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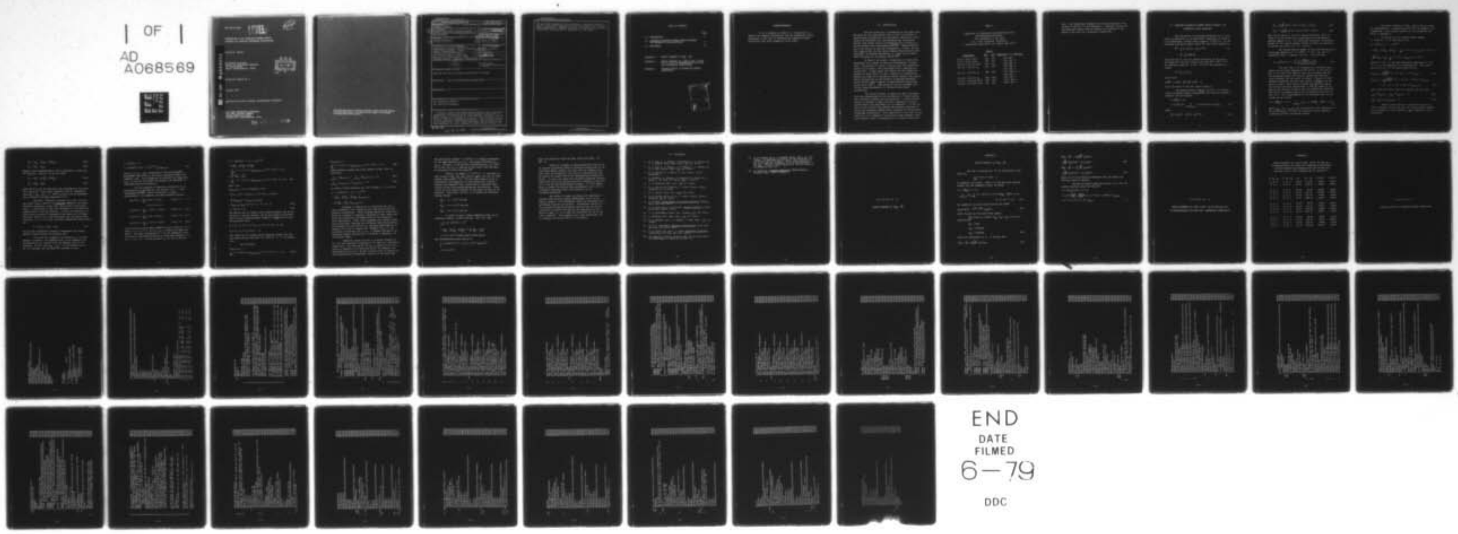

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COMPUTATION OF H_2O QUADRUPOLE MOMENT MATRIX ELEMENTS FOR PRESSURE BROADENING CALCULATIONS

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Recent tunable laser measurements indicate that theoretical linewidths, calculated for H_2O self-broadened transitions and based solely on the effects of dipole-dipole collisions, are too small at high and intermediate J values. This suggests neglect of other important scattering mechanisms, such as dipole-quadrupole interactions. This report discusses computational procedures necessary to obtain quadrupole moment matrix elements for

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H_2O and other asymmetric rotor molecules. Computer programs to obtain these matrix elements have been constructed and are presently operational. Numerical results for some low J quadrupole transitions are presented in Appendix B of the report.

TABLE OF CONTENTS

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1.0 INTRODUCTION

The work which will be presented in this report was motivated by our observations that, if only the effects of dipole-dipole interactions are considered, theoretical calculations of halfwidths for self-broadened H_2O transitions exhibit some rather serious discrepancies with recently reported tunable laser measurements.[1,2,3,4] These discrepancies occur mainly at high and intermediate J values, and obtain using either the well-known Anderson-Tsao-Curnutte (ATC) theory[5,6] of pressure broadening, or a more recent method (QFT) developed by the present author.[7,8]

In Table I we present a comparison of theory with experiment for a number of high and intermediate J transitions. The results in Table I indicate that the theoretical widths are too small, with percentage errors sometimes exceeding 50%. In most cases the results are only weakly dependent on which theory is used. However, all theoretical numbers are based on a calculation which includes only dipole-dipole interactions as the dominant scattering mechanism. These results suggest neglect of some important scattering mechanism at high J. Some possibilities are exchange scattering, dipole-quadrupole, or dipole-induced-dipole interactions.

Our initial efforts to remove the above discrepancies have concentrated on the contribution of dipole-quadrupole collisions between the H_2O molecules. A future journal article is planned in which detailed comparison of the expanded theory with experiment will be presented. In this report we will outline the computational methods necessary to obtain H_2O quadrupole moment matrix elements for the pressure-broadening calculations. This computation is far from trivial since H_2O is an asymmetric top molecule whose permanent quadrupole moment cannot be represented by a single scalar quan-

TABLE I

Comparison of Theoretical and Experimental H_2O
Self-Broadened Halfwidths
(All halfwidths in cm^{-1}/atm;
rot = pure rotational transition;
† measurement near 382°K, all others near 297°K)

Transition	Theory ATC	Theory QFT	Experiment and Reference
8,1,8 → 9,4,5 (rot)	.409	.402	.559, Ref. 3
8,3,6 → 9,6,3 (rot)	.343	.377	.611, Ref. 3
11,1,10 → 12,4,9 (rot)	.261	.257	.319, Ref. 3
12,2,11 → 13,1,12 ν_2	.160	.140	.228, Ref. 2
			.170, Ref. 4
15,1,15 → 16,0,16 ν_2	.098	.083	.177, Refs. 1, 2
			.166, Ref. 4
15,2,14 → 16,1,15 ν_2	.084	.085	.203, Ref. 2
17,0,17 → 18,3,16 (rot)	.085	.078	.125†, Ref. 3
19,0,19 → 20,3,18 (rot)	.063	.063	.089†, Ref. 3

tity. The theoretical framework for the calculations is developed in Section 2.0 and Appendix A. Numerical results for H_2O quadrupole moment matrix elements are presented in Appendix B for some low J quadrupole transitions.

2.0 PERMANENT QUADRUPOLE MOMENT MATRIX ELEMENTS FOR ASYMMETRIC ROTOR MOLECULES

The calculation of pressure broadening due to quadrupole interactions can be expressed[7] completely in terms of an m-independent, reduced matrix element, $\langle J||Q^t||J'\rangle$, of the traceless quadrupole moment tensor $\overleftrightarrow{Q}^t$, the latter defined as

$$\overleftrightarrow{Q}^t = \sum_i e_i \, [\vec{r}_i \, \vec{r}_i - \frac{1}{3} r_i^2 \, \overleftrightarrow{I}], \tag{1}$$

$$= \overleftrightarrow{Q} - \frac{1}{3} \mathrm{Tr}(\overleftrightarrow{Q}) \, \overleftrightarrow{I}, \tag{2}$$

where the sum is over all charged particles in the molecule, and where $\overleftrightarrow{I}$ is the unit tensor, such that $\overleftrightarrow{I} \cdot \vec{A} = \vec{A} \cdot \overleftrightarrow{I} = \vec{A}$ for an arbitrary vector $\vec{A}$. In Eq. (2), $\overleftrightarrow{Q}$ is the quadrupole moment tensor

$$\overleftrightarrow{Q} = \sum_i e_i \, \vec{r}_i \, \vec{r}_i, \tag{3}$$

and we note

$$\mathrm{Tr}(\overleftrightarrow{Q}^t) = \mathrm{Tr}(\overleftrightarrow{Q}) - \frac{1}{3} \mathrm{Tr}(\overleftrightarrow{Q}) \, \mathrm{Tr}(\overleftrightarrow{I}) = 0, \tag{4}$$

since the trace of the unit tensor equals 3.

The reduced matrix element $\langle J||Q^t||J'\rangle$ is defined using the Wigner-Eckhart theorem[9,10] for traceless symmetric tensors, via the equation

$$\langle J \; m|\overleftrightarrow{Q}^t|J' \; m'\rangle$$

$$= \langle J||Q^t||J'\rangle \sum_{M=0,\pm1,\pm2} (J'2{-}m'{-}M|J'2 \; J{-}m) \, \overleftrightarrow{T}_M, \tag{5}$$

where

$$\overleftrightarrow{T}_0 = \frac{2}{3} [\hat{Z} \, \hat{Z} - \frac{1}{2} \hat{X} \, \hat{X} - \frac{1}{2} \hat{Y} \, \hat{Y}], \tag{5a}$$

$$\vec{T}_{\pm 2} = \frac{1}{2}\sqrt{\frac{2}{3}}\,[(\hat{X}\,\hat{X} - \hat{Y}\,\hat{Y}) \mp i(\hat{X}\,\hat{Y} + \hat{Y}\,\hat{X})], \tag{5b}$$

$$\vec{T}_{\pm 1} = \mp\frac{1}{2}\sqrt{\frac{2}{3}}\,[(\hat{Z}\,\hat{X} + \hat{X}\,\hat{Z}) \mp i(\hat{Z}\,\hat{Y} + \hat{Y}\,\hat{Z})]. \tag{5c}$$

Here (X,Y,Z) refer to a set of spaced-fixed axes, and Z is taken to be the direction of quantization for the magnetic quantum numbers m, m'. For non-linear molecules $|J\rangle$ actually stands for all quantum numbers (except m) which are necessary to specify the state, i.e. $|J\rangle = |J\tau\cdots\rangle$.

