A COMPLETE FOURTH-ORDER VIBRATION-ROTATION HAMILTONIAN OF H_2O-TYPE MOLECULES

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ABSTRACT

A COMPLETE FOURTH-ORDER VIBRATION-ROTATION

HAMILTONIAN OF H_2O-TYPE MOLECULES

By

Liek Wilardjo

Starting with the Darling-Dennison Hamiltonian, a complete fourth-order vibration-rotation Hamiltonian for H_2O-type molecules has been obtained. It is in the form of a power series in the components of rotational angular momentum in the molecule-fixed frame. The coefficients of this power series include the equilibrium rotational constants, second-order and fourth-order centrifugal distortion constants and vibrational corrections to the rotational constants and to the second-order centrifugal distortion constants. Expressions for all the above coefficients in terms of the fundamental molecular parameters have been obtained and their relation to experimentally determinable quantities has been established. These fundamental parameters include the equilirium moments of inertia, the normal frequencies, and the potential constants of vibration of the molecule. The resulting Hamiltonian is appropriate for the calculation of ground-state energies of vibrating and rotating H_2O-type molecules to the fourth order of approximation. Such calculations may also be possible for those excited vibration states which are not subject to accidental vibrational and accidental vibration-rotation resonances.

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By

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I. INTRODUCTION

Among the microwave and infrared spectra of H_2O-type molecules, experiment has revealed many instances in which it is necessary to include in the Hamiltonian fourth-order centrifugal distortion terms in order to account for observed results to experimental accuracy. Molecules for which such a situation has been found to exist include the nonlinear triatomic molecules H_2O,[1] SO_2,[2] and F_2O.[3] Several workers have included on an ad hoc basis one or more fourth-order centrifugal distortion terms in their data analysis and thereby have obtained closer agreement between theory and experiment. Therefore it seems desirable to obtain fourth-order centrifugal distortion coefficients as a function of fundamental molecular parameters. The taking into account of the corresponding terms in the Hamiltonian should then give more satisfactory and theoretically meaningful fits to spectral data. To this end one can start from a general formalism of the Hamiltonian of polyatomic molecules such as that of Wilson and Howard,[4] or Darling and Dennison.[5] The two Hamiltonians are equivalent, but the latter is in more convenient form for expansion into terms according to orders of magnitude for perturbation calculations. Goldsmith, Amat, and Nielsen[6] have done such an expansion and development of the Darling-Dennison Hamiltonian up to the fourth order of approximation, but it is complicated, and one cannot use their results with complete confidence without duplicating the actual calculation. For this reason,

it seemed to us more advantageous to carry through the complete development of the Hamiltonian for the H_2O-type molecular configuration in particular rather than obtain the result as a special case of the general theory.In this way also the serious complications of the general theory due to degeneracy in the normal modes of vibration are absent since such degeneracies do not occur in asymmetric-top molecules and our calculation can avoid this complication from the start. Furthermore, a very recent paper by Watson[7] showed that the Darling-Dennison Hamiltonian can be written in a much simplified form. This was not known to Goldsmith, Amat, and Nielsen and therefore the details of the calculation in their expansion of the Hamiltonian are much more complicated than need be.

Chung and Parker[8] have studied the general vibration-rotation Hamiltonian of asymmetric-top molecules in the Goldsmith-Amat-Nielsen formulation. By subjecting the Hamiltonian to the symmetry restriction of the asymmetric-top point group, it was shown that there are only 105 independent fourth-order coefficients out of the possible 729. Watson's work[9] further reduced the number of independent fourth-order coefficients. This work also showed which parameters are determinable from experimental analysis, and how they relate to the theory. For these reasons, and since the number of independent fourth-order coefficients can be still further reduced and their expressions simplified by symmetry considerations, it was thought desirable to obtain a complete, fourth-order vibration-rotation Hamiltonian of H_2O-type molecules through a calculation specialized from the very start for

this configuration.

In this work we take as the starting point of our calculation the Watson-simplified Darling-Dennison Hamiltonian, written specifically for H_2O-type molecules. This Hamiltonian is expanded and subjected to two successive contact transformations of the Goldsmith-Amat-Nielsen type.[6] Pure vibrational terms of all orders are discarded since our interest lies in the detailed rotational structure for a given vibrational state. The resulting twice-transformed Hamiltonian is then subjected to extensive regrouping of terms based on the angular momentum commutation relations to put it in the final form cited by Yallabandi and Parker.[10,11] For a given vibrational state, it is in the form of a power series in the rotational angular momentum components with coefficients that are functions of the fundamental molecular parameters.

II. GENERAL VIBRATION-ROTATION HAMILTONIAN

We wish to consider vibration-rotation transitions during which the molecule remains in its electronic configuration. Consequently the part of the Hamiltonian coming directly from the electronic contribution to the total energy is of no interest here. To a very good degree of approximation[12] one may consider the electronic motion to be independent of the nuclear motion, and hence separate them and disregard the former in the formalism of the Hamiltonian. This procedure is known as the Born-Oppenheimer approximation.[12]

Within this approximation the Darling-Dennison[5] formulation of the vibration-rotation Hamiltonian of polyatomic molecules is:

$$H = (1/2)[\mu^{1/4}\sum_{\alpha\beta}(P_\alpha - p_\alpha)\mu_{\alpha\beta}\mu^{-1/2}(P_\beta - p_\beta)\mu^{1/4} + \mu^{1/4}\sum_{s\sigma}p^*_{s\sigma}\mu^{-1/2}\mu^{1/4}] + V \qquad (2.1)$$

where (1) and denote the principal axes of the equilibrium inertia tensor x, y, z of the molecule ; in general, Greek indices are assigned the range x,y,z except when they are used as normal modes' degeneracy indices in vibrational normal coordinates and momenta. Thus, for instance, α and β in (2.1) range over x,y and z, whereas σ ranges over the degrees of degeneracy.

(2) P_α and p_α are the components along the principal axes of inertia of the total and internal angular momentum, respectively.

(3) $p^*_{s\sigma}$ is the momentum conjugate to normal coordinate $Q_{s\sigma}$, i.e.,

$$p^*_{s\sigma} = -i\hbar\partial/\partial Q_{s\sigma} \tag{2.2}$$

(4) V is the potential energy of the molecular force field; it is a function of $Q_{s\sigma}$

(5)
$$\mu_{\alpha\alpha} = \mu(I'_{\beta\beta}I'_{\gamma\gamma} - I'^{2}_{\beta\gamma}) \tag{2.3}$$

$$\mu_{\alpha\beta} = \mu(I'_{\gamma\gamma}I'_{\alpha\beta} + I'_{\alpha\gamma}I'_{\gamma\beta}) \;;\alpha\neq\beta \tag{2.4}$$

$$\mu^{-1} = \det.\begin{vmatrix} I'_{xx} & -I'_{xy} & -I'_{xz} \\ -I'_{xy} & I'_{yy} & -I'_{yz} \\ -I'_{xz} & -I'_{yz} & I'_{zz} \end{vmatrix} \tag{2.5}$$

In (2.3) to (2.5), $I'_{\alpha\alpha}$ and $I'_{\alpha\beta}$ are the instantaneous moments and products of inertia, respectively. In terms of $Q_{s\sigma}$ they can be written as

$$I'_{\alpha\alpha} = I^{\circ}_{\alpha\alpha} + \sum_{s\sigma} a^{\alpha\alpha}_{s\sigma}Q_{s\sigma} + \sum_{s\sigma t\tau} A^{\alpha\alpha}_{s\sigma t\tau}Q_{s\sigma}Q_{t\tau} \tag{2.6}$$

$$-I'_{\alpha\beta} = -I^{\circ}_{\alpha\beta} + \sum_{s\sigma} a^{\alpha\beta}_{s\sigma}Q_{s\sigma} + \sum_{s\sigma t\tau} A^{\alpha\beta}_{s\sigma t\tau}Q_{s\sigma}Q_{t\tau} \tag{2.7}$$

where $a^{\alpha\beta}_{s\sigma}$ and $A'_{s\sigma s'\sigma'}(\alpha=\beta\,,\ \alpha\neq\beta)$ are constants for a given molecule whose explicit evaluations are given in Appendix I. Since we use the principal axes of inertia, we have

$$I^{\circ}_{\alpha\beta} = \delta_{\alpha\beta}I^{\circ}_{\alpha\alpha} \quad , \delta_{\alpha\beta} = \begin{cases} 1, \alpha=\beta \\ 0, \alpha\neq\beta \end{cases} \tag{2.8}$$

i.e., the equilibrium products of inertia $I^{\circ}_{\alpha\beta}$, $\alpha\neq\beta$ vanish. Using the defining formula of the internal vibrational angular momentum

$$p_{\alpha} = \sum_{s\sigma}\sum_{t\tau}\zeta^{\alpha}_{s\sigma t\tau}Q_{s\sigma}p^*_{t\tau} \tag{2.9}$$

where $\zeta^{\alpha}_{s\sigma t\tau}$ are Coriolis coupling coefficients defined in Appendix I, the Hamiltonian (2.1) can be written as

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$$H = (1/2)\sum_{\alpha\beta}\left\{[P_\alpha - p_\alpha]\mu_{\alpha\beta}[P_\beta - p_\beta] + \mu^{1/4}(p_\alpha\mu_{\alpha\beta}\mu^{-1/2}(p_\beta\mu^{1/4}))\right\}$$
$$+ (1/2)\sum_{s\sigma}\left\{p^{*2}_{s\sigma} + \mu^{1/4}(p^*_{s\sigma}\mu^{-1/2}(p^*_{s\sigma}\mu^{1/4}))\right\} + V \qquad (2.10)$$

In (2.10) an operator in parentheses acts only on quantities in the same parentheses, and not on the wavefunction.

The Hamiltonian (2.10) depends not only on $\mu_{\alpha\beta}$, but also on the determinant μ. Since the Schroedinger equation

$$(H - E)\psi = 0 \qquad (2.11)$$

is apparently impossible to solve in closed form, the Hamiltonian must be expanded in orders of magnitude to put it in a form suitable for perturbation calculations. Thus we would have to expand both $\mu_{\alpha\beta}$ and μ as power series in $Q_{s\sigma}$, which is quite a tedious calculation to do. Fortunately,however, it is not necessary to expand μ, as it has recently been shown by Watson[7] that the Hamiltonian (2.10) can be identically rewritten in the greatly simplified form:

$$H = (1/2)[\sum_{\alpha\beta}\{\mu_{\alpha\beta}P_\alpha P_\beta - [P_\alpha\mu_{\alpha\beta}p_\beta + p_\alpha\mu_{\alpha\beta}P_\beta] + p_\alpha\mu_{\alpha\beta}p_\beta\}$$
$$+ \sum_{s\sigma} p^{*2}_{s\sigma} - (\hbar^2/4)\sum_{\alpha}\mu_{\alpha\alpha}] + V \qquad (2.12)$$

If it is assumed that the displacements of the nuclei from their equilibrium positions are small relative to internuclear distances, we may expand $\mu_{\alpha\alpha}$ and $\mu_{\alpha\beta}$ in (2.12) into McLaurin series in dimensionless normal coordinates defined as

$$q_{s\sigma} = (\lambda_s/\hbar^2)^{1/4}Q_{s\sigma} \qquad (2.13a)$$

where λ_s is related to the normal frequency ω_s associated with $q_{s\sigma}$ by

$$H = (1/2)\sum_{\alpha\beta}\left\{[P_\alpha - p_\alpha]\mu_{\alpha\beta}[P_\beta - p_\beta] + \mu^{1/4}(p_\alpha\mu_{\alpha\beta}\mu^{-1/2}(p_\beta\mu^{1/4}))\right\}$$
$$+ (1/2)\sum_{s\sigma}\left\{p^{*2}_{s\sigma} + \mu^{1/4}(p^{*}_{s\sigma}\mu^{-1/2}(p^{*}_{s\sigma}\mu^{1/4}))\right\} + V \qquad (2.10)$$

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$$+ \sum_{s\sigma} p^{*2}_{s\sigma} - (\hbar^2/4)\sum_{\alpha}\mu_{\alpha\alpha}] + V \qquad (2.12)$$

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where λ_s is related to the normal frequency ω_s associated with $q_{s\sigma}$ by

$$\lambda_s = (2\pi c\omega_s)^2 \tag{2.13b}$$

Carrying through the procedure and collecting terms expected to be of the same order of magnitude, we obtain a Hamiltonian in the form:

$$H = H_0 + H_1 + H_2 + H_3 + H_4 \tag{2.14}$$

where H_0, H_1, H_2, H_3 and H_4 are the zeroth, first, second, third and fourth order portions of the vibration-rotation Hamiltonian, respectively. They are found to be of the form:

$$\begin{aligned}
H_0 &= \sum_{\alpha\beta}\sum_{s\sigma}\{(\alpha\beta*-*-)P_\alpha P_\beta + (\lambda_s^{1/2}/2\hbar)p_{s\sigma}^2\} + (\hbar/2)\sum_{s\sigma}\lambda_s^{1/2}q_s^2 \\
H_1 &= \sum_{\alpha\beta}\sum\{(\alpha\beta*-*s\sigma)q_{s\sigma}P_\alpha P_\beta + (\alpha*t\tau*s\sigma)(1/2)\{q_{s\sigma},p_{t\tau}\}P_\alpha\} \\
&\quad + 2\pi c\hbar\sum k_{rst}q_{r\rho}q_{s\sigma}q_{t\tau} \\
H_2 &= \sum_{\alpha\beta}\sum\{(\alpha\beta*-*s\sigma t\tau)q_{s\sigma}q_{t\tau}P_\alpha P_\beta + (\alpha*t\tau*r\rho s\sigma)(1/2)\{q_{r\rho}q_{s\sigma},p_{t\tau}\}P_\alpha \\
&\quad + (-*s\sigma t\tau*p\pi r\rho)(1/2)\{q_{p\pi}q_{r\rho},p_{s\sigma}p_{t\tau}\} - (\hbar^2/4)(\alpha\alpha*-*-)\} + \\
&\quad 2\pi c\hbar\sum k_{prst}q_{p\pi}q_{r\rho}q_{s\sigma}q_{t\tau} \\
H_3 &= \sum_{\alpha\beta}\sum\{(\alpha\beta*-*r\rho s\sigma t\tau)q_{r\rho}q_{s\sigma}q_{t\tau}P_\alpha P_\beta + \\
&\quad (\alpha*t\tau*p\pi r\rho s\sigma)(1/2)\{q_{p\pi}q_{r\rho}q_{s\sigma},p_{t\tau}\}P_\alpha + \\
&\quad (-*s\sigma t\tau*o\omega p\pi r\rho)(1/2)\{q_{o\omega}q_{p\pi}q_{r\rho},p_{s\sigma}p_{t\tau}\} - \\
&\quad -(\hbar^2/4)(\alpha\alpha*-*s\sigma)q_{s\sigma}\} + 2\pi c\hbar\sum k_{oprst}q_{o\omega}q_{p\pi}q_{r\rho}q_{s\sigma}q_{t\tau} \\
H_4 &= \sum_{\alpha\beta}\sum\{(\alpha\beta*-*p\pi r\rho s\sigma t\tau)q_{p\pi}q_{r\rho}q_{s\sigma}q_{t\tau}P_\alpha P_\beta + \\
&\quad (\alpha*t\tau*o\omega p\pi r\rho s\sigma)(1/2)\{q_{o\omega}q_{p\pi}q_{r\rho}q_{s\sigma},p_{t\tau}\}P_\alpha + \\
&\quad (-*s\sigma t\tau*n\nu o\omega p\pi r\rho)(1/2)\{q_{n\nu}q_{o\omega}q_{p\pi}q_{r\rho},p_{s\sigma}p_{t\tau}\} - \\
&\quad (\hbar^2/4)(\alpha\alpha*-*s\sigma t\tau)q_{s\sigma}q_{t\tau} + \\
&\quad 2\pi c\hbar\sum k_{noprst}q_{n\nu}q_{o\omega}q_{p\pi}q_{r\rho}q_{s\sigma}q_{t\tau}
\end{aligned} \tag{2.15}$$

where all summations are over all indices in the corresponding terms, $p_{s\sigma}$ is the momentum conjugate to the dimensionless normal coordinate

$q_{s\sigma}$, i.e.,

$$p_{s\sigma} = -i\hbar\partial/\partial q_{s\sigma} \qquad (2.16)$$

and the last term in each Hamiltonian represents the part of that Hamiltonian that comes from the potential energy V, also expanded as a McLaurin series in the dimensionless coordinates. The expansion of $\mu_{\alpha\alpha}$ and $\mu_{\alpha\beta}$ is outlined in Appendix II, and the derivation of (2.15), along with the definitions of the coefficients appearing therein, are given in Appendix III.

Except in cases of accidental resonance interaction,[13] H_1 in (2.15) has nonvanishing diagonal matrix elements arising only in the second term, which themselves vanish except for degenerate normal modes of vibration. Hence the second term is the only one in H_1 which can actually contribute to the first order energy. Therefore, one may partially diagonalize H by subjecting it to a contact transformation T[14] to get a transformed Hamiltonian H' of the form:

$$H' = THT^{-1} = H_0' + H_1' + H_2' + H_3' + H_4' \qquad (2.17)$$

where T is so chosen that

$$H_1' = \sum_{\alpha}\sum_{s\sigma}(\alpha{*}s\sigma{*}s\sigma)(1/2)\{q_{s\sigma}, p_{s\sigma}\}P_\alpha \qquad (2.18)$$

Here (2.18) is the same as the second term in H_1 with $t\tau = s\sigma$, i.e., it applies only to degenerate normal modes of vibration.

Choosing T to be of the exponential form:

$$T = \exp(i\lambda S) \qquad (2.19)$$

where T is a unitary operator which requires S to be a Hermitian

operator, and λ is a smallness parameter, we have

$$H' = \exp(i\lambda S)H\exp(-i\lambda S)$$
$$= (1 + i\lambda S - \lambda^2 S^2/2 - \ldots)(H_0 + \lambda H_1 + \lambda^2 H_2 + \ldots) \times$$
$$(1 - i\lambda S - \lambda^2 S^2/2 + \ldots)$$

Equating terms of the same order of magnitude we get

$$H_0' = H_0$$
$$H_1' = H_1 + i[S,H_0]$$
$$H_2' = H_2 + (1/2)[iS,(H_1 + H_1')]$$
$$H_3' = H_3 + i[S,H_2] - (1/3)[S,[S,(H_1 + (1/2)H_1')]]$$
$$H_4' = H_4 + i[S,H_3] - (1/4)[S,[S,(H_2 + H_2')]] + (1/12) \times$$
$$[iS,[S,[S,H_1']]] \qquad (2.20)$$

The proper Hermitian transformation function S has been found by Herman and Shaffer[15] and the treatment has been extended by Goldsmith, Amat, and Nielsen[16] to apply to energy calculations through the fourth order of approximation. If we perform the contact transformation, however, a part of the Hamiltonian formally belonging to H_n' becomes of the order of magnitude of H_{n+1}'. Hence after contact transforming the Hamiltonian we need to regroup the terms in true orders of magnitude. This transformed and regrouped Hamiltonian is

$$H' = h_0' + h_1' + h_2' + h_3' + h_4' \qquad (2.21)$$

where

$$h_n^{(m)} = H_n + (1/m)[iS,h_{n-1}^{(m+1)}]_V + (1/m)[iS,h_{n-2}^{(m+1)}]_R \qquad (2.22)$$

and
$$[iS,H]_V = (1/2)[iS_V,H_V]\{S_R,H_R\}$$
$$[iS,H]_R = (1/2)\{S_V,H_V\}[iS_R,H_R] \quad (2.23)$$

The subscripts V and R denote the vibrational and rotational part, respectively, of the corresponding operators. To be able to calculate vibration-rotation energies to the fourth order, we need to subject H' to a second contact transformation $\mathcal{T}$ such that h_0', h_1', and h_2' will be diagonal in the vibrational quantum numbers in the representation in which h_o' is diagonal in the vibrational quantum numbers. This contact transformation, too, will necessitate regrouping of terms in true orders of magnitude. Thus H' is once again transformed and once again regrouped to

$$H^{@} = \mathcal{T} H' \mathcal{T}^{-1} = \exp(i\sigma)H'\exp(-i\sigma) = h_0^{@} + h_1^{@} + h_2^{@} + h_3^{@} + h_4^{@} \quad (2.24)$$

where now $h_0^{@}$, $h_1^{@}$, and $h_2^{@}$ are diagonal in the vibrational quantum numbers in the representation in which h_0' is diagonal.The proper Hermitian transformation function σ has been found by Goldsmith, Amat and Nielsen.[17]

For the asymmetric-rotator case, and for given quantum number J, it has been found that through the fourth order of approximation the Hamiltonian in matrix form in a symmetric-top basis can be cast into the Wang form[18,19] as shown in Figure 2.1.For the orthorhombic point group symmetry to which H_2O-type molecules belong, all matrix elements outside the four diagonal blocks E^+, E^-, O^+,and O^- along the main diagonal vanish.[20] Thus when we specialize our Hamiltonian we need not retain terms that do not have matrix elements falling inside the blocks E^+, E^-, O^+ and O^-, i.e., we shall take into account only those terms that are of even power in the rotational angular momentum components P_α. We shall, moreover, not explicitly consider pure vibrational terms as our interest lies in the detailed rotational structure for given vibrational state. The third and fourth-order terms nondiagonal in any of the vibrational quantum numbers can be discarded as it is possible to show that these do not contribute to the vibration-rotation energy up to the fourth order.[21]

E^+	I_2	II_2	II_1
I_2	E^-	II_1	II_2
II_2	II_1	O^+	I_2
II_1	II_2	I_2	O^-

Figure 2.1

III. THE VIBRATION-ROTATION HAMILTONIAN OF H_2O -TYPE MOLECULES

Since any triatomic molecule is necessarily planar, we choose our molecular frame so that the x-y plane is also the plane of the molecule and the origin is at the instantaneous center of mass . We also hold this frame fixed with respect to the equilibrium configuration of the molecule. Thus we have:

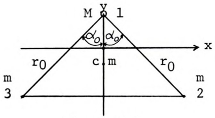

Figure 3.1
Equilibrium Configuration of the H_2O-type Molecule

$$z_1' = z_2' = z_3' = 0 \qquad (3.1a)$$

$$\begin{aligned} &m(x_2'+x_3') + Mx_1' = 0 \\ &m(y_2'+y_3') + My_1' = 0 \end{aligned} \qquad (3.1b)$$

$$mr_0\sin\alpha_0(y_2'-y_3') = (1/2)\ r_0\cos\alpha_0(2x_1'-x_2'-x_3') \qquad (3.1c)$$

where r_0, α_0, m and M are shown in Figure 3.1, and μ is the reduced mass

$$\mu = 2mM/(2m + M) \qquad (3.2)$$

Equation (3.1a) is the condition of planarity, and equations (3.1b) and (3.1c) are the Eckart conditions (see Appendix I).

From the geometry as shown in Figure 3.1 and equations (3.1b) we have

$$\begin{aligned} x_1^0 &= -x_2^0 = r_0\sin\alpha_0 \\ y_1^0 &= y_2^0 = -\ r_0\cos\alpha_0/2m \\ x_3^0 &= 0 \quad y_3^0 = \ r_0\cos\alpha_0/M \end{aligned} \qquad (3.3)$$

The transformation from the mass-adjusted coordinates $m_i^{1/2}\alpha_i$, ($m_1 = m_2 = m$, $m_3 = M$; $\alpha = x,y,z$) to normal coordinates Q_n ($n = 1,2,3$) is given in Appendix I. The coefficients l_{in}^{α} of this transformation are listed in Table I.

Table I. The coefficients l_{in}^{α} of the transformation to normal coordinates

$l_{11}^{x} = 0$	$l_{11}^{y} = (\mu/M)^{1/2}\sin\gamma$
$l_{21}^{x} = \cos\gamma/2^{1/2}$	$l_{21}^{y} = -1/2(\mu/m)^{1/2}\sin\gamma$
$l_{31}^{x} = -\cos\gamma/2^{1/2}$	$l_{31}^{y} = -1/2(\mu/m)^{1/2}\sin\gamma$
$l_{12}^{x} = 0$	$l_{12}^{y} = (\mu/M)^{1/2}\cos\gamma$
$l_{22}^{x} = -\sin\gamma/2^{1/2}$	$l_{22}^{y} = -1/2(\mu/m)^{1/2}\cos\gamma$
$l_{32}^{x} = \sin\gamma/2^{1/2}$	$l_{32}^{y} = -1/2(\mu/m)^{1/2}\cos\gamma$
$l_{13}^{x} = (\mu/M)(M/\mu_3)^{1/2}$	$l_{13}^{y} = 0$
$l_{23}^{x} = -(\mu/2m)(m/\mu_3)^{1/2}$	$l_{23}^{y} = (\mu/m)(m/\mu_3)^{1/2}\cot\alpha_0$
$l_{33}^{x} = -(\mu/2m)(m/\mu_3)^{1/2}$	$l_{33}^{y} = -(\mu/m)(m/\mu_3)^{1/2}\cot\alpha_0$
$l_{in}^{z} = 0$, $i = 1,2,3$; $n = 1,2,3$	

In Table I, μ_3 and γ are constants defined in the following equations:

$$\mu_3 = \mu[1 + (\mu/2)\cot^2\alpha_0] \quad (3.4)$$

$$\sin\gamma = +(1 - \{\Delta k/[(\Delta k)^2 + 4k_{12}^2]^{1/2}\})^{1/2}/2^{1/2}$$

$$\cos\gamma = +(1 - \sin^2\gamma)^{1/2} \quad ; \Delta k = k_{11} - k_{22} \quad (3.5)$$

The Coriolis coupling coefficients ζ_{mn}^{α} defined in Appendix I can now be constructed from the coefficients l_{in}^{α}. Those that are nonzero are listed in Table II. Since the only nonzero Coriolis coupling coefficients are those with superscript z, this superscript is superfluous and omitted henceforth.

Table II. Coriolis coupling coefficients ζ_{mn}^{α}

$$\zeta_{13} = -\zeta_{31} = (I_x/I_z)^{1/2}\cos\gamma - (I_y/I_z)^{1/2}\sin\gamma$$

$$\zeta_{23} = -\zeta_{32} = (I_x/I_z)^{1/2}\sin\gamma - (I_y/I_z)^{1/2}\cos\gamma$$

$$\zeta_{mn}^{\alpha} = -\zeta_{nm}^{\alpha} = 0, \quad \alpha = x, y \; ; \; m \;\&\; n = 1, 2, 3$$

ζ_{13} and ζ_{23} are related by

$$\zeta_{13}^{2} + \zeta_{23}^{2} = 1 \tag{3.6}$$

The equilibrium moments of inertia in Table II are:

$$I_x = \mu r_0^{2}\cos^{2}\alpha_0$$

$$I_y = 2mr_0^{2}\sin^{2}\alpha_0$$

$$I_z = I_x + I_y \tag{3.7}$$

With l_{in}^{α} from Table I and α_i^0, β_i^0, γ_i^0 from (3.2). the nonzero coefficients of expansion of the instantaneous moments and products of inertia $a_i^{\alpha\alpha}$, $a_i^{\alpha\beta}$, $A_{ij}^{\alpha\alpha}$, $A_{ij}^{\alpha\beta}$, $A_{ij}^{\prime\alpha\alpha}$ and $A_{ij}^{\prime\alpha\beta}$ are found to be as listed in Tables III and IV.

The H_2O-type molecular configuration belongs to the symmetry point group C_{2v}. With equilibrium geometry as in Figure 3.1, the components of the rotational angular momentum P_x, P_y and P_z, and the components of the internal angular momentum p_x, p_y and p_z belong to irreducible representations of species B_1, A_2 and B_2, respectively, as given in Table V. Of the three components of the internal angular momentum we need to consider only one, namely p_z, since the vanishing of ζ^{α}_{mn} (α = x,y) means that $p_x = p_y = 0$. The transformation (AI.6) with the coefficients of transformation as listed in Table I, moreover, is such that the normal coordinates q_1, q_2 and q_3 belong to species A_1,A_1 and B_2, respectively. Table V gives the character table of point group C_{2v}. We include the operators q_a, P_α and p_z in that table showing to which species each of them belongs.

