	9	4902.450	4903.071	-0.621								
13	2	11	4783.755	4784.096	-0.341								
13	0	13	4639.390	4639.491	-0.102								
								13	13	1	5161.552	5142.060	19.491
								13	11	3	5107.045	5114.840	-7.795
								13	9	5	5065.913	5067.705	-1.792
								13	7	7	4996.866	4997.808	-0.941
								13	5	9	4903.210	4903.758	-0.548
								13	3	11	4784.641	4784.906	-0.265
								13	1	13	4640.430	4640.446	-0.016
								13	12	1	5132.362	5136.930	-4.567
								13	10	3	5111.396	5111.685	-0.289
								13	8	5	5066.009	5067.564	-1.555

						12	7	5	4914.028	4915.258	-1.230
						12	5	7	4844.137	4844.837	-0.699
						12	3	9	4749.646	4750.022	-0.376
						12	1	11	4630.108	4630.238	-0.129
12	12	1	5005.140	4989.444	15.696						
12	10	3	4956.627	4962.178	-5.551						
12	8	5	4913.370	4914.786	-1.417						
12	6	7	4843.469	4844.229	-0.760						
12	4	9	4748.881	4749.320	-0.439						
12	2	11	4629.221	4629.423	-0.202						
13	13	0	5161.597	5142.758	18.840						
13	11	2	5131.466	5123.122	8.344						
13	9	4	5091.519	5092.498	-0.979						
13	7	6	5033.866	5035.176	-1.309						
13	5	8	4952.410	4953.207	-0.797						
13	3	10	4846.259	4846.732	-0.473						
13	1	12	4714.836	4715.055	-0.219						
						13	12	2	5117.340	5134.155	-16.814
						13	10	4	5090.027	5094.103	-4.076
						13	8	6	5034.480	5035.737	-1.257
						13	6	8	4953.118	4953.840	-0.722
						13	4	10	4847.079	4847.478	-0.399
						13	2	12	4715.796	4715.934	-0.138
						13	13	0	5161.586	5142.914	18.672
						13	11	2	5131.213	5123.496	7.717
						13	9	4	5091.721	5092.938	-1.217
						13	7	6	5034.499	5035.714	-1.215
						13	5	8	4953.118	4953.840	-0.722
						13	3	10	4847.079	4847.478	-0.399
						13	1	12	4715.796	4715.934	-0.138
13	12	2	5117.396	5133.484	-16.088						
13	10	4	5089.824	5093.595	-3.772						
13	8	6	5033.847	5035.196	-1.349						
13	6	8	4952.410	4953.207	-0.797						
13	4	10	4846.259	4846.732	-0.473						
13	2	12	4714.836	4715.055	-0.219						
13	12	1	5131.785	5136.193	-4.408						
13	10	3	5111.226	5111.178	0.047						
13	8	5	5065.375	5067.064	-1.689						
13	6	7	4996.203	4997.223	-1.020						
13	4	9	4902.450	4903.071	-0.621						
13	2	11	4783.755	4784.096	-0.341						
13	0	13	4639.390	4639.491	-0.102						
						13	13	1	5161.552	5142.060	19.491
						13	11	3	5107.045	5114.840	-7.795
						13	9	5	5065.913	5067.705	-1.792
						13	7	7	4996.866	4997.808	-0.941
						13	5	9	4903.210	4903.758	-0.548
						13	3	11	4784.641	4784.906	-0.265
						13	1	13	4640.430	4640.446	-0.016
						13	12	1	5132.362	5136.930	-4.567
						13	10	3	5111.396	5111.685	-0.289
						13	8	5	5066.009	5067.564	-1.555

						13	6	7	4996,868	4997,806	-0,938
						13	4	9	4903,210	4903,758	-0,548
						13	2	11	4784,641	4784,906	-0,265
						13	0	13	4640,430	4640,446	-0,016
13	13	1	5161,609	5142,005	19,604						
13	11	3	5107,059	5114,475	-7,415						
13	9	5	5065,278	5067,202	-1,924						
13	7	7	4996,202	4997,224	-1,022						
13	5	9	4902,450	4903,071	-0,621						
13	3	11	4783,755	4784,096	-0,341						
13	1	13	4639,390	4639,491	-0,102						
14	14	0	5329,782	5306,341	23,441						
14	12	2	5295,575	5285,033	10,542						
14	10	4	5254,345	5255,068	-0,723						
14	8	6	5197,131	5198,818	-1,686						
14	6	8	5116,557	5117,614	-1,057						
14	4	10	5011,390	5012,051	-0,661						
14	2	12	4881,100	4881,467	-0,366						
14	0	14	4724,854	4724,963	-0,109						
						14	13	2	5278,634	5298,888	-20,254
						14	11	4	5251,785	5257,446	-5,661
						14	9	6	5197,736	5199,366	-1,631
						14	7	8	5117,257	5118,214	-0,957
						14	5	10	5012,200	5012,777	-0,577
						14	3	12	4882,056	4882,338	-0,282
						14	1	14	4725,987	4726,005	-0,018
						14	14	0	5329,756	5306,503	23,253
						14	12	2	5295,220	5285,273	9,948
						14	10	4	5254,511	5255,419	-0,909
						14	8	6	5197,774	5199,308	-1,535
						14	6	8	5117,257	5118,214	-0,956
						14	4	10	5012,200	5012,777	-0,577
						14	2	12	4882,056	4882,338	-0,282
						14	0	14	4725,987	4726,005	-0,018
14	13	2	5278,577	5298,156	-19,579						
14	11	4	5251,597	5256,970	-5,372						
14	9	6	5197,091	5198,869	-1,778						
14	7	8	5116,557	5117,615	-1,058						
14	5	10	5011,390	5012,051	-0,661						
14	3	12	4881,100	4881,467	-0,366						
14	1	14	4724,854	4724,963	-0,109						
14	13	1	5295,543	5300,257	-4,714						
14	11	3	5273,540	5273,177	0,364						
14	9	5	5228,154	5230,311	-2,157						
14	7	7	5159,901	5161,236	-1,335						
14	5	9	5067,072	5067,912	-0,840						
14	3	11	4949,432	4949,938	-0,506						
14	1	13	4806,283	4806,518	-0,235						
						14	14	1	5329,736	5305,721	24,015
						14	12	3	5268,235	5277,969	-9,735
						14	10	5	5228,733	5231,043	-2,310
						14	8	7	5160,560	5161,785	-1,224
						14	6	9	5067,822	5068,572	-0,750
						14	4	11	4950,311	4950,734	-0,424
						14	2	13	4807,323	4807,471	-0,148

14	13	1	5296,148	5301.029	-4,881
14	11	3	5273,765	5273,628	0.137
14	9	5	5228,879	5230,757	-1,878
14	7	7	5160,564	5161,780	-1,216
14	5	9	5067,822	5068,572	-0,750
14	3	11	4950,311	4950,734	-0,424
14	1	13	4807,323	4807,471	-0,148

14	14	1	5329,791	5305,652	24,139
14	12	3	5268,255	5277,726	-9,471
14	10	5	5228,007	5230,591	-2,584
14	8	7	5159,897	5161,240	-1,343
14	6	9	5067,072	5067,912	-0,840
14	4	11	4949,432	4949,938	-0,506
14	2	13	4806,283	4806,518	-0,235

15	15	0	5509,618	5480,969	28,649
15	13	2	5470,867	5457,701	13,166
15	11	4	5428,034	5428,120	-0,087
15	9	6	5371,122	5373,243	-2,121
15	7	8	5291,534	5292,903	-1,369
15	5	10	5187,446	5188,331	-0,886
15	3	12	5058,387	5058,927	-0,540
15	1	14	4903,546	4903,797	-0,251