The reduced matrix element is then obtained by calculating <u>any</u> component of $\langle J\ \tau\ m|\vec{Q}^t|J'\ \tau'\ m'\rangle$, e.g. the $\hat{Z}\,\hat{Z}$ component, which is diagonal in m, m'. Thus, we have

$$\langle J\ \tau||Q^t||J'\ \tau'\rangle = \frac{3}{2}\,\frac{\langle J\ \tau\ m|\vec{Q}^t_{ZZ}|J'\ \tau'\ m\rangle}{(J'2{-}m\ 0|J'2\ J{-}m)}\,. \tag{6}$$

The next step is to transform to a principal axis system (x,y,z) which diagonalizes $\vec{Q}^t$ and $\vec{Q}$. In the case of H_2O, it is clear from symmetry that the principal axes for the quadrupole moment and inertial tensors are identical except possibly for the choice of origin. However, in most pressure-broadening theories this choice is <u>fixed</u> to be the center of mass. This results because one typically writes the various multipole interactions as $V(\vec{R}_i - \vec{R}_j)$ where $\vec{R}_i$, $\vec{R}_j$ specify the centers of mass of the two interacting molecules. This point is somewhat subtle and is discussed more fully in Ref. (17). The transformation to the principal axis (x,y,z) system can be written

$$\langle J\ \tau\ m|\vec{Q}^t_{ZZ}|J'\ \tau'\ m\rangle = \sum_{\alpha=x,y,z} Q_{\alpha\alpha}\,\langle J\ \tau\ m|[\Phi^2_{Z\alpha} - \tfrac{1}{3}]|J'\ \tau'\ m\rangle, \tag{7}$$

where $Q_{\alpha\alpha} = \sum_i e_i\, r_{i\alpha}\, r_{i\alpha}$ are the principal axis components of $\vec{Q}$, and where $\Phi_{Z\alpha} = \hat{Z}\cdot\hat{\alpha}$ are the direction cosine operators connecting the two coordinate systems.

The matrix elements of $[\Phi^2_{Z\alpha} - \frac{1}{3}]$ can be evaluated by transforming to a representation $|J\ K\ m\rangle$ of symmetric top eigenstates. Some further details of this evaluation are given in Appendix A.

The result for the reduced matrix element $\langle J\ \tau || Q^t || J'\ \tau' \rangle$ is then found to be

$$\langle J\ \tau || Q^t || J'\ \tau' \rangle = (-1)^{J+J'}$$

$$\cdot \{ (Q_{zz} - \frac{1}{2} Q_{xx} - \frac{1}{2} Q_{yy}) \cdot \sum_{KK'} \langle J\ \tau | J\ K \rangle A_{JK;J'K'} \langle J'\ K' | J'\ \tau' \rangle$$

$$- \sqrt{\frac{3}{4}} (Q_{xx} - Q_{yy}) \sum_{KK'} \langle J\ \tau | J\ K \rangle B_{JK;J'K'} \langle J'\ K' | J'\ \tau$$

where $\langle J'\ K' | J'\ \tau' \rangle$ are the eigenvector components of state $|J'\ \tau'\rangle$ in the symmetric top representation. The A and B matrices in Eq. (7) are given explicitly by

$$A_{JK;J'K'} = \sqrt{\frac{2J'+1}{2J+1}} (J'\ 2\ K'\ 0 | J'\ 2\ J\ K')\ \delta_{K,K'}, \qquad (9a)$$

$$B_{JK;J'K'} = \frac{1}{\sqrt{2}} \sqrt{\frac{2J'+1}{2J+1}} \{ (J'\ 2\ K'\ 2 | J'\ 2\ J(K'+2))\ \delta_{K,K'+2}$$

$$+ (J'\ 2\ K' - 2 | J'\ 2\ J(K'-2))\ \delta_{K,K'-2} \}, \qquad (9b)$$

and it may be verified that A, B satisfy the sum rules

$$\sum_{J'K'} A^2{}_{JK;J'K'} = \sum_{J'K'} B^2{}_{JK;J'K'} = 1, \qquad (10a)$$

$$\sum_{J'K'} A_{JK;J'K'} B_{JK;J'K'} = 0. \qquad (10b)$$

Several points should be noted before going on. First, from Eq. (8) we note that the reduced matrix element for an asymmetric rotor depends on two independent scalar parameters

$$Q_1 = (Q_{zz} - \frac{1}{2} Q_{xx} - \frac{1}{2} Q_{yy}), \quad (11a)$$

$$Q_2 = (Q_{xx} - Q_{yy}). \quad (11b)$$

However, this parameterization can be expressed in other useful fashions. From Eq. (2) we note that

$$Q_1 = (Q^t_{zz} - \frac{1}{2} Q^t_{xx} - \frac{1}{2} Q^t_{yy}), \quad (12a)$$

$$Q_2 = (Q^t_{xx} - Q^t_{yy}), \quad (12b)$$

where the Q^t's are the principal axis components of the traceless tensor $\overleftrightarrow{Q}^t$. These three components are not independent since $Q^t_{xx} + Q^t_{yy} + Q^t_{zz} = 0$. Hence Q_1 and Q_2 can be parameterized in terms of any <u>two</u> components of Q^t.

Secondly, it should be pointed out in Eq. (8) that the labels (x,y,z) refer to an <u>arbitrary</u> symmetric top representation (arbitrary, except that (x,y,z) must be principal axes). In particular, z need not correspond to the (two-fold) symmetry axis of the H_2O molecule. In fact the numerical results which we present in Appendix B are based on a IR representation, where (z,x,y) are associated with the lowest-order constants, A > B > C, in the rotational-vibrational Hamiltonian via

$$H = B J_x^2 + C J_y^2 + A J_z^2. \quad (13)$$

For H_2O the intermediate constant B represents the inverse moment of inertia about the symmetry axis.

Of course for a symmetric top molecule, it is most natural to choose z, the symmetry axis of the symmetric top representation, to coincide with the symmetry axis of the molecule. In this case $(Q_{xx} - Q_{yy}) = 0$, the second term in Eq. (8) vanishes, and the equation collapses to give

$$\langle J\ \tau || Q^t || J'\ \tau' \rangle$$

$$= \langle J\ K || Q^t || J'\ K' \rangle = (-1)^{J'+J}\ Q_1\ A_{JK;J'K'}, \quad (14)$$

where $Q_1 = (Q_{zz} - Q_{xx})$ corresponds to the Buckingham[11/], Birnbaum[12/] definition of the scalar quadrupole moment for symmetric tops. This definition is one-half the value used, e.g., by Tsao and Curnutte[6/] and Benedict and Kaplan[13/] in discussing pressure-broadening.

For the purposes of numerical computation it is advantageous to transform Eq. (8) further using the Wang transformation[14,15/], which corresponds to forming combinations of the symmetric top wave functions according

$$|E_+(J\ K)\rangle = \frac{1}{\sqrt{2}}\{\ |J\ K\rangle + |J{-}K\rangle\} \qquad K \text{ even} > 0, \quad (15a)$$

$$= |J\ 0\rangle \ (K = 0)$$

$$|E_-(J\ K)\rangle = \frac{1}{\sqrt{2}}\{-\ |J\ K\rangle + |J{-}K\rangle\} \qquad K \text{ even} > 0, \quad (15b)$$

$$|O_+(J\ K)\rangle = \frac{1}{\sqrt{2}}\{\ |J\ K\rangle + |J{-}K\rangle\} \qquad K \text{ odd} > 0, \quad (15c)$$

$$|O_-(J\ K)\rangle = \frac{1}{\sqrt{2}}\{-\ |J\ K\rangle + |J{-}K\rangle\} \qquad K \text{ odd} > 0. \quad (15d)$$

Let us write the above Wang (symmetric top) states as $|J\ K\ \nu\rangle$ where ν = 1, 2, 3, 4 = E_+, E_-, O_+, O_- denotes the Wang symmetry. The exact eigenstates $|J\ \tau\rangle$ of the asymmetric rotor can also be classified according to their Wang symmetry, i.e. $|J\ \tau\rangle = |J\ \tau\ \nu\rangle$. In this notation Eq. (8) can be written

$$<J\ \tau\ \nu||Q^t||J'\ \tau'\ \nu'> = (-1)^{J'+J}$$

$$\cdot \{(Q^t_{zz} - \frac{1}{2} Q^t_{xx} - \frac{1}{2} Q^t_{yy})$$

$$\cdot \sum_{K,K'} <J\ \tau\ \nu|J\ K\ \nu>\ A_{JK\nu;J'K'\nu'}\ <J'\ K'\ \nu'|J'\ \tau'\ \nu'>$$

$$-\sqrt{\frac{3}{4}}\ (Q^t_{xx} - Q^t_{yy})$$

$$\cdot \sum_{KK'} <J\ \tau\ \nu|J\ K\ \nu>\ B_{JK\nu;J'K'\nu'}\ <J'\ K'\ \nu'|J'\ \tau'\ \nu'>\}. \quad (16)$$

Here, e.g.,

$$A_{JK4;J'K'4} = <0_-(J\ K)|A|0_-(J'\ K')>$$

$$= \frac{1}{2}\ (-\ <J\ K|\ +\ <J-K|)\ A\ (-\ |J'\ K'>\ +\ |J'-K'>)$$

$$= \frac{1}{2}\ \{A_{JK;J'K} + A_{J-K;J'-K}\}\ \delta_{K,K'}$$

$$= A_{JK;J'K}\ \delta_{K,K'}\ \text{for}\ \Delta J = J - J' = 0,\ \pm 2 \quad (17a)$$

$$= 0\ \text{for}\ \Delta J = \pm 1. \quad (17b)$$

The results for all other A and B matrix elements can be obtained in a similar fashion, and it may readily be verified that the non-vanishing matrix elements of <u>both</u> A and B obey the selection rules

$$E_+ \rightleftarrows E_+,\ E_- \rightleftarrows E_-,\ 0_+ \rightleftarrows 0_+,\ 0_- \rightleftarrows 0_-\ \text{for}\ \Delta J = 0,\ \pm 2,$$

$$E_+ \rightleftarrows E_-,\ 0_+ \rightleftarrows 0_-\ \text{for}\ \Delta J = \pm 1.$$

That there are no allowed matrix elements between even and odd states follows from Eqs. (9) since $\Delta K = K - K'$ is always even.