Table III. First-order coefficients $a^{\alpha\alpha}_{ij}$, $a^{\alpha\beta}_{ij}$

$a^{xx}_1 = 2I_x{}^{1/2}\sin\gamma$	$a^{xx}_2 = 2I_x{}^{1/2}\cos\gamma$
$a^{yy}_1 = 2I_y{}^{1/2}\cos\gamma$	$a^{yy}_2 = -2I_y{}^{1/2}\sin\gamma$
$a^{zz}_1 = a^{xx}_1 + a^{yy}_1 = -2I_z{}^{1/2}\zeta_{23}$	$a^{zz}_2 = a^{xx}_2 + a^{yy}_2 = 2I_z{}^{1/2}\zeta_{13}$
$a^{xy}_3 = -2(I_xI_y/I_z)^{1/2} = a^{yx}_3$	

Since the Hamiltonian must be invariant under all symmetry operations of C_{2v}, terms in the Hamiltonian that do not satisfy this condition must vanish identically, i.e., their corresponding coefficients are zero. Thus, for instance, all operator terms in which q_3 appears in odd power have -a priori- zero coefficients if P_α and/or p_z appear in

Table IV. Second-order coefficients $A_{ij}^{\alpha\alpha}$, $A_{ij}^{\alpha\beta}$, $A_{ij}^{\prime\alpha\alpha}$, $A_{ij}^{\prime\alpha\beta}$

$A_{11}^{xx} = \sin^2\gamma$ $\qquad A_{11}^{yy} = \cos^2\gamma$ $\qquad A_{11}^{zz} = 1$

$A_{22}^{xx} = \cos^2\gamma$ $\qquad A_{22}^{yy} = \sin^2\gamma$ $\qquad A_{22}^{zz} = 1$

$A_{33}^{xx} = I_x/I_z$ $\qquad A_{33}^{yy} = I_y/I_z$ $\qquad A_{33}^{zz} = 1$

$A_{13}^{xy} = A_{31}^{yx} = -(I_x/I_z)^{1/2}\cos\gamma$ $\qquad A_{23}^{xy} = A_{32}^{yx} = -(I_x/I_z)^{1/2}\sin\gamma$

$A_{31}^{xy} = A_{13}^{yx} = -(I_y/I_z)^{1/2}\sin\gamma$ $\qquad A_{32}^{xy} = A_{23}^{yx} = -(I_y/I_z)^{1/2}\cos\gamma$

$A_{11}^{\prime zz} = \zeta_{23}^2$ $\qquad A_{22}^{\prime zz} = \zeta_{13}^2$ $\qquad A_{33}^{\prime zz} = 0$

$A_{12}^{\prime zz} = A_{21}^{\prime zz} = -\zeta_{13}\zeta_{23}$

$A_{ii}^{\prime\alpha\alpha} = A_{ii}^{\alpha\alpha}$; $\alpha = x,y \quad i = 1,2,3$

$A_{ij}^{\prime\alpha\beta} = A_{ij}^{\alpha\beta}$; $\alpha = x,y \quad \beta = x,y \quad ij = 13,23,31,32$

TableV. Character table of point group C_{2v} and symmetry species of the operators appearing in the Hamiltonian

Operators	Group elements				Species
	E	$C_2(y)$	$\sigma(xy)$	$\sigma(yz)$	
q_1, q_2	1	1	1	1	A_1
q_3, P_z, p_z	1	-1	1	-1	B_2
P_x	1	-1	-1	1	B_1
P_y	1	1	-1	-1	A_2

those terms in even power. Using this symmetry consideration, we can avoid evaluation of coefficients of expansion of $\mu_{\alpha\beta}$ which ultimately would be found to vanish. One notes also, that in the potential energy part of the Hamiltonian, q_1 and q_2 appear symmetrically, but not q_3. This is due to the fact that q_1 and q_2 both belong to the totally symmetric species A_1, while q_3 belongs to species B_2. Expanding $\mu_{\alpha\beta}$ in (AII.2) and using $I_{\alpha\alpha}$ and $I_{\alpha\beta}$ from (AI.13), the coefficients of the expansion can be shown to be as follows

$$\begin{aligned}
&\text{zeroth order:} && [\alpha\beta*] = \delta_{\alpha\beta}/I_{\alpha\beta} \\
&\text{first order:} && [\alpha\beta*a] = -a_a^{\alpha\beta}/I_\alpha I_\beta \\
&\text{second order:} && [\alpha\beta*ab] = [\textstyle\sum_\delta (a_a^{\alpha\delta} a_b^{\beta\delta} + a_b^{\alpha\delta} a_a^{\beta\delta})/I_\delta - (A'_{ab} + A'_{ba})]/2I_\alpha I_\beta(1+\delta_{ab}) \\
&\text{third order:} && [\alpha\beta*abc] = \textstyle\sum_P [\{ -\sum_{\delta\varepsilon} a_a^{\alpha\delta} a_b^{\beta\varepsilon} a_c^{\delta\varepsilon}/I_\delta I_\varepsilon + (a_a^{\alpha\delta} A'^{\beta\delta}_{bc} + a_a^{\beta\delta} A'^{\alpha\delta}_{bc})/I_\delta \}/6I_\alpha I_\beta]
\end{aligned} \tag{3.8}$$

In the expression for $[\alpha\beta*abc]$ $\sum_P$ denotes summation over all distinct permutations of a, b, and c.

Goldsmith et al,[6] and Watson[7] have obtained general expressions for the coefficients of expansion of $\mu_{\alpha\beta}$. Equations (3.8) above have been obtained from the general coefficients of expansion of $\mu_{\alpha\beta}$ of Goldsmith et al. The fourth-order coefficients $[\alpha\beta*abcd]$ which appear only in the fourth-order Hamiltonian are not needed since they appear in the final form of the Hamiltonian as corrections to the rotational constants of the rigid rotator. Since the latter are of order zero, these fourth-order corrections are negligible and hence discarded. The same argument also applies to other terms which originally stand in H_4. Therefore, although their detailed expressions have been obtained, we shall merely list them in a simplified version of the notation used in (2.15). The coefficients in (3.8) are not tabulated since what is really needed are not these coefficients, but the coefficients of the terms in the Hamiltonian (2.15). Of the latter, those that symmetry allows to be nonvanishing are included below:

$$H_0 = (1/2)[(P_x{}^2/I_x + P_y{}^2/I_y + P_z{}^2/I_z) + (p_1{}^2/\lambda_1{}^{1/2} + p_2{}^2/\lambda_2{}^{1/2} + p_3{}^2/\lambda_3{}^{1/2})/\hbar] + (\lambda_1{}^{1/2}q_1{}^2 + \lambda_2{}^{1/2}q_2{}^2 + \lambda_3{}^{1/2}q_3{}^2)/2\hbar \qquad (3.9a)$$

$$H_1 = [(xx*-*1)q_1 + (xx*-*2)q_2]P_x{}^2 + [(yy*-*1)q_1 + (yy*-*2)q_2]P_y{}^2 + [(zz*-*1)q_1 + (zz*-*2)q_2]P_z{}^2 + (xy*-*3)q_3(P_xP_y + P_yP_x) + 2\pi\hbar c(k_{111}q_1{}^3 + k_{112}q_1{}^2q_2 + k_{122}q_1q_2{}^2 + k_{133}q_1q_3{}^2 + k_{222}q_2{}^3 + k_{233}q_2q_3{}^2) \qquad (3.9b)$$

$$H_2 = [(xx*-*11)q_1{}^2 + (xx*-*12)q_1q_2 + (xx*-*22)q_2{}^2 + (xx*-*33)q_3{}^2]P_x{}^2 + [(yy*-*11)q_1{}^2 + (yy*-*12)q_1q_2 + (yy*-*22)q_2{}^2 + (yy*-*33)q_3{}^2]P_y{}^2 + [(zz*-*11)q_1{}^2 + (zz*-*12)q_1q_2 + (zz*-*22)q_2{}^2 + (zz*-*33)q_3{}^2]P_z{}^2 + [(xy*-*13)q_1q_3 + (xy*-*23)q_2q_3](P_xP_y + P_yP_x) + [(z*3*11)(q_1{}^2p_3 + p_3q_1{}^2) + (z*3*12)(q_1q_2p_3 + p_3q_1q_2) + (z*3*22)(q_2{}^2p_3 + p_3q_2{}^2) + (z*1*13)(q_1q_3p_1 + p_1q_1q_3) + (z*1*23)(q_2q_3p_1 + p_1q_2q_3) + (z*2*13)(q_1q_3p_2 + p_2q_1q_3) + (z*2*23)(q_2q_3p_2 + p_2q_2q_3)]P_z + -(\hbar^2/8)(1/I_x + 1/I_y + 1/I_z) + 2\pi\hbar c(k_{1111}q_1{}^4 + k_{1112}q_1{}^3q_2 + k_{1122}q_1{}^2q_2{}^2 + k_{1133}q_1{}^2q_3{}^2 + k_{1222}q_1q_2{}^3 + k_{1233}q_1q_2q_3{}^2 + \ldots..$$

$$\ldots + k_{2222}q_2^4 + k_{2233}q_2^2q_3^2 + k_{3333}q_3^4) +$$
$$(-*33*11)(q_1^2p_3^2+p_3^2q_1^2) + (-*33*12)(q_1q_2p_3^2+p_3^2q_1q_2) +$$
$$(-*33*22)(q_2^2p_3^2+p_3^2q_2^2) + (-*13*13)(q_1q_3p_1p_3+p_1p_3q_1q_3) +$$
$$(-*23*13)(q_1q_3p_2p_3+p_2p_3q_1q_3) + (-*13*23)(q_2q_3p_1p_3+p_1p_3q_2q_3) +$$
$$(-*23*23)(q_2q_3p_2p_3+p_2p_3q_2q_3) + (-*11*33)(q_3^2p_1^2+p_1^2q_3^2) +$$
$$(-*12*33)(q_3^2p_1p_2+p_1p_2q_3^2) + (-*22*33)(q_3^2p_2^2+p_2^2q_3^2) \qquad (3.9c)$$

$$H_3 = [(xx*-*111)q_1^3 + (xx*-*222)q_2^3 + (xx*-*112)q_1^2q_2 + (xx*-*122)q_1q_2^2$$
$$+ (xx*-*133)q_1q_3^2 + (xx*-*233)q_2q_3^2]P_x^2 + [(yy*-*111)q_1^3 +$$
$$(yy*-*222)q_2^3 + (yy*-*112)q_1^2q_2 + (yy*-*122)q_1q_2^2 +$$
$$(yy*-*133)q_1q_3^2 + (yy*-*233)q_2q_3^2]P_y^2 + [(zz*-*111)q_1^3 +$$
$$(zz*-*222)q_2^3 + (zz*-*112)q_1^2q_2 + (zz*-*122)q_1q_2^2 +$$
$$(zz*-*133)q_1q_3^2 + (zz*-*233)q_2q_3^2]P_z^2 + [(xy*-*113)q_1^2q_3 +$$
$$(xy*-*123)q_1q_2q_3 + (xy*-*223)q_2^2q_3 + (xy*-*333)q_3^3](P_xP_y + P_yP_x) +$$
$$(-\hbar^2/4)[((xx*-*1) + (yy*-*1) + (zz*-*1))q_1 +$$
$$((xx*-*2) + (yy*-*2) + (zz*-*2))q_2] +$$
$$[(z*3*111)(q_1^3p_3+p_3q_1^3) + (z*3*112)(q_1^2q_2p_3+p_3q_1^2q_2) + (z*3*122)\mathrm{X}$$
$$(q_1q_2^2p_3+p_3q_1q_2^2) + (z*3*222)(q_2^3p_3+p_3q_2^3) + (z*3*133)(q_1q_3^2p_3+$$
$$p_3q_1q_3^2) + (z*3*233)(q_2q_3^2p_3+p_3q_2q_3^2) + (z*1*113)(q_1^2q_3p_1+p_1q_1^2q_3)$$
$$+ (z*1*123)(q_1q_2q_3p_1+p_1q_1q_2q_3) + (z*1*223)(q_2^2q_3p_1+p_1q_2^2q_3) +$$
$$(z*1*333)(q_3^3p_1+p_1q_3^3) + (z*2*113)(q_1^2q_3p_2+p_2q_1^2q_3) + (z*2*123)\mathrm{X}$$
$$(q_1q_2q_3p_2+p_2q_1q_2q_3) + (z*2*223)(q_2^2q_3p_2+p_2q_2^2q_3) + (z*2*333)\mathrm{X}$$
$$(q_3^3p_2+p_2q_3^3)]P_z + 2\pi c\hbar[k_{11111}q_1^5+k_{22222}q_2^5+k_{11112}q_1^4q_2+k_{12222}q_1q_2^4$$
$$+k_{13333}q_1q_3^4+k_{23333}q_2q_3^4+k_{11122}q_1^3q_2^2+k_{11222}q_1^2q_2^3+k_{11133}q_1^3q_3^2+$$
$$k_{22233}q_2^3q_3^2+k_{11233}q_1^2q_2q_3^2+k_{12233}q_1q_2^2q_3^2] + \qquad \ldots\ldots$$

$$
\begin{aligned}
.. + [&(-*33*111)(q_1{}^3p_3{}^2+p_3{}^2q_1{}^3) + (-*33*112)(q_1{}^2q_2p_3{}^2+p_3{}^2q_1{}^2q_2) + \\
&(-*33*122)(q_1q_2{}^2p_3{}^2+p_3{}^2q_1q_2{}^2) + (-*33*222)(q_2{}^3p_3{}^2+p_3q_2{}^3) + \\
&(-*11*133)(q_1q_3{}^2p_1{}^2+p_1q_1q_3{}^2) + (-*11*233)(q_2q_3{}^2p_1{}^2+p_1{}^2q_2q_3{}^2) + \\
&(-*12*133)(q_1q_3{}^2p_1p_2+p_1p_2q_1q_3{}^2) + (-*12*233)(q_2q_3{}^2p_1p_2+p_1p_2q_2q_3^2) \\
&+ (-*22*133)(q_1q_3{}^2p_2{}^2+p_2{}^2q_1q_3{}^2) + (-*22*233)(q_2q_3{}^2p_2{}^2+p_2{}^2q_2q_3{}^2) \\
&+ (-*13*113)(q_1{}^2q_3p_1p_3+p_1p_3q_1{}^2q_3) + (-*13*223)(q_2^2q_3p_1p_3+p_1p_3q_2^2q_3) \\
&+ (-*13*123)(q_1q_2q_3p_1p_3+p_1p_3q_1q_2q_3)+(-*23*113)(q_1^2q_3p_2p_3+p_2p_3q_1^2q_3) \\
&+(-*23*123)(q_1q_2q_3p_2p_3+p_2p_3q_1q_2q_3)+(-*23*223)(q_2^2q_3p_2p_3+p_2p_3q_2^2q_3)]
\end{aligned}
\tag{3.9d}
$$

$$
\begin{aligned}
H_4 = &\sum_{\alpha\beta}\sum_{a\leqslant b\leqslant c\leqslant d}(\alpha\beta*-*abcd)q_aq_bq_cq_dP_\alpha P_\beta + \\
&\sum_{\alpha e}\sum_{;a\leqslant b\leqslant c\leqslant d}(\ *e*abcd)(q_aq_bq_cq_dp_e+ p_eq_aq_bq_cq_d)P_\alpha + \\
&\sum_{e\leqslant f;}\sum_{a\leqslant b\leqslant c\leqslant d}(-*ef*abcd)(q_aq_bq_cq_dp_ep_f + p_ep_fq_aq_bq_cq_d) + \\
&(-\hbar^2/4)\sum_{\alpha}\sum_{a\leqslant b}(\alpha\alpha*-*ab)q_aq_b + \\
&2\pi c\hbar\sum_{\substack{a\leqslant b\leqslant c\leqslant \\ d\leqslant e\leqslant f}}k_{abcdef}q_aq_bq_cq_dq_eq_f
\end{aligned}
\tag{3.9e}
$$

The detailed expressions of the coefficients in (3.9b) to (3.9d) are listed in Tables VI to X. Table XI lists the nonzero coefficients in the fourth-order Hamiltonian (3.9e)

Each of the coefficients in Tables VII to XI is equal to coefficient or coefficients of the same type, that could be obtained by permuting the indices of vibrational operators in the original one.

Table VI. Coefficients $(\alpha\beta$*-*a) and (z*b*a) in the first-order Hamiltonian H_1

(xx*-*1)	$= -(\hbar^2/\lambda_1)^{1/4} a_1^{xx}/2I_x^{\,2}$	(xx*-*2)	$= -(\hbar^2/\lambda_2)^{1/4} a_2^{xx}/2I_x^{\,2}$
(yy*-*1)	$= -(\hbar^2/\lambda_1)^{1/4} a_1^{yy}/2I_y^{\,2}$	(yy*-*2)	$= -(\hbar^2/\lambda_2)^{1/4} a_2^{yy}/2I_y^{\,2}$
(zz*-*1)	$= -(\hbar^2/\lambda_1)^{1/4} a_1^{zz}/2I_z^{\,2}$	(zz*-*2)	$= -(\hbar^2/\lambda_2)^{1/4} a_2^{zz}/2I_z^{\,2}$
(xy*-*3)	$= -(\hbar^2/\lambda_3)^{1/4} a_3^{xy}/2I_xI_y$	(yx*-*3)	$= -(\hbar^2/\lambda_3)^{1/4} a_3^{xy}/2I_xI_y$
(z*3*1)	$= -(\lambda_3/\lambda_1)^{1/4} \zeta_{13}/I_z$	(z*1*3)	$= +(\lambda_1/\lambda_3)^{1/4} \zeta_{13}/I_z$
(z*3*2)	$= -(\lambda_3/\lambda_2)^{1/4} \zeta_{23}/I_z$	(z*2*3)	$= +(\lambda_2/\lambda_3)^{1/4} \zeta_{23}/I_z$

Table VII. Coefficients $(\alpha\beta$*-*ab) in the second-order Hamiltonian H_2

(xx*-*11)	$= 3\hbar\sin^2\gamma/2I_x^{\,2}\lambda_1^{\,1/2}$	(yy*-*11)	$= 3\hbar\cos^2\gamma/2I_y^{\,2}\lambda_1^{\,1/2}$
(xx*-*12)	$= 4\hbar\sin\gamma\cos\gamma/I_x^2(\lambda_1\lambda_2)^{1/4}$	(zz*-*11)	$= 3\hbar\,\zeta_{23}^{\,2}/2I_z^{\,2}\lambda_1^{\,1/2}$
(yy*-*12)	$= -4\hbar\sin\gamma\cos\gamma/I_y^2(\lambda_1\lambda_2)^{1/4}$	(zz*-*22)	$= 3\hbar\,\zeta_{13}^{\,2}/2I_z^{\,2}\lambda_2^{\,1/2}$
(xx*-*22)	$= 3\hbar\cos^2\gamma/2I_x^{\,2}\lambda_2^{\,1/2}$	(yy*-*22)	$= 3\hbar\sin^2\gamma/2I_y^{\,2}\lambda_2^{\,1/2}$
(xx*-*33)	$= 3\hbar/2I_zI_x\lambda_3^{\,1/2}$	(yy*-*33)	$= 3\hbar/2I_zI_y\lambda_3^{\,1/2}$
(zz*-*12)	$= -3\hbar\,\zeta_{13}\zeta_{23}/I_z^{\,2}(\lambda_1\lambda_2)^{1/4}$	(zz*-*33)	$= 0$
(xy*-*13)	$= -3\hbar[(I_x/I_z)^{1/2}\cos\gamma+(I_y/I_z)^{1/2}\sin\gamma]/2I_xI_y(\lambda_1\lambda_3)^{1/4}$		
(xy*-*23)	$= \hbar[5(I_x/I_z)^{1/2}\sin\gamma-3(I_y/I_z)^{1/2}\cos\gamma]/2I_xI_y(\lambda_2\lambda_3)^{1/4}$		
(yx*-*13)	= (xy*-*13)	(yx*-*23)	= (xy*-*23)

Table VIII. Coefficients (α*c*ab) in the second-order Hamiltonian H_2

$(z*3*11) = \hbar^{1/2}\lambda_3^{1/4}a_1^{zz}\zeta_{13}/2\lambda_1^{1/2}I_z^2$
$(z*3*22) = \hbar^{1/2}\lambda_3^{1/4}a_2^{zz}\zeta_{23}/2\lambda_2^{1/2}I_z^2$
$(z*3*12) = \hbar^{1/2}\lambda_3^{1/4}(a_1^{zz}\zeta_{23} + a_2^{zz}\zeta_{13})/2(\lambda_1\lambda_2)^{1/4}I_z^2$
$(z*1*13) = -\hbar^{1/2}a_1^{zz}\zeta_{13}/2\lambda_3^{1/4}I_z^2$
$(z*1*23) = -\hbar^{1/2}\lambda_1^{1/4}a_2^{zz}\zeta_{13}/2(\lambda_2\lambda_3)^{1/4}I_z^2$
$(z*2*13) = -\hbar^{1/2}\lambda_2^{1/4}a_1^{zz}\zeta_{23}/2(\lambda_1\lambda_3)^{1/4}I_z^2$
$(z*2*23) = -\hbar^{1/2}a_2^{zz}\zeta_{23}/2\lambda_3^{1/4}I_z^2$

Table IX. Coefficients (-*cd*ab) in the second-order Hamiltonian H_2

$(-*33*11) = (\lambda_3/\lambda_1)^{1/2}\zeta_{13}^2/4I_z$	$(-*11*33) = (\lambda_1/\lambda_3)^{1/2}\zeta_{13}^2/4I_z$
$(-*33*12) = (\lambda_3^2/\lambda_1\lambda_2)^{1/4}\zeta_{13}\zeta_{23}/2I_z$	$(-*12*33) = (\lambda_1\lambda_2/\lambda_3^2)^{1/4}\zeta_{13}\zeta_{23}/2I_z$
$(-*33*22) = (\lambda_3/\lambda_2)^{1/2}\zeta_{23}^2/4I_z$	$(-*22*33) = (\lambda_2/\lambda_3)^{1/2}\zeta_{23}^2/4I_z$
$(-*23*13) = -(\lambda_2/\lambda_1)^{1/4}\zeta_{13}\zeta_{23}/2I_z$	$(-*13*23) = -(\lambda_1/\lambda_2)^{1/4}\zeta_{13}\zeta_{23}/2I_z$
$(-*23*23) = -\zeta_{23}^2/2I_z$	$(-*13*13) = -\zeta_{13}^2/2I_z$

Table X. Coefficients ($\alpha\beta$ *-*abc) in the third-order Hamiltonian H_3

$(xx*-*111) = -\hbar^{3/2}\sin^3\gamma/I_x^{5/2}\lambda_1^{3/4}2$
$(xx*-*222) = -\hbar^{3/2}\cos^3\gamma/I_x^{5/2}\lambda_2^{3/4}2$

Table X (cont'd)

$(xx^*\text{-}^*112) = -11\hbar^{3/2}\sin^2\gamma\cos\gamma/6I_x{}^{5/2}\lambda_1{}^{1/2}\lambda_2{}^{1/4}$

$(xx^*\text{-}^*122) = -11\hbar^{3/2}\sin\gamma\cos^2\gamma/6I_x{}^{5/2}\lambda_1{}^{1/4}\lambda_2{}^{1/2}$

$(xx^*\text{-}^*133) = -\hbar^{3/2}[2\sin\gamma + (I_x/I_y)^{1/2}\cos\gamma]/2I_zI_x{}^{3/2}\lambda_1{}^{1/4}\lambda_3{}^{1/2}$

$(xx^*\text{-}^*233) = -\hbar^{3/2}[2\cos\gamma + (I_x/I_y)^{1/2}\sin\gamma]/2I_zI_x{}^{3/2}\lambda_2{}^{1/4}\lambda_3{}^{1/2}$

$(yy^*\text{-}^*111) = -\hbar^{3/2}\cos^3\gamma/2I_y{}^{5/2}\lambda_1{}^{3/4}$

$(yy^*\text{-}^*222) = -5\hbar^{3/2}\sin^3\gamma/6I_y{}^{5/2}\lambda_2{}^{3/4}$

$(yy^*\text{-}^*112) = +11\hbar^{3/2}\sin\gamma\cos^2\gamma/6I_y{}^{5/2}\lambda_1{}^{1/2}\lambda_2{}^{1/4}$

$(yy^*\text{-}^*122) = -11\hbar^{3/2}\sin^2\gamma\cos\gamma/6I_y{}^{5/2}\lambda_1{}^{1/4}\lambda_2{}^{1/2}$

$(yy^*\text{-}^*133) = -\hbar^{3/2}[2\cos\gamma + (I_y/I_x)^{1/2}\sin\gamma]/2I_y{}^{3/2}I_z\lambda_1{}^{1/4}\lambda_3{}^{1/2}$

$(yy^*\text{-}^*233) = +\hbar^{3/2}[(8/3)\sin\gamma - (I_y/I_x)^{1/2}\cos\gamma]/2I_y{}^{3/2}I_z\lambda_2{}^{1/4}\lambda_3{}^{1/2}$

$(zz^*\text{-}^*111) = +\hbar^{3/2}\zeta_{23}{}^3/2I_z{}^{5/2}\lambda_1{}^{3/4}$

$(zz^*\text{-}^*222) = -\hbar^{3/2}\zeta_{13}{}^3/2I_z{}^{5/2}\lambda_2{}^{3/4}$

$(zz^*\text{-}^*112) = -3\hbar^{3/2}\zeta_{13}\zeta_{23}{}^2/2I_z{}^{5/2}\lambda_1{}^{1/2}\lambda_2{}^{1/4}$

$(zz^*\text{-}^*122) = +3\hbar^{3/2}\zeta_{23}\zeta_{13}{}^2/2I_z{}^{5/2}\lambda_1{}^{1/4}\lambda_2{}^{1/2}$

$(xy^*\text{-}^*113) = +\hbar^{3/2}[\sin\gamma\cos\gamma + (I_x/I_y)^{1/2}\cos^2\gamma + (I_y/I_x)^{1/2}\sin^2\gamma]/$
$2I_xI_yI_z{}^{1/2}\lambda_1{}^{1/2}\lambda_3{}^{1/4}$

$(xy^*\text{-}^*123) = +\hbar^{3/2}[3\cos^2\gamma + 7(I_y/I_x)^{1/2}\sin\gamma\cos\gamma - 8(I_x/I_y)^{1/2}\sin\gamma\cos\gamma -$
$4\sin^2\gamma]/6I_xI_yI_z{}^{1/2}(\lambda_1\lambda_2\lambda_3)^{1/4}$

$(xy^*\text{-}^*223) = +\hbar^{3/2}[\sin\gamma\cos\gamma + (I_x/I_y)^{1/2}\cos^2\gamma + (I_y/I_x)^{1/2}\sin^2\gamma]/$
$2I_xI_yI_z{}^{1/2}\lambda_3{}^{1/2}\lambda_3{}^{1/4}$

$(xy^*\text{-}^*333) = +\hbar^{3/2}/2(I_xI_yI_z{}^3)^{1/2}\lambda_3{}^{3/4}$

$(yx^*\text{-}^*113) = (xy^*\text{-}^*113)$, $(yx^*\text{-}^*223) = (xy^*\text{-}^*223)$

$(yx^*\text{-}^*123) = (xy^*\text{-}^*123)$, $(yx^*\text{-}^*333) = (xy^*\text{-}^*333)$

Table XI. Coefficients (α*d*abc) in the third-order Hamiltonian H_3

(z*3*111), (z*3*112), (z*3*122), (z*3*222), (z*3*133), (z*3*233), (z*1*113), (z*1*123), (z*1*223), (z*1*333), (z*2*113), (z*2*123), (z*2*223), (z*2*333)

The detailed forms of these coefficients are not required for our calculation.

Table XII. Nonvanishing coefficients in the fourth-order Hamiltonian H_4

(1) (αβ*-*abcd):

αβ	abcd
xx yy zz	1111, 1112, 1122, 1133, 1222, 2222, 2233, 3333
xy = yx	1113, 2223, 1123, 1223, 1333, 2333

(2) (α*e*abcd):

α	e	
z	1 2	1113, 2223, 1123, 1223, 1333, 2333
	3	1111, 1112, 1222, 2222, 1122, 1133, 1233, 2233

Table XII(cont'd)

(3) (-*ef*abcd):

ef	abcd
11	]
12 = 21	] 1133, 1233, 2233, 3333
22	]
13 = 31	]
23 = 32	] 1113, 1123, 1223, 2223, 1333, 2333
33	1111, 1112, 1122, 1222, 2222, 1133, 1233, 2233

(4) (αα*-*ab):

These coefficients have been listed in Table VII.