15	14	2	5450,725	5474,858	-24,132
15	12	4	5423,946	5431,685	-7,739
15	10	6	5371,720	5373,795	-2,075
15	8	8	5292,226	5293,454	-1,228
15	6	10	5188,240	5189,022	-0,782
15	4	12	5059,330	5059,779	-0,449
15	2	14	4904,677	4904,836	-0,159

15	15	0	5509,586	5481,190	28,396
15	13	2	5470,436	5457,758	12,678
15	11	4	5428,175	5428,339	-0,164
15	9	6	5371,792	5373,661	-1,870
15	7	8	5292,227	5293,452	-1,225
15	5	10	5188,240	5189,022	-0,782
15	3	12	5059,330	5059,779	-0,449
15	1	14	4904,677	4904,836	-0,159

15	14	2	5450,489	5474,041	-23,552
15	12	4	5423,738	5431,248	-7,510
15	10	6	5371,044	5373,360	-2,316
15	8	8	5291,533	5292,904	-1,371
15	6	10	5187,446	5188,331	-0,886
15	4	12	5058,387	5058,927	-0,540
15	2	14	4903,546	4903,797	-0,251

15	14	1	5440,150	5475,631	-35,481
15	12	3	5446,431	5445,799	0,632
15	10	5	5402,285	5404,247	-1,962
15	8	7	5334,379	5336,090	-1,711
15	6	9	5242,572	5243,674	-1,102
15	4	11	5126,082	5126,784	-0,702
15	2	13	4984,249	4984,641	-0,391
15	0	15	4816,139	4816,254	-0,115

15	15	1	5509,575	5480,476	29,099
15	13	3	5470,603	5451,763	18,840

15	11	5	5401,512	5405,156	-3,644
15	9	7	5335,037	5336,588	-1,551
15	7	9	5243,308	5244,291	-0,983
15	5	11	5126,946	5127,553	-0,607
15	3	13	4985,282	4985,582	-0,301
15	1	15	4817,379	4817,399	-0,020

15	14	1	5471,211	5476,465	-5,254
15	12	3	5446,781	5446,169	0,612
15	10	5	5402,467	5404,610	-2,142
15	8	7	5335,045	5336,576	-1,531
15	6	9	5243,308	5244,291	-0,983
15	4	11	5126,946	5127,553	-0,607
15	2	13	4985,282	4985,582	-0,301
15	0	15	4817,379	4817,399	-0,020

15	15	1	5509,625	5480,335	29,290
15	13	3	5440,130	5451,698	-11,568
15	11	5	5401,326	5404,780	-3,455
15	9	7	5334,371	5336,101	-1,731
15	7	9	5242,572	5243,674	-1,102
15	5	11	5126,082	5126,784	-0,702
15	3	13	4984,249	4984,641	-0,391
15	1	15	4816,139	4816,254	-0,115

APPENDIX VI

LISTING OF PROGRAM SPEC-FIT 1

This program is set up for the simultaneous analysis of the two interacting bands $\nu_1+\nu_2$ and $\nu_2+\nu_3$. To set the program up for the analysis of any other two interacting bands (v_1,v_2,v_3) and (v_1',v_2',v_3'), the only changes that must be made are in the calculation of the vibrational matrix elements, PQ and QQ, of the interaction terms.

$$PQ = \langle v_1,v_2,v_3|q_1q_3|v_1',v_2',v_3'\rangle$$

$$QQ = \langle v_1,v_2,v_3|q_1p_3-q_3p_1|v_1',v_2',v_3'\rangle$$

For $(v_1,v_2,v_3) = (1,1,0)$ and $(v_1',v_2',v_3') = (0,1,1)$, PQ = -1.0 and QQ = +0.5 as can be seen in the program. It is necessary that the unprimed quantum numbers (v_1,v_2,v_3) represent the type B band, and the primed represent the type A band.