We now define

$$A_{J\tau\nu;J'\tau'\nu'} =$$

$$\sum_{KK'} <J\ \tau\ \nu|J\ K\ \nu>\ A_{JK\nu;J'K'\nu'}\ <J'\ K'\ \nu'|J'\ \tau'\ \nu'>, \quad (18a)$$

$B_{J\tau\nu;J'\tau'\nu'} =$

$$\sum_{KK'} \langle J\ \tau\ \nu | J\ K\ \nu\rangle\ B_{JK\nu;J'K'\nu'}\ \langle J'\ K'\ \nu' | J'\ \tau'\ \nu'\rangle. \qquad 18b)$$

These matrices satisfy sum rules similar to Eqs. (10), in particular

$$\sum_{J'\tau'\nu'} A^2_{J\tau\nu;J'\tau'\nu'} = \sum_{J'\tau'\nu'} B^2_{J\tau\nu;J'\tau'\nu'} = 1, \qquad (19a)$$

$$\sum_{J'\tau'\nu'} A_{J\tau\nu;J'\tau'\nu'}\ B_{J\tau\nu;J'\tau'\nu'} = 0. \qquad (19b)$$

In terms of these matrices, Eq. (16) assumes its final form

$$\langle J\ \tau\ \nu || Q^t || J'\ \tau'\ \nu'\rangle = (-1)^{J+J'}$$

$$\cdot \{(Q^t_{zz} - \tfrac{1}{2} Q^t_{xx} - \tfrac{1}{2} Q^t_{yy})\ A_{J\tau\nu;J'\tau'\nu'}$$

$$- \tfrac{3}{4} (Q^t_{xx} - Q^t_{yy})\ B_{J\tau\nu;J'\tau'\nu'}\}. \qquad (20)$$

Programs to compute the A, B matrices for H_2O and other asymmetric rotor molecules have been written and are presently operational. These programs operate as subroutines which are attached to programs, developed at AFGL, which generate the eigenvalues and eigenvectors of the asymmetric rotor Hamiltonian. These latter programs also include vibrational-rotational coupling via the Watson Hamiltonian method. The programs are quite efficient, requiring approximately 60 seconds of CP time to compute the strongest ($\Delta K_a = 0, \pm 2$) quadrupole transitions for $J \leq 22$. A program listing of our quadrupole moment subroutines is furnished in Appendix C of the present report.

Numerical results for the A, B matrix elements in Eq. (20) are presented in Appendix B for some low J quadrupole transitions. The labeling of the K_a, K_c states in the tabulation of Appendix B is consistent with a IR symmetric top representation for H_2O. We have verified that our methods do give representation-independent results, in the sense that the same matrix element $\langle J\ \tau||Q^t||J'\ \tau'\rangle$ always corresponds to the same energies $E_{J\tau}$, $E_{J'\tau'}$ and energy difference $E_{J\tau} - E_{J'\tau'}$. However, if one switches representations, e.g. from IR to IIR, the K_a, K_c labeling of the states also switches, as discussed in Allen and Cross.[16]

Finally, to compute $\langle J\ \tau||Q^t||J'\ \tau'\rangle$, one needs to know values of Q^t_{xx}, Q^t_{yy}, Q^t_{zz} (which, again, are not all independent since $Tr(Q^t) = 0$). For H_2O there appears to be no experimental determination of these quantities, however, Stogryn and Stogryn[17] have listed fairly consistent theoretical values from quantum mechanical calculations. Their values are also quoted relative to the center of mass of the molecule. From Table 3 of Ref. 17 we deduce the following average values:

$$Q^t_{xx} = .12 \times 10^{-26} \text{ esu-cm}^2$$

$$Q^t_{yy} = -.72 \times 10^{-26} \text{ esu-cm}^2$$

$$Q^t_{zz} = .60 \times 10^{-26} \text{ esu-cm}^2$$

In order to make a simple comparison with the N_2 quadrupole moment, we note from Eqs. (19), (20) that

$$\sum_{J'\tau'} |\langle J\ \tau||Q^t||J'\ \tau'\rangle|^2$$

$$= (Q^t_{zz} - \tfrac{1}{2} Q^t_{xx} - \tfrac{1}{2} Q^t_{yy})^2 + \tfrac{3}{4} (Q^t_{xx} - Q^t_{yy})^2$$

$$= 1.34 \times 10^{-52} \text{ (from values listed above).}$$

The corresponding result for N_2 is

$$\sum_{J'} |\langle J||Q^t||J'\rangle|^2 = (1.52 \times 10^{-26} \text{ esu-cm}^2)^2$$

$$= 2.31 \times 10^{-52},$$

where the numerical value has been taken from Table 1 of Ref. 17.

Since the strength of dipole-quadrupole scattering in pressure broadening theory is directly proportional to the quadrupole moment squared, we infer from the numbers given above that the strength of this type of scattering for H_2O-H_2O should be roughly 60% of the corresponding strength for H_2O-N_2. In turn, one knows from pressure broadening calculations that the H_2O-N_2 dipole-quadrupole strength is typically 20% of the H_2O-H_2O dipole-dipole strength. On this simple basis we expect the H_2O-H_2O dipole-quadrupole collisions to contribute something like a 10% correction to the broadened halfwidths.

The effect of these collisions will sometimes be enhanced when resonant energy denominators occur in the theory, however, this enhancement cannot be estimated without performing detailed calculations. Preliminary results from our pressure broadening programs indicate that the dipole-quadrupole collisions for H_2O-H_2O are negligible at low J, while at high J ($J \gtrsim 12$) they can contribute 10-15% of the total linewidth. This suggests that other mechanisms such as exchange scattering need to be considered.

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A P P E N D I X   A

MATRIX ELEMENTS OF $[\Phi_{z\alpha}^2 - \frac{1}{3}]$

APPENDIX A

Matrix Elements of $[\Phi^2_{Z\alpha} - \frac{1}{3}]$

We wish to evaluate Eq. (7) by introducing a complete set

$$\sum_{JKm} |J\ K\ m\rangle \langle J\ K\ m| = 1$$

of symmetric top states. Since J, m are also good quantum numbers for the asymmetric rotor, we obtain

$$\langle J\ \tau\ m|\hat{Q}^t_{ZZ}|J'\ \tau'\ m\rangle$$

$$= \sum_{\alpha=x,y,z} Q_{\alpha\alpha} \sum_{KK'} \langle J\ \tau\ m|J\ K\ m\rangle \langle J\ K\ m|[\Phi^2_{Z\alpha} - \tfrac{1}{3}]|J'\ K'\ m\rangle$$
$$\langle J'\ K'\ m|J'\ \tau'\ m\rangle. \quad \text{(A1)}$$

The symmetric top wave functions have the form[6]

$$\psi_{JKm}(\theta,\psi,\phi) = e^{im\phi}\, e^{iK\psi}\, f_{JKm}(\theta), \quad \text{(A2)}$$

where (θ,ψ,ϕ) are the three Euler angles.

The direction cosines $(\Phi_{Zx}, \Phi_{Zy}, \Phi_{Zz})$ can be expressed as[18]

$$\Phi_{Zz} = \cos\theta$$

$$\Phi_{Zx} = \sin\theta\sin\psi$$

$$\Phi_{Zy} = \sin\theta\cos\psi \quad , \quad \text{(A3)}$$

which are independent of ϕ. It follows that

$$[\Phi^2_{Zz} - \tfrac{1}{3}] = \tfrac{2}{3}\sqrt{\tfrac{4\pi}{5}}\, Y_{20}(\theta,\psi) \ , \quad \text{(A4)}$$

$$[\Phi_{Zx}^2 - \frac{1}{3}] = -\frac{1}{3}\sqrt{\frac{4\pi}{5}}\, Y_{20}(\theta,\psi)$$

$$-\sqrt{\frac{2\pi}{15}}\,(Y_{22}(\theta,\psi) + Y_{2-2}(\theta,\psi)) \;, \qquad (A5)$$

$$[\Phi_{Zy}^2 - \frac{1}{3}] = -\frac{1}{3}\sqrt{\frac{4\pi}{5}}\, Y_{20}(\theta,\psi)$$

$$+\sqrt{\frac{2\pi}{15}}\,(Y_{22}(\theta,\psi) + Y_{2-2}(\theta,\psi)) \;, \qquad (A6)$$

where the Y's are spherical harmonics with the Condon and Shortley choice of phases.

The matrix element which are needed in Eq. (A1) are readily obtained using the formula[6]

$$\langle J\ K\ m|Y_{jk}(\theta,\psi)|J'\ K'\ m'\rangle$$

$$= (-1)^k\sqrt{\frac{2j+1}{4\pi}}\sqrt{\frac{2J'+1}{2J+1}}\,(J'\ j\ K'\ k|J'\ j\ J(k+K'))\ \delta_{K,k+K'}$$

$$\cdot\ (J'\ j\ m'\ 0|J'\ j\ J\ m')\ \delta_{m,m'}\,. \qquad (A7)$$

APPENDIX B

MATRIX ELEMENTS OF A AND B (EQS. 18-20) FOR H_2O IN A IR REPRESENTATION FOR SOME LOW J QUADRUPOLE TRANSITIONS.

APPENDIX B

Matrix Elements of A and B (Eqs. 18-20) for H_2O in a IR Representation for Some Low J Quadrupole Transitions. (A and B elements are dimensionless and satisfy the sum rules in Eq. (19); energies are in units cm^{-1}.)