(5) k_{abcdef}:

abcdef = 111111, 222222, 333333, 111112, 122222, 111122, 112222,
111133, 113333, 222233, 223333, 111222, 111233, 122233,

The detailed forms of all these coefficients are not required for our calculation.

4. ONCE-TRANSFORMED HAMILTONIAN

The terms in H_1 that truly contribute to the first-order energy are absent in the case of asymmetric rotators. This is because there are no degenerate modes of vibration. The S function of Herman and Shaffer may expressed as[16]

$$S = \sum_{\alpha\beta}\Big\{ \sum_{a}[S;\alpha\beta;a;-]p_a P_\alpha P_\beta + \sum_{ab}([S;\alpha;-;ab]q_a q_b + [S;\alpha;ab;-]p_a p_b)P_\alpha\Big\} + \sum_{a\leqslant b\leqslant c}[S;-abc;-]p_a p_b p_c + \sum_{c;a\leqslant b}[S;-c;ab](q_a q_b p_c + p_c q_a q_b)/2 \tag{4.1}$$

the coefficients $[S;\alpha\beta;a;-]$, $[S;\alpha;-;ab]$, etc. being given in Tables XIII to XVI. We obtained H' of (2.21) from (2.20), (2.22), (2.23a) and (2.23b) with the aid of the commutation relations

$$[q_a, p_b] = i\hbar\delta_{ab} \quad ; \quad [P_\alpha, P_\beta] = -i\hbar P_\gamma, \text{ cyclic}$$

Throughout the calculations the vibrational operators were written in symmetric form as $(1/2)(q_a q_b \cdots p_n p_m \cdots + p_n p_m \cdots q_a q_b \cdots)$, but the rotational operators are not symmetrized. They will be symmetrized in the final stage of the calculations, and the symmetrized final results will be Hermitian. Since in (2.23a) the anti-commutator $\{S_R, H_R\}$ yields rotational operators in symmetric form, we "desymmetrized" them by subjecting the second terms to proper permutations of the indices. This procedure leads to terms having coefficients that consist of two parts, the second being a certain permutation of the first. Thus, for instance, a symmetric form

$$[Y;xy;11;12](1/2)(q_1q_2p_1^2 + p_1^2q_1q_2)(P_xP_y + P_yP_x)$$

would be desymmetrized to

$$([Y;xy;11;12] + [Y;yx;11;12])(1/2)(q_1q_2p_1^2 + p_1^2q_1q_2)P_xP_y$$

Table XIII. Coefficients $[S;\alpha\beta;a;-]$ in the first contact transformation

$[S;xx;1;-] = a_1^{xx}/2I_x^2\hbar^{3/2}\lambda_1^{3/4}$	$[S;yy;1;-] = a_1^{yy}/2I_y^2\hbar^{3/2}\lambda_1^{3/4}$
$[S;xx;2;-] = a_2^{xx}/2I_x^2\hbar^{3/2}\lambda_2^{3/4}$	$[S;yy;2;-] = a_2^{yy}/2I\ ^2\hbar^{3/2}\lambda_2^{3/4}$
$[S;zz;1;-] = a_1^{zz}/2I_z^2\hbar^{3/2}\lambda_1^{3/4}$	$[S;xy;3;-] = a_3^{xy}/2I_xI_y\hbar^{3/2}\lambda_3^{3/4}$
$[S;zz;2;-] = a_2^{zz}/2I_z^2\hbar^{3/2}\lambda_2^{3/4}$	$[S;yx;3;-] = a_3^{xy}/2I_xI_y\hbar^{3/2}\lambda_3^{3/4}$

Table XIV. Coefficients $[S;\alpha;-;ab]$ and $[S;\alpha;ab;-]$ in the first contact transformation

$$[S;z;-;13] = [S;z;-;31] = \zeta_{13}(\lambda_1+\lambda_3)/(\lambda_1-\lambda_3)I_z\lambda_1^{1/4}\lambda_3^{1/4}$$

$$[S;z;-;23] = [S;z;-;32] = \zeta_{23}(\lambda_2+\lambda_3)/(\lambda_2-\lambda_3)I_z\lambda_2^{1/4}\lambda_3^{1/4}$$

$$[S;z;13;-] = [S;z;31;-] = 2\zeta_{13}\lambda_1^{1/4}\lambda_3^{1/4}/(\lambda_1-\lambda_3)I_z\hbar^2$$

$$[S;z;23;-] = [S;z;32;-] = 2\zeta_{23}\lambda_2^{1/4}\lambda_3^{1/4}/(\lambda_2-\lambda_3)I_z\hbar^2$$

The once-transformed Hamiltonians, regrouped in true orders of magnitude with the aid of (2.22), are found to be as in (2.21), where

Table XV. Coefficients [S;-;abc;-] in the first contact transformation

$[S;-;111;-] = -4\pi c k_{111}/3\hbar^3\lambda_1^{1/2}$ $\quad$ $[S;-;222;-] = -4\pi c k_{222}/3\hbar^3\lambda_2^{1/2}$

$[S;-;112;-] = -4\pi c k_{112}\lambda_1/\hbar^3\lambda_2^{1/2}(4\lambda_1-\lambda_2) = [S;-;121;-] = [S;-;211;-]$

$[S;-;122;-] = -4\pi c k_{122}\lambda_2/\hbar^3\lambda_1^{1/2}(4\lambda_2-\lambda_1) = [S;-;212;-] = [S;-;221;-]$

$[S;-;133;-] = -4\pi c k_{133}\lambda_3/\hbar^3\lambda_1^{1/2}(4\lambda_3-\lambda_1) = [S;-;313;-] = [S;-;331;-]$

$[S;-;233;-] = -4\pi c k_{233}\lambda_3/\hbar^3\lambda_2^{1/2}(4\lambda_3-\lambda_2) = [S;-;323;-] = [S;-;332;-]$

Table XVI. Coefficients [S;-;c;ab] in the first contact transformation

$[S;-;1;11] = -2\pi c k_{111}/\hbar\lambda_1^{1/2}$ $\quad$ $[S;-;2;22] = -2\pi c k_{222}/\hbar\lambda_2^{1/2}$

$[S;-;2;11] = -2\pi c k_{112}(2\lambda_1-\lambda_2)/\hbar\lambda_2^{1/2}(4\lambda_1-\lambda_2)$

$[S;-;1;12] = -4\pi c k_{112}\lambda_1^{1/2}/\hbar(4\lambda_1-\lambda_2) = [S;-;1;21]$

$[S;-;2;12] = -4\pi c k_{122}\lambda_2^{1/2}/\hbar(4\lambda_2-\lambda_1) = [S;-;2;21]$

$[S;-;3;13] = -4\pi c k_{133}\lambda_3^{1/2}/\hbar(4\lambda_3-\lambda_1) = [S;-;3;31]$

$[S;-;1;22] = -2\pi c k_{122}(2\lambda_2-\lambda_1)/\hbar\lambda_1^{1/2}(4\lambda_2-\lambda_1)$

$[S;-;3;23] = -4\pi c k_{233}\lambda_3^{1/2}/\hbar(4\lambda_3-\lambda_2) = [S;-;3;32]$

$[S;-;1;33] = -2\pi c k_{133}(2\lambda_3-\lambda_1)/\hbar\lambda_1^{1/2}(4\lambda_3-\lambda_1)$

$[S;-;2;33] = -2\pi c k_{233}(2\lambda_3-\lambda_2)/\hbar\lambda_2^{1/2}(4\lambda_3-\lambda_2)$

$$h_0' = H_o \tag{4.2}$$

H_o is given in (3.9a)

$$h_1' = H_1 + [iS, H_0]_V = 0 \tag{4.3}$$

$$\begin{aligned} h_2' = {} & H_2 + [iS, H_1/2]_V + [iS, H_0]_R = \\ & \sum_{\alpha\beta\gamma\delta} (2;\alpha\beta\gamma\delta;-;-) P_\alpha P_\beta P_\gamma P_\delta + \sum_{\alpha\beta\gamma} \sum_a (2;\alpha\beta\gamma;a;-) p_a P_\alpha P_\beta P_\gamma + \\ & \sum_{\alpha\beta} \sum_{a \leqslant b} [(2;\alpha\beta;ab;-) p_a p_b + (2;\alpha\beta;-;ab) q_a q_b] P_\alpha P_\beta + \\ & \sum_\alpha \sum_{a \leqslant b \leqslant c} (2;\alpha;abc;-) p_a p_b p_c P_\alpha + \\ & \sum_{\alpha c;} \sum_{a \leqslant b} (2;\alpha;c;ab)(1/2)(q_a q_b p_c + p_c q_a q_b) P_\alpha + \\ & \sum_{a \leqslant b;} \sum_{c \leqslant d} (2;-;cd;ab)(1/2)(q_a q_b p_c p_d + p_c p_d q_a q_b) + \\ & \sum_{a \leqslant b \leqslant c \leqslant d} (2;-;-;abcd) q_a q_b q_c q_d \end{aligned} \tag{4.4}$$

Coefficients in the first sum are listed in Table XVII, and the rest of the coefficients are listed in Appendixes IV to X.

$$\begin{aligned} h_3' = {} & H_3 + [iS, (H_2 + (2/3)[iS, H_1/2]_V + (1/2)[iS, H_0]_R)]_V + \\ & [iS, H_1/2]_R = \\ & \sum_{\alpha\beta\gamma\delta} \sum_a (3;\alpha\beta\gamma\delta;-;a) q_a P_\alpha P_\beta P_\gamma P_\delta + \\ & \sum_{\alpha\beta\gamma} \sum_{ab} (3;\alpha\beta\gamma;b;a)(1/2)(q_a p_b + p_b q_a) P_\alpha P_\beta P_\gamma + \\ & \sum_{\alpha\beta} \sum_{a; b \leqslant c} (3;\alpha\beta;bc;a)(1/2)(q_a p_b p_c + p_b p_c q_a) P_\alpha P_\beta + \\ & \sum_{a \leqslant b \leqslant c} (3;\alpha\beta;-;abc) q_a q_b q_c P_\alpha P_\beta + h_3^* \end{aligned} \tag{4.5}$$

The coefficients appearing in (4.5) above are listed in Appendixes XI to XIV. h_3^* is the portion of h_3' that is discarded henceforth; it consists of terms of the types $\{q_a, p_b p_c p_d\} P_\alpha$, $\{q_a q_b q_c, p_d\} P_\alpha$ and pure vibrational terms which do not contribute to the energy through the fourth order of approximation.

$$
\begin{aligned}
h_4' = {} & H_4 + [iS,(H_3 + [iS/2,(H_2 + [iS,H_1/4]_V + [iS,H_0/3]_R]_V)]_V + \\
& [iS,H_1/3]_R)]_V + [iS,(H_2 + [iS,H_1/3]_V + [iS,H_0/2]_R)]_R \\
= {} & \sum_{\alpha\beta\gamma\delta\varepsilon\rho} (4;\alpha\beta,\gamma\delta\varepsilon\rho;-;-)\{P_\alpha P_\beta P_\gamma P_\delta P_\varepsilon P_\rho + P_\gamma P_\delta P_\varepsilon P_\rho P_\alpha P_\beta\} + \\
& \sum_{\alpha\beta\gamma\delta} \sum_{a\leq b} \{(4;\alpha\beta\gamma\delta;-;ab)q_a q_b + (4;\alpha\beta\gamma\delta;ab;-)p_a p_b\} P_\alpha P_\beta P_\gamma P_\delta \\
& + h_4^* \qquad (4.6)
\end{aligned}
$$

The coefficients appearing in (4.6) are listed in Appendixes XV to XVII. h_4^* is the portion of h_4' that is discarded henceforth; it consists of pure vibrational terms, terms whose matrix elements in a symmetric-top basis fall outside the diagonal blocks E^+, E^-, O^+, O^-, and terms quadratic in the components of rotational angular momentum P_α. These terms either do not contribute to the energy through the fourth order of approximation, or represent negligible corrections to the terms retained in the final form of the Hamiltonian.

The first sum in (4.6) is not desymmetrized in the components of rotational angular momentum since h_4' is already in the form in which it will enter the final form of the Hamiltonian.One could also symmetrize the second sum at this point,but instead of doing so now, we shall symmetrize this sum later (Appendix XVI). We expect that identical coefficients in that appendix will automatically symmetrize the corresponding terms in this sum, and this is, in fact, the case.

Table XVII. Coefficients $(2;\alpha\beta\gamma\delta;-;-)$ in the second-order Hamiltonian h_2'

$$(2;xxyy;-;-) = -[(a_1^{xx}\,a_1^{yy})/\lambda_1 + (a_2^{xx}\,a_2^{yy})/\lambda_2]/8I_x^2I_y^2$$

$$(2;yyzz;-;-) = -[(a_1^{yy}a_1^{zz})/\lambda_1 + (a_2^{yy}a_2^{zz})/\lambda_2]/8I_y^2I_z^2$$

$$(2;zzxx;-;-) = -[(a_1^{zz}a_1^{xx})/\lambda_1 + (a_2^{zz}a_2^{xx})/\lambda_2]/8I_z^2I_x^2$$

$$(2;xyxy;-;-) = -(a_3^{xy})^2/8I_x^2\,I_y^2\,\lambda_3$$

$$(2;xxxx;-;-) = -[(a_1^{xx})^2/\lambda_1 + (a_2^{xx})^2/\lambda_2]/8I_x^4$$

$$(2;yyyy;-;-) = -[(a_1^{yy})^2/\lambda_1 + (a_2^{yy})^2/\lambda_2]/8I_y^4$$

$$(2;zzzz;-;-) = -[(a_1^{zz})^2/\lambda_1 + (a_2^{zz})^2/\lambda_2]/8I_z^4$$

$$(2;yyxx;-;-) = (2;xxyy;-;-)$$

$$(2;zzyy;-;-) = (2;yyzz;-;-)$$

$$(2;xxzz;-;-) = (2;zzxx;-;-)$$

$$(2;xyyx;-;-) = (2;yxxy;-;-) = (2;yxyx;-;-) = (2;xyxy;-;-)$$

5. TWICE-TRANSFORMED HAMILTONIAN

The second contact transformation that diagonalizes H in the vibrational quantum numbers through the second order of approximation has been constructed by Amat and Nielsen[16] from the basic Herman-Shaffer functions. The portion of this function that is needed in our case can be written as follows:

$$\begin{aligned}\sigma = &\sum_{\alpha\beta\gamma}\sum_{a}[\sigma;\alpha\beta\gamma;-;a]q_a P_\alpha P_\beta P_\gamma + \sum_{\alpha\beta}\sum_{ab}[\sigma;\alpha\beta;b;a](1/2)(q_a p_b + p_b q_a)P_\alpha P_\beta \\ &+\sum_{\alpha}\sum_{c;a\leqslant b}[\sigma;\alpha;ab;c](1/2)(q_c p_a p_b + p_a p_b q_c)P_\alpha + \\ &\sum_{a\leqslant b\leqslant c}\sum_{\alpha}[\sigma;\alpha;-;abc]q_a q_b q_c P_\alpha \end{aligned} \tag{5.1}$$

The coefficients $[\sigma;\alpha\beta\gamma;-;a]$, $[\sigma;\alpha\beta;b;a]$, etc., are given in Tables XVIII to XXI, with the constants A_{abc} and B_{abc} appearing in $[\sigma;\alpha;c;ab]$ and $[\sigma;\alpha;-;abc]$ as listed in Table XXII.

Expanding $\tau = \exp.(i\lambda^2\sigma)$ and $\tau^{-1} = \exp.(-i\lambda^2\sigma)$ in power series in σ and collecting terms of the same order of magnitude in $H^{@} = \tau H' \tau^{-1}$ we obtain:

$$\begin{aligned} H_0^{@} &= h_0' \\ H_1^{@} &= h_1' \\ H_2^{@} &= h_2' + i[\sigma, h_0'] \\ H_3^{@} &= h_3' + i[\sigma, h_1'] \\ H_4^{@} &= h_4' + i[\sigma, h_2'] - (1/2)[\sigma,[\sigma,h_0']] \end{aligned} \tag{5.2}$$

In (5.2) h_0' , h_1' , h_2' , etc., are the zeroth, first, second-order portion, etc., of the once-transformed Hamiltonian regrouped to true oreders of magnitude which we have obtained in Chapter 4 from the original once-transformed Hamiltonian with the aid of (2.22).

Table XVIII. Coefficients $[\sigma;\alpha\beta\gamma;-;a]$ in the second contact transformation.

$$[\sigma;zzz;-;3] = (2;zzz;3;-)/\lambda_3^{1/2}$$

$$[\sigma;xxz;-;3] = (2;xxz;3;-)/\lambda_3^{1/2} \qquad [\sigma;zxx;-;3] = (2;zxx;3;-)/\lambda_3^{1/2}$$

$$[\sigma;yyz;-;3] = (2;yyz;3;-)/\lambda_3^{1/2} \qquad [\sigma;zyy;-;3] = (2;zyy;3;-)/\lambda_3^{1/2}$$

$$[\sigma;xzx;-;3] = (2;xzx;3;-)/\lambda_3^{1/2} \qquad [\sigma;yzy;-;3] = (2;yzy;3;-)/\lambda_3^{1/2}$$

$$[\sigma;xyz;-;j] = [\sigma;zyx;-;j] = (2;xyz;j;-)/\lambda_j^{1/2}$$

$$[\sigma;xzy;-;j] = [\sigma;yzx;-;j] = (2;xzy;j;-)/\lambda_j^{1/2}$$

$$[\sigma;yxz;-;j] = [\sigma;zxy;-;j] = (2;yxz;j;-)/\lambda_j^{1/2}$$

$$j = 1,2$$

Table XIX. Coefficients $[\sigma;\alpha\beta;b;a]$ in the second contact transformation.

$$[\sigma;\alpha\alpha;j;j] = [(2;\alpha\alpha;jj;-) - (2;\alpha\alpha;-;jj)/\hbar^2]/2\lambda_j^{1/2} \quad ; \ \alpha = x,y,z$$

$$[\sigma;\alpha\alpha;2;1] = [(2;\alpha\alpha;12;-)\lambda_1^{1/2} + (2;\alpha\alpha;-;12)\lambda_2^{1/2}/\hbar^2]/(\lambda_1 - \lambda_2)$$

$$[\sigma;\alpha\alpha;1;2] = [(2;\alpha\alpha;12;-)\lambda_2^{1/2} + (2;\alpha\alpha;-;12)\lambda_1^{1/2}/\hbar^2]/(\lambda_2 - \lambda_1)$$

$$[\sigma;xy;3;j] = [(2;xy;j3;-)\lambda_j^{1/2} + (2;xy;-;j3)\lambda_3^{1/2}/\hbar^2]/(\lambda_j - \lambda_3)$$

$$[\sigma;xy;j;3] = [(2;xy;j3;-)\lambda_3^{1/2} + (2;xy;-;j3)\lambda_j^{1/2}/\hbar^2]/(\lambda_3 - \lambda_j)$$

$$[\sigma;yx;3;j] = [\sigma;xy;3;j] \qquad j = 1,2 \qquad [\sigma;yx;j;3] = [\sigma;xy;j;3]$$

Table XX. Coefficients $[\sigma;\alpha;c;ab]$ in the second contact transformation.

$$[\sigma;z;jj;3] = -(2;z;3;jj)A_{jj3}/\hbar^2 + (2;z;j;j3)B_{j3,j}/\hbar^2 -(2;z;jj3;-)B_{jj,3}(1+2\delta_{j3}) \quad ; \; j = 1,2,3$$

$$[\sigma;z;12;3] = -(2;z;3;12)A_{123}/\hbar^2 + (2;z;1;23)B_{13,2}/\hbar^2 +(2;z;2;13)B_{23,1}/\hbar^2 - (2;z;123;-)B_{12,3}$$

$$[\sigma;z;13;1] = -(2;z;1;13)A_{113}/\hbar^2 + (2;z;1;13)B_{11,3}/\hbar^2 +2(2;z;3;11)B_{13,1}/\hbar^2 - 2(2;z;113;-)B_{13,1}$$

$$[\sigma;z;23;2] = -(2;z;2;23)A_{223}/\hbar^2 + (2;z;2;23)B_{22,3}/\hbar^2 +2(2;z;3;22)B_{23,2}/\hbar^2 - 2(2;z;223;-)B_{23,2}$$

$$[\sigma;z;13;2] = -(2;z;2;13)A_{123}/\hbar^2 + (2;z;1;23)B_{12,3}/\hbar^2 +(2;z;3;12)B_{23,1}/\hbar^2 - (2;z;123;-)B_{13,2}$$

$$[\sigma;z;23;1] = -(2;z;1;23)A_{123}/\hbar^2 + (2;z;2;13)B_{12,3}/\hbar^2 +(2;z;3;12)B_{13,2}/\hbar^2 - (2;z;123;-)B_{23,1}$$

$$[\sigma;z;21;3] = [\sigma;z;12;3] \qquad [\sigma;z;31;j] = [\sigma;z;13;j]$$

$$[\sigma;z;32;j] = [\sigma;z;23;j] \qquad j = 1,2$$

Table XXI. Coefficients $[\sigma;\alpha;-;abc]$ in the second contact transformation.

$$[\sigma;z;-;113] = -(2;z;1;13)B_{13,1} - (2;z;3;11)B_{11,3} - \hbar^2(2;z;113;-)A_{113}$$

$$[\sigma;z;-;223] = -(2;z;2;23)B_{23,2} - (2;z;3;22)B_{22,3} - \hbar^2(2;z;223;-)A_{223}$$

$$[\sigma;z;-;123] = -(2;z;1;23)B_{23,1} - (2;z;2;13)B_{13,2} - (2;z;3;12)B_{12,3} - \hbar^2(2;z;123;-)A_{123}$$

$$[\sigma;z;-;333] = -(2;z;3;33)B_{33,3} - \hbar^2(2;z;333;-)A_{333}$$

Here, too, it is advantageous to regroup $H^@$ in true orders of magnitude. Upon subjecting $H^@$ to regrouping of terms according to true orders of magnitude we have:

$$H^@ = h^@ = h_0{}^@ + h_1{}^@ + h_2{}^@ + h_3{}^@ + h_4{}^@$$

where
$$h_0{}^@ = H_0$$
$$h_1{}^@ = 0$$
$$h_2{}^@ = h_2{}' + i[\sigma,H_0]_V$$
$$h_3{}^@ = h_3{}' + i[\sigma,H_0]_R$$
$$h_4{}^@ = h_4{}' + i[\sigma,h_2{}']_V - (1/2)[\sigma,[\sigma,h_0{}']_V]_V$$

The last two terms in $h_4{}'$ can be written as follows:

$$i[\sigma,h_2{}']_V - (1/2)[\sigma,[\sigma,h_0{}']_V]_V = i[\sigma,(h_2{}' + (i/2)[\sigma,h_0{}']_V)]_V$$
$$= i[\sigma,(h_2{}'/2 + (1/2)(h_2{}' + i[\sigma,h_0{}']_V))]_V$$
$$= i[\sigma,(1/2)(h_2{}' + h_2{}^@)]_V = (i/2)[\sigma,(h_2{}' + h_2{}^@)]_V$$

Moreover, it can be shown that $i[\sigma,h_2{}^@]_V$ does not contribute to the energy through the fourth order of approximation except in cases of accidental near-degeneracy.[22] The same is true of $h_3{}^@$. Thus for the calculation of energies through the fourth order of approximation we only need to consider:

$$h_0{}^@ = H_0$$
$$h_2{}^@ = h_2{}' + i[\sigma,H_0]_V$$
$$h_4{}^@ = h_4{}' + i[\sigma,h_2{}']_V$$
$$h^@ = h_0{}^@ + h_2{}^@ + h_4{}^@ \qquad (5.4)$$

Table XXII. The constants A_{abc} and $B_{ab,c}$

$$A_{aaa} = -2\lambda_a^{1/2}/3; \quad a = 1,2,3$$

$$A_{112} = -2\lambda_1/\lambda_2^{1/2}(4\lambda_1 - \lambda_2) \qquad A_{122} = -2\lambda_2/\lambda_1^{1/2}(4\lambda_2 - \lambda_1)$$

$$A_{113} = -2\lambda_1/\lambda_3^{1/2}(4\lambda_1 - \lambda_3) \qquad A_{133} = -2\lambda_3/\lambda_1^{1/2}(4\lambda_3 - \lambda_1)$$

$$A_{223} = -2\lambda_2/\lambda_3^{1/2}(4\lambda_2 - \lambda_3) \qquad A_{233} = -2\lambda_3/\lambda_2^{1/2}(4\lambda_3 - \lambda_2)$$

$$A_{123} = 2(\lambda_1\lambda_2\lambda_3)^{1/2}D_{123} \quad ;$$ (and all permutations of indices.)

$$B_{aa,a} = -(1/3)\lambda_a^{1/2} \quad ; \; a = 1,2,3 \qquad B_{12,3} = -\lambda_3^{1/2}(\lambda_3 - \lambda_1 - \lambda_2)D_{123}$$

$$B_{13,2} = -\lambda_2^{1/2}(\lambda_2 - \lambda_1 - \lambda_3)D_{123} \qquad B_{23,1} = -\lambda_1^{1/2}(\lambda_1 - \lambda_2 - \lambda_3)D_{123}$$

$$B_{12,1} = -\lambda_1^{1/2}/(4\lambda_1 - \lambda_2) \qquad B_{12,2} = -\lambda_2^{1/2}/(4\lambda_2 - \lambda_1)$$

$$B_{13,3} = -\lambda_3^{1/2}/(4\lambda_3 - \lambda_1) \qquad B_{23,3} = -\lambda_3^{1/2}/(4\lambda_3 - \lambda_2)$$

$$B_{13,1} = -\lambda_1^{1/2}/(4\lambda_1 - \lambda_3) \qquad B_{23,2} = -\lambda_2^{1/2}/(4\lambda_2 - \lambda_3)$$

$$B_{11,2} = (\lambda_2 - 2\lambda_1)/\lambda_2^{1/2}(4\lambda_1 - \lambda_2) \qquad B_{22,1} = (\lambda_1 - 2\lambda_2)/\lambda_1^{1/2}(4\lambda_2 - \lambda_1)$$

$$B_{11,3} = (\lambda_3 - 2\lambda_1)/\lambda_3^{1/2}(4\lambda_1 - \lambda_3) \qquad B_{33,1} = (\lambda_1 - 2\lambda_3)/\lambda_1^{1/2}(4\lambda_3 - \lambda_1)$$

$$B_{22,3} = (\lambda_3 - 2\lambda_2)/\lambda_3^{1/2}(4\lambda_2 - \lambda_3) \qquad B_{33,2} = (\lambda_2 - 2\lambda_3)/\lambda_2^{1/2}(4\lambda_3 - \lambda_2)$$

In A_{123} , $B_{12,3}$ and the corresponding constants obtained through permutations of indices,

$$D_{123} = [(\lambda_1^{1/2}+\lambda_2^{1/2}+\lambda_3^{1/2})(\lambda_1^{1/2}-\lambda_2^{1/2}-\lambda_3^{1/2})(\lambda_1^{1/2}-\lambda_2^{1/2}+\lambda_3^{1/3})$$
$$\times(\lambda_1^{1/2}+\lambda_2^{1/2}-\lambda_3^{1/2})]^{-1} \quad ;$$ (all permutations of indices)

Of the terms in H_0 in (3.9a) only the first three will be kept in $h_0^@$ since the remaining terms are purely vibrational and of no interest here. However, in the second term of $h_2^@$ in (5.4) the pure-vibrational operator-terms in H_0 must be included in the commutator $[\sigma,H_0]_V$ for it is precisely these terms that contribute to $h_2^@$, since for the pure-rotational operator-terms in H_0 (2-23b) yields

$$
\begin{aligned}
i[\sigma,H_o]_V &= i[\sigma_V,H_{0V}](1/2)(\sigma_R H_{0R} + H_{0R}\sigma_R) \\
&= i[\sigma_V,1](1/2)(\sigma_R H_{0R} + H_{0R}\sigma_R) = 0
\end{aligned}
$$