BELOW IS A LISTING OF PROGRAM SPEC-FIT 1

```
 JOB,151154,NKM, 5, MONCUR,       SPEC-FIT 1
 FTN,X,L
       PROGRAM SPEC FIT 1
       DIMENSION AV(14,2),AA(2),BB(2),CC(2),T1(2),T2(2),T3(2),T4(2),H1(2)
      1,H2(2),H3(2),H4(2),VO(2),NPTS(2),PX(3),PY(3),PZ(3),PXZ(3),PYZ(3),
      2PXY(3),PX2(21,21),PZ2(21,21),P1(21,21),P2(21,21),P3(21,21),P4(21,
      321),A(21,21),SS(21,21),PBXY(21,21),PBZ(21,21),JJU(800),KKU(800),
      4LLU(800),JJG(800),KKG(800),LLG(800),OBS(800),ENG(800),WHT(2,800),
      5IFUSE(800),CAP(2)
       COMMON JJU,KKU,LLU,JJG,KKG,LLG,OBS,ENG,WHT
       COMPLEX A,SS,PBXY,PBZ
C THIS PROGRAM IS SET UP FOR THE SIMULTANEOUS ANALYSIS OF THE BANDS
C (1,1,0) AND (0,1,1)
C  THE VIBRATIONAL MATRIX ELEMENTS USED ARE (1,1,0 Q1Q3 0,1,1) =
C    (0,1,1 Q1Q3 1,1,0) = 1./2.
C    (1,1,0 Q1P3-Q3P1 0,1,1) = -1*I
C  (0,1,1 Q1P3-Q3P1 1,1,0) = +1*I
       REWIND 51
       RT2=SQRT(2.)
       QQ= 0.5
       PQ = -1.0
       NM=21
       BH0=1.0E-06
       IER=0
       READ 500, AA(1),BB(1),CC(1),T1(1),T2(1),T3(1),T4(1),VO(1),H1(1),
      1H2(1),H3(1),H4(1)
  500 FORMAT(3F15.6/4F10.6,F10.5/4F20.12)
       CAP(1)=(2.*BB(1)-AA(1)-CC(1))/(AA(1)-CC(1))
       AA(2)=AA(1) $ BB(2)=BB(1) $ CC(2)=CC(1) $ T1(2)=T1(1)
       T2(2)=T2(1) $ T3(2)=T3(1) $ T4(2)=T4(1) $H1(2)=H1(1) $ H2(2)=H2(1)
       H3(2)=H3(1) $ H4(2)=H4(1) $ VO(2) = VO(1)
       PRINT 501,(AA(1),BB(1),CC(1),T1(1),T2(1),T3(1),T4(1),H1(1),H2(1),
      1H3(1),H4(1),CAP(1))
       R=BB(1)**2/(AA(1)+BB(1))**2  $ S=AA(1)**2/(AA(1)+BB(1))**2
       NPTS(1)=NPTS(2)=I=0
  501 FORMAT(*1GROUND STATE CONSTANTS*//* A= *F15.10/* B = *F15.10/
      1* C = *F15.10//* TAAAA = *F15.9/* TBBBB = *F15.9/* TAABB = *F15.9/
      2 * TABAB = *F15.9/,* HJ  = *F20.12/* HJK = *F20.12/* HKJ = *F20.12
      3 / * HK  = *F20.12//* KAPPA = *F10.4)
       DO 12 J=1,2
       DO 10 K=1,800
       I=I+1
       READ 504,JJU(I),KKU(I),LLU(I),JJG(I),KKG(I),LLG(I),OBS(I),WHT(1,
      1  I),LASTDATA
  504 FORMAT(1X,6I3,F13.4,7X,F4.2,29X,A8)
       IF(LASTDATA,EQ.8HEND DATA)GO TO 12
       WHT(2,I)=WHT(1,I)
       ENG(I)=0.0
       NPTS(J)=NPTS(J)+1
   10 CONTINUE
```

```
 12 I=I-1
    NSUM = NPTS(1)*NPTS(2)
    DO 298 NTMS =1,2
    IOPT=0
    IF(NTMS,EQ,1) GO TO 503
    IOPT = 1
    READ 502, (AA(I),BB(I),CC(I),T1(I),T2(I),T3(I),T4(I),VO(I),
   1 H1(I),H2(I),H3(I),H4(I),I=1,2), GZ,GXY
502 FORMAT(2(3F15,6/4F10,7,F10,5/4F20,12/),2F20,10)
    CAP(1)=(2,*BB(1)-AA(1)-CC(1))/(AA(1)-CC(1))
    CAP(2)=(2,*BB(2)-AA(2)-CC(2))/(AA(2)-CC(2))
    PRINT 555,(AA(I),BB(I),CC(I),T1(I),T2(I),T3(I),T4(I),H1(I),H2(I),
   1H3(I),H4(I),VO(I),CAP(I),I=1,2),GZ,GXY
555 FORMAT(///* UPPER STATE CONSTANTS*2(//* A = *F15,10/* B = *F15,10/
   1* C = *F15,10//* TAAAA = *F15,9/* TBBBB = *F15,9/* TAABB = *F15,9/
   2 * TABAB = *F15,9/,* HJ  = *F20,12/* HJK = *F20,12/* HKJ = *F20,12
   3 / * HK  = *F20,12//* BAND CENTER = *F15,6/*0KAPPA = *F10,4)/*=GZ
   4 = *F15,6/* GXY = *F15,6)
503 CONTINUE
    DO 201 KKK=1,NSUM
201 IFUSE(KKK)=0
    NBAND =0
    DO 290 MM=1,NSUM
    IF( IFUSE(MM),NE,0)GO TO 290
    IF(NTMS,EQ,2)GO TO 2
    J=JJG(MM)
    IF(J,EQ,0) GO TO 290
    IF(LLG(MM)-(LLG(MM)/2)*2)206,204
204 JEO=2
    EO=0,
    GO TO 208
206 JEO=4
    EO=1,
208 IF(J,EQ,KKG(MM)+LLG(MM))JEO=JEO-1
    GO TO 3
  2 J=JJU(MM)
    IF (J,NE,0) GO TO 404
    DO 401 NN=1,14
401 AV(NN,1)=AV(NN,2)=0,0
    NB=1
    NLM=1
    MB=2
    IF(MM,LE,NPTS(1)) GO TO 402
    NLM=2
    NB=2
    MB=1
402 IF(NBAND,NE,(NBAND/2)*2)NB=MB
    AV(1,NLM)=1
    ENGU=VO(NB)
    WRITE TAPE 51,JJU(MM),KKU(MM),LLU(MM),JJG(MM),KKG(MM),LLG(MM),
   1 OBS(MM),ENGU,ENG(MM),WHT(1,MM),((AV(II,JJ),II=1,12),JJ=1,2),
   2 AV(13,1),AV(14,1),MM
    GO TO 290
404 CONTINUE
```

```
      IF(LLU(MM)-(LLU(MM)/2)*2)210,209
  209 JEO=2
      GO TO 211
  210 JEO=4
  211 IF(J.EQ.KKU(MM)+LLU(MM))JEO=JEO-1
      IF(MM.LE.NPTS(1))GO TO 145
      GO TO(140,141,140,141),JEO
  140 JEO=JEO+1
      GO TO 142
  141 JEO=JEO-1
  142 CONTINUE
  145 GO TO(146,147,146,147),JEO
  146 IF(NBAND.EQ.(NBAND/2)*2)GO TO 3
      GO TO 148
  147 IF(NBAND -  (NBAND/2)*2)3,148
  148 ASV=AA(1)$BSV=BB(1)$CSV=CC(1)                    $ VOSV=VO(1)
      T1SV=T1(1) $ T2SV=T2(1) $ T3SV=T3(1)$T4SV=T4(1)
      H1SV=H1(1) $ H2SV=H2(1) $ H3SV=H3(1) $ H4SV=H4(1)
      PQ=-PQ
      AA(1)=AA(2) $ BB(1)=BB(2) $ CC(1)=CC(2)                $VO(1)=VO(2)
      T1(1)=T1(2) $ T2(1)=T2(2) $T3(1)=T3(2) $ T4(1)=T4(2)
      H1(1)=H1(2) $ H2(1)=H2(2) $ H3(1)=H3(2) $ H4(1)=H4(2)