J, K_a, K_c	J', K'_a, K'_c	E_J	$E_J - E_{J'}$	<J|A|J'>	<J|B|J'>
0, 0, 0	2, 0, 2	00.00	- 70.09	.99040	.13822
0, 0, 0	2, 2, 0	00.00	-136.16	-.13822	.99040
1, 0, 1	1, 0, 1	23.79	00.00	-.63246	.00000
1, 0, 1	2, 2, 1	23.79	-111.11	.00000	-.81650
1, 0, 1	3, 0, 3	23.79	-112.97	.74391	.16089
1, 0, 1	3, 2, 1	23.79	-188.36	-.21586	.55448
1, 1, 0	1, 1, 0	42.37	00.00	.31623	-.54772
1, 1, 0	2, 1, 2	42.37	- 37.13	.70711	.40825
1, 1, 0	3, 1, 2	42.37	-130.99	.62988	-.11805
1, 1, 0	3, 3, 0	42.37	-243.05	-.05704	.72069
1, 1, 1	1, 1, 1	37.14	00.00	.31623	.54772
1, 1, 1	2, 1, 1	37.14	- 58.04	.70711	-.40825
1, 1, 1	3, 1, 3	37.14	-105.14	.63088	.23203
1, 1, 1	3, 3, 1	37.14	-248.08	-.04465	.69245