Thus we have

$$
h_2^@ = h_2' + i[\sigma_V,H_{0V}](1/2)(\sigma_R.1 + 1.\sigma_R) = h_2' + i[\sigma_V,H_{0V}]\sigma_R
$$

and with σ from (5.1) and the last six terms in (3.9a) for H_{0V}, one can show that

$$
\begin{aligned}
h_2^@ = &\sum_{\alpha\beta\gamma\delta}(2;\alpha\beta\gamma\delta;-;-)P_\alpha P_\beta P_\gamma P_\delta + \\
&\sum_{\alpha\beta}\sum_a [\hbar^2(2;\alpha\beta;aa;-) + (2;\alpha\beta;-;aa)](q_a{}^2 + p_a{}^2/\hbar^2)P_\alpha P_\beta + h_2^*
\end{aligned} \tag{5.5}
$$

i.e., except for h_2^*, $h_2^@$ is diagonal in all vibrational quantum numbers; h_2^* consists of pure-vibrational operator-terms originating from h_2'. Even though this portion of $h_2^@$ is not diagonal in the vibrational quantum numbers, it can be disregarded as it can be shown that the pure-vibrational operator-terms in $h_2^@$ would be diagonal if the complete transformation function of Goldsmith et al had been used. Substituting (4.6) for h_4', (4.4) for h_2' and (5.1) for σ into the last equation in (5.4), we obtain

$$h_4{}^{@} = \sum_{\alpha\beta\gamma\delta\varepsilon\rho} (\mathrm{IV};\alpha\beta\gamma\delta\varepsilon\rho;-;-)P_\alpha P_\beta P_\gamma P_\delta P_\varepsilon P_\rho \; + $$
$$\sum_{\alpha\beta\gamma\delta}\sum_{a\leq b} [(\mathrm{IV};\alpha\beta\gamma\delta;-;ab)q_a q_b + (\mathrm{IV};\alpha\beta\gamma\delta;ab;-)p_a p_b]P_\alpha P_\beta P_\gamma P_\delta$$
$$+ h_4{}^{*} \tag{5.6}$$

where $h_4{}^{*}$ includes terms of the type r^4P^2 and r^kP^{6-k}, $k = 1,3,5$. Following the notation introduced by Amat and Nielsen,[22] r^n and P^m are used to denote products of any n vibrational and any m rotational operators, respectively; $h_4{}^{*}$ is discarded henceforth since herein terms of the first type represent fourth-order corrections to zeroth-order rotational constants of rigid rotator, while terms of the second type would contribute only to the energy in an order higher than the fourth.[21] The coefficients in $h_4{}^{@}$ can be shown to be the following:

$$(\mathrm{IV};\alpha\beta\gamma\delta\varepsilon\rho;-;-) = (4;\underline{\alpha\beta},\underline{\gamma\delta\varepsilon\rho};-;-) + (4!\underline{\alpha\beta\gamma};\underline{\delta\varepsilon\rho}!-!-)$$
$$(\mathrm{IV};\alpha\beta\gamma\delta;-;ab) = (4;\alpha\beta\gamma\delta;-;ab) + (4!\underline{\alpha\beta\gamma},\underline{\delta}!-!ab) + (4!\underline{\alpha\beta},\underline{\gamma\delta}!-!ab) + (4!\underline{\alpha},\underline{\beta\gamma\delta}!-!ab)$$
$$(\mathrm{IV};\alpha\beta\gamma\delta;ab;-) = (4;\alpha\beta\gamma\delta;ab;-) + (4!\underline{\alpha\beta\gamma},\underline{\delta}!ab!-) + (4!\underline{\alpha\beta},\underline{\gamma\delta}!ab!-) + (4!\underline{\alpha},\underline{\beta\gamma\delta}!ab!-) \tag{5.7}$$

$(4;\underline{\alpha\beta},\underline{\gamma\delta\varepsilon\rho};-;-)$, $(4;\alpha\beta\gamma\delta;-;ab)$ and $(4;\alpha\beta\gamma\delta;ab;-)$ are the coefficients in $h_4{}'$, the underlining on the groups of indices indicating how they can be constructed from the original coefficients to accomplish the desymmetrization of the corresponding rotational operators. Thus, for instance,

$$(4;\underline{\alpha\beta},\underline{\gamma\delta\varepsilon\rho};-;-) = (1/2)[(4;\alpha\beta,\gamma\delta\varepsilon\rho;-;-) + (4;\varepsilon\rho,\alpha\beta\gamma\delta;-;-)]$$

since the corresponding rotational operator-term

$(1/2)(P_\alpha P_\beta P_\gamma P_\delta P_\varepsilon P_\rho + P_\gamma P_\delta P_\varepsilon P_\rho P_\alpha P_\beta)$ is desymmetrized to

$P_\alpha P_\beta P_\gamma P_\delta P_\varepsilon P_\rho$.

The rest of the coefficients in (5.7), i.e., $(4!\underline{\alpha\beta\gamma},\underline{\delta\varepsilon\rho}!-!-)$, etc., belong to the terms in $i[\sigma,h_2']_V$. Again, the underlines are used here to show how they can be constructed from the original coefficients. These original coefficients are given in Appendixes XVIII to XXIV. The desymmetrization procedure mentioned above was used merely to facilitate writing the coefficients of $h_4^@$ in (5.6) in general form. In our actual calculation all terms were left in their original symmetric-form since they are already in the correct form in which they enter the final form of the Hamiltonian.

We now summarize the final result. From (5.4) we have

$$h^@ = h_0^@ + h_2^@ + h_4^@ \qquad (5.8)$$

Excluding the pure vibrational terms in H_0, we have, from (5.4) and (3.9a),

$$h_0^@ = (1/2)[\, P_x^2/I_x + P_y^2/I_y + P_z^2/I_z \,] \qquad (5.9)$$

No further rearrangement is required in (5.9) since it is already in the desired final form. One identifies the coefficients therein as being proportional to the equilibrium rotational constants A_0, B_0 and C_0. The coefficients $(2;\alpha\beta\gamma\delta;-;-)$ in the first sum of (5.5) have been listed in Table XVII. Following the notation of Chung and Parker[23] we write

$$(2;\alpha\beta\gamma\delta;-;-) = (1/4)\tau_{\alpha\beta\gamma\delta}$$

and in terms of the coefficients $\tau_{\alpha\beta\gamma\delta}$, the first sum of (5.5) and Table XVII yield

$$(1/4)[\,\tau_{xxxx}P_x^4 + \tau_{yyyy}P_y^4 + \tau_{zzzz}P_z^4 + \tau_{xxyy}(P_x^2P_y^2 + P_y^2P_x^2) + \tau_{yyzz}(P_y^2P_z^2 + P_z^2P_y^2) + \tau_{zzxx}(P_z^2P_x^2 + P_x^2P_z^2) + \tau_{xyxy}(P_xP_yP_xP_y + P_yP_xP_yP_x + P_xP_y^2P_x + P_yP_x^2P_y)\,]$$

With the aid of the commutation relations $[P_\alpha, P_\beta] = -i\hbar P_\gamma$, cyclic, the last term can be written as

$$(1/4)[\,2(P_x^2P_y^2 + P_y^2P_x^2) + 3\hbar^2P_z^2 - 2\hbar^2P_x^2 - 2\hbar^2P_y^2\,]\tau_{xyxy}$$

Thus we have, from the first sum in (5.5),

$$(1/4)[\,\tau_1P_x^4 + \tau_2P_y^4 + \tau_3P_z^4 + \tau_4(P_y^2P_z^2 + P_z^2P_y^2) + \tau_5(P_z^2P_x^2 + P_x^2P_z^2) + \tau_6{*}(P_x^2P_y^2 + P_y^2P_x^2) + \tau_9\hbar^2(3P_z^2 - 2P_x^2 - 2P_y^2)\,]$$

The last term is of the second order but will now be grouped with $h_0^{@}$, and the coefficients of P_x^2, P_y^2 and P_z^2 therein represent centrifugal distortion corrections to the rotational constants A_0, B_0 and C_0, respectively. The coefficients τ_{xxxx}, τ_{yyyy}, etc., or their numerical-subscript forms τ_1, τ_2, etc., are listed in Table XXIII.

The coefficients $(2;\alpha\beta;aa;-)$ and $(2;\alpha\beta;-;aa)$ in the second sum of (5.5) are given in Appendixes V and VI, respectively, along with the coefficients of the off-diagonal terms in h_2'. We note that for a = b $(2;\alpha\beta;ab;-)$ and $(2;\alpha\beta;-ab)$ vanish if $\alpha \neq \beta$. Hence the second sum of (5.5) can be written as follows:

$$\sum_{\alpha} \sum_{a=1}^{3} [\, \hbar^2(2;\alpha\alpha;aa;-) + (2;\alpha\alpha;-;aa)\,](\, q_a{}^2 + p_a{}^2/\hbar^2\,)P_\alpha^2$$

Table XXIII. The coefficients $\tau_{\alpha\beta\gamma\delta}$.

$$\tau_{xxxx} = \tau_1 = -[(a_1{}^{xx})^2/\lambda_1 + (a_2^{xx})^2/\lambda_2]/2I_x{}^4$$

$$\tau_{yyyy} = \tau_2 = -[(a_1{}^{yy})^2/\lambda_1 + (a_2^{yy})^2/\lambda_2]/2I_y{}^4$$

$$\tau_{zzzz} = \tau_3 = -[(a_1{}^{zz})^2/\lambda_1 + (a_2^{zz})^2/\lambda_2]/2I_z{}^4$$

$$\tau_{yyzz} = \tau_{zzyy} = \tau_4 = -[(a_1{}^{yy}a_1{}^{zz}/\lambda_1) + (a_2^{yy}a_2{}^{zz}/\lambda_2)]/2I_y{}^2I_z{}^2$$

$$\tau_{zzxx} = \tau_{xxzz} = \tau_5 = -[(a_1{}^{zz}a_1{}^{xx}/\lambda_1) + (a_2^{zz}a_2{}^{xx}/\lambda_2)]/2I_z{}^2I_x{}^2$$

$$\tau_{xxyy} = \tau_{yyxx} = \tau_6 = -[(a_1{}^{xx}a_1{}^{yy}/\lambda_1) + (a_2^{xx}a_2{}^{yy}/\lambda_2)]/2I_x{}^2I_y{}^2$$

$$\tau_{xyxy} = \tau_{yxyx} = \tau_{xyyx} = \tau_{yxxy} = \tau_9 = -(a_3{}^{xy})^2/(2I_x{}^2I_y{}^2\lambda_3)$$

$$\tau_6{}^* = \tau_6 + 2\tau_9$$

If for a given vibrational state the eigenvalues of $p_a{}^2$ and $q_a{}^2$ are written as

$$\langle p_a{}^2 \rangle = (\, v_a + 1/2\,)\hbar^2\,, \quad \langle q_a{}^2 \rangle = (\, v_a + 1/2\,)$$

$$a = 1,2,3$$

respectively, where v_a is the harmonic oscillator quantum number corresponding to normal mode a, we can write the above double sum as

$$\mathcal{H}_1P_x{}^2 + \mathcal{H}_2P_y{}^2 + \mathcal{H}_3P_z{}^2$$

where

$$\mathcal{H}_1 = \sum_{a=1}^{3} (v_a + 1/2)[\hbar^2(2;xx;aa;-) + (2;xx;-;aa)]$$

$$\mathcal{H}_2 = \sum_{a=1}^{3} (v_a + 1/2)[\hbar^2(2;yy;aa;-) + (2;yy;-;aa)]$$

$$\mathcal{H}_3 = \sum_{a=1}^{3} (v_a + 1/2)[\hbar^2(2;zz;aa;-) + (2;zz;-;aa)] \qquad (5.10)$$

Since $\mathcal{H}_j$; j = 1,2,3 are the coefficients of terms quadratic in the components of angular momentum, these terms, although of the second order, are now also grouped into $h_0{}^{@}$. Therefore, they will be added to $h_0{}^{@}$ along with the centrifugal distortion terms from the first sum of (5.5). The $\mathcal{H}_j$'s represent the vibration-rotation coupling corrections to the equilibrium rotational constants A_0, B_0, C_0 .

The first sum in (5.6) contains terms sextic in the components of rotational angular momentum, the coefficients of which are given in (5.7). Since there are no sextic terms in $h_0{}^{@}$ or $h_2{}^{@}$, no ambiguities will be introduced if the "IV" and "4" are omitted from the coefficients. Thus we simplify the notation and write $(\alpha\beta\gamma\delta\varepsilon\rho)$, $(\alpha\beta,\gamma\delta\varepsilon\rho)$ and $(\alpha\beta\gamma*\delta\varepsilon\rho)$ for $(IV;\alpha\beta\gamma\delta\varepsilon\rho;-;-)$, $(4;\alpha\beta,\gamma\delta\varepsilon\rho)$ and $(4!\alpha\beta\gamma,\delta\varepsilon\rho!-!-)$, respectively. Comma and asterisk are used in the second and third coefficients, respectively, to show which group of indices originates from the transformation function, and which one from the Hamiltonian. In our notation the group of indices preceding the separating comma or asterisk is the one coming from the transformation function. We use the comma when the function is S, and the asterisk when the function is σ. The detailed expressions of the coefficients $(\alpha\beta,\gamma\delta\varepsilon\rho)$ are given in Appendix XV. These are the coefficients of the sextic terms P^6 in $h_4{}'$. The coefficients $(\alpha\beta\gamma*\delta\varepsilon\rho)$ are given in Appendix XVIII. One can see in these appendixes that the operators P_x, P_y and P_z always appear in even power in all the sextic pure-rotational terms. To have the sextic terms in the form arrived at by Yallabandi and Parker,[10] the original form

$(\alpha\beta,\gamma\delta\varepsilon\rho)(\,P_\alpha P_\beta P_\gamma P_\delta P_\varepsilon P_\rho + P_\gamma P_\delta P_\varepsilon P_\rho P_\alpha P_\beta\,) +$

$(\alpha\beta\gamma{*}\delta\varepsilon\rho)(\,P_\alpha P_\beta P_\gamma P_\delta P_\varepsilon P_\rho + P_\delta P_\varepsilon P_\rho P_\alpha P_\beta P_\gamma\,)$

was subjected to rearrangement based on the angular momentum commutation relations. In carrying out this rearrangement, Table II of Kneizys, Freedman and Clough[11] was very useful. Entries 58 through 105 in this table were subjected to permutations of indices to obtain operators with P_z symmetrically placed with respect to P_x and P_y. As a result of extensive rearrangement we obtain sixteen new coefficients, of which ten belong to P^6-terms and the other six belong to P^4-terms. Three of the former stay in their original form; they are the coefficients of $P_x{}^6$, $P_y{}^6$ and $P_z{}^6$. The rest of the coefficients are found to be certain linear combinations of the original coefficients. Actually we also obtained terms quadratic in the components of angular momentum, but these were discarded since they are negligible relative to the coefficients A_0, B_0 and C_0 in the $P_\alpha{}^2$-terms. Following Yallabandi and Parker,[10] these sixteen coefficients are called ϕ_1 to ϕ_{16}. They are listed in Table XXIV. Where these coefficients stand in the final form of the Hamiltonian will be shown later.

The coefficients of the r^2P^4-terms in (5.6) comprise eight different coefficients, two coming from $h_4{}'$ and six from $i[\sigma,h_2{}']_V$. The notation in (5.7) will now be simplified as follows:

$(4;\alpha\beta\gamma\delta;-;ab) \dashrightarrow (\alpha\beta\gamma\delta ab)$ $\qquad$ $(4;\alpha\beta\gamma\delta;ab;-) \dashrightarrow (ab\alpha\beta\gamma\delta)$

$(4!\alpha\beta\gamma,\delta!-!ab) \rightarrow (\alpha\beta\gamma{*}\delta ab)$ $\qquad$ $(4!\alpha\beta\gamma,\delta!ab!-) \rightarrow (ab\alpha\beta\gamma{*}\delta)$

$(4!\alpha\beta,\gamma\delta!-!ab) \rightarrow (\alpha\beta{*}\gamma\delta ab)$ $\qquad$ $(4!\alpha\beta,\gamma\delta!ab!-) \rightarrow (ab\alpha\beta{*}\gamma\delta)$

$(4!\alpha,\beta\gamma\delta!-!ab) \rightarrow (\alpha{*}\beta\gamma\delta ab)$ $\qquad$ $(4!\alpha,\beta\gamma\delta!ab!-) \rightarrow (ab\alpha{*}\beta\gamma\delta)$

Table XXIV. Coefficients ϕ_j

ϕ_1 = (xx,xxxx)

ϕ_2 = (yy,yyyy)

ϕ_3 = (zz,zzzz) + (zzz*zzz)

ϕ_4 = (yy,yyxx) + 2(yy,xyxy) + 4(xy,xyyy) + (1/2)(xx,yyyy)

ϕ_5 = (xx,xxyy) + 2(xx,xyxy) + 4(xy,xyxx) + (1/2)(yy,xxxx)

ϕ_6 = (zz,zzyy) + (zz,zyzy) + (1/2)(yy,zzzz) + 2(zzz*yyz) + (zzz*yzy)

ϕ_7 = (yy,yyzz) + (yy,zyzy) + (1/2)(zz,yyyy) + 2(yyz*yyz) +
2(yyz*yzy) + (1/2)(yzy*yzy)

ϕ_8 = (xx-xxzz) + (xx,zxzx) + (1/2)(zz,xxxx) + 2(xxz*xxz) +
2(xxz*xzx) + (1/2)(xzx*xzx)

ϕ_9 = (zz,zzxx) + (zz,zxzx) + (1/2)(xx,zzzz) + 2(zzz*xxz) + (zzz*xzx)

ϕ_{10}= 2(zz,xxyy) + (xx,yyzz) + (yy,zzxx) + 2(zz,xyxy) + 4(xy,xyzz) +
(yy,zxzx) + (xx,zyzy) + 4(xy,zxzy) + 4(xxz*yyz) + 2(xxz*yzy) +
2(yyz*xzx) + (xzx*yzy) + 2(xzy*xzy) + 2(zxy*zxy) +4(xyz*xzy) +
4(xyz*zxy) + 4(xzy*zxy)

ϕ_{11}= -2(xx,xyxy) - 8(xy,xyxx) + 4(xy,xyzz) - (xx,zxzx) + (xx,zyzy) +
4(xy,zxzy) - 4(xxz*xxz) + 4(xxz*yyz) - 4(xxz*xzx) + 2(xxz*yzy) +
2(yyz*xzx) + (xzx*yzy) - (xzx*xzx) + 3(xzy*xzy) + 3(xyz*xyz) +
3(zxy*zxy) + 6(xyz*xzy) + 6(xyz*zxy) + 6(xzy*zxy)

ϕ_{12}= -2(yy,xyxy) - 8(xy,xyyy) + 4(xy,xyzz) + (yy,zxzx) - (yy,zyzy) +
4(xy,zxzy) + 4(xxz*yyz) - 4(yyz*yyz) - 4(yyz*yzy) + 2(xxz*yzy) +
2(yyz*xzx) + (xzx*yzy) - (yzy*yzy) + 3(xzy*xzy) + 3(xyz*xyz) +
3(zxy*zxy) + 6(xyz*xzy) + 6(xyz*zxy) + 6(xzy*zxy)

ϕ_{13}= (5/2)(zz,xyxy) + 6(xy,xyzz) - (zz,zxzx) - (zz,zyzy) +
6(xy,zxzy) - (zzz*xzx) - (zzz*yzy) + 3(xzy*xzy) + 3(xyz*xyz) +
3(zxy*zxy) + 6(xyz*xzy) + 6(xyz*zxy) + 6(xzy*zxy)

Table XXIV (cont'd)

$$
\begin{aligned}
\Phi_{14} = {} & 2(yy,-yxx) + 2(zz,zzxx) - 2(yy,yyzz) - 2(zz,zzyy) - 4(zz,xxyy) \\
& -2(y-,zzxx) + (11/2)(yy,xyxy) - 5(zz,xyxy) + 15(xy,xyyy) - \\
& 14(xy,xyzz) - (5/2)(yy,zxzx) + (5/2)(zz,zxzx) - (5/2)(yy,zyzy) \\
& -(5/2)(zz,zyzy) - 14(xy,zxzy) + 3(zzz*xxz) - 3(zzz*yyz) - \\
& (3/2)(zzz*xzx) + (3/2)(zzz*yzy) - 4(xxz*yyz) - 4(yyz*yyz) - \\
& -3(yyz*xzx) - 5(yyz*yzy) - (3/2)(xzx*yzy) - (3/2)(yzy*yzy) - \\
& 7(xzy*xzy) - 7(xyz*xyz) - 7(zxy*zxy) - 14(xyz*xzy) - \\
& 14(xyz*zxy) - 14(xzy*zxy)
\end{aligned}
$$

$$
\begin{aligned}
\Phi_{15} = {} & 2(xx,xxyy) - 2(xx,xxzz) - 2(zz,zzxx) + 2(zz,zzyy) - 4(zz,xxyy) \\
& -2(xx,yyzz) + (11/2)(xx,xyxy) - 5(zz,xyxy) + 15(xy,xyxx) - \\
& 14(xy,xyzz) -(5/2)(xx,zxzx) - (5/2)(zz,zxzx) - (5/2)(xx,zyzy) \\
& + (5/2)(zz,zyzy) - 14(xy,zxzy) -3(zzz*xxz) + 3(zzz*yyz) - \\
& (3/2)(zzz*xzx) + (3/2)(zzz*yzy) - 4(xxz*xxz) - 4(xxz*yyz) - \\
& 5(xxz*xzx) - 3(xxz*yzy) - 2(yyz*xzx) - (3/2)(xzx*yzy) - \\
& (3/2)(xzx*xzx) - 7(xzy*xzy) - 7(xyz*xyz) - 7(zxy*zxy) - \\
& 14(xyz*xzy) - 14(xyz*zxy) - 14(xzy*zxy)
\end{aligned}
$$

$$
\begin{aligned}
\Phi_{16} = {} & -2(xx,xxyy) - 2(yy,yyxx) - 2(xx,xxzz) + 2(yy,yyzz) + 8(zz,xxyy) \\
& +2(xx,yyzz) + 2(yy,zzxx) - 5(xx,xyxy) - 5(yy,xyxy) + 8(zz,xyxy) \\
& -8(xy,xyxx) - 8(xy,xyyy) + 12(xy,xyzz) + (5/2)(xx,zxzx) + \\
& (3/2)(yy,zxzx) + (3/2)(xx,zyzy) + (5/2)(yy,zyzy) + 8(xy,zxzy) + \\
& 2(xxz*xxz) + 8(xxz*xzx) + 8(yyz*yyz) + 8(yyz*yzy) + 2(xzx*xzx) \\
& +2(yzy*yzy) + (xzy*xzy) + (xyz*xyz) + (zxy*zxy) + 2(xyz*xzy) + \\
& 2(xyz*zxy) = 2(xzy*zxy)
\end{aligned}
$$

Herein $(\alpha\beta,\gamma\delta\epsilon\rho)$ and $(\alpha\beta\gamma*\delta\epsilon\rho)$ are as given in Appendixes XV and XVIII, respectively.

In the simplified notation above, rotational operators' indices, $\alpha\beta\gamma\delta$, either precede the indices of vibrational normal coordinates, or follow those of the momenta conjugate to the normal coordinates. Again, an asterisk is used to separate rotational operators' indices coming from σ and from H'. The two contact transformations, S and σ, diagonalize H in the vibrational quantum numbers through second order only. Thus we have both diagonal and off-diagonal elements in the

matrix representation of $h_4^{@}$. It can be shown,[21] however, that the terms that are off-diagonal in the vibrational quantum numbers v_a do not contribute to the energy through the fourth order of approximation unless the vibrational states are spaced so closely that an accidental near-degeneracy results. For this reason we have not included in Appendixes XVIII through XXIV the coefficients of terms off-diagonal in v_a. The regrouping of the r^2P^4-terms into the final form of the Hamiltonian can be accomplished either through commutator algebra with the aid of the commutation relations $[P_\alpha, P_\beta] = -i\hbar P_\gamma$, cyclic, or by using the relations among the angular momentum operators of Olson and Allen.[24] This rearrangement has been done by Yallabandi and Parker,[10] and their results were used. Following their notation, we have, from the coefficients in Appendixes XVIII to XXIV,

$$\rho_1 = \rho_{xxxx} = \sum_a (v_a + 1/2)[\ (xxxxaa) + (aaxxxx)\hbar^2 + (xx{*}xxaa) + (aaxx{*}xx)\hbar^2\ ]$$

$$\rho_2 = \rho_{yyyy} = \sum_a (v_a + 1/2)[\ (yyyyaa) + (aayyyy)\hbar^2 + (yy{*}yyaa) + (aayy{*}yy)\hbar^2\ ]$$

$$\rho_3 = \rho_{zzzz} = \sum_a (v_a + 1/2)[\ (zzzzaa) + (aazzzz)\hbar^2 + (zzz{*}zaa) + (aazzz{*}z)\hbar^2 + (zz{*}zzaa) + (aazz{*}zz)\hbar^2 + (z{*}zzzaa) + (aaz{*}zzz)\hbar^2\ ]$$

$$\rho_4 = \rho_{yyzz} = \sum_a (v_a + 1/2)[\ (yyzzaa) + (aayyzz)\hbar^2 + (yyz{*}zaa) + (aayyz{*}z)\hbar^2 + (yy{*}zzaa) + (aayy{*}zz)\hbar^2 + (zz{*}yyaa) + (aazz{*}yy)\hbar^2 + (z{*}yyzaa) + (aaz{*}yyz)\hbar^2]$$

$$= \rho_{zzyy}$$

$$\rho_5 = \rho_{zzxx} = \sum_a (v_a + 1/2)[\ (xxzzaa) + (aaxxzz)\hbar^2 + (xxz^*zaa) + (aaxxz^*z)\hbar^2 + (xx^*zzaa) + (aaxx^*zz)\hbar^2 + (zz^*xxaa) + (aazz^*xx)\hbar^2 + (z^*xxzaa) + (aaz^*xxz)\hbar^2]$$

$$= \rho_{xxzz}$$

$$\rho_6 = \rho_{xxyy} = \sum_a (v_a + 1/2)[\ (xxyyaa) + (aaxxyy)\hbar^2 + (xx^*yyaa) + (aaxx^*yy)\hbar^2 + (yy^*xxaa) + (aayy^*xx)\hbar^2\ ]$$

$$= \rho_{yyxx}$$

$$\rho_7 = \rho_{yzyz} = \sum_a (v_a + 1/2)[\ (zyzyaa) + (aazyzy)\hbar^2 + (yzy^*zaa) + (aayzy^*z)\hbar^2 + (z^*yzyaa) + (aaz^*yzy)\hbar^2\ ]$$

$$= \rho_{zyzy}$$

$$\rho_8 = \rho_{zxzx} = \sum_a (v_a + 1/2)[\ (zxzxaa) + (aazxzx)\hbar^2 + (xzx^*zaa) + (aaxzx^*z)\hbar^2 + (z^*xzxaa) + (aaz^*xzx)\hbar^2\ ]$$

$$= \rho_{xzxz}$$

$$\rho_9 = \rho_{xyxy} = \sum_a (v_a + 1/2)[\ (xyxyaa) + (aaxyxy)\hbar^2 + (xy^*xyaa) + (aaxy^*xy)\hbar^2\ ]$$

$$= \rho_{yxyx}$$

$$\rho_{10} = \rho_{zyyz} = \sum_a (v_a + 1/2)[\ (zyyzaa) + (aazyyz)\hbar^2 + (zyy^*zaa) + (aazyy^*z)\hbar^2 + (z^*yyzaa) + (aaz^*yyz)\hbar^2\ ]$$

$$\rho_{11} = \rho_{yzzy} = \sum_a (v_a + 1/2)[\ (aayzzy)\hbar^2\ ]$$

$$\rho_{12} = \rho_{zxxz} = \sum_a (v_a + 1/2)[\ (zxxzaa) + (aazxxz)\hbar^2 + (zxx^*zaa) + (aazxx^*z)\hbar^2 + (z^*xxzaa) + (aaz^*xxz)\hbar^2\ ]$$

$$\rho_{13} = \rho_{xzzx} = \sum_a (v_a + 1/2)[\ (aaxzzx)\hbar^2\ ]$$

$$\rho_{14} = \rho_{xyyx} = \sum_a (v_a + 1/2)[\ (xyyxaa) + (aaxyyx)\hbar^2 + (xy^*yxaa) + (aaxy^*yx)\hbar^2\ ]$$

$$\rho_{15} = \rho_{yxxy} = \rho_{14} \qquad (5.11)$$

After all these rearrangements, the Hamiltonian $h^@$ in (5.4) can be written as

$$h^@ = h_2 + h_4 + h_6 \tag{5.12}$$

where

$$h_2 = (A_0 - \tau_9\hbar^2/2 + \mathcal{H}_1)P_x{}^2 + (B_0 - \tau_9\hbar^2/2 + \mathcal{H}_2)P_y{}^2 + (C_0 + 3\tau_9\hbar^2/2 + \mathcal{H}_3)P_z{}^2 \tag{5.13}$$

$$\begin{aligned} h_4 = {} & [(\tau_1 + \rho_1)/4 + \hbar^2\phi_{11}]P_x{}^4 + [(\tau_2 + \rho_2)/4 + \hbar^2\phi_{12}]P_y{}^4 + \\ & [(\tau_3 + \rho_3)/4 + \hbar^2\phi_{13}]P_z{}^4 + [(\tau_4 + \rho_4^*)/4 + \hbar^2\phi_{14}](P_y^2P_z^2 + P_z^2P_y^2) \\ & [(\tau_5 + \rho_5^*)/4 + \hbar^2\phi_{15}](P_z{}^2P_x{}^2 + P_x{}^2P_z{}^2) + \\ & [(\tau_6^* + \tau_6^*)/4 + \hbar^2\phi_{16}](P_x{}^2P_y{}^2 + P_y{}^2P_x{}^2) \end{aligned} \tag{5.14}$$

$$\begin{aligned} h_6 = {} & \phi_1P_x{}^6 + \phi_2P_y{}^6 + \phi_3P_z{}^6 + \phi_4(P_x{}^2P_y{}^4 + P_y{}^4P_x{}^2) + \\ & \phi_5(P_y{}^2P_x{}^4 + P_x{}^4P_y{}^2) + \phi_6(P_y{}^2P_z{}^4 + P_z{}^4P_y{}^2) + \\ & \phi_7(P_z{}^2P_y{}^4 + P_y{}^4P_z{}^2) + \phi_8(P_z{}^2P_x{}^4 + P_x{}^4P_z{}^2) + \\ & \phi_9(P_x{}^2P_z{}^4 + P_z{}^4P_x{}^2) + \phi_{10}(P_x{}^2P_z{}^2P_y{}^2 + P_y{}^2P_z{}^2P_x{}^2) \end{aligned} \tag{5.15}$$

In (5.14)

$$\begin{aligned} \rho_4{}^* &= \rho_4 + \rho_7 + (1/2)\rho_{10} + (1/2)\rho_{11} \\ \rho_5{}^* &= \rho_5 + \rho_8 + (1/2)\rho_{12} + (1/2)\rho_{13} \\ \rho_6{}^* &= \rho_6 + \rho_9 + (1/2)\rho_{14} + (1/2)\rho_{15} \end{aligned} \tag{5.16}$$

$h^@$ is a complete fourth-order vibration-rotation Hamiltonian for H_2O-type molecules. The detailed expressions for the coefficients therein have been obtained and are given in the tables and appendixes referred to in this chapter. The expressions for all coefficients ρ_j and the expressions for ϕ_{11} through ϕ_{16} are original with this investigation.