      AA(2)=ASV $ BB(2)=BSV $ CC(2)=CSV                 $VO(2)=VOSV
      T1(2)=T1SV $ T2(2)=T2SV $T3(2)=T3SV $T4(2)=T4SV
      H1(2)=H1SV $ H2(2)=H2SV $ H3(2)=H3SV $ H4(2)=H4SV
      NBAND = NBAND+1
    3 F=J*(J+1)
      IF(JEO-2)119,119,123
  119 NSZ=2*(J/2)+1
      N=J/2+2
      GO TO 124
  123 NSZ=2*((J+1)/2)
      N=(J+1)/2
  124 CONTINUE
      DO 4 I=1,NSZ
      DO 4 JJ=1,NSZ
    4 A(I,JJ)= (0.,0.)
      DO 70 I=1,2
      IF(JEO-2)126,126,127
  126 N=N-1
  127 CONTINUE
      IF(N.EQ.0) GO TO 70
      NN=0
      IF(I.EQ.2)NN=(NSZ+1)/2
      DO 70 L=1,N
      IF(JEO-2)130,130,135
  130 IF(I-2)16,15
   15 K=2*L
      GO TO 17
   16 K=2*L-2
      GO TO 17
  135 K=2*L-1
   17 CONTINUE
      M=L+NN
```

```
      PX2(M,M)=(F-K*K)/2.
      PZ2(M,M)=K*K
      PX(1)=(3.*F*F-2.*F-6.*F*K*K+5.*K*K+3*(K*K*K*K)/8.
      PY(1)=PX(1)
      PZ(1)=K*K*K*K
      PX7(1)=K*K*(F-K*K)
      PY7(1)=PXZ(1)
      PXY(1)=(F*F+2.*F-2.*F*K*K-5.*K*K*K*K*(K)/4.
      IF(L.EQ.N)GO TO 18
      PX2(M,M+1)=-SQRT((F-K*(K+1))*(F-(K+1)*(K+2)))/4.
      PZ2(M,M+1)=0.0
      PX(2)=-(2.*F-K*K-(K+2.)**2)*SQRT((F-K*(K+1))*(F-(K+1)*(K+2)))/8.
      PY(2)=-PX(2)
      PZ(2)=PZ(3)=0.
      PX7(2)=-(K*K+(K+2)**2)*SQRT((F-K*(K+1))*(F-(K+1)*(K+2)))/4.
      PY7(2)=-PXZ(2)
      PXY(2)=0.
      IF(L.EQ.N-1)GO TO 18
      PZ2(M,M+2)=PX2(M,M+2)=0.0
      PX(3)=SQRT((F-K*(K+1))*(F-(K+1)*(K+2))*(F-(K+2)*(K+3))*(F-(K+3)*(K
     1+4)))/16.
      PY(3)=PX(3)
      PX7(3)=0.
      PY7(3)=0.
      PXY(3)=-2.*PX(3)
18    CONTINUE
      IF(JE0-2)19,19,47
19    IF(K)25,20
20    PX2(M,M+1)=RT2*PX2(M,M+1)
      PX(2)=PX(2)*RT2
       PY(2)=-PX(2)
      PXZ(2)=PXZ(2)*RT2
      PY7(2)=-PXZ(2)
      PX(3)=PX(3)*RT2
      PY(3)=PX(3)
      PXY(3)=-2.*PX(3)
      GO TO 53
25    IF(K-2)53,30
30    IF(I-2)40,45
40    PX(1)=PX(1)+F*(F-2.)/16.
      PY(1)=PX(1)
      PXY(1)=PXY(1)+F*(F-2.)/8.
      GO TO 53
45    PX(1)=PX(1)-F*(F-2.)/16.
      PY(1)=PX(1)
      PXY(1)=PXY(1)+F*(F-2.)/8.
      GO TO 53
47    IF(K-1)53,48
48    XM=1.
      IF(I.EQ.2)XM=-1.
      PX2(M,M)=PX2(M,M)-XM*F/4.
      PX(1)=PX(1)-XM*F*(F-1.)/4.
      PY(1)=PY(1)+XM*F*(F-1.)/4.
      PX(2)=PX(2)+XM*F*SQRT((F-2.)*(F-6.))/16.
```

```
      PY(2)=PY(2)+XM*F*SQRT((F-2.)*(F-6.))/16.
      PXZ(1)=PXZ(1)+YM*F/2.
      PYZ(1)=PYZ(1)+XM*F/2.
      PXY(2)=-XM*F*SQRT((F-2.)*(F-6.))/8.
   53 CONTINUE
      NS=3
      IF(L.EQ.N-1)NS=2
      IF(L.EQ.N)NS=1
      DO 55 KK=1,NS
      JJ=M+KK-1
      P1(M,JJ)=(PX(KK)+R*R*PZ(KK)+R*PXZ(KK))/4.
      P2(M,JJ)=(PY(KK)+S*S*PZ(KK)+S*PYZ(KK))/4.
      P3(M,JJ)=(2.*R*S*PZ(KK)+PXY(KK)+S*PXZ(KK)+R*PYZ(KK))/4.
      P4(M,JJ)=PXY(KK)/2.
      IF(M.EQ.JJ)P4(M,M)=P4(M,M)+(5.*PZ2(M,M)-2.*F)/4.
      A(M,JJ)=(AA(I)-BB(I))*PX2(M,JJ)+CC(I)*PZ2(M,JJ)+T1(I)*P1(M,JJ) +
     1 T2(I)*P2(M,JJ)+T3(I)*P3(M,JJ)+T4(I)*P4(M,JJ)
      IF(M.NE.JJ)GO TO 55
      A(M,JJ)=A(M,JJ)+BB(I)*(F-K*K)+V0(I)+H1(I)*F*F+F+H2(I)*F*F*K*K+
     1 H3(I)*F*K**4+H4(I)*K**6
   55 A(JJ,M)=A(M,JJ)
   70 CONTINUE
      IF(NTMS.EQ.1)GO TO 116
C THE FOLLOWING SETS UP THE INTERACTION MATRIX ELEMENTS
      IF(JEO.GT.2 ) GO TO 105
      PBXY(1,N+2)=QQ*SQRT(F*(F-2.)/2.)*(0.,1.)
      A(1,N+2)=GXY*PBXY(1,N+2)
      A(N+2,1)=-A(1,N+2)
  105 DO 115 M=1,N
      K=2*N-1
      II=M
      JJ=M+N
      IF(JEO.GT.2) GO TO 110
      K=K+1
      II=II+1
      JJ=JJ+1
  110 CONTINUE
      PBZ2=0.
      PBZ1=K
      PBXY1=0.
      PBXY2=SQRT((F-K*(K+1))*(F-(K+1)*(K+2)))/2.
      IF(K-1)112,111,112
  111 PBXY1=F/2.
  112 PBZ1=PQ*PBZ1
      PBXY1=QQ*PBXY1
      PBXY2=QQ*PBXY2
      ICNT = II+1
      JCNT = JJ+1
      IF(M.EQ.N) GO TO 114
      PBXY(II,JCNT)=PBXY(JJ,ICNT)=PBXY2*(0.,1.)
      A(II,JCNT)=A(JJ,ICNT) =GXY*PBXY(II,JCNT)
      A(JCNT,II) = A(ICNT,JJ) = CONJG(A(II,JCNT))
  114 PBZ(II,JJ)=PBZ1*(0.,1.)
      PBXY(II,JJ)=PBXY1*(0.,1.)
```

```
      A(II,JJ)=GZ*PBZ(II,JJ)+GXY*PRXY(II,JJ)
      A(JJ,II)= CONJG(A(II,JJ))
  115 CONTINUE
  116 CONTINUE
  302 FORMAT(*0*)
      CALL JHERMX(A,MM,NSZ,IOPT,RHO,IER,SS)
      MM1=MM+1
      IF(NTMS,EQ,2)GO TO 228
      GO TO(120,120,122,122),JEO
  120 NN=LLG(MM)/2 + 1
      IF(JEO,EQ,2)NN=NN+J/2
      GO TO 125
  122 NN=(LLG(MM)+1)/2
      IF(JEO,EQ,4)NN=NN+(J+1)/2
  125 ENG(MM)= A(NN,NN)
      IFUSE(MM)=1
      IF(MM,EQ,NSUM)GO TO 290
      DO 226 MMM=MM1,NSUM
      IF(IFUSE(MM1),NE.0)GO TO 226
      IF(JJG(MMM),NE,J)GO TO 226
      IF(LLG(MMM)+(LLG(MMM)/2)*2)216,214
  214 ID=2
      EOE=0,
      GO TO 218
  216 ID=4
      EOE=1,