A P P E N D I X C

PROGRAM LISTING OF QUADRUPOLE MOMENT SUBROUTINES

```
RUN(S,,1011,,,,77777)
ATTACH(SAC,ASMROTUPDATE,ID=CLOUGH,MR=1.
UPDATE(P=SAC,F)
REWIND,COMPILE.
RUN(S,,,COMPILE)
RETURN,SAC,COMPILE.
ATTACH(SAC,QUADM,ID=DAVIES,MR=1.)
RUN(S,,,SAC)
LDSET(PRESET=INDEF)
MAP,PART.
REQUEST,TAPE8,*PF.
LOAD(LGO)
EXECUTE.
EXIT.
```

```
*ID QUADMO
*I ASMROT.1
                    NOLIST
*I ASMROT.18
      COMMON/QUADOF/IFQDEV,IFQDOD
*I ASMROT.46
      READ(INTAPE,921) IFQDEV,IFQDOD
  921 FORMAT(2I5)
*I ASMROT.114
      IF(IFQDEV.EQ.0) CALL QUADEV
      IF(IFQDOD.EQ.0) CALL QUADOD
```

```
      PROGRAM CRLAS (INPUT,OUTPUT,TAPE7,TAPE1,TAPE5=INPUT,TAPE6=OUTPUT,
     1  TAPE2,TAPE8)
      COMMON /XYZ/ INTAPE,LEAVE,JUGGLE,JPUNCH,LSTOR,LOUT,LTAPES(4)
      COMMON/WRTCNT/IWRTCN
      LOUT=6
      JUGGLE=0
      JUGGLE=6
      JUGGLE=1
      LSTOR=0
      LSTOR=7
      LSTOR=6
      LSTOR=2
      CALL FTNBIN(1,0,DUMMY)
   10 CONTINUE
      INTAPE=5
      JPUNCH=1
      LEAVE=1
      LEAVE=6
      CALL ASMROT
      WRITE(6,900) IWRTCN
  900 FORMAT(10X,*IWRITECOUNT=*,I10)
C     CALL LSTSQ
      STOP
      END
      SUBROUTINE PHITOP (G,V)
      DIMENSION G(39),V(39)
      COMMON /CONSTID/ OPID(40),SYMID(40)
      DATA (SYMID(I),I=1,39)                   /6H  100 ,6H  0[illegible] ,6H  001 ,
     $ 6H  200 ,6H  110 ,6H  020 ,6H  101 ,6H  011 ,6H  0[illegible] ,
     $ 6H  300 ,6H  210 ,6H  120 ,6H  030 ,6H  201 ,6H  [illegible] ,6H  021 ,
     $ 6H  102 ,6H  012 ,6H  003 ,
     $ 6H  040 ,6H  130 ,6H  220 ,6H  310 ,6H  [illegible] ,6H  [illegible] ,6H  230 ,
     $ 6H  320 ,6H  060 ,6H  150 ,6H  240 ,6H  330 ,6H  [illegible] ,
     $ 6H  031 ,6H  121 ,6H  211 ,6H  301 ,6H  041 ,6H  [illegible] ,6H  090 /
      DO 30 J=1,39
```

```
      OPID(J)=SYMID(J)
   30 V(J)=G(J)
      RETURN
      END
      SUBROUTINE QUADEV
C     SUBROUTINES QUADMOMENT
C     THESE SUBROUTINES COMPUTE REDUCED MATRIX ELEMENTS OF THE
C     TRACELESS QUADRUPOLE MOMENT OPERATOR FOR ASYMMETRIC ROTOR
C     MOLECULES POSSESSING AN AXIS OF SYMMETRY
C
C     THE REDUCED MATRIX ELEMENTS ARE GIVEN BY
C     (J,TAU//Q//JP,TAUP)=(-1)**(JP-J)*((Q(Z,Z)-Q(X,X)/2-Q(Y,Y)/2)*AWIG
C     -SQRT(3/4)*(Q(X,X)-Q(Y,Y))*BWIG) , WHERE Q(Z,Z),Q(X,X),Q(Y,Y) ARE
C     THE PRINCIPAL AXIS COMPONENTS OF THE PERMANENT QUADRUPOLE MOMENT
C     TENSOR , AND WHERE THE MATRIX ELEMENTS
C     AWIG=(J,TAU/A/JP,TAUP)
C     BWIG=(J,TAU/B/JP,TAUP)
C     ARE COMPUTED IN THE SUBROUTINES WHICH FOLLOW .
C
C     SUM RULES FOR AWIG,BWIG
C     LET A2=AWIG**2 , B2=BWIG**2 , AB=AWIG*BWIG
C     A2 SUMMED OVER JP,TAUP EQUALS ONE .
C    A2 MULTIPLIED BY (2*J+1)/(2*JP+1) AND SUMMED OVER J,TAU EQUALS ONE
C     B2 SUMMED OVER JP,TAUP EQUALS ONE
C    B2 MULTIPLIED BY (2*J+1)/(2*JP+1) AND SUMMED OVER J,TAU EQUALS ONE
C     AB SUMMED OVER JP,TAUP VANISHES
C    AB MULTIPLIED BY (2*J+1)/(2*JP+1) AND SUMMED OVER J,TAU VANISHES
C
      COMMON /XYZ/ INTAPE,LEAVE,JUGGLE,JPUNCH,LSTOR,LOUT,LTAPES(4)
      COMMON IFEDIG,IFTRFS,IFTRQS,IFTRRW,IFTRQW,IFEXPP,IFFSUM,IFLIST,
     1       IFSTAR,IFCHOY,IFCLOK,IFPUNC,INDSUR(20)
      COMMON W0,CXX,CYY,CZZ,T1,T2,T3,T4,T5,T6,PHI(30)
      COMMON    BPC,COEEK,BMC,D1,D2,D3,D4,D5,D6,HH(30)
      COMMON JJ, JMIN, JMAX, JSYM,KDIM(4,2),LSYM(4,2),DEGEN(2), WJMAX
      COMMON NDIM,KP(31,4),KO(31,4),WJHI(31,4),WJLO(31,4),HLAMD(31,4,2),
```

```
     2    BOLTZ(31,4,2),MAT1(31,31),MAT2(31,31),MAT3(31,31),MAT4(31,31),
     3        TJHI(31,31,4)
      COMMON /INT/ ITEMP,TEMP(3),OSUM,BOTLIM,UPLIM,RFREQ,KDIP,
     C              IDIP(3),DIPOLE(3),DPHI(9,3),DIPSQ(3)
      COMMON /VECLO/ TJLO(31,31,4)
      COMMON /XRC/ RC,RELO,SUMINT1,SUMINT2,SUMINT3
      COMMON /FN03/ EJ,P2,P4,P6
      COMMON /SELEC/ XDIP,XTYP
      COMMON/QUADOF/IFQDEV,IFQDOD
      COMMON/QUAD/ KDIM3(4),LSYM3(4),AQD(31,31),BQD(31,31),WJLOO(31,4),
     1    HLAMD3(31,4),BOLTZ3(31,4),TJLOO(31,31,4)
      IF(INDSUB(3).NE.0) GO TO 20
      INDSUB(3)=1
      CALL FREQQD(0,0,0,0,0)
      READ(INTAPE,900) JFREMN,JFREMX,(IDIP(I),I=1,3),BOTLIM,UPLIM,RELOR
  900 FORMAT(2I5,5X,3I5,2F10.3,E10.3)
      IF(JFREMN.LE.JMIN) JFREMN=JMIN+1
      IF(JFREMX.GT.JMAX) JFREMX=JMAX
      IF(LOUT.EQ.JUGGLE) RETURN
   20 CONTINUE
      IF(JJ.LT.JFREMN-1) RETURN
      IF(JJ.LT.0) RETURN
      IF(JJ.EQ.JMIN) WRITE(LOUT,901) JJ,JMIN,JMAX,JFREMN,JFREMX
  901 FORMAT(10X,*JJ=*,I3,2X,*JMIN=*,I3,2X,*JMAX=*,I3,2X,*JFREMN=*,I3,
     1     2X,*JFREMX=*,I3,2X,*FOR DELTAJ EVEN*)
C     JJ=0 GIVES NO MATRIX ELEMENTS
      IF(JJ.EQ.0)RETURN
      IF(JJ.EQ.JFREMX) IFQDEV=1
C      QINTNS=QINTNS(L,LP,ITYPE)
C     FREQQD=FREQQD(L,LP,ITYPE,INCKPA,INCKPB)  .  THE LA   TWO
C     PARAMETERS IN FREQQD REPRESENT VALUES FOR THE A,B    RICES WHICH
C     ENTER INTO SUBROUTINE CSOM13 IN THE FORM IDEL=(KD    INCKP)/2 .
C     CAUTION....INCKPA,INCKPB MUST BE EVEN. PRESENT P    DURE
C     LIMITS TRANSITIONS TO DELTA(KA)=0,2,-2
C     DO JP=J TRANSITIONS FOR A AND B
```

```
C     IN JP=J CASE , A AND B ARE HERMITIAN , IT IS ONLY NECESSARY TO
C     CALL FREQOD FOR INCKPA AND INCKB VALUES GREATER OR EQUAL ZERO.
      CALL QINTNS(1,1,0)
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .
      CALL FREQOD(1,1,0,0,2)
C     NOW ADD SOME WEAKER TRANSITIONS .
      CALL FREQOD(1,1,0,2,0)
C     E- DOESNT EXIST FOR JJ LESS THAN OR EQUAL TO ONE .
      IF(JJ.EQ.1) GO TO 85
      CALL QINTNS(2,2,0)
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .
      CALL FREQOD(2,2,0,0,2)
C     NOW ADD SOME WEAKER TRANSITIONS .
      CALL FREQOD(2,2,0,2,0)
   85 CONTINUE
      CALL QINTNS(3,3,0)
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .
      CALL FREQOD(3,3,0,0,2)
      CALL FREQOD(3,3,0,-99,0)
C     NOW ADD SOME WEAKER TRANSITIONS .
      CALL FREQOD(3,3,0,2,-99)
      CALL QINTNS(4,4,0)
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .
      CALL FREQOD(4,4,0,0,2)
      CALL FREQOD(4,4,0,-99,0)
C     NOW ADD SOME WEAKER TRANSITIONS .
      CALL FREQOD(4,4,0,2,-99)
      IF(JJ.LT.JFREQMN+1) GO TO 2000
C     DO JP=J-2 TRANSITIONS FOR A,B  .
C     SKIP CALCULATION FOR J=1 .
      IF(JJ.LE.1) GO TO 2000
      CALL QINTNS(1,1,2)
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .
      CALL FREQOD(1,1,2,0,2)
      CALL FREQOD(1,1,2,-99,-2)
```

```
C     NOW ADD SOME WEAKER TRANSITIONS .
      CALL FREQOD(1,1,2,2,0)
      CALL FREQOD(1,1,2,-2,-99)
C     E- DOESNT EXIST FOR JP=JJ-2=0
      IF(JJ.EQ.2) GO TO 88
      CALL QINTNS(2,2,2)
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .
      CALL FREQOD(2,2,2,0,2)
      CALL FREQOD(2,2,2,-99,-2)
C     NOW ADD SOME WEAKER TRANSITIONS .
      CALL FREQOD(2,2,2,2,0)
      CALL FREQOD(2,2,2,-2,-99)
   88 CONTINUE
      CALL QINTNS(3,3,2)
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .
      CALL FREQOD(3,3,2,0,2)
      CALL FREQOD(3,3,2,-99,-2)
      CALL FREQOD(3,3,2,-99,0)
C     NOW ADD SOME WEAKER TRANSITIONS .
      CALL FREQOD(3,3,2,2,-99)
      CALL FREQOD(3,3,2,-2,-99)
      CALL QINTNS(4,4,2)
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .
      CALL FREQOD(4,4,2,0,2)
      CALL FREQOD(4,4,2,-99,-2)