The fact that two Hamiltonians H and $\underline{H}$ have identical eigenvalues if they are related by any arbitrary unitary transformation U has been utilized by Watson[9] along with an order-of-magnitude argument, to deduce the form of a rotational Hamiltonian devoid of experimentally indeterminable coefficients. This theory has been extended by Yallabandi and Parker,[10] who, in their order-of-magnitude argument, included second-order corrections of the P^2-type and fourth-order corrections of the P^4-type in the zeroth and second-order terms, respectively, of the transformed Hamiltonian. In this way it was shown that one can impose one constraint and thereby reduce the number of independent coefficients of the quartic terms to five, and three further constraints to reduce the number of independent coefficients of the sextic terms to seven. Subject to certain restrictions[25] one can choose these constraints in several ways. For further information, the original papers[9,10,25] should be consulted.

In this thesis, a complete Hamiltonian was developed through the fourth order of approximation for the vibrating and rotating H_2O-type molecular configuration. Explicit expressions were calculated for all coefficients occurring in the Hamiltonian in terms of fundamental molecular constants, viz., the equilibrium principal moments of inertia (which are related to the equilibrium geometry of the molecule), the normal frequencies of vibration, and the qubic and quartic potential constants of the molecule. Since vibrational and vibration-rotational accidental resonances have not been considered, the theory at the present stage is applicable to the ground state, and to bands not subject to such resonances.

APPENDICES

APPENDIX I

Coefficients $a_{s\sigma}^{\alpha\beta}$, $A_{s\sigma s'\sigma'}^{\alpha\beta}$ and Coriolis Coupling Coefficients ζ_{ab}^{α}

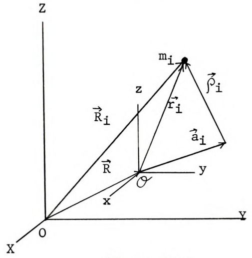

Figure AI-1

To show how the constants $a_{s\sigma}^{\alpha\alpha}$, $a_{s\sigma}^{\alpha\beta}$, $A_{s\sigma s'\sigma'}^{\alpha\alpha}$ and $A_{s\sigma s'\sigma'}^{\alpha\beta}$ relate to the Hamiltonian (2.1) it suffices to consider the classical Hamiltonian of a rotating and vibrating polyatomic molecule--specifically the part of the Hamiltonian coming from the kinetic energy.

If the i^{th} nucleus, whose mass is m_i, is denoted by the radius vectors $\vec{R}_i(X,Y,Z)$ and $\vec{r}_i(x,y,z)$ in the inertial or space-fixed and moving or molecule-fixed frames, respectively, and if $\vec{\rho}_i$ is its displacement relative to its equilibrium position $\vec{a}_i$ in the latter frame, we have

$$\vec{R}_i = \vec{R} + \vec{r}_i \tag{AI.1}$$

$$\vec{\rho}_i = \vec{r}_i - \vec{a}_i \tag{AI.2}$$

where $\vec{R}$ is the radius vector of the moving frame's origin $\mathcal{O}$ in the inertial frame. In the moving frame $\vec{a}_i$ is a constant vector. If T is the kinetic energy of the molecular framework,

$$2T = \sum_i m_i\dot{\vec{R}}_i\cdot\dot{\vec{R}}_i = \sum_i m_i\vec{V}_i\cdot\vec{V}_i = \sum_i m_i[\vec{V} + \vec{v}_i + (\vec{\omega} \times \vec{v}_i)]^2 \tag{AI.3}$$

where $\vec{V}_i$ is the velocity of the i^{th} nucleus in the inertial frame,

$\vec{v}_i$ is the velocity of the i^{th} nucleus in the moving frame, $\vec{V}$ is the velocity of the moving frame relative to the inertial frame and $\vec{\omega}$ is the angular velocity of the moving frame relative to the inertial frame. Use has been made of the operator relation

$$d/dt\Big|_{\text{inertial}} = d/dt\Big|_{\text{moving}} + \vec{\omega}\,X$$

(AI.3) can be written as

$$2T = V^2M + \sum_i m_i(\vec{\omega}\,X\,\vec{r}_i).(\vec{\omega}\,X\,\vec{r}_i) + \sum_i m_i v_i{}^2 + 2\sum_i m_i(\vec{V}.\vec{v}_i) +$$
$$2\sum_i m_i(\vec{\omega}\,X\,\vec{r}_i.\vec{V}) + 2\sum_i m_i(\vec{v}_i.\vec{\omega}\,X\,\vec{r}_i),$$

where M is the mass of the molecule. The rules of vector algebra allow rearrangement to

$$2T = MV^2 + \sum_i m_i[\vec{r}_i{}^2.\vec{\omega}^2 - (\vec{r}_i.\vec{\omega})^2] + \sum_i m_i v_i{}^2 + 2V.\sum_i m_i v_i +$$
$$2\vec{V}\,X\vec{\omega}.\sum_i m_i\vec{r}_i + 2\vec{\omega}.\sum_i m_i\vec{r}_i\,X\,\vec{v}_i$$

Choosing the origin of the moving frame to be at the center of mass of the molecule makes the fourth and fifth terms vanish identically. Thus

$$\sum_i m_i r_i = 0 \qquad \text{(AI.4)}$$

and

$$T = (1/2)MV^2 + (1/2)\sum_i m_i[\vec{r}_i^{\,2}.\vec{\omega}^2 - (\vec{r}_i.\vec{\omega})^2] + (1/2)\sum_i m_i v_i{}^2 +$$
$$\vec{\omega}.\sum_i m_i\vec{r}_i\,X\,\vec{v}_i$$

The first term in the above is the kinetic energy of the overall translation which we shall discard as it leads only to an additive constant in the total energy, the second term represents the rotational kinetic energy T_{rot}, the third term represents the vibrational kinetic energy T_{vib} and the last term represents the Coriolis energy, the energy of rotation-vibration interaction, T_c. Equation (AI.4) is called the first Eckart condition.

The rotational kinetic energy can be written

$$T_{rot} = (1/2)\sum_i m_i[\vec{r}_i{}^2\vec{\omega}^2 - (\vec{r}_i\cdot\vec{\omega})^2] = (1/2)\sum_{\alpha\beta} I_{\alpha\beta}\omega_\alpha\omega_\beta \qquad \text{(AI.5)}$$

where

$$\begin{aligned}
I_{\alpha\alpha} &= \sum_i m_i[(\beta_i{}^0 + \beta_i{}')^2 + (\gamma_i{}^0 + \gamma_i{}')^2] \\
&= \sum_i m_i(\beta_i{}^{02} + \gamma_i{}^{02}) + 2\sum_i m_i(\beta_i{}^0\beta_i{}' + \gamma_i{}^0\gamma_i{}') + \\
&\quad \sum_i m_i(\beta_i{}'^2 + \gamma_i{}'^2) \\
&= I^0_{\alpha\alpha} + 2\sum_i m_i(\beta_i{}^0\beta_i{}' + \gamma_i{}^0\gamma_i{}') + \sum_i m_i(\beta_i{}'^2 + \gamma_i{}'^2), \text{ cyclic} \\
-I_{\alpha\beta} &= -\sum_i m_i\alpha_i\beta_i + \sum_i m_i(\alpha_i{}^0\beta_i{}' + \beta_i{}^0\alpha_i{}') - \sum_i m_i\alpha_i{}'\beta_i{}' \\
&= -I^0_{\alpha\beta} + \sum_i m_i(\alpha_i{}^0\beta_i{}' + \beta_i{}^0\alpha_i{}') - \sum_i m_i\alpha_i{}'\beta_i{}', \text{ cyclic}
\end{aligned}$$

$I_{\alpha\alpha}$ and $I_{\alpha\beta}$ are the instantaneous moments and products of inertia, respectively, and $I^0_{\alpha\alpha}$ and $I^0_{\alpha\beta}$ the corresponding equilibrium values; $\alpha_i{}'$, $\beta_i{}'$ and $\gamma_i{}'$ are the components of $\vec{\rho}_i$ and $\alpha_i{}^0$, $\beta_i{}^0$ and $\gamma_i{}^0$ the components of $\vec{a}_i$.

If normal coordinates $Q_{s\sigma}$ are introduced by the following:

$$m_i{}^{1/2}\alpha_i{}' = l^\alpha_{is\sigma}Q_{s\sigma} \qquad \text{(AI.6)}$$

where $\alpha_i{}'$ are the x, y or z-component of $\vec{\rho}_i$ (i = 1,2,......N) and $l^\alpha_{is\sigma}$ are the elements of the matrix of transformation to normal coordinates, then $I_{\alpha\alpha}$ and $I_{\alpha\beta}$ can be written as

$$\begin{aligned}
I_{\alpha\alpha} &= I^0_{\alpha\alpha} + \sum_{s\sigma} a^{\alpha\alpha}_s Q_{s\sigma} + \sum_{s\sigma}\sum_{s'\sigma'} A^{\alpha\alpha}_{s\sigma s'\sigma'} Q_{s\sigma}Q_{s'\sigma'} \\
I_{\alpha\beta} &= 0 + \sum_{s\sigma} a^{\alpha\beta}_s Q_{s\sigma} + \sum_{s\sigma}\sum_{s'\sigma'} A^{\alpha\beta}_{s\sigma s'\sigma'} Q_{s\sigma}Q_{s'\sigma'}
\end{aligned} \qquad \text{(AI.7)}$$

where

$$\begin{aligned}
a^{\alpha\alpha}_{s\sigma} &= 2\sum_i m_i{}^{1/2}(\beta_i{}^0 l^\beta_{is} + \gamma_i{}^0 l^\gamma_{is}) \\
a^{\alpha\beta}_s &= -\sum_i m_i{}^{1/2}(\alpha_i{}^0 l^\beta_{is} + \beta_i{}^0 l^\alpha_{is}) \; ; \; \alpha \neq \beta \\
A^{\alpha\alpha}_{s\sigma s'\sigma'} &= \sum_i (l^\beta_{is\sigma} l^\beta_{is'\sigma'} + l^\gamma_{is\sigma} l^\gamma_{is'\sigma'}) \\
A^{\alpha\beta}_{s\sigma s'\sigma'} &= -\sum_i l^\alpha_{is\sigma} l^\beta_{is'\sigma'} = A^{\beta\alpha}_{s'\sigma' s\sigma} \; ; \; \alpha \neq \beta \\
&\alpha,\ \beta,\ \gamma \text{ cyclic}
\end{aligned} \qquad \text{(AI.8)}$$

This defines the constants $a^{\alpha\alpha}_{s\sigma}$, $a^{\alpha\beta}_{s\sigma}$, $A^{\alpha\alpha}_{s\sigma s'\sigma'}$ and $A^{\alpha\beta}_{s\sigma s'\sigma'}$.

Using the second Eckart condition

$$\sum_i m_i(\vec{a}_i \times \vec{v}_i) = 0 \qquad \text{(AI.9)}$$

the kinetic energy of Coriolis interaction can be simplified to

$$T_c = \vec{\omega}.\sum_i m_i\vec{\rho}_i \times \vec{v}_i$$

Again, using the transformation to normal coordinates (AI.6) to express $\vec{\rho}_i$ and $\vec{v}_i$ in terms of normal coordinates, the α-component of the sum in T_c can be written as

$$\begin{aligned}\sum_i(m_i\vec{\rho}_i \times \vec{v}_i)_\alpha &= \sum_i m_i(\beta_i\dot{\gamma}_i - \gamma_i\dot{\beta}_i)\\ &= \sum_{is\sigma}\sum_{s'\sigma'}(l^\beta_{is\sigma}l^\gamma_{is'\sigma'}Q_{s\sigma}\dot{Q}_{s'\sigma'} - l^\gamma_{is'\sigma'}l^\beta_{is\sigma}Q_{s'\sigma'}\dot{Q}_{s\sigma})\end{aligned}$$

Interchanging $s\sigma$ and $s'\sigma'$ in the second term, we have

$$\begin{aligned}(m_i\vec{\rho}_i \times \vec{v}_i)_\alpha &= \sum_{is\,s'\sigma'}(l^\beta_{is}l^\gamma_{is'\sigma'} - l^\beta_{is'\sigma'}l^\gamma_{is\sigma})Q_{s\sigma}\dot{Q}_{s'\sigma'}\\ &= \sum_{s\sigma s'\sigma'}\zeta^\alpha_{s\sigma s'\sigma'}Q_{s\sigma}\dot{Q}_{s'\sigma'}\end{aligned}$$

and the Coriolis interaction energy becomes

$$T_c = \sum_\alpha \omega_\alpha \zeta^\alpha_{s\sigma s'\sigma'}Q_{s\sigma}\dot{Q}_{s'\sigma'} \qquad \text{(AI.10)}$$

The coefficients

$$\zeta^\alpha_{s\sigma s'\sigma'} = \sum_i(l^\beta_{is\sigma}l^\gamma_{is'\sigma'} - l^\beta_{is'\sigma'}l^\gamma_{is\sigma})\ ,\ \text{cyclic} \qquad \text{(AI.11)}$$

are called Coriolis coupling coefficients since the Coriolis term T_c in the kinetic energy, and hence in the Hamiltonian, couples the vibrational and rotational motions.

Now, if we <u>define</u>

$$\begin{aligned}I'_{\alpha\alpha} &= I_{\alpha\alpha} - \sum_{s''}\zeta^\alpha_{s\sigma s'\sigma'}\zeta^\alpha_{s\sigma s''\sigma''}Q_{s'\sigma'}Q_{s''\sigma''}\\ I'_{\alpha\beta} &= I_{\alpha\beta} - \sum_{s''}\zeta^\alpha_{s\sigma s'\sigma'}\zeta^\beta_{s\sigma s''\sigma''}Q_{s'\sigma'}Q_{s''\sigma''}\end{aligned} \qquad \text{(AI.12)}$$

we then have, using (AI.7),

$$\begin{aligned}I'_{\alpha\alpha} &= I^0_{\alpha\alpha} + \sum_{s\sigma}a^{\alpha\alpha}_{s\sigma}Q_{s\sigma} + \sum_{s\sigma}\sum_{s'\sigma'}A^{\alpha\alpha}_{s\sigma s'\sigma'}Q_{s\sigma}Q_{s'\sigma'}\\ I'_{\alpha\beta} &= 0 - \sum_{s\sigma}a^{\alpha\beta}_{s\sigma}Q_{s\sigma} - \sum_{s\sigma}\sum_{s'\sigma'}A^{\alpha\beta}_{s\sigma s'\sigma'}Q_{s\sigma}Q_{s'\sigma'}\end{aligned} \qquad \text{(AI.13)}$$

where

$$A^{\alpha\alpha}_{s\sigma s'\sigma'} = A^{\alpha\alpha}_{s\sigma s'\sigma'} - \sum_{s''\sigma''} \zeta^{\alpha}_{s\sigma s''\sigma''} \zeta^{\alpha}_{s'\sigma' s''\sigma''}$$

$$A_{s\sigma s'\sigma'} = A_{s\sigma s'\sigma'} - \sum_{s''\sigma''} \zeta^{\alpha}_{s\sigma s''\sigma''} \zeta^{\beta}_{s'\sigma' s''\sigma''} \qquad \text{(AI.14)}$$

This defines the coefficients $A^{\alpha\alpha}_{s\sigma s'\sigma'}$ and $A^{\alpha\beta}_{s\sigma s'\sigma'}$.

APPENDIX II

The Expansion of $\mu_{\alpha\alpha}$, $\mu_{\alpha\beta}$

The determinant in (2.5) can be expanded into

$$\mu^{-1} = [I'_{xx}I'_{yy}I'_{zz} - I'_{xx}I'^{2}_{yz} - I'_{yy}I'^{2}_{xz} - I'_{zz}I'^{2}_{xy} - 2I'_{xy}I'_{yz}I'_{xz}]$$

Thus

$$\mu = [I'_{xx}I'_{yy}I'_{zz} - I'_{xx}I'^{2}_{yz} - I'_{yy}I'^{2}_{xz} - I'_{zz}I'^{2}_{xy} - 2I'_{xy}I'_{yz}I'_{xz}]^{-1} \tag{AII.1}$$

Substituting (AII.1) into (2.3) and (2.4) we get

$$\mu_{\alpha\alpha} = (I'_{\beta\beta}I'_{\gamma\gamma} - I'^{2}_{\beta\gamma})/(I'_{xx}I'_{yy}I'_{zz} - I'_{xx}I'^{2}_{yz} - I'_{yy}I'^{2}_{xz} - I'_{zz}I'^{2}_{xy} - 2I'_{xy}I'_{yz}I'_{xz}) \; ; \; \alpha, \beta, \gamma = x, y, z \text{ cyclic}$$

$$\mu_{\alpha\beta} = (I'_{\gamma\gamma}I'_{\alpha\beta} - I'_{\alpha\gamma}I'_{\gamma\beta})/(I'_{xx}I'_{yy}I'_{zz} - I'_{xx}I'^{2}_{yz} - I'_{yy}I'^{2}_{xz} - I'_{zz}I'^{2}_{xy} - 2I'_{xy}I'_{yz}I'_{xz}) \; ; \; \alpha, \beta, \gamma = x, y, z \text{ cyclic} \tag{AII.2}$$

It has been shown in Appendix I that $I'_{\alpha\alpha}$ and $I'_{\alpha\beta}$ ($\alpha, \beta = x, y, z$) are functions of the normal coordinates $Q_{s\sigma}$. Hence $u_{\alpha\alpha}$ and $u_{\alpha\beta}$ are also functions of $Q_{s\sigma}$. Since the nuclei are assumed to move about their equilibrium positions with small displacements $\vec{\rho}_i$, the $Q_{s\sigma}$'s are small relative to internuclear distances. Therefore, we may expand $\mu_{\alpha\alpha}$ and $u_{\alpha\beta}$ into McLaurin series in $Q_{s\sigma}$,

$$\mu_{\alpha\beta} = (u_{\alpha\beta})_0 + \sum_{s\sigma} (\partial u_{\alpha\beta}/\partial Q_{s\sigma})_0 Q_{s\sigma} + (1/2)\sum_{s\sigma}\sum_{s'\sigma'} (\partial^2 u_{\alpha\beta}/\partial Q_{s\sigma}\partial Q_{s'\sigma'})_0 \times Q_{s\sigma}Q_{s'\sigma'} + (1/6)\sum_{s\sigma s'\sigma' s''\sigma''} (\partial^3 u_{\alpha\beta}/\partial Q_{s\sigma}\partial Q_{s'\sigma'}\partial Q_{s''\sigma''})_0 Q_{s\sigma}Q_{s'\sigma'}Q_{s''\sigma''} + \ldots\ldots \; ; \; \alpha = \beta \text{ and } \alpha \neq \beta \tag{AII.3}$$

or, in terms of dimensionless normal coordinates

$$q_{s\sigma} = (\lambda_s/\hbar^2)^{1/4} Q_{s\sigma} \tag{AII.4}$$

$$\mu_{\alpha\beta} = [\alpha\beta*] + \sum_{s\sigma} [\alpha\beta*s\sigma] q_{s\sigma} + \sum_{s\sigma}\sum_{s'\sigma'} [\alpha\beta*s\sigma s'\sigma'] q_{s\sigma}q_{s'\sigma'} + \ldots \tag{AII.5}$$

where $[\alpha\beta*] = (u_{\alpha\beta})_0$

$$[\alpha\beta*s\sigma] = (\hbar^{1/2}/1!)(\partial u_{\alpha\beta}/\partial Q_{s\sigma})_0/\lambda_s^{1/4}$$

$$[\alpha\beta*s\sigma s'\sigma'] = \sum_P(\hbar/2!)(\partial^2 u_{\alpha\beta}/\partial Q_{s\sigma}\partial Q_{s'\sigma'})_0/(\lambda_s\lambda_{s'})^{1/4}$$

$$[\alpha\beta*s\sigma s'\sigma' s''\sigma''] = \sum_P(\hbar^{3/2}/3!)(\partial^3 u_{\alpha\beta}/\partial Q_{s\sigma}\partial Q_{s'\sigma'}\partial Q_{s''\sigma''})_0/(\lambda_s\lambda_{s'}\lambda_{s''})^{1/4},$$

etc., (AII.6)

In (AII.6) $\sum_P$ = sum over all distinct permutations of s, s', s", etc., and in (AII.5) all summations are restricted, i.e., subject to $s \lessgtr s' \lessgtr s''$ ... etc.

APPENDIX III

The Untransformed Hamiltonian

It will be understood that throughout this appendix there is a degeneracy index associated with each normal mode. The Watson-simplified Darling-Dennison Hamiltonian in (2.12) has the following terms:

(1) $(1/2)\sum_{\alpha\beta} \mu_{\alpha\beta} P_\alpha P_\beta$ — We shall call this "term-1"; this term contributes to H_0 through H_4.

(2) $-(1/2)\sum_{\alpha\beta} [p_\alpha \mu_{\alpha\beta} + \mu_{\beta\alpha} p_\alpha] P_\beta$ — We shall call this "term-2"; this term contributes to H_1 through H_4.

(3) $(1/2)\sum_{\alpha\beta} p_\alpha \mu_{\alpha\beta} p_\beta$ — We shall call this "term-3"; this term contributes to H_2, H_3 and H_4.

(4) $(1/2)\sum_{s} p_s^{*2}$ — We shall call this "term-4"; this term contributes to H_0.

(5) $-(\hbar^2/8)\sum_{\alpha} \mu_{\alpha\alpha}$ — We shall call this "term-5"; this term contributes to H_2, H_3 and H_4.

(6) V — We shall call this "term-6"; this potential-energy term contributes to H_0 through H_4.

In general we shall use the notation $H_m{}^{(n)}$, n = 1, 2, ..., 6; m = 1, 2, 3, 4, to denote the $m^{\underline{th}}$-order Hamiltonian coming from term-n. Thus we have:

$$H_0 = H_0{}^{(1)} + H_0{}^{(4)} + H_0{}^{(6)}$$
$$H_1 = H_1{}^{(1)} + H_1{}^{(2)} + H_1{}^{(6)}$$
$$H_m = H_m{}^{(1)} + H_m{}^{(2)} + H_m{}^{(3)} + H_m{}^{(5)} + H_m{}^{(6)}, \quad m = 2, 3, 4 \tag{AIII.1}$$

Using the expansion of $\mu_{\alpha\beta}$ (see Appendix II, equation (AII.5)), one has

$$H_0{}^{(1)} = (1/2)\sum_{\alpha\beta}[\alpha\beta *]P_\alpha P_\beta$$
$$H_0{}^{(4)} = (1/2\hbar)\sum_a \lambda_a{}^{1/2}p_a{}^2$$
$$H_0{}^{(6)} = V_0 = (\hbar/2)\sum_a \lambda_a{}^{1/2}q_a{}^2 \qquad \text{(AIII.2)}$$
$$H_1{}^{(1)} = (1/2)\sum_{\alpha\beta a}[\alpha\beta *a]q_aP_\alpha P_\beta$$
$$H_1{}^{(2)} = \sum_{\alpha ab}(\alpha *b*a)(1/2)\{q_a,p_b\}P_\alpha$$
$$H_1{}^{(6)} = 2\pi\hbar c\sum_{abc}k_{abc}q_aq_bq_c \qquad \text{(AIII.3)}$$
$$H_2{}^{(1)} = (1/2)\sum_{\alpha\beta ab}[\alpha\beta *ab]q_aq_bP_\alpha P_\beta$$
$$H_2{}^{(2)} = -\sum_{\alpha abc}(\alpha *c*ab)(1/2)\{q_aq_b,p_c\}P_\alpha$$
$$H_2{}^{(3)} = \sum_{abcd}(-*cd*ab)(1/2)\{q_aq_b,p_cp_d\}$$
$$H_2{}^{(5)} = -(\hbar^2/8)\sum_\alpha[\alpha\alpha *]$$
$$H_2{}^{(6)} = 2\pi\hbar c\sum_{abcd}k_{abcd}q_aq_bq_cq_d \qquad \text{(AIII.4)}$$
$$H_3{}^{(1)} = (1/2)\sum_{\alpha\beta abc}[\alpha\beta *abc]q_aq_bq_cP_\alpha P_\beta$$
$$H_3{}^{(2)} = -\sum_{\alpha abcd}(\alpha *d*abc)(1/2)\{q_aq_bq_c,p_d\}P_\alpha$$
$$H_3{}^{(3)} = \sum_{abcde}(-*de*abc)(1/2)\{q_aq_bq_c,p_dp_e\}$$
$$H_3{}^{(5)} = -(\hbar^2/8)\sum_a[\alpha\alpha *a]q_a$$
$$H_3{}^{(6)} = 2\pi\hbar c\sum_{abcde}k_{abcde}q_aq_bq_cq_dq_e \qquad \text{(AIII.5)}$$
$$H_4{}^{(1)} = (1/2)\sum_{\alpha\beta abcd}[\alpha\beta *abcd]q_aq_bq_cq_dP_\alpha P_\beta$$
$$H_4{}^{(2)} = -\sum_{\alpha abcde}(\alpha *e*abcd)(1/2)\{q_aq_bq_cq_d,p_e\}P_\alpha$$
$$H_4{}^{(3)} = \sum_{abcdef}(-*ef*abcd)(1/2)\{q_aq_bq_cq_d,p_ep_f\}$$
$$H_4{}^{(5)} = -(\hbar^2/8)\sum_{\alpha ab}[\alpha\alpha *ab]q_aq_b$$
$$H_4{}^{(6)} = 2\pi\hbar c\sum_{abcdef}k_{abcdef}q_aq_bq_cq_dq_eq_f \qquad \text{(AIII.6)}$$

In equations (AIII.2) through (AIII.6) the "bracket coefficients" are those directly arising from the expansion of $\mu_{\alpha\beta}$, with the factor of conversion from normal coordinates and momenta Q_s, p_s* to dimensionless coordinates and momenta q_s, p_s absorbed into them. They are defined in Appendix II.