  218 IF(EO,NE,EOE)GO TO 226
      IF(J,EQ,KKG(MMM)+LLG(MMM))ID=ID+1
      GO TO(220,220,222,222),ID
  220 NN=LLG(MMM)/2+1
      IF(ID,EQ.2)NN=NN+J/2
      GO TO 225
  222 NN=(LLG(MMM)+1)/2
      IF(ID,EQ,4)NN=NN+(J+1)/2
  225 ENG(MMM)=A(NN,NN)
      IFUSE(MMM)=1
  226 CONTINUE
      GO TO 290
  228 CONTINUE
      ID=JEO
      IS=-1
      IF(MM,GT,NPTS(1)) ID=ID+IS**ID
      GO TO (230,230,234,234),ID
  230 NN=LLU(MM)/2+1
      IF(ID,EQ,2)NN=NN+J/2
      GO TO 236
  234 NN=(LLU(MM)+1)/2
      IF(ID,EQ,4)NN=NN+(J+1)/2
  236 CONTINUE
      DO 280 IJ=MM,NSUM
      IF(IJ,EQ,MM)GO TO 249
      IF(IFUSE(IJ).NE.0)GO TO 280
      IF(JJU(IJ),NE,J)GO TO 280
      IF(LLU(IJ)+(LLU(IJ)/2)*2)239,238
```

```
  238 ID=2
      GO TO 240
  239 ID=4
  240 IF(J.EQ.KKU(IJ)+LLU(IJ))ID=ID-1
      IDR=ID
      IF(IJ.LE.NPTS(1))GO TO 243
      GO TO(241,242,241,242),ID
  241 ID=ID+1
      GO TO 243
  242 ID=ID-1
  243 CONTINUE
      IF(ID.NE.JEO)GO TO 280
      GO TO(246,246,248,248),IDR
  246 NN=LLU(IJ)/2+1
      IF(IDR.EQ.2)NN=NN+J/2
      GO TO 249
  248 NN=(LLU(IJ)+1)/2
      IF(IDR.EQ.4)NN=NN+(J+1)/2
  249 ENGU=A(NN,NN)
      IFUSE(IJ)=1
C THE FOLLOWING CALCULATES THE AVERAGE VALUES OF THE OPERATORS
  250 DO 149 I=1,14
  149 AV(I,1)=AV(I,2)=0.
      LSZ=(NSZ+1)/2
      NB=1
      MB=2
      IF(JEO.NE.(JEO/2)*2)GO TO 153
      NB=2
      MB=1
  153 CONTINUE
      DO 150 II=1,NSZ
      IF(I).EQ.LSZ+1)NB=MB
      KSZ=II+2
      IF(II.EQ.NSZ-1)KSZ=II+1
      IF(II.EQ.NSZ)KSZ=II
      DO 150 JJ=II,KSZ
      VSQ = CONJG(SS(II,NN))*SS(JJ,NN)
      IF(II-JJ)121,151
  151 AV(1,NB)=AV(1,NB)+VSQ
      AV(9,NB)=VSQ*F**3 + AV(9,NB)
      AV(10,NB)=AV(10,NB)+VSQ*F**2+PZ2(II,II)
      AV(11,NB)= AV(11,NB)+VSQ*F*PZ2(II,II)**2
      AV(12,NB)=AV(12,NB)+VSQ*PZ2(II,II)**3
      AV(3,NB)=VSQ*(F-PX2(II,II)-PZ2(II,II))+AV(3,NB)
      GO TO 152
  121 VSQ=2.*VSQ
      AV(3,NB)=AV(3,NB)-VSQ*PX2(II,JJ)
  152 AV(2,NB)=AV(2,NB)+VSQ*PX2(II,JJ)
      AV(4,NB)=AV(4,NB)+VSQ*PZ2(II,JJ)
      AV(5,NB)=AV(5,NB)+VSQ*P1(II,JJ)
      AV(6,NB)=AV(6,NB)+VSQ*P2(II,JJ)
      AV(7,NB)=AV(7,NB)+VSQ*P3(II,JJ)
      AV(8,NB)=AV(8,NB)+VSQ*P4(II,JJ)
  150 CONTINUE
```

```
      IF(JEO.GT.2)GO TO 155
      NP=LSZ+1
      AV(14,1)=AV(14,1)+2.*CONJG(SS(1,NN))*SS(NP,NN)*PBXY(1,NP)
  155 CONTINUE
      DO 160 M=1,N
      II=M
      JJ=M+N
      IF(JEO.GT.2)GO TO 158
      II=II+1
      JJ=JJ+1
  158 CONTINUE
      ICNT = II+1
      JCNT = JJ+1
      IF(M.EQ.N)GO TO 159
      AV(13,1)=AV(13,1)+2.*CONJG(SS(II,NN))*SS(JCNT,NN)*PBZ(II,JCNT)+2.*
     1CONJG(SS(JJ,NN))*SS(ICNT,NN)*PBZ(JJ,ICNT)
      AV(14,1)=AV(14,1)+2.*CONJG(SS(II,NN))*SS(JCNT,NN)*PBXY(II,JCNT)+
     1 2.*CONJG(SS(JJ,NN))*SS(ICNT,NN)*PBXY(JJ,ICNT)
  159 AV(13,1)=AV(13,1)+2.*CONJG(SS(II,NN))*SS(JJ,NN)*PBZ(II,JJ)
      AV(14,1)=AV(14,1)+2.*CONJG(SS(II,NN))*SS(JJ,NN)*PBXY(II,JJ)
  160 CONTINUE
  405 WRITE TAPE 51,JJG(IJ),KKU(IJ),LLU(IJ),JJG(IJ),KKG(IJ),LLG(IJ),
     1 OBS(IJ),ENGU,ENG(IJ),WHT(1,IJ), ((AV(II,JJ),II=1,12),JJ=1,2),
     2 AV(13,1),AV(14,1),IJ
  240 CONTINUE
  290 CONTINUE
  298 CONTINUE
      CALL REGRESS(NSUM)
      END
      SUBROUTINE JHERMX (A,NM,N,IOPT,RHO,IER,S)
      DIMENSION A(21,21), S(21,21)
      COMPLEX A, S, V1, V2, V3, CSNT, SNT, TEMP
      IOC = 0
      IER = 0
      EPI2 = 0.000000000001
      EN = FLOATF(N)
      DO 1 I=1,N
      DO 1 J=1,N
      S(I,J) = (0.0,0.0)
      IF(I.EQ.J)S(I,J) =(1.0,0.0)
    1 CONTINUE
      IF(N.LE.1)GO TO 12
      SOFFD = 0.0
      NM1 = N-1
      DO 2 I=1,NM1
      IJ = I+1
      DO 2 J=IJ,N
      X1=A(I,J)
      X2=A(I,J)*(0.0,-1.0)
    2 SOFFD = SOFFD + 2.0*(X1*X1+X2*X2)
      IF(SOFFD .LT. 0.1E-10)GO TO 12
      THR = SQRTF(SOFFD)
      FTHR = (RHO/EN)*THR
      IND = 0
```

```
  3 THR = THR / EN
  4 DO 10 L=2,N
    LM1 = L-1
    DO 10 K=1,LM1
    X1=A(L,K)
    X2=A(L,K)*(0.0, 1.0)
    IF(SQRT(X1*X1 + X2*X2) ,LT, THR) GO TO 10
    IND = 1
    V1 = A(K,K)
    V2 = CONJG( A(L,K) )
    V3 = A(L,L)
    C = -AIMAG( A(L,K) )
    B = REAL( A(L,K) )
    E = REAL( A(L,L) )
    D = REAL( A(K,K) )
    THET = 0.0
    IF(ABSF(C),LT, EPI2)GO TO 13
    THET = 1.5707963
    IF(ABSF(B),LT, EPI2)GO TO 13
    T = C / B
    THET = ATANF(T)
 13 CONTINUE
    PHI = 0.78539818
    ED = ABSF(E-D)
    IF(ED ,LT, EPI2)GO TO 15
    TAO = 2.0*(B*COSF(THET) + C*SINF(THET)) / (E-D)
    PHI = 0.5 * ATANF(TAO)
 15 CONTINUE
    CSNT =COSF(PHI) + (0.0,0.0)
    CS = COSF(THET) * SINF(PHI)
    SS = SINF(THET) * SINF(PHI)
    SNT = CS + (0.0,1.0) * SS