      CALL FREQOD(4,4,2,-99,0)
C     NOW ADD SOME WEAKER TRANSITIONS .
      CALL FREQOD(4,4,2,2,-99)
      CALL FREQOD(4,4,2,-2,-99)
 2000 CONTINUE
      RETURN
      END
      SUBROUTINE QUADOD
      COMMON /XYZ/ INTAPE,LEAVE,JUGGLE,JPUNCH,LSTOR,LO[illegible] TAPES(4)
      COMMON IFEDIG,IFTRRS,IFTRQS,IFTRRW,IFTRQW,IF[illegible]XP[illegible] SUM,IFLIST,
```

```
     1      IFSTAR,IFCHOY,IFCLOK,IFPUNC,INDSUB(20)
      COMMON W0,CXX,CYY,CZZ,T1,T2,T3,T4,T5,T6,PHI(30)
      COMMON    BPC,COEEK,BMC,D1,D2,D3,D4,D5,D6,HH(30)
      COMMON JJ, JMIN, JMAX, JSYM,KDIM(4,2),LSYM(4,2),DEGEN(2), WJMAX
      COMMON NDIM,KP(31,4),KO(31,4),WJHI(31,4),WJLO(31,4),HLAMD(31,4,2),
     2   BOLTZ(31,4,2),MAT1(31,31),MAT2(31,31),MAT3(31,31),MAT4(31,31),
     3      TJHI(31,31,4)
      COMMON /INT/ ITEMP,TEMP(3),QSUM,BOTLIM,UPLIM,RFREG,KDIP,
     C           IDIP(3),DIPOLE(3),DPHI(9,3),DIPSQ(3)
      COMMON/VECLO/TJLO(31,31,4)
      COMMON /XRC/ RC,RELO,SUMINT1,SUMINT2,SUMINT3
      COMMON /FN00/ EJ,P2,P4,P6
      COMMON /SELEC/ XDIP,XTYP
      COMMON/QUADOF/IFQDEV,IFQDOD
      COMMON/QUAD/ KDIM3(4),LSYM3(4),AOD(31,31),BOD(31,31),WJLOO(31,4),
     1   HLAMD3(31,4),BOLTZ3(31,4),TJLOO(31,31,4)
      IF(INDSUB(2).NE.0) GO TO 20
      INDSUB(2)=1
      CALL FREQQD(0,0,0,0,0)
      READ(INTAPE,900) JFREMN,JFREMX,(IDIP(I),I=1,3),BOTLIM,UPLIM,RELOQ
  900 FORMAT(2I5,5X,3I5,2F10.3,E10.3)
      IF(JFREMN.LE.JMIN) JFREMN=JMIN+1
      IF(JFREMX.GT.JMAX) JFREMX=JMAX
      IF(LOUT.EQ.JUGGLE) RETURN
   20 CONTINUE
C     ONLY STORE FOR J=0,DON'T COMPUTE TRANSITIONS.
      IF(JJ.LT.JFREMN) GO TO 4000
      IF(JJ.EQ.JMIN+1) WRITE(LOUT,901) JJ,JMIN,JMAX,JFREMN,JFREMX
  901 FORMAT(10X,*JJ=*,I3,2X,*JMIN=*,I3,2X,*JMAX=*,I3,2X,*JFREMN=*,I3,
     1     2X,*JFREMX=*,I3,2X,*FOR DELTAJ ODD*)
C     J=1 GIVES NO DELTAJ=ODD TRANSITIONS.IF J=1 ONLY STORE
      IF(JJ.EQ.JFREMN)GO TO 2000
      IF(JJ.EQ.JFREMX) IFQDOD=1
C     DO JP=J-1 TRANSITIONS FOR A,B
C     E- DOESNT EXIST FOR JP=JJ-1=1
```

```
      IF(JJ.LE.2) GO TO 85                                              001890
      CALL QINTNS(1,2,1)                                                001900
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .                           001910
      CALL FREQQD(1,2,1,0,2)                                            001920
      CALL FREQQD(1,2,1,-99,-2)                                         001930
C     NOW ADD SOME WEAKER TRANSITIONS .                                 001940
      CALL FREQQD(1,2,1,2,0)                                            001950
      CALL FREQQD(1,2,1,-2,-99)                                         001960
   85 CONTINUE                                                          001980
      CALL QINTNS(2,1,1)                                                001990
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .                           002000
      CALL FREQQD(2,1,1,0,2)                                            002010
      CALL FREQQD(2,1,1,-99,-2)                                         002020
C     NOW ADD SOME WEAKER TRANSITIONS .                                 002030
      CALL FREQQD(2,1,1,2,0)                                            002040
      CALL FREQQD(2,1,1,-2,-99)                                         002050
      CALL QINTNS(3,4,1)                                                002070
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .                           002080
      CALL FREQQD(3,4,1,0,2)                                            002090
      CALL FREQQD(3,4,1,-99,-2)                                         002100
      CALL FREQQD(3,4,1,-99,0)                                          002110
C     NOW ADD SOME WEAKER TRANSITIONS .                                 002120
      CALL FREQQD(3,4,1,2,-99)                                          002130
      CALL FREQQD(3,4,1,-2,-99)                                         002140
      CALL QINTNS(4,3,1)                                                002150
C     DO STRONG (SYMMETRIC TOP) TRANSITIONS .                           002160
      CALL FREQQD(4,3,1,0,2)                                            002170
      CALL FREQQD(4,3,1,-99,-2)                                         002180
      CALL FREQQD(4,3,1,-99,0)                                          002190
C     NOW ADD SOME WEAKER TRANSITIONS .                                 002200
      CALL FREQQD(4,3,1,2,-99)                                          002210
      CALL FREQQD(4,3,1,-2,-99)                                         002220
 2000 CONTINUE                                                          002240
C     STORE SMALLER J EIGENVECTOR ARRAYS                                002250
      IF(JJ.EQ.JFREMN-1) GO TO 4000                                     002260
```

```
      DO 3100 L=1,4
      IF(LSYM(L,2).NE.0) GO TO 3100
      LIM=KDIM(L,2)
      LSYM3(L)=LSYM(L,2)
      KDIM3(L)=KDIM(L,2)
      IF(LIM.LT.1) GO TO 3100
      DO 3020 I=1,LIM
      WJLOO(I,L)=WJLO(I,L)
      HLAMD3(I,L)=HLAMD(I,L,2)
      BOLTZ3(I,L)=BOLTZ(I,L,2)
      DO 3010 J=1,LIM
 3010 TJLOO(I,J,L)=TJLO(I,J,L)
 3020 CONTINUE
 3100 CONTINUE
 4000 CONTINUE
      DO 2100 L=1,4
      IF(LSYM(L,1).NE.0) GO TO 2100
      LIM=KDIM(L,1)
      IF(LIM.LT.1) GO TO 2100
      DO 2020 I=1,LIM
      WJLO(I,L)=WJHI(I,L)
      HLAMD(I,L,2)=HLAMD(I,L,1)
      BOLTZ(I,L,2)=BOLTZ(I,L,1)
      DO 2010 J=1,LIM
 2010 TJLO(I,J,L)=TJHI(I,J,L)
 2020 CONTINUE
 2100 CONTINUE
      RETURN
      END
      SUBROUTINE FREQOD(L,LP,ITYPE,INCKPA,INCKPB)
      COMMON /XYZ/ INTAPE,LEAVE,JUGGLE,JPUNCH,LSTOR,LOUT,LTAPES(4)
      COMMON IFEDIG,IFTRRS,IFTROS,IFTRRW,IFTROW,IFEXPP,IFPSUM,IFLIST,
     1       IFSTAR,IFCHOY,IFCLOK,IFPUNC,INDSUB(20)
      COMMON W0,CXX,CYY,CZZ,T1,T2,T3,T4,T5,T6,PHICON(30)
      COMMON    BPC,COEFK,BMC,D1,D2,D3,D4,D5,D6,HH(30)
```

```
      COMMON JJ, JMIN, JMAX, JSYM,KDIM(4,2),LSYM(4,2),DEGEN(2), WJMAX
      COMMON NDIM,KP(31,4),KO(31,4),WJ(31,4,2),            HLAMD(31,4,2),
     1    BOLTZ(31,4,2),
     2 H(31,31),PHI(31,31),CO(31,31),MAT4(31,29),TENSIT(31),TENS2(31),
     3       TJHI(31,31,4)
      COMMON /VFCLO/ TJLO(31,31,4)
      COMMON /FN00/ EJ,P2,P4,P6
      COMMON /SELEC/ XDIP,XTYP
      COMMON /INT/ ITEMP,TEMP(3),QSUM,BOTLIM,UPLIM,RFREQ,KDIP,
     C            IDIF(3),DIPOLE(3),DPHI(9,3),DIPSQ(3)
      COMMON /XPC/ RC,RELO,SUMINT1,SUMINT2,SUMINT3
      COMMON /SSS/ SO(200),KPLO(4),KCDEL(4),XX11(4)
      COMMON/QUAD/ KDIM3(4),LSYM3(4),AQD(31,31),BQD(31,31),WJLOO(31,4),
     1    HLAMD3(31,4),BOLTZ3(31,4),TJLOO(31,31,4)
      COMMON/WRTCNT/IWRTCN
      IF(INDSUB(10).NE.0) GO TO 70
      IWRTCN=0
      INDSUB(10)=1
      READ(INTAPE,900) IPN,INTIND
  900 FORMAT(2I5)
   70 IF(L.LE.0) RETURN
      LO=ITYPE+1
      JP=JJ-ITYPE
      INCA=(KPLO(L)-KPLO(LP)+INCKPA)/2
      INCB=(KPLO(L)-KPLO(LP)+INCKPB)/2
C     INCA,INCB PLAY THE ROLE OF IDEL IN SUBROUTINE CSQM13
      IF(LO.EQ.3) GO TO 71
      IF((LSYM(L,1).NE.0).OR.(LSYM(LP,LO).NE.0)) RETURN
      GO TO 72
   71 IF((LSYM(L,1).NE.0).OR.(LSYM3(LP).NE.0)) RETURN