The "parentheses coefficients" are related to the corresponding "bracket coefficients" by a normal-mode depending factor that arises from expressing the components of the internal vibrational momentum p_α in terms of normal coordinates and momenta.

Substituting (AIII.2) into the first equation in (AIII.1) we obtain the H_0 in (2.15). Similarly, we obtain the H_1, H_2, H_3 and H_4 in (2.15) by substituting (AIII.3), (AIII.4), (AIII.5) and (AIII.6) into the second, third, fourth and fifth equation in (AIII.1), respectively.

APPENDIX IV

Coefficients $(2;\alpha\beta\gamma;a;-)$ in h_2'

Herein are given the coefficients $(2;\alpha\beta\gamma;a;-)$ in the second sum of (4.4). Throughout this appendix the condensed notation $(\alpha\beta\gamma a)$ will be used to denote $(2;\alpha\beta\gamma;a;-)$, and $j = 1, 2$.

$$(zz z3) = -(\lambda_3^{1/4}/2I_z^3\hbar^{1/2})(a_1^{zz}\zeta_{13} + a_2^{zz}\zeta_{23})[(\lambda_1 + \lambda_2 - 2\lambda_3)/(\lambda_1 - \lambda_3)(\lambda_2 - \lambda_3) - (\lambda_1 + \lambda_2)/2\lambda_1\lambda_2]$$

$$(xxz3) = -(\lambda_3^{1/4}/8I_x^2I_z\hbar^{1/2})(a_1^{xx}\zeta_{13}/\lambda_1 + a_2^{xx}\zeta_{23}/\lambda_2) + a_3^{xy}(I_z - I_x)/4I_x^2I_yI_z\lambda_3^{3/4}\hbar^{3/2} - (\lambda_3^{1/4}/4I_x^2I_z\hbar^{1/2}) \times [a_1^{xx}\zeta_{13}/(\lambda_1 - \lambda_3) + a_2^{xx}\zeta_{23}/(\lambda_2 - \lambda_3)]$$

$$(zxx3) = (xxz3)$$

$$(yyz3) = -(\lambda_3^{1/4}/8I_y^2I_z\hbar^{1/2})(a_1^{yy}\zeta_{13}/\lambda_1 + a_2^{yy}\zeta_{23}/\lambda_2) + a_3^{xy}(I_y - I_z)/4I_xI_y^2I_z\,{}_3^{3/4}\hbar^{3/2} - (\lambda_3^{1/4}/4I_y^2I_z\hbar^{1/2}) \times [a_1^{yy}\zeta_{13}/(\lambda_1 - \lambda_3) + a_2^{yy}\zeta_{23}/(\lambda_2 - \lambda_3)]$$

$$(zyy3) = (yyz3)$$

$$(xzx3) = a_3^{xy}(I_z - I_x)/2I_x^2I_yI_z\lambda_3^{3/4}\hbar^{3/2}$$

$$(yzy3) = a_3^{xy}(I_y - I_z)/2I_xI_y^2I_z\lambda_3^{3/4}\hbar^{3/2}$$

$$(xyzj) = (\lambda_j^{1/4}a_3^{xy}\zeta_{j3}/4I_xI_yI_z\hbar^{1/2})[(\lambda_j - 3\lambda_3)/2\lambda_3(\lambda_j - \lambda_3)] + [a_j^{xx}(I_y - I_z)/I_x + a_j^{zz}(I_x - I_y)/I_z]/4I_xI_yI_z\lambda_j^{3/4}\hbar^{3/2}$$

$$(zyxj) = (xyzj)$$

$$(xzyj) = [a_j^{xx}(I_y - I_z)/I_x + a_j^{yy}(I_z - I_x)/I_y]/4I_xI_yI_z\lambda_j^{3/4}\hbar^{3/2}$$

$$(yzxj) = (xzyj)$$

$$(zxyj) = (yxzj) = (\lambda_j^{1/4}a_3^{xy}\zeta_{j3}/4I_xI_yI_z\hbar^{1/2})[(\lambda_j - 3\lambda_3)/2\lambda_3(\lambda_j - \lambda_3)] + [a_j^{yy}(I_z - I_x)/I_y + a_j^{zz}(I_x - I_y)/I_z]/4I_xI_yI_z\lambda_j^{3/4}\hbar^{3/2}$$

APPENDIX V

Coefficients $(2;\alpha\beta;ab;-)$ in h_2'

Herein are given the coefficients $(2;\alpha\beta;ab;-)$ of the first term in the third sum of (4.4). Throughout this appendix the condensed notation $(\alpha\beta ab)$ will be used to denote $(2;\alpha\beta;ab;-)$, and $\alpha = x, y$.

$$(\alpha\alpha 11) = (\pi c/I_\alpha^2\hbar^{3/2})[a_1^{\alpha\alpha}k_{111}/\lambda_1^{3/4} + \lambda_1 a_2^{\alpha\alpha}k_{112}/\lambda_2^{3/4}(4\lambda_1 - \lambda_2)]$$

$$(\alpha\alpha 12) = (\alpha\alpha 21) = (2\pi c/I_\alpha^2\hbar^{3/2})[\lambda_2^{3/4}a_2^{\alpha\alpha}k_{122}/\lambda_1^{1/2}(4\lambda_2 - \lambda_1) + \lambda_1^{3/4}a_1^{\alpha\alpha}k_{112}/\lambda_2^{1/2}(4\lambda_1 - \lambda_2)]$$

$$(\alpha\alpha 22) = (\pi c/I_\alpha^2\hbar^{3/2})[a_2^{\alpha\alpha}k_{222}/\lambda_2^{3/4} + \lambda_2 a_1^{\alpha\alpha}k_{122}/\lambda_1^{3/4}(4\lambda_2 - \lambda_1)]$$

$$(\alpha\alpha 33) = (\pi c\lambda_3/I_\alpha^2\hbar^{3/2})[a_1^{\alpha\alpha}k_{133}/\lambda_1^{3/4}(4\lambda_3 - \lambda_1) + a_2^{\alpha\alpha}k_{233}/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$$

$$(zz11) = (\pi c/I_z^2\hbar^{3/2})[a_1^{zz}k_{111}/\lambda_1^{3/4} + \lambda_1 a_2^{zz}k_{112}/\lambda_2^{3/4}(4\lambda_1 - \lambda_2)] - \lambda_1^{1/2}\zeta_{13}^2/I_z^2\hbar(\lambda_1 - \lambda_3)$$

$$(zz12) = (zz21) = (2\pi c/I_z^2\hbar^{3/2})[\lambda_1^{3/4}a_1^{zz}k_{112}/\lambda_2^{1/2}(4\lambda_1 - \lambda_2) + \lambda_2^{3/4}a_2^{zz}k_{122}/\lambda_1^{1/2}(4\lambda_2 - \lambda_1)] - (\lambda_1\lambda_2)^{1/4}(\lambda_1 + \lambda_2 - 2\lambda_3)\zeta_{13}\zeta_{23}/I_z^2\hbar(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)$$

$$(zz22) = (\pi c/I_z^2\hbar^{3/2})[a_2^{zz}k_{222}/\lambda_2^{3/4} + \lambda_2 a_1^{zz}k_{122}/\lambda_1^{3/4}(4\lambda_2 - \lambda_1) - \lambda_2^{1/2}\zeta_{23}^2/I_z^2\hbar(\lambda_2 - \lambda_3)$$

$$(zz33) = (\pi c/I_z^2\hbar^{3/2})[a_1^{zz}k_{133}/\lambda_1^{3/4}(4\lambda_3 - \lambda_1) + a_2^{zz}k_{233}/\lambda_2^{3/4}(4\lambda_3-\lambda_2)] - (\lambda_3^{1/2}/I_z^2\hbar)[\zeta_{13}^2/(\lambda_1 - \lambda_3) + \zeta_{23}^2/(\lambda_2 - \lambda_3)]$$

$$(xy13) = 2\pi c\lambda_3^{3/4}a_3^{xy}k_{133}/I_xI_y\hbar^{3/2}\lambda_1^{1/2}(4\lambda_3 - \lambda_1) + (\lambda_1\lambda_3)^{1/4}\zeta_{13}^2(I_y - I_x)/I_x^2I_y^2(\lambda_1 - \lambda_3)$$

$$(xy23) = 2\pi c\lambda_3^{3/4}a_3^{xy}k_{233}/I_xI_y\hbar^{3/2}\lambda_2^{1/2}(4\lambda_3 - \lambda_2) + (\lambda_2\lambda_3)^{1/4}\zeta_{23}(I_y - I_x)/I_x^2I_y^2(\lambda_2 - \lambda_3)$$

$(xy31) = (yx13) = (yx31) = (xy13)$; $(xy32) = (yx23)$ $(yx32) = (xy23)$

APPENDIX VI

Coefficients $(2;\alpha\beta;-;ab)$ in h_2'

Herein are given the coefficients $(2;\alpha\beta;-;ab)$ of the second term in the third sum of (4.4). Throughout this appendix $(2;\alpha\beta;-;ab)$ will be written in the condensed form $(\alpha\beta ab)$.

$$(xx11) = 3\hbar\sin^2\gamma/2I_x^2\lambda_1^{1/2} + (\pi c\hbar^{1/2}/I_x^2)[2a_1^{xx}k_{111}/\lambda_1^{3/4} + a_2^{xx}k_{112}(3\lambda_1-\lambda_2)/\lambda_2^{3/4}(4\lambda_1-\lambda_2)]$$

$$(xx22) = 3\hbar\cos^2\gamma/2I_x^2\lambda_1^{1/2} + (\pi c\hbar^{1/2}/I_x^2)[2a_2^{xx}k_{222}/\lambda_2^{3/4} + a_1^{xx}k_{122}(3\lambda_2-\lambda_1)/\lambda_1^{3/4}(4\lambda_2-\lambda_1)]$$

$$(xx33) = 3\hbar/2I_xI_z\lambda_3^{1/2} + (\pi c\hbar^{1/2}/I_x^2)[a_1^{xx}k_{133}(3\lambda_3-\lambda_1)/\lambda_1^{3/4}(4\lambda_3-\lambda_1) + a_2^{xx}k_{233}(3\lambda_3-\lambda_2)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$$

$$(xx12) = (xx21) = 3\hbar\sin\gamma\cos\gamma/2I_x^2(\lambda_1\lambda_2)^{1/4} + (\pi ch^{1/2}/I_x^2)\ X\ [a_1^{xx}k_{112}(5\lambda_1-\lambda_2)/\lambda_1^{3/4}(4\lambda_1-\lambda_2)+a_2^{xx}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{3/4}(4\lambda_2-\lambda_1)]$$

$$(yy11) = 3\hbar\cos^2\gamma/2I_y^2\lambda_1^{1/2} + (\pi c\hbar^{1/2}/I_y^2)[2a_1^{yy}k_{111}/\lambda_1^{3/4} + a_2^{yy}k_{112}(3\lambda_1-\lambda_2)/\lambda_2^{3/4}(4\lambda_1-\lambda_2)]$$

$$(yy22) = 3\hbar\sin^2\gamma/2I_y^2\lambda_2^{1/2} + (\pi c\hbar^{1/2}/I_y^2)[2a_2^{yy}k_{222}/\lambda_2^{3/4} + a_1^{yy}k_{122}(3\lambda_2-\lambda_1)/\lambda_1^{3/4}(4\lambda_2-\lambda_1)]$$

$$(yy33) = 3\hbar/2I_yI_z\lambda_3^{1/2} + (\pi c\hbar^{1/2}/I_y^2)[a_1^{yy}k_{133}(3\lambda_3-\lambda_1)/\lambda_1^{3/4}(4\lambda_3-\lambda_1) + a_2^{yy}k_{233}(3\lambda_3-\lambda_2)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$$

$$(yy12) = (yy21) = -3\hbar\sin\gamma\cos\gamma/2I_y^2(\lambda_1\lambda_2)^{1/4} + (\pi c\hbar^{1/2}/I_y^2)\ X\ [a_1^{yy}k_{112}(5\lambda_1-\lambda_2)/\lambda_1^{3/4}(4\lambda_1-\lambda_2)+a_2^{yy}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{3/4}(4\lambda_2-\lambda_1)]$$

$$(zz11) = (\hbar/2I_z^2\lambda_1^{1/2})[3\zeta_{23}^2 + \zeta_{13}^2(\lambda_1+\lambda_3)/(\lambda_1-\lambda_3)] + (\pi c\hbar^{1/2}/I_z^2)[2a_1^{zz}k_{111}/\lambda_1^{3/4} + a_2^{zz}k_{112}(3\lambda_1-\lambda_2)/\lambda_2^{3/4}(4\lambda_1-\lambda_2)]$$

$$(zz22) = (\hbar/2I_z^2\lambda_2^{1/2})[3\zeta_{13} + \zeta_{23}(\lambda_2+\lambda_3)/(\lambda_2-\lambda_3)] + (\pi c\hbar^{1/2}/I_z^2)[2a_2^{zz}k_{222}/\lambda_2^{3/4} + a_1^{zz}k_{122}(3\lambda_2-\lambda_1)/\lambda_1^{3/4}(4\lambda_2-\lambda_1)]$$

$$(zz33) = (\hbar/2I_z^2\lambda_3^{1/2})[\zeta_{13}^2(\lambda_1+\lambda_3)/(\lambda_1-\lambda_3) + \zeta_{23}^2(\lambda_2+\lambda_3)/(\lambda_2-\lambda_3)] + (\pi c\hbar^{1/2}/I_z^2)[a_1^{zz}k_{133}(3\lambda_3-\lambda_1)/\lambda_1^{3/4}(4\lambda_3-\lambda_1) + a_2^{zz}k_{233}(3\lambda_3-\lambda_2)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$$

$$(zz12) = (zz21) = (\hbar\zeta_{13}\zeta_{23}/2I_z^2\lambda_1^{1/4}\lambda_2^{1/4})[-3 + 2(\lambda_1+\lambda_3)(\lambda_1+\lambda_2-2\lambda_3)/(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)] + (\pi c\hbar^{1/2}/I_z^2)[a_1^{zz}k_{112}(5\lambda_1-\lambda_2)/\lambda_1^{3/4}(4\lambda_1-\lambda_2) + a_2^{zz}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{3/4}(4\lambda_2-\lambda_1)]$$

$$(xy13) = (yx13) = (xy31) = (yx31) = \pi c\hbar^{1/2}k_{133}(5\lambda_3-\lambda_1)/I_xI_y\lambda_3^{3/4}(4\lambda_3-\lambda_1) - (\hbar/4I_x^2I_y^2\lambda_1^{1/4}\lambda_3^{1/4})[3(I_x/I_z)^{1/2}\cos\gamma + 3(I_y/I_z)^{1/2}\sin\gamma - - 2\zeta_{13}(I_y-I_x)(\lambda_1+\lambda_3)/(\lambda_1-\lambda_3)]$$

$$(xy23) = (yx23) = (xy32) = (yx32) = \pi c\hbar^{1/2}k_{233}(5\lambda_3-\lambda_2)/I_xI_y\lambda_3^{3/4}(4\lambda_3-\lambda_2) + (\hbar/4I_x^2I_y^2\lambda_2^{1/4}\lambda_3^{1/4})[5(I_x/I_z)^{1/2}\sin\gamma - (I_y/I_z)^{1/2}\cos\gamma + + 2\zeta_{23}(I_y-I_x)(\lambda_2+\lambda_3)/(\lambda_2-\lambda_3)]$$

APPENDIX VII

Coefficients $(2;\alpha;abc;-)$ in $h_2^{\prime}$ and All Possible Permutations

The following is the list of the coefficients (2; ;abc;-), written in the condensed form (αabc), appearing in the fourth sum of (4.4) :

$$(z113) = (2\pi c\lambda_3{}^{1/4}/I_z\hbar^2)[\ {}_{13}k_{111}/\lambda_1{}^{3/4} - 2\zeta_{13}k_{133}\lambda_3{}^{1/2}/\lambda_1{}^{1/4}(4\lambda_3-\lambda_1)$$
$$+ \zeta_{23}k_{112}\lambda_1/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)]$$

$$(z223) = (2\pi c\lambda_3{}^{1/4}/I_z\hbar^2)[\zeta_{23}k_{222}/\lambda_2{}^{3/4} - 2\zeta_{23}k_{233}\lambda_3{}^{1/2}/\lambda_2{}^{1/4}(4\lambda_3-\lambda_2)$$
$$+ \zeta_{13}k_{122}\lambda_2/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)]$$

$$(z123) = (4\pi c\zeta_{23}\lambda_2{}^{1/4}\lambda_3{}^{1/4}/I_z\hbar^2\lambda_1{}^{1/2})[k_{122}\lambda_2{}^{1/2}/(4\lambda_2-\lambda_1) - k_{133}\lambda_3{}^{1/2}/$$
$$(4\lambda_3-\lambda_1)] + (4\pi c\zeta_{13}\lambda_1{}^{1/4}\lambda_3{}^{1/4}/I_z\hbar^2\lambda_2{}^{1/2})[k_{112}\lambda_1{}^{1/2}/(4\lambda_1-\lambda_2)$$
$$- k_{233}\lambda_3{}^{1/2}/(4\lambda_3-\lambda_2)]$$

$$(z333) = (2\pi c\lambda_3{}^{5/4}/I_z\hbar^2)[\zeta_{13}k_{133}/\lambda_1{}^{3/4}(4\lambda_3-\lambda_1) + \zeta_{23}k_{233}/\lambda_2{}^{3/4}(4\lambda_3-\lambda_2)]$$

APPENDIX VIII

Coefficients $(2;\alpha;c;ab)$ in h_2'

Listed herein are the coefficients $(2;\alpha;c;ab)$, written in the condensed form (αcab), appearing in the fifth sum of (4.4) :

$$(z311) = \hbar^{1/2}\lambda_3^{1/4}a_1^{zz}\zeta_{13}/\lambda_1^{1/2}I_z^{2} + (\pi c\lambda_3^{1/4}/I_z)[k_{111}\zeta_{13}(\lambda_3-7\lambda_1)/$$
$$\lambda_1^{3/4}(\lambda_3-\lambda_1) + k_{112}\zeta_{23}((2\lambda_1-\lambda_2)/\lambda_2^{3/4}(4\lambda_1-\lambda_2) -2\lambda_2^{1/4}/(\lambda_3-\lambda_2))$$
$$- 2\lambda_3^{1/2}\zeta_{13}k_{133}/\lambda_1^{1/4}(4\lambda_3-\lambda_1)]$$

$$(z322) = \hbar^{1/2}\lambda_3^{1/4}a_2^{zz}\zeta_{23}/\lambda_2^{1/2}I_z^{2} + (\pi c\lambda_3^{1/4}/I_z)[k_{222}\zeta_{23}(\lambda_3-7\lambda_2)/$$
$$\lambda_2^{3/4}(\lambda_3-\lambda_2) + k_{122}\zeta_{13}((2\lambda_2-\lambda_1)/\lambda_1^{3/4}(4\lambda_2-\lambda_1) -2\lambda_1^{1/4}/(\lambda_3-\lambda_1))$$
$$- 2\lambda_3^{1/2}\zeta_{23}k_{233}/\lambda_2^{1/4}(4\lambda_3-\lambda_2)]$$

$$(z312) = (z321) = \hbar^{1/2}\lambda_3^{1/4}(a_1^{zz}\zeta_{23} + a_2^{zz}\zeta_{13})/\lambda_1^{1/4}\lambda_2^{1/4}I_z^{2} +$$
$$(2\pi c\lambda_3^{1/4}/I_z)[(\lambda_3-9\lambda_1+2\lambda_2)\lambda_1^{1/4}\zeta_{13}k_{112}/(4\lambda_1-\lambda_2)(\lambda_3-\lambda_1) +$$
$$(\lambda_3-9\lambda_2+2\lambda_1)\lambda_2^{1/4}\zeta_{23}k_{122}/(4\lambda_2-\lambda_1)(\lambda_3-\lambda_2) -$$
$$\lambda_3^{1/2}\zeta_{23}k_{133}/\lambda_2^{1/4}(4\lambda_3-\lambda_1) - \lambda_3^{1/2}\zeta_{13}k_{233}/\lambda_1^{1/4}(4\lambda_3-\lambda_2)]$$

$$(z333) = (\pi c\lambda_3^{1/4}/I_z)[\zeta_{13}k_{133}(2\lambda_1^{2}+2\lambda_3^{2}-7\lambda_1\lambda_3)/\lambda_1^{3/4}\ (4\lambda_3-\lambda_1)(\lambda_3-\lambda_1) +$$
$$\zeta_{23}k_{233}(2\lambda_2^{2}+2\lambda_3^{2}-7\lambda_2\lambda_3)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)(\lambda_3-\lambda_2)]$$

$$(z113) = (z131) = -\hbar^{1/2}a_1^{zz}\zeta_{13}/\lambda_3^{1/4}I_z^{2} - (2\pi c/I_z)[2\lambda_3^{5/4}(2\lambda_1+\lambda_3)\zeta_{13}\ \times$$
$$k_{133}/(4\lambda_3-\lambda_1)(\lambda_3-\lambda_1)\lambda_1^{3/4} - (\lambda_1^{2}\lambda_2)^{1/4}\zeta_{23}k_{112}/\lambda_3^{1/4}(4\lambda_1-\lambda_2) -$$
$$\zeta_{13}k_{111}/(\lambda_1\lambda_3)^{1/4}]$$

$$(z223) = (z232) = -\hbar^{1/2}a_2^{zz}\zeta_{23}/\lambda_3^{1/4}I_z^{2} - (2\pi c/I_z)[2\lambda_3^{5/4}(2\lambda_2+\lambda_3)\zeta_{23}\ \times$$
$$k_{233}/(4\lambda_3-\lambda_2)(\lambda_3-\lambda_2)\lambda_2^{3/4} - (\lambda_2^{2}\lambda_1)^{1/4}\zeta_{13}k_{122}/\lambda_3^{1/4}(4\lambda_2-\lambda_1) -$$
$$\zeta_{23}k_{222}/(\lambda_2\lambda_3)^{1/4}]$$

$$(z123) = (z132) = -\hbar^{1/2}a_2^{zz}\lambda_1^{1/4}\zeta_{13}/(\lambda_2\lambda_3)^{1/4}I_z^2 - (2\pi c/I_z)[(\lambda_1\lambda_3)^{1/4} \times \zeta_{13}k_{233}(\lambda_1+2\lambda_2-9\lambda_3)/(4\lambda_3-\lambda_2)(\lambda_1-\lambda_3) + \lambda_3^{1/4}\zeta_{23}k_{133} \times (2\lambda_3-\lambda_1)/(\lambda_1^2\lambda_2)^{1/4}(4\lambda_3-\lambda_1) - \lambda_2^{1/4}\zeta_{23}k_{122}(2\lambda_2-\lambda_1)/(\lambda_1^2\lambda_3)^{1/4}(4\lambda_2-\lambda_1) - \lambda_1^{3/4}\zeta_{23}k_{112}/\lambda_3^{1/4}(4\lambda_1-\lambda_2)]$$

$$(z213) = (z231) = -\hbar^{1/2}a_1^{zz}\lambda_2^{1/4}\zeta_{23}/(\lambda_1\lambda_3)^{1/4}I_z^2 - (2\pi c/I_z)[(\lambda_2\lambda_3)^{1/4} \times \zeta_{23}k_{133}(\lambda_2+2\lambda_1-9\lambda_3)/(4\lambda_3-\lambda_1)(\lambda_2-\lambda_3) + \lambda_3^{1/4}\zeta_{13}k_{233} \times (2\lambda_3-\lambda_2)/(\lambda_2^2\lambda_1)^{1/4}(4\lambda_3-\lambda_2) - \lambda_1^{1/4}\zeta_{13}k_{112}(2\lambda_1-\lambda_2)/(\lambda_2^2\lambda_3)^{1/4}(4\lambda_1-\lambda_2) - \lambda_2^{3/4}\zeta_{13}k_{122}/\lambda_3^{1/4}(4\lambda_2-\lambda_1)]$$

APPENDIX IX

Coefficients (2;-;cd;ab) in h_2'

Herein are given the coefficients (2;-;cd;ab) appearing in the sixth sum of (4.4). Throughout this appendix (2;-;cd;ab) will be written in the condensed form (cdab).

$$(1111) = (-4\pi^2c^2/\hbar)[3k_{111}^2/\lambda_1^{1/2} + \lambda_1k_{112}^2/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$$

$$(1112) = (1121) = (-8\pi^2c^2k_{112}/\hbar)[k_{111}/\lambda_1^{1/2} + k_{122}\lambda_1/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$$

$$(1122) = (-4\pi^2c^2/\hbar)[3\lambda_2k_{111}k_{122}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + k_{112}k_{222}/\lambda_2^{1/2}]$$

$$(1133) = (-4\pi^2c^2/\hbar)[k_{111}k_{133}/\lambda_1^{1/2} + k_{112}k_{233}\lambda_1/\lambda_2^{1/2}(4\lambda_1-\lambda_2)] + (\lambda_1/\lambda_3)^{1/2}\zeta_{13}^2/2I_z$$

$$(1211) = (2111) = (-8\pi^2c^2k_{112}/\hbar)[3k_{111}\lambda_1/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + k_{122}\lambda_2/\lambda_1^{1/2}(4\lambda_2-\lambda_1)]$$

$$(1212) = (1221) = (2112) = (2121) = (-16\pi^2c^2/\hbar)[\lambda_1k_{112}^2/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + \lambda_2k_{122}^2/\lambda_1^{1/2}(4\lambda_2-\lambda_1)]$$

$$(1222) = (2122) = (-8\pi^2c^2k_{122}/\hbar)[k_{112}\lambda_1/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + 3k_{222}\lambda_2/\lambda_1^{1/2}(4\lambda_2-\lambda_1)]$$

$$(1233) = (2133) = (-8\pi^2c^2/\hbar)[\lambda_1k_{112}k_{133}/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + \lambda_2k_{122}k_{233}/\lambda_1^{1/2}(4\lambda_2-\lambda_1)] + (\lambda_1\lambda_2/\lambda_3^2)^{1/4}\zeta_{13}\zeta_{23}/I_z$$

$$(2211) = (-4\pi^2c^2/\hbar)[3\lambda_2k_{111}k_{122}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + k_{112}k_{222}/\lambda_2^{1/2}]$$

$$(2212) = (2221) = (-8\pi^2c^2k_{122}/\hbar)[k_{112}\lambda_2/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + k_{222}/\lambda_2^{1/2}]$$

$$(2222) = (-4\pi^2c^2/\hbar)[\lambda_2k_{122}^2/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + 3k_{222}^2/\lambda_2^{1/2}]$$

$$(2233) = (-4\pi^2c^2/\hbar)[\lambda_2k_{122}k_{133}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + k_{222}k_{233}/\lambda_2^{1/2}] + (\lambda_2/\lambda_3)^{1/2}\zeta_{23}^2/2I_z$$

$(3311) = (-4\pi^2c^2/\hbar)[3\lambda_3k_{111}k_{133}/\lambda_1{}^{1/2}(4\lambda_3-\lambda_1) + \lambda_3k_{112}k_{233}/\lambda_2{}^{1/2}(4\lambda_3-\lambda_2)] + (\lambda_3/\lambda_1)^{1/2}\zeta_{13}^2/2I_z$