    DO 8 I=1,N
    TEMP = A(I,K)*CSNT - A(I,L)*CONJG(SNT)
    A(I,L) = A(I,K)*SNT + A(I,L)*CSNT
    A(I,K) = TEMP
    IF(IOPT ,EQ, 0)GO TO 8
    TEMP = S(I,K)*CSNT - S(I,L)*CONJG(SNT)
    S(I,L) = S(I,K)*SNT + S(I,L)*CSNT
    S(I,K) = TEMP
  8 CONTINUE
    DO 9 I=1,N
    A(K,I) = CONJG( A(I,K) )
    A(L,I) = CONJG( A(I,L) )
  9 CONTINUE
    A(K,K) = SNT*CONJG(SNT)*V3 + CSNT*CSNT*V1-SNT*CSNT*CONJG(V2)
   1 -CSNT*CONJG(SNT)*V2
    A(L,L) = CSNT*CSNT*V3 + CONJG(SNT)*SNT*V1 + SNT*CSNT*
   2 CONJG(V2) + CONJG(SNT)*CSNT*V2
    A(K,L) = CSNT*CSNT*V2 - SNT*SNT*CONJG(V2) + CSNT*SNT*V1
   1  -CSNT*SNT*V3
    A(L,K) = CONJG( A(K,L) )
 10 CONTINUE
    IOC = IOC + 1
```

```
      IF(ICC .GE. 100)GO TO 21
      IF(IND .LE. 0)GO TO 11
      IND = 0
      GO TO 4
   11 IF(THR-FTHR)12,12,3
   12 RETURN
   21 IER = 1
      RETURN
      END
      SUBROUTINE REGRESS(NODATA)
      DIMENSION DATA(35), VECTOR(36,36),AVE(35),AV(26),
     1SIGMA(35),COEN(35),SIGMCO(35),INDEX(35),CONST(35),NK(35),WT(  800)
     2  ,JJU(800),KKU(800),LLU(800), JJG(800), KKG(800),LLG(800),
     3 OBS(800),ENG(800),DV(800),WHT(2,800)
      COMMON JJU,KKU,LLU,JJG,KKG,LLG,OBS,ENG,WHT
      TYPE DOUBLE VECTOR, AVE, SIGMA, COEN, SIGMCO, SIGY
      TOL=.001  $ EPIN=EPOUT=.000000001
      IFWT=IFSTEP=IFAVE=IFCOEN=IFPRED=IFREV=0
      IFSTEP=1
  100 READ 33, (NK(I), I=1,33),XDEVMAX,LNOUT,BDLN,LAST
   33 FORMAT(33I2, F5.1, I2, F5.1, I2)
      XDEVMAX=XDEVMAX*XDEVMAX
      NOPROB=INVAR=IFRAW=IFRESD=IFCNST=1
      OBSNO=SUMWHT=0.
      LNCNT = 0
      IF(BDLN)36,34
   34 BDLN = 10.
   36 CONTINUE
      DO 38 I=1,33  $ IF(NK(I))37,38
   37 INVAR=INVAR+1
   38 CONTINUE
      REWIND 50
      REWIND 51
C     IFWT = 1,THEN ALL WHTS = 1.0
C     IFSTEP = 1, DO NOT PRINT EACH STEP
C     IFRAW  = 1   DO NOT PRINT RAW SUMS AND SQUARES
C     IFAVE  = 1   DO NOT PRINT AVERAGES
C     IFRESD = 1   DO NOT PRINT RESIDUAL SUMS SQUARES
C     IFCOEN = 1   DO NOT PRINT PARTIAL COEFFICIENTS
C     IFPRED = 1   DO NOT CALC PREDICTED VALUES
C     IFCNST = 1   DO NOT HAVE CONST TERM IN EQUATION
      NOVAR = INVAR
      NVP1 = NOVAR + 1
  495 CONTINUE
      LNCNT = LNCNT+1
      NOIN = 0
      VAR = 0.0
      K    = 0
      FLEVEL = 0.0
      NOENT = 0
      NOMIN = 0
      NOMAX = 0
  110 DO 120 I = 1, NVP1
  130 DO 120 J = 1, NVP1
```

```
  120 VECTOR(I,J) = 0.0
      IF(LNCNT.GT.1)GO TO 506
  519 DO 235M=1,NODATA
      READ TAPE 51,J1,LL1,KK1,JJ,LL,KK,OBSFREQ,ENG1,EG,WT(   M),
     1 (AV(II),II=1,26),IJ
      FREQ=ENG1-EG
      ENG(IJ)=FREQ
      DATA(NOVAR)= OBSFREQ-FREQ
      IF(WT(   M))206,206,204
  204 IF(ABSF(OBSFREQ-FREQ)-BDLN)264,264,205
  205 PRINT 218,J1,LL1,KK1,JJ,LL,KK,OBSFREQ,FREQ,IJ
  218 FORMAT(     *THE WEIGHT OF THIS LINE IS BEING SET EQUAL TO ZERO*//
     1 2(2X,3I3),     2F11.5,I11)
      WHT(1,IJ)=0.
      WT(M)=0.
      GO TO 206
  264 SUMWHT=SUMWHT+WT(   M)
      OBSNO=OBSNO+1.
  206 NUM=0
      DO 220 I=1,26
      IF(NK(I))220,220,210
  210 NUM=NUM+1
      DATA(NUM)=AV(I)
  220 CONTINUE
  230 WRITE TAPE50,J1,LL1,KK1,JJ,LL,KK,OBSFREQ,FREQ,
     1 (DATA(L), L=1,NOVAR), M,IJ
  235 CONTINUE
  506 CONTINUE
      REWIND 50
      AVEWHT=SUMWHT/OBSNO
      DO 511 N=1,NODATA
      READ TAPE50,J1,LL1,KK1,J,LL,KK,OBSFREQ,FREQ,    (DATA(L),L=1,NOVAR
     1 ),NRUN
      WGT=WT(   N)/AVEWHT
      IF(WGT)530,511
  530 DO 540 I = 1, NOVAR
  550 VECTOR (I,NOVAR + 1) = VECTOR (I, NOVAR + 1) + DATA (I) * WGT
  560 DO 540 J = I, NOVAR
  540 VECTOR (I, J) = VECTOR (I, J) + DATA (I) * DATA (J) * WGT
  510 VECTOR (NVP1, NVP1)           = VECTOR (NVP1, NVP1)           +WGT
  511 CONTINUE
C     COMPLETED SUMS OF SQUARES AND CROSS PRODUCTS,  THESE ARE IN
C    1STORAGE IN LOCATION, VECTOR (I, J),  THESE WILL BE PRINTED OUT ON
C    2TAPE 6 UNDER CONTROL OF STATEMENT 100
  565 NOVMI = NOVAR + 1
  566 NOVPL = NOVAR + 1
  568 PRINT 90, NOPROB, NODATA,NOVAR, VECTOR(NOVPL,NOVPL), EPIN, EPOUT
  570 IF (IPRAW) 900, 580, 650
  580 WRITE OUTPUT TAPE61, 15
  590 WRITE OUTPUT TAPE61, 20,(I,VECTOR(I,NOVPL),I=1,NOVMI)
  600 WRITE OUTPUT TAPE61,25, VECTOR(NOVAR,NOVPL)
  610 WRITE OUTPUT TAPE61, 30
  620 WRITE OUTPUT TAPE61, 35, ((I,J,VECTOR(I,J),J=1,NOVMI),I=1,NOVMI)
  630 WRITE OUTPUT TAPE61, 40, (I,VECTOR(I,NOVAR),I=1,NOVMI)
```

```
  640 WRITE OUTPUT TAPE61, 45, VECTOR(NOVAR,NOVAR)
      GO TO 650
C     CALCULATION OF RESIDUAL SUMS OF SQUARES AND CROSS PRODUCTS
  650 IF(IFCNST) 900,651,735
  651 IF(VECTOR(NOVPL,NOVPL)) 652,652,655