   72 CONTINUE
      MINA=1
      MINB=1
      IF(INCA.LT.0) MINA=1-INCA
      IF(INCB.LT.0) MINB=1-INCB
```

```
      LIM1=KDIM(L,1)
      IF(LO.EQ.3) GO TO 73
      LIM2=KDIM(LP,LO)
      GO TO 74
   73 LIM2=KDIM3(LP)
   74 CONTINUE
      MAXA=LIM1
      MAXB=LIM1
      IF(MAXA+INCA.GT.LIM2) MAXA=LIM2-INCA
      IF(MAXB+INCB.GT.LIM2) MAXB=LIM2-INCB
      JPKO=JP+KCDEL(LP)
      LTAUA=KP(MINA,L)-KO(MINA,L)
      LTAUB=KP(MINB,L)-KO(MINB,L)
      LLSYMA=((-1)**LTAUA+3)/2
      LLSYMB=((-1)**LTAUB+3)/2
      RENOA=SQRT(2.*JP+1)/SQRT(2.*JJ+1)
      RENOB=RENOA/SQ(2+1)
      IATYPE=1000
      IBTYPE=2000
      IF(INCKPA.EQ.-99) GO TO 590
      IF(MINA.GT.MAXA) GO TO 590
      DO 600 K=MINA,MAXA
      KINC=K+INCA
      HHI=WJ(K,L,1)
      IF(LO.EQ.3) GO TO 500
      HLO=WJ(KINC,LP,LO)
      GO TO 501
  500 HLO=WJLOO(KINC,LF)
  501 CONTINUE
C     XLINE IS NOW THE FREQUENCY .
      XLINE=HHI-HLO
C     WE COMPARE XLINE WITH THE UPPER AND LOWER LIMITS AND DISCARD
C     IT IF IT DOES NOT PASS THE TESTS .
      ABSLIN=ABS(XLINE)
      IF((ABSLIN.LT.BOTLIM).OR.(ABSLIN.GT.UPLIM)) GO TO 590
```

```
      KPP=KP(K,L)+INCKPA
      KOP=JPKO-KPP
      IF(KPP.LT.0.OR.KOP.LT.0) GO TO 600
      IF(KPP.GT.JP.OR.KOP.GT.JP)GO TO 600
      IF(IFLIST.NE.0) RETURN
C     OBTAIN A RESULTS FOR JP=J
      IF(ITYPE.EQ.0) AWIG=TRANSM(K,KINC,TJHI,AQD,TJHI,L,LIM1,LP,LIM2)
C     OBTAIN A RESULTS FOR JP=J-1
      IF(ITYPE.EQ.1) AWIG=TRANSM(K,KINC,TJHI,AQD,TJLO,L,LIM1,LP,LIM2)
C     OBTAIN A RESULTS FOR JP=J-2
      IF(ITYPE.EQ.2) AWIG=TRANSM(K,KINC,TJHI,AQD,TJLOO,L,LIM1,LP,LIM2)
      IF(AWIG.EQ.0.0) GO TO 600
C     OBTAIN REVERSED MATRIX ELEMENT
C     FIRST CHECK THAT REVERSED MATRIX ELEMENT IS NOT A REPEAT .
      IHI=KO(K,L)+1000*KP(K,L)+1000000*JJ
      ILO=KOP+1000*KPP+1000000*JP
      IF(ILO.EQ.IHI) GO TO 51
      AWIGRV=((-1)**ITYPE)*AWIG
   51 CONTINUE
      AWIG=RENOA*AWIG
C     SQUARE MATRIX ELEMENTS TO GIVE A MATRIX LINE STRENGTHS .
      AWIG2=AWIG**2
      IF(ILO.EQ.IHI) GO TO 52
      AWIGR2=AWIGRV**2
   52 CONTINUE
      WRITE(8) IATYPE,JJ,KP(K,L),KO(K,L),JP,KPP,KOP,XLINE, HI,
     1    AWIG,AWIG2
      WRITE(LEAVE,904) IATYPE,JJ,KP(K,L),KO(K,L),JP,KPP,KOP,XLINE,HHI,
     1    AWIG,AWIG2
      IWRTCN=IWRTCN+1
  904 FORMAT(10X,I5,3X,3I3,4X,3I3,4(2X,E15.5))
      IF(ILO.EQ.IHI) GO TO 600
C     WRITE REVERSED TRANSITION
      XLINE=-XLINE
      WRITE(8) IATYPE,JP,KPP,KOP,JJ,KP(K,L),KO(K,L),XLINE,HLO,
```

```
     1     AWIGRV,AWIGR2
      WRITE(LEAVE,904) IATYPE,JP,KPP,KOP,JJ,KP(K,L),KO(K,L),XLINE,HLO,
     1     AWIGRV,AWIGR2
      IWRTCN=IWRTCN+1
  600 CONTINUE
  590 CONTINUE
      IF(INCKPB.EQ.-99) GO TO 850
      IF(MINB.GT.MAXB) RETURN
      DO 800 K=MINB,MAXB
      KINC=K+INCB
      HHI=WJ(K,L,1)
      IF(LO.EQ.3) GO TO 700
      HLO=WJ(KINC,LP,LO)
      GO TO 701
  700 HLO=WJLOO(KINC,LP)
  701 CONTINUE
C     XLINE IS NOW THE FREQUENCY .
      XLINE=HHI-HLO
C     WE COMPARE XLINE WITH THE UPPER AND LOWER LIMITS AND DISCARD
C     IT IF IT DOES NOT PASS THE TESTS .
      ABSLIN=ABS(XLINE)
      IF((ABSLIN.LT.BOTLIM).OR.(ABSLIN.GT.UPLIM)) RETURN
      KPP=KP(K,L)+INCKPB
      KOP=JPKO-KPP
      IF(KPP.LT.0.OR.KOP.LT.0) GO TO 800
      IF(KPP.GT.JP.OR.KOP.GT.JP)GO TO 800
      IF(IFLIST.NE.0) RETURN
C     OBTAIN B RESULTS FOR JP=J
      IF(ITYPE.EQ.0) BWIG=TRANSM(K,KINC,TJHI,BQD,TJHI,L,LIM1,LP,LIM2)
C     OBTAIN B RESULTS FOR JP=J-1
      IF(ITYPE.EQ.1) BWIG=TRANSM(K,KINC,TJHI,BQD,TJLO,L,LIM1,LP,LIM2)
C     OBTAIN B RESULTS FOR JP=J-2
      IF(ITYPE.EQ.2) BWIG=TRANSM(K,KINC,TJHI,BQD,TJLOO,L,LIM1,LP,LIM2)
      IF(BWIG.EQ.0.0) GO TO 800
C     OBTAIN REVERSED MATRIX ELEMENT
```

```
C      FIRST CHECK THAT REVERSED MATRIX ELEMENT IS NOT A REPEAT .
       IHI=KO(K,L)+1000*KP(K,L)+1000000*JJ
       ILO=KOP+1000*KPP+1000000*JP
       IF(ILO.EQ.IHI) GO TO 61
       BWIGRV=((-1)**ITYPE)*BWIG/SQ(2+1)
   61  CONTINUE
       BWIG=RENOB*BWIG
C      SQUARE MATRIX ELEMENTS TO GIVE B MATRIX LINE STRENGTHS .
       BWIG2=BWIG**2
       IF(ILO.EQ.IHI) GO TO 62
       BWIGR2=BWIGRV**2
   62  CONTINUE
       WRITE(8) IBTYPE,JJ,KP(K,L),KO(K,L),JP,KPP,KOP,XLINE,HHI,
      1   BWIG,BWIG2
       WRITE(LEAVE,904) IBTYPE,JJ,KP(K,L),KO(K,L),JP,KPP,KOP,XLINE,HHI,
      1    BWIG,BWIG2
       IWRTCN=IWRTCN+1
       IF(ILO.EQ.IHI) GO TO 800
C      WRITE REVERSED TRANSITION
       XLINE=-XLINE
       WRITE(8) IBTYPE,JP,KPP,KOP,JJ,KP(K,L),KO(K,L),XLINE,HLO,
      1    BWIGRV,BWIGR2
       WRITE(LEAVE,904) IBTYPE,JP,KPP,KOP,JJ,KP(K,L),KO(K,L),XLINE,HLO,
      1     BWIGRV,BWIGR2
       IWRTCN=IWRTCN+1
  800  CONTINUE
  850  CONTINUE
       RETURN
       END
       FUNCTION TRANSM(I,J,UA,CO,UB,LA,LIMA,LB,LIMB)
       DIMENSION UA(31,31,4),CO(31,31),UB(31,31,4)
       AA=0.
       DO 20 IA=1,LIMA
       BB=0.
       DO 10 IB=1,LIMB
```

```
10 BB=BB+CO(IA,IB)*UB(IB,J,LB)
20 AA=AA+UA(IA,I,LA)*BB
   TRANSM=AA
   RETURN
   END
   SUBROUTINE QINTNS(LA,LB,ITYPE)
   COMMON /XYZ/ INTAPE,LEAVE,JUGGLE,JPUNCH,LSTOR,LOUT,LTAPES(4)
   COMMON IFEDIG,IFTRQS,IFTRPS,IFTRQW,IFTRRW,IFEXPF,IFFSUM,IFLIST,
  1       IFSTAR,IFCHOY,IFCLOK,IFPUNC,INDSUB(20)
   COMMON W0,CXX,CYY,CZZ,T1,T2,T3,T4,T5,T6,PHICON(30)
   COMMON     BPC,COEEK,BMC,D1,D2,D3,D4,D5,D6,HH(30)
   COMMON JJ, JMIN, JMAX, JSYM,KDIM(4,2),LSYM(4,2),DEGEN(2), WJMAX
   COMMON NDIM,KP(31,4),KO(31,4),WJHI(31,4),WJLO(31,4),HLAMD(31,4,2),
  2    BOLTZ(31,4,2),    H(31,31),PHI(31,31),CO (31,31),MAT4(31,31),
  3       TJHI(31,31,4)
   COMMON /INT/ ITEMP,TEMP(3),QSUM,BOTLIM,UPLIM,RFREQ,KDIP,
  C             IDIF(3),DIPOLE(3),DPHI(9,3),DIPSQ(3)
   COMMON /SSS/ SQ(200),KPLO(4),KCDEL(4),XX11(4)
   COMMON/QUAD/ KDIM3(4),LSYM3(4),AQD(31,31),BQD(31,31),WJLOO(31,4),
  1    HLAMD3(31,4),BOLTZ3(31,4),TJLOO(31,31,4)
   IF(IFLIST.EQ.1) RETURN
   LO=ITYPE+1
   IF(LO.EQ.3) GO TO 50
   IF((LSYM(LA,1).NE.0).OR.(LSYM(LB,LO).NE.0)) RETURN
   LIMB=KDIM(LB,LO)
   GO TO 51
50 IF((LSYM(LA,1).NE.0).OR.(LSYM3(LB).NE.0)) RETURN
   LIMB=KDIM3(LB)
51 LIMA=KDIM(LA,1)
   CALL CSQM13(AQD,BQD,JJ,ITYPE,LA,LIMA,LB,LIMB)
   RETURN
   END
   SUBROUTINE CSQM13(A,B,J,ITYPE,L,LIM,L1,LIM1)
C  SUBROUTINE CSQM13(A,B,J,ITYPE,L,LIM,L1,LIM1)
C  PROGRAM SETS UP THE WANG TRANSFORMED MATRICES
```

```
C      AQD(J,K:JF,KP)   , BQD(J,K:JP,KP) FOR USE WITH CALCULATION
C      OF ASYMMETRIC ROTOR QUADRUPOLE MOMENT MATRIX ELEMENTS .
C      THE SYMMETRIC TOP MATRIX ELEMENTS OF AQD, BQD (I.E. BEFORE
C      WANG TRANSFORMATION ) ARE GIVEN BY%
C      AQD(J,K;JF,KP)=(JP 2 KP 0/JP 2 J KP) FOR K=KP =ZERO OTHERWISE.
C      BQD(J,K:JP,KP)=(JP 2 KP 2/JP 2 J (KP+2)) FOR K=KP+2
C           =(JP 2 KP -2/JP 2 J (KP-2)) FOR K=KP-2
C           =ZERO OTHERWISE
C      THE CLEBSCH-GORDON COEFFS. ARE DEFINED AS IN CONDON-SHORTLY P.77.
C      PARAMETERS IN CALL LIST .
C      A,B=WANG TRANSFORMED MATRICES
C      J=J IN COMMENTS ABOVE .
C      ITYPE=0(JP=J),   1(JP=J-1) ,  2(JP=J-2) .
C      L,L1=1(E+) ,  2(E-) ,  3(O+) ,  4(O-)
C      THE COLUMN INDEX OF A,B RUNS OVER L1 TYPE STATES .
C      THE ROW INDEX OF A,B RUNS OVER L TYPE STATES .
C      LIM1=WANG ROW DIMENSION ,I.E. THE NUMBER OF COLUMNS .