$(3312) = (3321) = (-8\pi^2c^2/\hbar)[\lambda_3k_{112}k_{133}/\lambda_1{}^{1/2}(4\lambda_3-\lambda_1) + \lambda_3k_{122}k_{233}/\lambda_2{}^{1/2}(4\lambda_3-\lambda_2)] + (\lambda_3{}^2/\lambda_1\lambda_2)^{1/4}\zeta_{13}\zeta_{23}/I_z$

$(3322) = (-4\pi^2c^2/\hbar)[\lambda_3k_{122}k_{133}/\lambda_1{}^{1/2}(4\lambda_3-\lambda_1) + 3\lambda_3k_{222}k_{233}/\lambda_2{}^{1/2}(4\lambda_3-\lambda_2)] + (\lambda_3/\lambda_2)^{1/2}\zeta_{23}^2/2I_z$

$(3333) = (-4\pi^2c^2/\hbar)[\lambda_3k_{133}^2/\lambda_1{}^{1/2}(4\lambda_3-\lambda_1) + \lambda_3k_{233}^2/\lambda_2{}^{1/2}(4\lambda_3-\lambda_2)]$

$(1313) = (1331) = (3113) = (3131) = [-16\pi^2c^2\lambda_3k_{133}k_{133}/\hbar\lambda_1{}^{1/2}(4\lambda_3-\lambda_1) - \zeta_{13}^2/I_z]$

$(1323) = (1332) = (3123) = (3132) = [-16\pi^2c^2\lambda_3k_{133}k_{233}/\hbar\lambda_1{}^{1/2}(4\lambda_3-\lambda_1) - (\lambda_1/\lambda_2)^{1/4}\zeta_{13}\zeta_{23}/I_z]$

$(2313) = (2331) = (3213) = (3231) = [-16\pi^2c^2\lambda_3k_{133}k_{233}/\hbar\lambda_2{}^{1/2}(4\lambda_3-\lambda_2) - (\lambda_2/\lambda_1)^{1/4}\zeta_{13}\zeta_{23}/I_z]$

$(2323) = (2332) = (3223) = (3232) = [-16\pi^2c^2\lambda_3k_{233}k_{233}/\hbar\lambda_2{}^{1/2}(4\lambda_3-\lambda_2) - \zeta_{23}^2/I_z$

APPENDIX X

Coefficients (2;-;-;abcd) and All Possible Permutations

Listed herein are the coefficients (2;-;-;abcd) in the seventh sum of (4.4). Throughout this appendix (2;-;-;abcd) will be written in the condensed form (abcd).

$$(1111) = 2\pi\hbar c k_{1111} - 2\pi^2c^2\hbar[3k_{111}^2/\lambda_1^{1/2} + k_{112}^2(2\lambda_1-\lambda_2)/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$$

$$(2222) = 2\pi\hbar c k_{2222} - 2\pi^2c^2\hbar[3k_{222}^2/\lambda_2^{1/2} + k_{122}^2(\lambda_2-\lambda_1)\lambda_1^{1/2}(4\lambda_2-\lambda_1)]$$

$$(3333) = 2\pi\hbar c k_{3333} - 2\pi^2c^2\hbar[k_{133}^2(2\lambda_3-\lambda_1)/\lambda_1^{1/2}(4\lambda_3-\lambda_1) + k_{233}^2(2\lambda_3-\lambda_2)/\lambda_2^{1/2}(4\lambda_3-\lambda_2)]$$

$$(1122) = 2\pi\hbar c k_{1122} - 4\pi^2c^2\hbar[k_{112}k_{222}(3\lambda_1-\lambda_2)/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + k_{111}k_{122}(3\lambda_2-\lambda_1)/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + 2k_{112}^2\lambda_1^{1/2}/(4\lambda_1-\lambda_2) + 2k_{122}^2\lambda_2^{1/2}/(4\lambda_2-\lambda_1)]$$

$$(1133) = 2\pi\hbar c k_{1133} - 2\pi^2c^2\hbar[k_{111}k_{133}(5\lambda_3-2\lambda_1)/\lambda_1^{1/2}(4\lambda_3-\lambda_1) + k_{112}k_{233}((2\lambda_1-\lambda_2)/2\lambda_2^{1/2}(4\lambda_1-\lambda_2) + (2\lambda_3-\lambda_2)/2\lambda_2^{1/2}(4\lambda_3-\lambda_2)) + 2k_{133}^2\lambda_3^{1/2}/(4\lambda_3-\lambda_1)]$$

$$(2233) = 2\pi\hbar c k_{2233} - 2\pi^2c^2\hbar[k_{222}k_{233}(5\lambda_3-2\lambda_2)/\lambda_2^{1/2}(4\lambda_3-\lambda_2) + (k_{122}k_{133}/\lambda_1^{1/2})((2\lambda_2-\lambda_1)/(4\lambda_2-\lambda_1) + (2\lambda_3-\lambda_1)/(4\lambda_3-\lambda_1)) + 2k_{233}^2\lambda_3^{1/2}/(4\lambda_3-\lambda_2)]$$

$$(1112) = 2\pi\hbar c k_{1112} - 2\pi^2c^2\hbar[k_{111}k_{112}(7\lambda_1-\lambda_2)/\lambda_1^{1/2}(4\lambda_1-\lambda_2) + k_{112}k_{122}(13\lambda_1\lambda_2-2\lambda_1^2-5\lambda_2^2)/\lambda_2^{1/2}(4\lambda_1-\lambda_2)(4\lambda_2-\lambda_1)]$$

$$(1222) = 2\pi\hbar c k_{1222} - 2\pi^2c^2\hbar[k_{122}k_{222}(7\lambda_2-\lambda_1)/\lambda_2^{1/2}(4\lambda_2-\lambda_1) + k_{112}k_{122}(13\lambda_1\lambda_2-2\lambda_2^2-5\lambda_1^2)/\lambda_1^{1/2}(4\lambda_1-\lambda_2)(4\lambda_2-\lambda_1)]$$

$$(1233) = 2\pi\hbar c k_{1233} - 4\pi^2c^2\hbar[k_{122}k_{233}((2\lambda_3-\lambda_2)/\lambda_2^{1/2}(4\lambda_3-\lambda_2) + \lambda_2^{1/2}/(4\lambda_2-\lambda_1)) + k_{112}k_{133}((2\lambda_3-\lambda_1)/\lambda_1^{1/2}(4\lambda_3-\lambda_1) + \lambda_1^{1/2}/(4\lambda_1-\lambda_2)) + 2k_{133}k_{233}\lambda_3^{1/2}(8\lambda_3-\lambda_1-\lambda_2)/(4\lambda_3-\lambda_1)(4\lambda_3-\lambda_2)]$$

APPENDIX XI

Coefficients $(3;\alpha\beta\gamma\delta;-;a)$ in h_3'

Listed herein are the coefficients $(3;\alpha\beta\gamma\delta;-;a)$ appearing in the first sum of (4.5). They are expressed in terms of the auxiliary coefficients $(T;\alpha,\beta\gamma\delta;-;a)$ and $(U;\alpha\beta,\gamma\delta;-;a)$ as follows:

$$(3;\alpha\beta\gamma\delta;-;a) = (T;\underline{\alpha,\beta\gamma\delta};-;a) + (U;\underline{\alpha\beta,\gamma\delta};-;a) \qquad \text{(A XI.1)}$$

The detailed expressions for $(T;\alpha,\beta\gamma\delta;-;a)$ and $(U;\alpha\beta,\gamma\delta;-;a)$ are given in this appendix following the list of $(3;\alpha\beta\gamma\delta;-;a)$. Throughout this appendix the condensed notations $(\alpha\beta\gamma\delta a)$, $(\alpha,\beta\gamma\delta a)$ and $(\alpha\beta,\gamma\delta a)$ are used to represent $(3;\alpha\beta\gamma\delta;-;a)$, $(T;\alpha,\beta\gamma\delta;-;a)$ and $(U;\alpha\beta,\gamma\delta;-;a)$, respectively.

(1) <u>Coefficients $(\alpha\beta\gamma\delta a)$:</u>

(xxxx1) = (xx,xx1) (xxxx2) = (xx,xx2)

(yyyy1) = (yy,yy1) (yyyy2) = (yy,yy2)

(zzzz1) = (z,zzz1) + (zz,zz1) (zzzz2) = (z,zzz2) = (zz,zz2)

(xxyy1) = (yyxx1) = [(xx,yy1) + (yy,xx1)]/2

(xxyy2) = (yyxx2) = [(xx,yy2) + (yy,xx2)]/2

(yyzz1) = (zzyy1) = [(z,yyz1) + (yy,zz1) + (zz,yy1)]/2

(yyzz2) = (zzyy2) = [(z,yyz2) + (yy,zz2) + (zz,yy2)]/2

(zzxx1) = (xxzz1) = [(z,xxz1) + (xx,zz1) + (zz,xx1)]/2

(zzxx2) = (xxzz2) = [(z,xxz2) + (xx,zz2) + (zz,xx2)]/2

(zxzx1) = (xzxz1) = (z,xzx1)/2

(zxzx2) = (xzxz2) = (z,xzx2)/2

(zyz-1) = (yzyz1) = (z,yzy1)/2

(zyzy2) = (yzyz2) = (z,yzy2)/2

(xyxy1) = (xyyx1) = (yxxy1) = (yxyx1) = (xy,xy1)

(xyxy2) = (xyyx2) = (yxxy2) = (yxyx2) = (xy,xy2)

(xxxy3) = (xxyx3) = (xyxx3) = (yxxx3) = [(xx,xy3) + (xy,xx3)]/2

(yyxy3) = (yyyx3) = (xyyy3) = (yxyy3) = [(yy,xy3) + (xy,yy3)]/2

(zzxy3) = (zzyx3) = [(z,zxy3) + (zz,xy3) + (xy,zz3)]/2

(xyzz3) = (yxzz3) = [(z,xyz3) + (xy,zz3) + (zz,xy3)]/2

(zxzy3) = (xzyz3) = zyzx3) = (yzxz3) = (z,xzy3)/2

(zyyz3) = (z,yyz3)/2 (zxxz3) = (z,xxz3)/2

(2) <u>Auxiliary coefficients $(\alpha,\beta\gamma\delta a)$:</u>

$$(z,zzz1) = [\hbar^{1/2}\zeta_{13}(\lambda_1+\lambda_3)/3(\lambda_1-\lambda_3)\lambda_1{}^{1/4}I_z{}^4](a_1^{zz}\zeta_{13} + a_2^{zz}\zeta_{23})\ X$$
$$[(\lambda_1+\lambda_2-2\lambda_3)/(\lambda_1-\lambda_2)(\lambda_2-\lambda_3) - (\lambda_1+\lambda_2)/2\lambda_1\lambda_2]$$

$$(z,zzz2) = [\hbar^{1/2}\zeta_{23}(\lambda_2+\lambda_3)/3(\lambda_2-\lambda_3)\lambda_2{}^{1/4}I_z{}^4](a_1^{zz}\zeta_{13} + a_2^{zz}\zeta_{23})\ X$$
$$[(\lambda_1+\lambda_2-2\lambda_3)/(\lambda_1-\lambda_2)(\lambda_2-\lambda_3) - (\lambda_1+\lambda_2)/2\lambda_1\lambda_2]$$

$$(z,xxz1) = (z,zxx1) = [\hbar^{1/2}\zeta_{13}(\lambda_1+\lambda_3)/12(\lambda_1-\lambda_3)\lambda_1{}^{1/4}I_x{}^2I_z{}^2]\ X$$
$$[a_1^{xx}\zeta_{13}(3\lambda_1-\lambda_3)/\lambda_1(\lambda_1-\lambda_3) + a_2^{xx}\zeta_{23}(3\lambda_2-\lambda_3)/\lambda_2(\lambda_2-\lambda_3)]$$
$$-a_3^{xy}\zeta_{13}(\lambda_1+\lambda_3)/8(\lambda_1-\lambda_3)\lambda_1{}^{1/4}\lambda_3I_x{}^2I_z{}^2\hbar^{1/2}$$

$$(z,xxz2) = (z,zxx2) = [\hbar^{1/2}\zeta_{23}(\lambda_2+\lambda_3)/12(\lambda_2-\lambda_3)\lambda_2{}^{1/4}I_x{}^2I_z{}^2]\ X$$
$$-a_3^{xy}\zeta_{23}(\lambda_2+\lambda_3)/8(\lambda_2-\lambda_3)\lambda_2{}^{1/4}\lambda_3I_x{}^2I_z{}^2\hbar^{1/2}$$

$$(z,yyz1) = (z,zyy1) = [\hbar^{1/2}\zeta_{13}(\lambda_1+\lambda_3)/12(\lambda_1-\lambda_3)\lambda_1{}^{1/4}I_y{}^2I_z{}^2]\ X$$
$$+a_3^{xy}\zeta_{13}(\lambda_1+\lambda_3)/8(\lambda_1-\lambda_3)\lambda_1{}^{1/4}\lambda_3I_y{}^2I_z{}^2\hbar^{1/2}$$

$$(z,yyz2) = (z,zyy2) = [\hbar^{1/2}\zeta_{23}(\lambda_2+\lambda_3)/12(\lambda_2-\lambda_3)\lambda_2{}^{1/4}I_y{}^2I_z{}^2]\ X$$
$$+a_3^{xy}\zeta_{23}(\lambda_2+\lambda_3)/8(\lambda_2-\lambda_3)\lambda_2{}^{1/4}\lambda_3I_y{}^2I_z{}^2\hbar^{1/2}$$

$$(z,xzx1) = -a_3^{xy}\zeta_{13}(\lambda_1+\lambda_3)/4I_x{}^2I_z{}^2(\lambda_1-\lambda_3)\lambda_1{}^{1/4}\lambda_3\hbar^{1/2}$$

$$(z,xzx2) = -a_3^{xy}\zeta_{23}(\lambda_2+\lambda_3)/4I_x{}^2I_z{}^2(\lambda_2-\lambda_3)\lambda_2{}^{1/4}\lambda_3\hbar^{1/2}$$

$$(z,yzy1) = +a_3^{xy}\zeta_{13}(\lambda_1+\lambda_3)/4I_y{}^2I_z{}^2(\lambda_1-\lambda_3)\lambda_1{}^{1/4}\lambda_3\hbar^{1/2}$$

$$(z,yzy2) = +a_3^{xy}\zeta_{23}(\lambda_2+\lambda_3)/4I_y{}^2I_z{}^2(\lambda_2-\lambda_3)\lambda_2{}^{1/4}\lambda_3\hbar^{1/2}$$

$$(z,xyz3) = (z,zyx3) = [-\hbar^{1/2}a_3^{xy}\zeta_{13}^2(\lambda_1+\lambda_3)/6(\lambda_1-\lambda_3)\lambda_3{}^{1/4}I_xI_yI_z{}^2] \times$$
$$[(\lambda_1-3\lambda_3)/2\lambda_3(\lambda_2-\lambda_3)] + [-\hbar^{1/2}a_3^{xy}\zeta_{23}^2(\lambda_2+\lambda_3)/6(\lambda_2-\lambda_3) \times$$
$$\lambda_3{}^{1/4}I_xI_yI_z{}^2][(\lambda_2-3\lambda_3)/2\lambda_3(\lambda_2-\lambda_3)] + [a_1^{xx} - a_1^{yy}(I_x-I_y)/$$
$$I_z][\zeta_{13}(\lambda_1+\lambda_3)/8I_xI_yI_z{}^2\lambda_1\lambda_3{}^{1/4}(\lambda_1-\lambda_3)\hbar^{1/2}] + [a_2^{xx}-a_2^{yy}\times$$
$$(I_x-I_y)/I_z][\zeta_{23}(\lambda_2+\lambda_3)/8I_xI_yI_z{}^2\lambda_2\lambda_3{}^{1/4}(\lambda_2-\lambda_3)\hbar^{1/2}]$$

$$(z,xzy3) = (z,yzx3) = (a_1^{yy}-a_1^{xx})\zeta_{13}(\lambda_1+\lambda_3)/8\ {}_1\ {}_3{}^{1/4}(\lambda_1-\lambda_3)I_xI_yI_z^2h^{1/2}$$

$$(z,zxy3) = (z,yxz3) = [-\hbar^{1/2}a_3^{xy}/12\lambda_3{}^{5/4}I_xI_yI_z{}^2][\zeta_{13}^2(\lambda_1+\lambda_3) \times$$
$$(\lambda_1-3\lambda_3)/(\lambda_1-\lambda_3) + \zeta_{23}^2(\lambda_2+\lambda_3)(\lambda_2-3\lambda_3)/(\lambda_2-\lambda_3)] - [a_1^{yy} +$$
$$a_1^{zz}(I_x-I_y)/I_z]\zeta_{13}(\lambda_1+\lambda_3)/8\lambda_1\lambda_3{}^{1/4}(\lambda_1-\lambda_3)I_xI_yI_z{}^2\hbar^{1/2} -$$
$$[a_2^{yy} + a_2^{zz}(I_x-I_y)/I_z]\zeta_{23}(\lambda_2+\lambda_3)/8\lambda_2\lambda_3^{1/4}I_xI_yI_z^2(\lambda_2-\lambda_3)\hbar^{1/2}$$

(3) <u>Auxiliary coefficients $(\alpha\beta,\gamma\delta a)$:</u>

$$(xx,xx1) = (3\hbar^{1/2}/2I_x{}^4\lambda_1{}^{1/4})[a_1^{xx}\sin^2\gamma/\lambda_1 + a_2^{xx}\sin\gamma\cos\gamma/2\lambda_2] +$$
$$(2\pi c a_1^{xx}/3I_x{}^4\lambda_1{}^{3/4})[2a_1^{xx}k_{111}/\lambda_1{}^{3/4} + a_2^{xx}k_{112}(3\lambda_1-\lambda_2)/$$
$$\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] + (\pi c a_2^{xx}/3I_x{}^4\lambda_2{}^{3/4})[a_1^{xx}k_{112}(5\lambda_1-\lambda_2)/$$
$$\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{xx}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]$$

$$(xx,xx2) = (3\hbar^{1/2}/2I_x{}^4\lambda_2{}^{1/4})[a_2^{xx}\cos^2\gamma/\lambda_2 + a_2^{xx}\sin\gamma\cos\gamma/2\lambda_1] +$$
$$(2\pi c a_2^{xx}/3I_x{}^4\lambda_2{}^{3/4})[2a_2^{xx}k_{222}/\lambda_2{}^{3/4} + a_1^{xx}k_{122}(3\lambda_2-\lambda_1)/$$
$$\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] + (\pi c a_1^{xx}/3I_x{}^4\lambda_1{}^{3/4})[a_1^{xx}k_{112}(5\lambda_1-\lambda_2)/$$
$$\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{xx}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]$$

$$(xx,yy1) = (3\hbar^{1/2}/2I_x{}^2I_y{}^2\lambda_1{}^{1/4})[a_1^{xx}\cos^2\gamma/\lambda_1 - a_2^{xx}\sin\gamma\cos\gamma/2\lambda_2] + (2\pi c a_1^{xx}/3I_x^2I_y^2\lambda_1^{3/4})[2a_1^{yy}k_{111}/\lambda_1 + a_2^{yy}k_{112}(3\lambda_1-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] + (\pi c a_2^{xx}/3I_x{}^2I_y{}^2\lambda_2{}^{3/4})[a_1^{yy}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{yy}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]$$

$$(xx,yy2) = (3\hbar^{1/2}/2I_x{}^2I_y{}^2\lambda_2{}^{1/4})[a_2^{xx}\cos^2\gamma/\lambda_2 - a_1^{xx}\sin\gamma\cos\gamma/2\lambda_1] + (2\pi c a_2^{xx}/3I_x{}^2I_y{}^2\lambda_2{}^{1/4})[2a_2^{yy}k_{222}/\lambda_2 + a_1^{yy}k_{122}(3\lambda_2-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] + (\pi c a_1^{xx}/3I_x{}^2I_y{}^2\lambda_1{}^{3/4})[a_1^{yy}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{yy}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]$$

$$(xx,zz1) = (3\hbar^{1/2}a_1^{zz}/8I_x{}^2I_z{}^3\lambda_1{}^{1/4})[a_1^{xx}a_1^{zz}/\lambda_1 + a_2^{xx}a_2^{zz}/2\lambda_2] + [\hbar^{1/2}\zeta_{13}(\lambda_1+\lambda_3)/3I_x{}^2I_z{}^2\lambda_1{}^{1/4}(\lambda_1-\lambda_3)][\zeta_{13}/\lambda_1 + 2\zeta_{23} \times (\lambda_1+\lambda_2-2\lambda_3)/\lambda_2(\lambda_2-\lambda_3)] + (2\pi c a_1^{xx}/3I_x{}^2I_z{}^2\lambda_1{}^{3/4})[2a_1^{zz} \times k_{111}/\lambda_1{}^{3/4} + a_2^{zz}k_{112}(3\lambda_1-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] + (\pi c a_2^{xx}/3I_x{}^2I_z{}^2\lambda_2{}^{3/4})[a_1^{zz}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{zz}k_{122} \times (5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]$$

$$(xx,zz2) = (3\hbar^{1/2}a_2^{zz}/8I_x{}^2I_z{}^3\lambda_2{}^{1/4})[a_2^{xx}a_2^{zz}/\lambda_2 + a_1^{xx}a_1^{zz}/2\lambda_1] + [\hbar^{1/2}\zeta_{23}(\lambda_2+\lambda_3)/3I_x{}^2I_z{}^2\lambda_2{}^{1/4}(\lambda_2-\lambda_3)][\zeta_{23}/\lambda_2 + 2\zeta_{13} \times (\lambda_1+\lambda_2-2\lambda_3)/\lambda_1(\lambda_1-\lambda_3)] + (2\pi c a_2^{xx}/3I_x{}^2I_z{}^2\lambda_2{}^{3/4})[2a_2^{zz} \times k_{222}/\lambda_2{}^{3/4} + a_1^{zz}k_{122}(3\lambda_2-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] + (\pi c a_1^{xx}/3I_x{}^2I_z{}^2\lambda_1{}^{3/4})[a_1^{zz}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{zz}k_{122} \times (5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]$$

$$(xx,xy3) = (xx,yx3) = (-3\hbar^{1/2}a_1^{xx}/8\lambda_1\lambda_3{}^{1/4}I_x{}^4I_y{}^2)[(I_x/I_z)^{1/2}\cos\gamma + (I_y/I_z)^{1/2}\sin\gamma] + (\hbar^{1/2}a_2^{xx}/8\lambda_2\lambda_3{}^{1/4}I_x{}^4I_y{}^2)[5(I_x/I_z)^{1/2} \times \sin\gamma - (I_y/I_z)^{1/2}\cos\gamma] + (\pi c/3I_x{}^3I_y\lambda_3{}^{3/4})[a_1^{xx}k_{133} \times (5\lambda_3-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_3-\lambda_1) + a_2^{xx}k_{233}(5\lambda_3-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_3-\lambda_2)] [\hbar^{1/2}(I_y-I_x)/8I_x{}^4I_y^2\lambda_3{}^{1/4}][a_1^{xx}\zeta_{13}(\lambda_1+\lambda_3)/\lambda_1(\lambda_1-\lambda_3) + a_2^{xx}\zeta_{23}(\lambda_2+\lambda_3)/\lambda_2(\lambda_2-\lambda_3)]$$

$$
\begin{aligned}
(yy,xx1) = {} & (3\hbar^{1/2}/2I_x{}^2I_y{}^2\lambda_1{}^{1/4})[a_1^{yy}\sin^2\gamma/\lambda_1 + a_2^{yy}\sin\gamma\cos\gamma/2\lambda_2] + \\
& (2\pi c a_1^{yy}/3I_x{}^2I_y{}^2\lambda_1{}^{3/4})[2a_1^{xx}k_{111}/\lambda_1{}^{3/4} + a_2^{xx}k_{112}(3\lambda_1-\lambda_2)/ \\
& \lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] + (\pi c a_2^{yy}/3I_x{}^2I_y{}^2\lambda_2{}^{3/4})[a_1^{xx}k_{112}(5\lambda_1-\lambda_2)/ \\
& \lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{xx}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]
\end{aligned}
$$

$$
\begin{aligned}
(yy,xx2) = {} & (3\hbar^{1/2}/2I_x{}^2I_y{}^2\lambda_2{}^{1/4})[a_2^{yy}\cos^2\gamma/\lambda_2 + a_1^{yy}\sin\gamma\cos\gamma/2\lambda_1] + \\
& (2\pi c a_2^{yy}/3I_x{}^2I_y{}^2\lambda_2{}^{3/4})[2a^{xx}k_{222}/\lambda_2{}^{3/4} + a_1^{xx}k_{122}(3\lambda_2-\lambda_1)/ \\
& \lambda_2{}^{3/4}(4\lambda_2-\lambda_1)] + (\pi c a_1^{yy}/3I_x{}^2I_y{}^2\lambda_1{}^{3/4})[a_1^{xx}k_{112}(5\lambda_1-\lambda_2)/ \\
& \lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{xx}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]
\end{aligned}
$$

$$
\begin{aligned}
(yy,yy1) = {} & (3\hbar^{1/2}/2I_y{}^4\lambda_1{}^{1/4})[a_1^{yy}\cos^2\gamma/\lambda_1 - a_2^{yy}\sin\gamma\cos\gamma/2\lambda_2] + \\
& (2\pi c a_1^{yy}/3I_y{}^4\lambda_1{}^{3/4})[2a_1^{yy}k_{111}/\lambda_1{}^{3/4} + a_2^{yy}k_{112}(3\lambda_1-\lambda_2)/ \\
& \lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] + (\pi c a_2^{yy}/3I_y{}^4\lambda_2{}^{3/4})[a_1^{yy}k_{112}(5\lambda_1-\lambda_2)/ \\
& \lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{yy}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]
\end{aligned}
$$

$$
\begin{aligned}
(yy,yy2) = {} & (3\hbar^{1/2}/2I_y{}^4\lambda_2{}^{1/4})[a_2^{yy}\sin^2\gamma/\lambda_2 - a_1^{yy}\sin\gamma\cos\gamma/2\lambda_1] + \\
& (2\pi c a_2^{yy}/3I_y{}^4\ {}_2{}^{3/4})[2a_2^{yy}k_{222}/\lambda_2{}^{3/4} + a_1^{yy}k_{122}(3\lambda_2-\lambda_1)/ \\
& \lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] + (\pi c a_1^{yy}/3I_y{}^4\lambda_1{}^{3/4})[a_1^{yy}k_{112}(5\lambda_1-\lambda_2)/ \\
& \lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{yy}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]
\end{aligned}
$$

$$
\begin{aligned}
(yy,zz1) = {} & (3\hbar^{1/2}a_1^{zz}/8I_y{}^2I_z{}^3\lambda_1{}^{1/4})[a_1^{yy}a_1^{zz}/\lambda_1 + a_2^{yy}a_2^{zz}/2\lambda_2] + \\
& [\hbar^{1/2}\zeta_{13}(\lambda_1+\lambda_3)/3I_y{}^2I_z{}^2\lambda_1{}^{1/4}(\lambda_1-\lambda_3)][a_1^{yy}\zeta_{13}/\lambda_1 + 2a_2^{yy} \times \\
& \zeta_{23}(\lambda_1+\lambda_2-2\lambda_3)/\lambda_2(\lambda_2-\lambda_3)] + (2\pi c a_1^{yy}/3I_y{}^2I_z{}^2\lambda_1{}^{3/4})[2a_1^{zz}\times \\
& k_{111}/\lambda_1{}^{3/4} + a_2^{zz}k_{112}(3\lambda_1-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] + (\pi c a_2^{yy}/ \\
& 3I_y{}^2I_z{}^2\lambda_2{}^{3/4})[a_1^{zz}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{zz}k_{122} \times \\
& (5\lambda_2-\lambda_1)/\ {}_2{}^{3/4}(4\lambda_2-\lambda_1)]
\end{aligned}
$$