  652 PRINT 654
      GO TO 910
  655 DO 660 I = 1, NOVAR
  670 DO 660 J = I, NOVAR
  660 VECTOR (I,J) = VECTOR (I,J) - (VECTOR(I,NOVPL) * VECTOR (J,NOVPL)
     - / VECTOR (NOVPL, NOVPL))
  680 DO 690  I = 1, NOVAR
  690 AVE(I)  = VECTOR(I,NOVPL) / VECTOR(NOVPL,NOVPL)
  700 IF (IFAVE)   900, 710, 735
  710 WRITE OUTPUT TAPE61, 50
  720 WRITE OUTPUT TAPE61, 20, (I,AVE(I),I=1,NOVMI)
  730 WRITE OUTPUT TAPE61, 25, AVE(NOVAR)
  735 IF (IFRESD)  900, 740, 780
  740 WRITE OUTPUT TAPE61, 55
  750 WRITE OUTPUT TAPE61, 35,((I,J,VECTOR(I,J),J=1,NOVMI),I=1,NOVMI)
  760 WRITE OUTPUT TAPE61, 40, (I,VECTOR(I,NOVAR),I=1,NOVMI)
  770 WRITE OUTPUT TAPE61, 45, VECTOR(NOVAR,NOVAR)
  780 NOSTEP = -1
  781 ASSIGN  1320  TO NUMBER
  782 DEFR   = VECTOR(NOVPL,NOVPL) - 1.0
  790 DO 800  I = 1,NOVAR
  791 IF(VECTOR(I,I)) 792,794,810
  792 PRINT  793, I
      GO TO 910
  793 FORMAT (31H ERROR RESIDUAL SQUARE VARIABLE I4,31H IS NEGATIVE,PROB
     1LEM TERMINATED )
  794 WRITE OUTPUT TAPE61, 795, I
  796 SIGMA(I) =     1.0
  797 GO TO 800
  795 FORMAT (1H010H VARIABLE I5,13H IS CONSTANT )
  810 SIGMA(I) =DSQRT  (VECTOR (I,I))
  800 VECTOR(I,I) = 1.0
  820 DO 830  I = 1,NOVMI
  840 IP1 = I + 1
  841 DO 830 J = IP1, NOVAR
  850 VECTOR(I,J) = VECTOR(I,J) /( SIGMA(I)* SIGMA(J))
  830 VECTOR(J,I) = VECTOR(I,J)
  860 IF (IFCOEN)  900, 870, 1000
  870 WRITE OUTPUT TAPE61, 60
  874 NOVM2  = NOVMI  - 1
  875 DO 885  I = 1, NOVM2
  880 IP1 =  I + 1
  885 WRITE OUTPUT TAPE61, 35,(I,J,VECTOR(I,J),J=IP1,NOVMI)
  890 WRITE OUTPUT TAPE61, 40,(I,VECTOR(I,NOVAR),I=1,NOVMI)
 1000 NOSTEP = NOSTEP + 1
 1001 IF (VECTOR( NOVAR,NOVAR)) 1002,1002,1010
 1002 NSTPM1 = NOSTEP - 1
      PRINT 1004, NSTPM1
      GO TO 1381
```

```
1010 SIGY =  SIGMA(NOVAR) *DSQRT  (VECTOR(NOVAR,NOVAR)/ DEFR)
1015 DEFR =DEFR-1.0
1016 IF (DEFR )  1017,1017, 1020
1017 PRINT  1019 ,NOSTEP
     GO TO 1381
1020 VMIN = 0.0
1030 VMAX = 0.0
1035 NOIN = 0
1040 DO 1050  I = 1,NOVMI
1041 IF (VECTOR(I,I)) 1042, 1050, 1060
1042 PRINT 1044, I, NOSTEP
1045 GO TO 1381
1060 IF(VECTOR(I,I)-TOL) 1050, 1080, 1080
1080 VAR=VECTOR(I,NOVAR)*VECTOR(NOVAR,I)/VECTOR(I,I)
1090 IF(VAR)1100, 1050, 1110
1100 NOIN = NOIN + 1
1120 INDEX(NOIN) = I
1130 COEN(NOIN)  = VECTOR(I,NOVAR) * SIGMA(NOVAR) / SIGMA (I)
1140 SIGMCO(NOIN) = (SIGY / SIGMA(I)) *DSQRT (VECTOR(I,I))
1150 IF (VMIN) 1160,1170,904
 904 WRITE OUTPUT TAPE61, 906
     GO TO 910
1170 VMIN = VAR
1180 NOMIN = I
1190 GO TO 1050
1160 IF(VAR - VMIN)1050,1050,1170
1110 IF (VAR - VMAX)1050,1050,1210
1210 VMAX = VAR
1220 NOMAX = I
1050 CONTINUE
1230 IF (NOIN) 903,1240,1245
 903 WRITE OUTPUT TAPE61, 907
     GO TO  910
1240 WRITE OUTPUT TAPE61, 65,SIGY
1260 GO TO 1350
1245 IF (IFCNST) 900,1250,1246
1246 CNST = 0.0
1247 GO TO 1300
1250 CNST = AVE(NOVAR)
1270 DO 1280 I = 1,NOIN
1290 J = INDEX(I)
1260 CNST = CNST - (COEN(I) * AVE(J))
1300 IF(IFSTEP) 900,1310,1320
1310 IF (NOENT) 1311,1311,1313
1311 WRITE OUTPUT TAPE61, 91,NOSTEP,K
1312 GO TO 1314
1313 WRITE OUTPUT TAPE61, 92,NOSTEP,K
1314 WRITE OUTPUT TAPE61, 70,FLEVEL,SIGY,CNST,
    1(INDEX(J),COEN(J),SIGMCO(J),J=1,NOIN)
1315 GO TO NUMBER, (1320,1580)
1320 FLEVEL = VMIN + DEFR / VECTOR (NOVAR,NOVAR)
1330 IF(EFOUT + FLEVEL) 1350, 1350, 1340
1340 K =  NOMIN
1345 NOENT = 0
```

```
      GO  TO  1391
1350  FLEVEL = VMAX * DEFR / (VECTOR(NOVAR,NOVAR)*  VMAX)
1360  IF (EFIN - FLEVEL) 1370,1361,1380
1361  IF (EFIN) 1380,1380,1370
1370  K=NOMAX
1390  NOENT =  K
1391  IF(K) 1392,1392,1400
1392  WRITE OUTPUT TAPE61,1395,NOSTEP
1394  GO TO 910
1400  DO 1410   I = 1,NOVAR
1420  IF (I-K) 1430,1410,1430
1430  DO 1440   J = 1, NOVAR
1450  IF (J-K) 1460,1440,1460
1460  VECTOR(I,J) = VECTOR(I,J) - (VECTOR(I,K) * VECTOR (K,J) / VECTOR
     -(K,K))
1440  CONTINUE
1410  CONTINUE
1470  DO 1480  I = 1, NOVAR
1490  IF (I-K) 1500,1480,1500
1500  VECTOR (I,K)  =  -  VECTOR (I,K) / VECTOR (K,K)
1480  CONTINUE
1510  DO 1520 J = 1, NOVAR
1530  IF (J-K) 1540,1520,1540
1540  VECTOR(K,J) =   VECTOR (K,J) / VECTOR (K,K)
1520  CONTINUE
1550  VECTOR(K,K) =  1.0 / VECTOR(K,K)
1560  GO TO 1000
1380  PRINT 75, NOSTEP
1381  IF (IFSTEP) 900, 1580,1570
1570  ASSIGN  1580  TO NUMBER
1571  GO TO  1310
1580  WRITE OUTPUT TAPE61, 1586,(L,VECTOR(L,L),L=1,NOVMI)
1581  IF( IFPRED)  900,1582,910
1582  REWIND 50
      PRINT 930,(NK(I),I=1,26)
 930  FORMAT(*-THE FOLLOWING CONSTANTS WERE VARIED*//* UPPER STATE*//
     1* BAND NO. 1*/  * VO   A   B   C   TAAAA   TBBBB   TAABB   TABAB