C       LIM=WANG COLUMN DIMENSION ,I.E. THE NUMBER OF ROWS .
C      L1,LIM1 GO WITH RIGHT HAND EIGENVECTOR ARRAY .
C      L,LIM GO WITH (TRANSPOSE) OF LEFT HAND EIGENVECTOR ARRAY .
C
C
C      IN THE PROGRAM JP TAKES ON VALUES J , J-1 , J-2
C      THE FOLLOWING TRANSITIONS ARE STRICTLY EXCLUDED .
C      J=0 .
C      JP NEGATIVE .
C      JP=0 IS ALLOWED ONLY FOR J=2 ,IS UNALLOWED FOR J=1.
C
C
C      IN MAIN PROGRAM MULTIPLY A BY FACT1 AND MULTIPLY B  / FACT2
C      TO GIVE SIMPLE SUM RULES .
C      FACT1=SQRT(2.*JP+1)/SQRT(2.*J+1) ,FACT2=FACT1/SQF    )
C
       DIMENSION A(31,31),B(31,31)
       COMMON /SSS/ SQ(200),KPLO(4),KCDEL(4),XX11  )
```

```
      KP(I,L)=KPLO(L)+2.*(I-1)
C     CAUTION...IN THE PROGRAM KP(I,L) PLAYS THE ROLE OF  K IN THE
C     COMMENT SECTION .
C     KPLO(1)=0  (E+) ,KPLO(2)=2  (E-) ,KPLO(3)=1  (O+)  KPLO(4)=1  (O-)
C     THE ARRAYS ARE INITIALLY SET TO ZERO ,THUS ELEMENTS NOT
C     RESET REMAIN ZERO.
      DO 8 I1=1,31
      DO 8 I=1,31
      A(I,I1)=0.0
    8 B(I,I1)=0.0
      IF(J.EQ.0) GO TO 700
      KDEL=KPLO(L)-KPLO(L1)
      IF(ITYPE.EQ.1) GO TO 300
C     DO DELTA(J) EVEN TRANSITIONS , THE SELECTION RULES FOR A,B ARE
C     (O-,O-) , (O+,O+) , (E-,E-) , (E+,E+)
C     KDEL=0 THROUGHOUT THIS SECTION .
      JP=J-2
      IDEL=KDEL/2
      LIMLO=MAX0(1,1-IDEL)
      LIMHI=MIN0(LIM,LIM1-IDEL)
      IF(LIMHI.LT.LIMLO) GO TO 102
      DO 100 I=LIMLO,LIMHI
      I1=I+IDEL
      IF(ITYPE.EQ.2) GO TO 101
C     DO JP=J TRANSITIONS FOR A MATRIX
      SNUM=3.*KP(I,L)**2-J*(J+1)
      NA=2*J-1
      NB=J
      NC=J+1
      ND=2*J+3
C     REMEMBER SQ(I+1)=SQRT(I)
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
      GO TO 100
C     DO JP=J-2 TRANSITIONS FOR A MATRIX
  101 IF(JP.LT.0) GO TO 102
```

```
      IA=JP-KP(I,L)+2
      IB=JP-KP(I,L)+1
      IC=JP+KP(I,L)+2
      ID=JP+KP(I,L)+1
      SNUM=SQ(3+1)*SQ(IA+1)*SQ(IB+1)*SQ(IC+1)*SQ(ID+1)
      NA=2*JP+1
      NB=2*JP+2
      NC=2*JP+3
      ND=JP+2
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
  100 A(I,I1)=SNUM/DENOM
  102 CONTINUE
C     OBTAIN B(1,1) MATRIX ELEMENTS
      IF(L.EQ.1.OR.L.EQ.2)GO TO 106
      IF(ITYPE.EQ.2)GO TO 103
C  B(1,1) FOR JP=J
      SNUM=SQ(3+1)*SQ(J+1)*SQ(J+2)*SQ(J+1)*SQ(J+2)
      NA=2*J-1
      NB=J
      NC=2*J+2
      ND=2*J+3
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
      GO TO 105
C  B(1,1) FOR JP=J-2
103   IF(JP.LT.0) GO TO 106
      SNUM=SQ(JP+1)*SQ(JP+2)*SQ(JP+3)*SQ(JP+4)
      NA=2*JP+1
      NB=2*JP+2
      NC=2*JP+3
      ND=2*JP+4
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
105   B(1,1)=SNUM/DENOM
      IF(L.EQ.4) B(1,1)=-B(1,1)
106   CONTINUE
C  OBTAIN REMAINING B(I,I1) MATRIX ELEMENTS
```

```
C  FIRST DO UPPER SUPEFDIAGONAL (K/K+2)
      IDEL=(KDEL+2)/2
      LIMLO=MAX0(1,1-IDEL)
      LIMHI=MIN0(LIM,LIM1-IDEL)
      IF(LIMHI.LT.LIMLO)GO TO 111
      DO 110 I=LIMLO,LIMHI
      I1=I+IDEL
      IF(ITYPE.EQ.2) GO TO 108
C  DO JP=J TRANSITIONS FOR B MATRIX
      IA=J-KP(I,L)-1
      IB=J-KP(I,L)
      IC=J+KP(I,L)+1
      ID=J+KP(I,L)+2
      SNUM=SQ(3+1)*SQ(IA+1)*SQ(IB+1)*SQ(IC+1)*SQ(ID+1)
      NA=2*J-1
      NB=J
      NC=2*J+2
      ND=2*J+3
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
      GO TO 109
C  DO JP=J-2 TRANSITIONS FOR B MATRIX
108   IF(JP.LT.0)GO TO 111
      IA=JP-KP(I,L)-1
      IB=JP-KP(I,L)
      IC=JP-KP(I,L)+1
      ID=JP-KP(I,L)+2
      SNUM=SQ(IA+1)*SQ(IB+1)*SQ(IC+1)*SQ(ID+1)
      NA=2*JP+1
      NB=2*JP+2
      NC=2*JP+3
      ND=2*JP+4
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
109   B(I,I1)=SNUM/DENOM
C  INSERT WANG SQRT(2) FACTOR FOR E+
110   IF(L.EQ.1.AND.I.EQ.1)B(I,I1)=SQ(2+1)*B(I,I1)
```

```
111   CONTINUE
C     NOW DO LOWER SUPERDIAGONAL
      IDEL=(KDEL-2)/2
      LIMLO=MAX0(1,1-IDEL)
      LIMHI=MIN0(LIM,LIM1-IDEL)
      IF(LIMHI.LT.LIMLO) GO TO 116
      DO 115 I=LIMLO,LIMHI
      I1=I+IDEL
      IF(ITYPE.EQ.2) GO TO 112
C     DO JP=J TRANSITIONS FOR B MATRIX
      IA=J+KP(I,L)-1
      IB=J+KP(I,L)
      IC=J-KP(I,L)+1
      ID=J-KP(I,L)+2
      SNUM=SQ(3+1)*SQ(IA+1)*SQ(IB+1)*SQ(IC+1)*SQ(ID+1)
      NA=2*J-1
      NB=2*J
      NC=J+1
      ND=2*J+3
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
      GO TO 113
C     DO JP=J-2 TRANSITIONS FOR B MATRIX
  112 IF(JP.LT.0) GO TO 116
      IA=JP+KP(I,L)-1
      IB=JP+KP(I,L)
      IC=JP+KP(I,L)+1
      ID=JP+KP(I,L)+2
      SNUM=SQ(IA+1)*SQ(IB+1)*SQ(IC+1)*SQ(ID+1)
      NA=2*JP+1
      NB=2*JP+2
      NC=2*JP+3
      ND=2*JP+4
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
  113 B(I,I1)=SNUM/DENOM
C     INSERT WANG SQRT(2) FOR E+
```

```
  115 IF(L.EQ.1.AND.I1.EQ.1) B(I,I1)=SQ(2+1)*B(I,I1)
  116 CONTINUE
      GO TO 700
C     NOW DO DELTA(J) ODD TRANSITIONS, IN PARTICULAR DO JP=J-1
C     THE SELECTION RULES ARE (O+,O-) , (O-,O+) , (E+,E-) , (E-,E+)
  300 JP=J-1
C     J=1 , JP=0 IS EXCLUDED
      IF(JP.LE.0) GO TO 700
      IDEL=KDEL/2
      LIMLO=MAX0(1,1-IDEL)
      LIMHI=MIN0(LIM,LIM1-IDEL)
      IF(LIMHI.LT.LIMLO) GO TO 401
      DO 400 I=LIMLO,LIMHI
      I1=I+IDEL
C     OBTAIN JP=J-1 MATRIX ELEMENTS OF A
      IA=JP-KP(I,L)+1
      IB=JP+KP(I,6)+1
      SNUM=KP(I,L)*SQ(3+1)*SQ(IA+1)*SQ(IB+1)
      NA=JP
      NB=2*JP+1
      NC=JP+1
      ND=JP+2
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
      A(I,I1)=SNUM/DENOM
C     CHANGE SIGN
400   A(I,I1)=-A(I,I1)
  401 CONTINUE
C     OBTAIN JP=J-1 MATRIX ELEMENTS OF B
C     FIRST OBTAIN B(1,1) MATRIX ELEMENT
      IF(L.EQ.1.OR.L.EQ.2) GO TO 406
      IA=JP
      IB=JP+1
      IC=JP+2
      ID=JP+1
      SNUM=SQ(IA+1)*SQ(IB+1)*SQ(IC+1)*SQ(ID+1)
```

```
      NA=JP
      NB=2*JP+1
      NC=JP+1
      ND=2*JP+4
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
      B(1,1)=SNUM/DENOM
      IF(L.EQ.3) B(1,1)=-B(1,1)
  406 CONTINUE
C     OBTAIN REMAINING B MATRIX ELEMENTS
C     FIRST DO UPPER SUPERDIAGONAL
      IDEL=(KDEL+2)/2
      LIMLO=MAX0(1,1-IDEL)
      LIMHI=MIN0(LIM,LIM1-IDEL)
      IF(LIMHI.LT.LIMLO) GO TO 411
      DO 410 I=LIMLO,LIMHI
      I1=I+IDEL
      IA=JP-KP(I,L)-1
      IB=JP-KP(I,L)
      IC=JP-KP(I,L)+1
      ID=JP+KP(I,L)+2
      SNUM=SQ(IA+1)*SQ(IB+1)*SQ(IC+1)*SQ(ID+1)
      NA=JP
      NB=2*JP+1
      NC=JP+1
      ND=2*JP+4
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
      B(I,I1)=SNUM/DENOM
C     INSERT WANG SQRT(2) FACTOR
      IF(L.EQ.1.AND.I.EQ.1) B(I,I1)=SQ(2+1)*B(I,I1)
C     CHANGE SIGNS
  410 B(I,I1)=-B(I,I1)
  411 CONTINUE
C     NOW DO LOWER SUPERDIAGONAL
      IDEL=(KDEL-2)/2
      LIMLO=MAX0(1,1-IDEL)
```

```
      LIMHI=MIN0(LIM,LIM1-IDEL)
      IF(LIMHI.LT.LIMLO) GO TO 700
      DO 415 I=LIMLO,LIMHI
      I1=I+IDEL
      IA=JP+KP(I,L)-1
      IB=JP+KP(I,L)
      IC=JP+KP(I,L)+1
      ID=JP-KP(I,L)+2
      SNUM=-SQ(IA+1)*SQ(IB+1)*SQ(IC+1)*SQ(ID+1)
      NA=2*JP
      NB=JP+1
      NC=JP+2
      ND=2*JP+1
      DENOM=SQ(NA+1)*SQ(NB+1)*SQ(NC+1)*SQ(ND+1)
      B(I,I1)=SNUM/DENOM
C     INSERT WANG SQRT(2) FACTOR
      IF(L.EQ.2.AND.I.EQ.1) B(I,I1)=SQ(2+1)*B(I,I1)
C     CHANGE SIGN
  415 B(I,I1)=-B(I,I1)
  700 CONTINUE
      RETURN
      END
```