     2 HJ   HJK   HKJ   HK  */I3,3I4,4(3X,I3,2X),2I5,2I6/*-BAND NO. 2*/
     3* VO   A   B   C   TAAAA   TBBBB   TAABB   TABAB   HJ   HJK   HKJ
     4  HK */I3,3I4,4(3X,I3,2X),2I5,2I6/*-PERTURBATION TERMS*/* GZ   GXY
     5*/I3,2X,I3)
1583  WRITE OUTPUT TAPE61, 85
1586  FORMAT (24H0      DIAGONAL  ELEMENTS //20H   VAR.NO.      VALUE//
     1(1H  I 7, F16.6))
      DEVMAX=0.
      SRFS2WT = 0.
1590  DO  1660   N = 1, NODATA
1600  READ TAPE 50,J1, LL1,KK1, J, LL, KK, OBSFREQ, FREQ,
     1 (DATA(L),L=1,NOVAR),NRUN,IJ
1610  YPRED = CNST
1620  DO 1630  I = 1,NCIN
1640  K = INDEX(I)
1630  YPRED=  YPRED +  COEN(I) * DATA(K)
1650  DEV  =  DATA(NOVAR) -  YPRED
```

```
      DV(IJ)=DEV
   81 FORMAT(2(2X,3I3), 3F10.3,2F11.3,F9.2,I10)
      SRES2WT = SRES2WT+ DEV**2*WT(  N)
      DEV=WT(  N)*DEV*DEV
      IF(DEVMAX-DEV)912,912,1660
  912 DEVMAX=DEV
      NRUNX=NRUN
      IJM=IJ
 1660 CONTINUE
      DO 1664 N=1,NODATA
      FREQPRD=OBS(N)-DV(N)
      DIFF=OBS(N)-ENG(N)
 1664 PRINT 81,JJU(N),KKU(N),LLU(N),JJG(N),KKG(N),LLG(N),FREQPRD,
     1  OBS(N),ENG(N),DIFF,DV(N),WHT(1,N),N
C          STANDARD DEVIATION FROM RESIDUALS
      S2=OBSNO*SRES2WT/((OBSNO-NOIN)*SUMWHT)
 1770 PRINT 1775, S2
 1775 FORMAT (//24H SUM SQ. OF RESIDUALS = , F14.8)
 1780 STDDEV = SQRTF(S2)
 1785 PRINT 1790, STDDEV
 1790 FORMAT (39H STD. DEV. CALCULATED FROM RESIDUALS = , F10.8)
      IF(LNCNT-LNOUT)1665, 910, 910
 1665 IF(DEVMAX-XDEVMAX)910,910,913
  913 PRINT 918,IJM
  918 FORMAT(///////* THE WEIGHT OF LINE NO.  *I3* IS BEING SET EQUAL TO
     1ZERO*)
      OBSNO=OBSNO-1,
      SUMWHT=SUMWHT-WT(  NRUNX)
      WT(  NRUNX)=0,
      WHT(1,IJM)=0.
      GO TO 495
  910 IF(LAST)911,911,960
  960 DO 961 N=1,NODATA
  961 WHT(1,N)=WHT(2,N)
      GO TO 100
  900 PRINT 905
  911 CONTINUE
      PRINT 3
    3 FORMAT(1H1)
C     END...
    5 FORMAT (3F10.5,3I5,1H 9I2,5X,F6.4)
   10 FORMAT (6(F12.5))
   15 FORMAT (1H 49H                                          SUM  OF  VARIABLES//)
   20 FORMAT (1H 11H      SUM X( I2,3H) = F12.4,8H  SUM X( I2,3H) =F12.4,
     1 8H  SUM X( I2,3H) =F12.4,8H  SUM X(I2,3H) =F12.4 )
   25 FORMAT (17H       SUM    Y   =F12.4)
   30 FORMAT(1H0 70H                                    RAW  SUM  OF  SQUARES  A
     1ND  CROSS PRODUCTS// )
   35 FORMAT (1H 7H      X(I2,7H) VS X(I2,3H) = F15.6,
     1         6H     X(I2,7H) VS X(I2,3H) = F15.6,
     2         6H     X(I2,7H) VS X(I2,3H) = F15.6  )
   40 FORMAT (1H 7H      X(I2,12H) VS    Y   =F15.6,
     1         6H     X(I2,12H) VS    Y   =F15.6,
     2         6H     X(I2,12H) VS    Y   =F15.6  )
```

```
   45 FORMAT (1H 21H      Y      VS    Y    =F15,6)
   50 FORMAT (1H063H                                          AVERAGE  VALUE  OF
     -  VARIABLES// )
   55 FORMAT(1H077H                                      RESIDUAL  SUMS  OF  SQUA
     -RES  AND  CROSS PRODUCTS//)
   60 FORMAT(1H069H                                          PARTIAL  CORRELATI
     -ON  COEFFICIENTS//)
   65 FORMAT (25H0  STANDARD ERROR OF Y = F12,6 )
   70 FORMAT (11H   F LEVEL  F12,4/25H   STANDARD ERROR OF Y = F12,4/12H
     1   CONSTANT F13,5/56H                VARIABLE   COEFFICIENT   STD ERR
     2OR OF COEF //  (16H               X=I3,F18,11,F15,11))
   75 FORMAT (10H COMPLETED I5,20H STEPS OF REGRESSION)
   80 FORMAT (8H        F6,0,2H  F12,5,3H   F12,5,2H  F12,5)
   85 FORMAT(//4x* UPPER      GROUND   PREDICTED      OBS      CALC       O
     1BS-CALC     DEV          WHT*//)
   90 FORMAT (22H1STEPWISE  REGRESSION //12H PROBLEM NO I10 //13H NO OF
     1DATA = I5 //16H NO OF VARIABLES = I10 //30H WEIGHTED DEGREES OF FR
     2EEDOM = F12,2 //28H F LEVEL TO ENTER VARIABLE = F12,9 //29H F LEVE
     3L TO REMOVE VARIABLE = F13,9 /// )
   91 FORMAT (9H0STEP NO,I5 /19H   VARIABLE REMOVED I8)
   92 FORMAT (9H0STEP NO,I5 /20H   VARIABLE ENTERING I8)
   93 FORMAT (5H RUN  F6,0,3H   F10,5,3H   F10,5,3H   F10,5,3H   F10,5,
     13H   F10,5/(14H              F10,5,3H   F10,5,3H   F10,5,3H   F10,
     25,3H   F10,5))
  654 FORMAT (31H  ZERO NUMBER OF DATA, SO LONG.)
  905 FORMAT (42H ERROR IN CONTROL CARD, PROBLEM TERMINATED)
  906 FORMAT (25H ERROR, VMIN PLUS. SOLONG)
  907 FORMAT (26H  ERROR,NOIN MINUS, SOLONG )
 1004 FORMAT (1H037HY SQUARE NON-POSITIVE,TERMINATE STEP  I 5)
 1019 FORMAT (1H029H NO MORE DEGREES FREEDOM STEP I 5 )
 1044 FORMAT (1H010H SQUARE X=I5,17H NEGATIVE, SOLONG I5,6H STEPS)
 1395 FORMAT (12H  K=0, STEP I6, 7H SOLONG)
      END
RUN, 5, 2100
```