$$
\begin{aligned}
(zz,xx1) = {} & (3\hbar^{1/2}/2I_x{}^2I_z{}^2\lambda_1{}^{1/4})[a_1^{zz}\sin^2\gamma/\lambda_1 + a_2^{zz}\sin\gamma\cos\gamma/2\lambda_2] + \\
& (2\pi c a_1^{zz}/3I_x{}^2I_z{}^2\lambda_1{}^{3/4})[2a_1^{xx}k_{111}/\lambda_1{}^{3/4} + a_2^{xx}k_{112}(3\lambda_1-\lambda_2)/ \\
& \lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] + (\pi c a_2^{zz}/3I_x{}^2I_z{}^2\lambda_2{}^{3/4})[a_1^{xx}k_{112}(5\lambda_1-\lambda_2)/ \\
& \lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{xx}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]
\end{aligned}
$$

$$\begin{aligned}(yy,zz2) = {} & (3\hbar^{1/2}a_2^{zz}/8I_y{}^2I_z{}^3\lambda_2{}^{1/4})[a_2^{yy}a_2^{zz}/\lambda_2 + a_1^{yy}a_1^{zz}/2\lambda_1] + \\ & [\hbar^{1/2}\zeta_{23}/3I_y{}^2I_z{}^2\lambda_2{}^{1/4}(\lambda_2-\lambda_3)][a_2^{yy}\zeta_{23}(\lambda_2+\lambda_3)/\lambda_2 + \\ & 2a_1^{yy}\zeta_{13}(\lambda_1+\lambda_3)(\lambda_1+\lambda_2-2\lambda_3)/\lambda_1(\lambda_1-\lambda_3)] + (2\pi c a_2^{yy}/3I_y{}^2I_z{}^2 \times \\ & \lambda_2{}^{3/4})[2a_2^{zz}k_{222}/\lambda_2{}^{3/4} + a_1^{zz}k_{122}(3\lambda_2-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] + \\ & (\pi c a_1^{yy}/3I_y{}^2I_z{}^2\lambda_1{}^{3/4})[a_1^{zz}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + \\ & a_2^{zz}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]\end{aligned}$$

$$\begin{aligned}(zz,xx2) = {} & (3\hbar^{1/2}/2I_x{}^2I_z{}^2\lambda_2{}^{1/4})[a_2^{zz}\cos^2\gamma/\lambda_2 + a_1^{zz}\sin\gamma\cos\gamma/2\lambda_1] + \\ & (2\pi c a_2^{zz}/3I_x{}^2I_z{}^2\lambda_2{}^{3/4})[2a_2^{xx}k_{222}/\lambda_2{}^{3/4} + a_1^{xx}k_{122}(3\lambda_2-\lambda_1)/ \\ & \lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] + (\pi c a_1^{zz}/3I_x{}^2I_z{}^2\lambda_1{}^{3/4})[a_1^{xx}k_{112}(5\lambda_1-\lambda_2)/ \\ & \lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{xx}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]\end{aligned}$$

$$\begin{aligned}(yy,xy3) = {} & (yy,yx3) = (-3\hbar^{1/2}a_1^{yy}/8I_x{}^2I_y{}^4\lambda_1\lambda_3{}^{1/4})[(I_x/I_z)^{1/2}\cos\gamma + \\ & (I_y/I_z)^{1/2}\sin\gamma] + (\hbar^{1/2}a_2^{yy}/8I_x{}^2I_y{}^4\lambda_2\lambda_3{}^{1/4})[5(I_x/I_z)^{1/2} \\ & \times \sin\gamma - (I_y/I_z)^{1/2}\cos\gamma] + (\pi c/3I_xI_y{}^3\lambda_3{}^{3/4})[a_1^{yy}k_{133} \times \\ & (5\lambda_3-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_3-\lambda_1) + a_2^{yy}k_{233}(5\lambda_3-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_3-\lambda_2)] \\ & [\hbar^{1/2}(I_y-I_x)/8I_x{}^2I_y{}^4\lambda_3{}^{1/4}][a_1^{yy}\zeta_{13}(\lambda_1+\lambda_3)/\lambda_1(\lambda_1-\lambda_3) + \\ & a_2^{yy}\zeta_{23}(\lambda_2+\lambda_3)/\lambda_2(\lambda_2-\lambda_3)]\end{aligned}$$

$$\begin{aligned}(zz,yy1) = {} & (3\hbar^{1/2}/2I_y{}^2I_z{}^2\lambda_1{}^{1/4})[a_1^{zz}\cos^2\gamma/\lambda_1 - a_2^{zz}\sin\gamma\cos\gamma/2\lambda_2] + \\ & (2\pi c a_1^{zz}/3I_z{}^2I_y^2\lambda_1{}^{3/4})[2a_1^{yy}k_{111}/\lambda_1{}^{3/4} + a_2^{yy}k_{112}(3\lambda_1-\lambda_2)/ \\ & \lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] + (\pi c a_2^{zz}/3I_z{}^2I_y{}^2\lambda_2{}^{3/4})[a_1^{yy}k_{112}(5\lambda_1-\lambda_2)/ \\ & \lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{yy}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]\end{aligned}$$

$$\begin{aligned}(zz,yy2) = {} & (3\hbar^{1/2}/2I_y{}^2I_z{}^2\lambda_2{}^{1/4})[a_2^{zz}\sin^2\gamma/\lambda_2 - a_1^{zz}\sin\gamma\cos\gamma/2\lambda_1] + \\ & (2\pi c a_2^{zz}/3I_z{}^2I_y{}^2\lambda_2{}^{3/4})[2a_2^{yy}k_{222}/\lambda_2{}^{3/4} + a_1^{yy}k_{122}(3\lambda_2-\lambda_1)/ \\ & \lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] + (\pi c a_1^{zz}/3I_z{}^2I_y{}^2\lambda_1{}^{3/4})[a_1^{yy}k_{112}(5\lambda_1-\lambda_2)/ \\ & \lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{yy}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]\end{aligned}$$

$$
\begin{aligned}
(zz,zz1) = {} & (3\hbar^{1/2}a_1^{zz}/2I_z{}^5\lambda_1{}^{1/4})[(a_1^{zz})^2/\lambda_1 + (a_2^{zz})^2/2\lambda_2] + [\hbar^{1/2} \times \\
& \zeta_{13}(\lambda_1+\lambda_3)/3I_z^4\,\lambda_1{}^{1/4}(\lambda_1-\lambda_3)][a_1^{zz}\zeta_{13}/\lambda_1 + 2a_2^{zz}\zeta_{23} \times \\
& (\lambda_1+\lambda_2-2\lambda_3)/\lambda_2(\lambda_2-\lambda_3)] + (2\pi c a_1^{zz}/3I_z{}^4\lambda_1{}^{3/4})[2a_1^{zz}k_{111}/ \\
& \lambda_1{}^{3/4} + a_2^{zz}k_{112}(3\lambda_1-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] + (\pi c a_2^{zz}/3I_z \times \\
& \lambda_2{}^{3/4})[a_1^{zz}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{zz}k_{122}(5\lambda_2-\lambda_1)/ \\
& \lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]
\end{aligned}
$$

$$
\begin{aligned}
(zz,zz2) = {} & (3\hbar^{1/2}a_2^{zz}/2I_z{}^5\lambda_2{}^{1/4})[(a_2^{zz})^2/\lambda_2 + (a_1^{zz})^2/2\lambda_1] + [\hbar^{1/2} \times \\
& \zeta_{23}(\lambda_1+\lambda_3)/3I_z{}^4\lambda_2{}^{1/4}(\lambda_2-\lambda_3)][a_2^{zz}\zeta_{23}/\lambda_2 + 2a_1^{zz}\zeta_{13} \times \\
& (\lambda_1+\lambda_2-2\lambda_3)/\lambda_1(\lambda_1-\lambda_3)] + (2\pi c a_2^{zz}/3I_z{}^4\lambda_2{}^{3/4})[2a_2^{zz}k_{222}/ \\
& \lambda_2{}^{3/4} + a_1^{zz}k_{122}(3\lambda_2-\lambda_1)/\lambda_1{}^{3/4}\ (4\lambda_2-\lambda_1)] + (\pi c a_1^{zz}/3I_z{}^4 \times \\
& \lambda_1{}^{3/4})[a_1^{zz}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{zz}k_{122}(5\lambda_2-\lambda_1)/ \\
& \lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]
\end{aligned}
$$

$$
\begin{aligned}
(zz,xy3) = (zz,yx3) = {} & (-3\hbar^{1/2}a_1^{zz}/8I_x{}^2I_y{}^2I_z{}^2\lambda_1\lambda_3{}^{1/4})[(I_x/I_z)^{1/2}\cos\gamma \\
& + (I_y/I_z)^{1/2}\sin\gamma] + (\hbar^{1/2}a_2^{zz}/8I_x{}^2I_y{}^2I_z{}^2\lambda_2\lambda_3{}^{1/4}) \times \\
& [5(I_x/I_z)^{1/2}\sin\gamma - (I_y/I_z)^{1/2}\cos\gamma] + [\hbar^{1/2}(I_y-I_x)/ \\
& 8I_x{}^2I_y{}^2I_z{}^2\lambda_3{}^{1/4}][a_1^{zz}\zeta_{13}(\lambda_1+\lambda_3)/\lambda_1(\lambda_1-\lambda_3) + a_2^{zz}\zeta_{23} \times \\
& (\lambda_2+\lambda_3)/\lambda_2(\lambda_2-\lambda_3)] + (\pi c/3I_xI_yI_z{}^2\lambda_3{}^{3/4})[a_1^{zz}k_{133} \times \\
& (5\lambda_3-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_3-\lambda_1) + a_2^{zz}k_{233}(5\lambda_3-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_3-\lambda_2)]
\end{aligned}
$$

$$
\begin{aligned}
(xy,xy1) = (xy,yx1) = (yx,xy1) = (yx,yx1) = {} & (-3\hbar^{1/2}a_3^{xy}/8I_x{}^3I_y{}^3\lambda_3 \times \\
& \lambda_1{}^{1/4})[(I_x/I_z)^{1/2}\cos\gamma + (I_y/I_z)^{1/2}\sin\gamma] + [\pi c a_3^{xy}k_{133} \times \\
& (5\lambda_3-\lambda_1)/3I_x{}^2I_y{}^2\ {}_3{}^{3/2}(4\lambda_3-\lambda_1)] + [\hbar^{1/2}\zeta_{13}(I_y-I_x) \times \\
& a_3^{xy}(\lambda_1+\lambda_3)/8I_x{}^3I_y{}^3\lambda_3\lambda_1{}^{1/4}(\lambda_1-\lambda_3)]
\end{aligned}
$$

$$
\begin{aligned}
(xy,xy2) = (xy,yx2) = (yx,xy2) = (yx,yx2) = {} & (\hbar^{1/2}a_3^{xy}/8I_x{}^3I_y{}^3\lambda_3 \times \\
& \lambda_2{}^{1/4})[5(I_x/I_z)^{1/2}\sin\gamma-(I_y/I_z)^{1/2}\cos\gamma] + (\pi c a_3^{xy}k_{233} \times \\
& (5\lambda_3-\lambda_2)/3I_x{}^2I_y{}^2\lambda_3{}^{3/2}(4\lambda_3-\lambda_2)] + [\hbar^{1/2}\zeta_{23}(I_y-I_x) \times \\
& a_3^{xy}(\lambda_2+\lambda_3)/8I_x{}^3I_y{}^3\lambda_3\lambda_2^{1/4}(\lambda_2-\lambda_3)]
\end{aligned}
$$

$$(xy,xx3) = (yx,xx3) = (3\hbar^{1/2}a_3^{xy}/2I_yI_zI_x{}^2\lambda_3{}^{5/4}) + (\pi ca_3^{xy}/3I_x{}^3I_y \times \lambda_3{}^{3/4})[a_1^{xx}k_{133}(3\lambda_3-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_3-\lambda_1) + a_2^{xx}k_{233}(3\lambda_3-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_3-\lambda_2)]$$

$$(xy,yy3) = (yx,yy3) = (3\hbar^{1/2}a_3^{xy}/2I_zI_xI_y{}^2\lambda_3{}^{5/4}) + (\pi ca_3^{xy}/3I_y{}^3I_x \times \lambda_3{}^{3/4})[a_1^{yy}k_{133}(3\lambda_3-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_3-\lambda_1) + a_2^{yy}k_{233}(3\lambda_3-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_3-\lambda_2)]$$

$$(xy,zz3) = (yx,zz3) = (\hbar^{1/2}a_3^{xy}/4I_xI_yI_z{}^2\lambda_3{}^{5/4})[\zeta_{13}{}^2/(\lambda_1-\lambda_3)+\zeta_{23}{}^2/(\lambda_2-\lambda_3)] + (\pi ca_3^{xy}/I_xI_yI_z{}^2\lambda_3{}^{3/4})[a_1^{zz}k_{133}(3\lambda_3-\lambda_1)/\lambda_1{}^{3/4}\times(4\lambda_3-\lambda_1) + a_2^{zz}k_{233}(3\lambda_3-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_3-\lambda_2)]$$

APPENDIX XII

Coefficients $(3;\alpha\beta\gamma;b;a)$ in h_3'

Expressed in terms of the auxiliary coefficients $(T;\alpha\beta\gamma;b;a)$, $(U;\alpha,\beta\gamma;b;a)$, $(N;\alpha,\beta\gamma;b;a)$, $(X;\alpha\beta,\gamma;b;a)$ and $(G;\alpha\beta\gamma;b;a)$, the coefficients $(3;\alpha\beta\gamma;b;a)$ appearing in the second sum of (4.5) are listed in this appendix. The detailed expressions for the auxiliary coefficients $(T;\alpha\beta\gamma;b;a)$, $(U;\alpha,\beta\gamma;b;a)$, etc., are given successively thereafter. For simplicity, the symbol "3" and all separating semicolons will be omitted , and the symbols "T", "U", etc., in the auxiliary coefficients will be kept only in the list of $(3;\alpha\beta\gamma;b;a)$.

(1) <u>Coefficients $(3;\alpha\beta\gamma;b;a)$</u> $\equiv (\alpha\beta\gamma ba) = (T\alpha\beta\gamma ba) + (U\underline{\alpha},\underline{\beta\gamma}ba) + (N\underline{\alpha},\underline{\beta\gamma}ba) + (X\underline{\alpha\beta},\underline{\gamma}ba) + (G\alpha\beta\gamma ba)$

In the following first ten entries j= 1, 2 :

(zzz3j) = (Tzzz3j) + (Uz,zz3j) + (Nz,zz3j) + (Xzz,z3j)

(zzzj3) = (Tzzzj3) + (Uz,zzj3) + (Nz,zzj3) + (Xzz,zj3)

(zxx3j) = (xxz3j) = (Tzxx3j) + [(Uz,xx3j) + (Nz,xx3j) + (Xxx,z3j)]/2 + (Gzxx3j)

(zxxj3) = (xxzj3) = (Tzxxj3) + [(Uz,xxj3) + (Nz,xxj3) + (Xxx,zj3)]/2 + (Gzxxj3)

(zyy3j) = (yyz3j) = (Tzyy3j) + [(Uz,yy3j) + (Nz,yy3j) + (Xyy,z3j)]/2 + (Gzyy3j)

(zyyj3) = (yyzj3) = (Tzyyj3) + [(Uz,yyj3) + (Nz,yyj3) + (Xyy-zj3)]/2 + (Gzyyj3) (xzx3j) = (Txzx3j) + (Gxzx3j)   (xzxj3) = (Txzxj3) + (Gxzxj3)

(yzy3j) = (Tyzy3j) + (Gyzy3j)   (yzyj3) = (Tyzyj3) + (Gyzyj3)

In the following three entries i = 1, 2 ; j = 1, 2 :

(xyzij) = (zyxij) = (Txyzij) + [(Uz,xyij) + (Nz,xyij) + (Xxy,zij)]/2 + (Gxyzij)

(zxyij) = (yxzij) = (Tzxyij) + [(Uz,xyij) + (Nz,xyij) + (Xxy,zij)]/2 + (Gzxyij)

(xzyij) = (yzxij) = (Txzyij) + (Gxzyij)

These last three entries are for a = b = 3 :

(xyz33) = (zyx33) = (Txyz33) + [(Uz,xy33) + (Nz,xy33) + (Xxy,z33)]/2 + (Gxyz33)

(zxy33) = (yxz33) = (Tzxy33) + [(Uz,xy33) + (Nz,xy33) + (Xxy,z33)]/2 + (Gzxy33)

(xzy33) = (yzx33) = (Txzy33)

(2) <u>Auxiliary coefficients $(T;\alpha\beta\gamma;b;a) \equiv (\alpha\beta\gamma\,ba)$:</u>

j = 1, 2

$$(zzz3j) = [-4\pi c k_{j33}\lambda_3^{3/4}/3I_z^3\hbar^{1/2}(4\lambda_3-\lambda_j)][a_1^{zz}\zeta_{13} + a_2^{zz}\zeta_{23}] \times [(\lambda_1+\lambda_2-2\lambda_3)/(\lambda_1-\lambda_3)(\lambda_2-\lambda_3) - (\lambda_1+\lambda_2)/2\lambda_1\lambda_2]$$

$$(zzzj3) = [-4\pi c k_{j33}\lambda_3^{1/4}(2\lambda_3-\lambda_j)/3I_z^3\hbar^{1/2}\lambda_j^{1/2}(4\lambda_3-\lambda_j)][a_1^{zz}\zeta_{13} + a_2^{zz}\zeta_{23}][(\lambda_1+\lambda_2-2\lambda_3)/(\lambda_1-\lambda_3)(\lambda_2-\lambda_3) - (\lambda_1+\lambda_2)/2\lambda_1\lambda_2]$$

$$(xxz3j) = (zxx3j) = [-\ c k_{j33}\ {}_3^{3/4}/3I_x^2 I_z h^{1/2}(4\ {}_3-\ {}_j)][a_1^{xx}\ {}_{13} \times (3\lambda_1-\lambda_3)/(\lambda_1-\lambda_3)\lambda_1 + a_2^{xx}\zeta_{23}(3\lambda_2-\lambda_3)/(\lambda_2-\lambda_3)\lambda_2] + \pi c k_{j33}a_3^{xy}/2I_x^2 I_z(4\lambda_3-\lambda_j)\lambda_3^{1/4}\hbar^{3/2}$$

$$\begin{aligned}
(xxzj3) = (zxxj3) = {} & [-\pi ck_{j33}(2\lambda_3-\lambda_j)\lambda_3^{1/4}/3I_x^2 I_z\lambda_j^{1/2}(4\lambda_3-\lambda_j)\hbar^{1/2}] \\
& \times [a_1^{xx}\zeta_{13}(3\lambda_1-\lambda_3)/(\lambda_1-\lambda_3)\lambda_1 + a_2^{xx}\zeta_{23}(3\lambda_2-\lambda_3)/(\lambda_2-\lambda_3)\lambda_2] \\
& + \pi ck_{j33}a_3^{xy}(2\lambda_3-\lambda_j)/2I_x^2 I_z\lambda_j^{1/2}(4\lambda_3-\lambda_j)\lambda_3^{3/4}\hbar^{3/2}
\end{aligned}$$

$$\begin{aligned}
(yyz3j) = (zyy3j) = {} & [-\pi ck_{j33}\;3^{3/4}/3I_y^2 I_z\hbar^{1/2}(4\lambda_3-\lambda_j)][a_1^{yy}\zeta_{13} \times \\
& (3\lambda_1-\lambda_3)/(\lambda_1-\lambda_3)\lambda_1 + a_2^{yy}\zeta_{23}(3\lambda_2-\lambda_3)/(\lambda_2-\lambda_3)\lambda_2] - \\
& \pi ck_{j33}a_3^{xy}/2I_y^2 I_z(4\lambda_3-\lambda_j)\lambda_3^{1/4}\hbar^{3/2}
\end{aligned}$$

$$\begin{aligned}
(yyzj3) = (zyyj3) = {} & [-\pi ck_{j33}(2\lambda_3-\lambda_j)\lambda_3^{1/4}/3I_y^2 I_z\lambda_j^{1/2}(4\lambda_3-\lambda_j)\hbar^{1/2}] \\
& \times [a_1^{yy}\zeta_{13}(3\lambda_1-\lambda_3)/(\lambda_1-\lambda_3)\lambda_1 + a_2^{yy}\zeta_{23}(3\lambda_2-\lambda_3)/(\lambda_2-\lambda_3)\lambda_2] \\
& - \pi ck_{j33}a_3^{xy}(2\lambda_3-\lambda_j)/2I_y^2 I_z\lambda_j^{1/2}(4\lambda_3-\lambda_j)\lambda_3^{3/4}\hbar^{3/2}
\end{aligned}$$

$$(xzx3j) = \pi ck_{j33}a_3^{xy}/I_x^2 I_z\lambda_3^{1/4}(4\lambda_3-\lambda_j)\hbar^{3/2}$$

$$(xzxj3) = \pi ck_{j33}a_3^{xy}(2\lambda_3-\lambda_j)/I_x^2 I_z\lambda_j^{1/2}\lambda_3^{3/4}(4\lambda_3-\lambda_j)\hbar^{3/2}$$

$$(yzy3j) = -\pi ck_{j33}a_3^{xy}/I_y\ I_z\lambda_3^{1/4}(4\lambda_3-\lambda_j)\hbar^{3/2}$$

$$(yzyj3) = -\pi ck_{j33}a_3^{xy}(2\lambda_3-\lambda_j)/I_y^2 I_z\lambda_j^{1/2}\lambda_3^{3/4}(4\lambda_3-\lambda_j)\hbar^{3/2}$$

$$\begin{aligned}
(xyz11) = (zyx11) = {} & \pi ck_{111}a_3^{xy}\zeta_{13}(\lambda_1-3\lambda_3)/3I_xI_yI_z\lambda_1^{1/4}(\lambda_1-\lambda_3)\hbar^{1/2} + \\
& (\pi ck_{111}/2I_xI_yI_z\lambda_1^{5/4}\hbar^{3/2})[a_1^{zz}(I_x-I_y)/I_z - a_1^{xx}] + \pi ck_{112} \times \\
& \lambda_1^{1/2}\lambda_2^{1/4}a_3^{xy}\zeta_{23}(\lambda_2-3\lambda_3)/3I_xI_yI_z(\lambda_2-\lambda_3)(4\lambda_1-\lambda_2)\lambda_3\hbar^{1/2} + \\
& (\pi ck_{112}\lambda_1^{1/2}/2I_xI_yI_z\lambda_2^{3/4}(4\lambda_1-\lambda_2)\hbar^{3/2})[a_2^{zz}(I_x-I_y)/I_z-a_2^{xx}]
\end{aligned}$$

$$\begin{aligned}
(xyz22) = (zyx22) = {} & \pi ck_{222}a_3^{xy}\zeta_{23}(\lambda_2-3\lambda_3)/3I_xI_yI_z\lambda_2^{1/4}(\lambda_2-\lambda_3)\hbar^{1/2} + \\
& (\pi ck_{222}/2I_xI_yI_z\lambda_2^{5/4}\hbar^{3/2})[a_2^{zz}(I_x-I_y)/I_z - a_2^{xx}] + \pi ck_{122} \times \\
& \lambda_2^{1/2}\lambda_1^{1/4}a_3^{xy}\zeta_{13}(\lambda_1-3\lambda_3)/3I_xI_yI_z(\lambda_1-\lambda_3)(4\lambda_2-\lambda_1)\lambda_3\hbar^{1/2} + \\
& (\pi ck_{122}\lambda_2^{1/2}/2I_xI_yI_z\lambda_1^{3/4}(4\lambda_2-\lambda_1)\hbar^{3/2})[a_1^{zz}(I_x-I_y)/I_z-a_1^{xx}]
\end{aligned}$$

$$\begin{aligned}
(xyz21) = (zyx21) = {} & \pi ck_{112}a_3^{xy}\zeta_{13}\lambda_1^{1/4}(2\lambda_1-\lambda_2)(\lambda_1-3\lambda_3)/3I_xI_yI_z \times \\
& \lambda_2^{1/2}(4\lambda_1-\lambda_2)(\lambda_1-\lambda_3)\hbar^{1/2} + (\pi ck_{112}(2\lambda_1-\lambda_2)/2I_xI_yI_z\lambda_2^{1/2} \times \\
& \lambda_1^{3/4}(4\lambda_1-\lambda_2)\hbar^{3/2})[a_1^{zz}(I_x-I_y)/I_z - a_1^{xx}] + \pi ck_{122}\lambda_1^{1/4} \times \\
& \lambda_2^{1/2}a_3^{xy}\zeta_{23}(\lambda_2-3\lambda_3)/3I_xI_yI_z\lambda_3(\lambda_2-\lambda_3)(4\lambda_2-\lambda_1)\hbar^{1/2} + (\pi c \times \\
& k_{122}/2I_xI_yI_z\lambda_2^{1/4}(4\lambda_2-\lambda_1)\hbar^{3/2})[a_2^{zz}(I_x-I_y)/I_z - a_2^{xx}]
\end{aligned}$$

$$(xyz12) = (zyx12) = \pi c k_{122}(2\lambda_2-\lambda_1)\lambda_2{}^{1/4}(\lambda_2-3\lambda_3)a_3^{xy}\zeta_{23}/3I_xI_yI_z \times$$
$$\lambda_1{}^{1/2}\lambda_3(\lambda_2-\lambda_3)(4\lambda_2-\lambda_1)\hbar^{1/2} + (\pi c k_{122}(2\lambda_2-\lambda_1)/2I_xI_yI_z \times$$
$$\lambda_1{}^{1/2}{}_2{}^{3/4}(4\lambda_2-\lambda_1)\hbar^{3/2})[a_2^{zz}(I_x-I_y)/I_z - a_2^{xx}] + \pi c k_{112} \times$$
$$\lambda_1{}^{3/4}a_3^{xy}\zeta_{13}(\lambda_1-3\lambda_3)/3I_xI_yI_z\lambda_3(\lambda_2-\lambda_3)(4\lambda_1-\lambda_2)\hbar^{1/2} + (\pi c \times$$
$$k_{112}/2I_xI_yI_z\ {}_1{}^{1/4}(4\lambda_1-\lambda_2)\hbar^{3/2})[a_1^{zz}(I_x-I_y)/I_z - a_1^{xx}]$$

$$(zxy11) = (yxz11) = \pi c k_{111}a_3^{xy}\zeta_{13}(\lambda_1-3\lambda_3)/3I_xI_yI_z\lambda_1{}^{1/4}\lambda_3(\lambda_1-\lambda_3)\hbar^{1/2}$$
$$+ (\pi c k_{111}/2I_xI_yI_z\lambda_1{}^{5/4}\hbar^{3/2})[a_1^{zz}(I_x-I_y)/I_z + a_1^{yy}] + \pi c \times$$
$$k_{112}\lambda_1{}^{1/2}\lambda_2{}^{1/4}a_3^{xy}\zeta_{13}(\lambda_2-3\lambda_3)/3I_xI_yI_z\lambda_3(\lambda_2-\lambda_3)(4\lambda_1-\lambda_2)\hbar^{1/2}$$
$$+ (\pi c k_{112}\lambda_1{}^{1/2}/2I_xI_yI_z\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)\hbar^{3/2})[a_2^{zz}(I_x-I_y)/I_z$$
$$+ a_2^{yy}]$$

$$(zxy22) = (yxz22) = \pi c k_{222}a_3^{xy}\zeta_{23}(\lambda_2-3\lambda_3)/3I_xI_yI_z\lambda_2{}^{1/4}\lambda_3(\lambda_2-\lambda_3)\hbar^{1/2}$$
$$+ (\pi c k_{222}/2I_xI_yI_z\lambda_2{}^{5/4}\hbar^{3/2})[a_2^{zz}(I_x-I_y)/I_z + a_2^{yy}] + \pi c \times$$
$$k_{122}\lambda_2{}^{1/2}\lambda_1{}^{1/4}a_3^{xy}\zeta_{23}(\lambda_1-3\lambda_3)/3I_xI_yI_z\lambda_3(\lambda_1-\lambda_3)(4\lambda_2-\lambda_1)\hbar^{1/2}$$
$$+ (\pi c k_{122}\lambda_2{}^{1/2}/2I_xI_yI_z\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)\hbar^{3/2})[a_1^{zz}(I_x-I_y)/I_z$$
$$+ a_1^{yy}]$$

$$(zxy21) = (yxz21) = \pi c k_{112}\lambda_1{}^{1/4}(2\lambda_1-\lambda_2)(\lambda_1-3\lambda_3)a_3^{xy}\zeta_{13}/3I_xI_yI_z\lambda_3 \times$$
$$\lambda_2{}^{1/2}(\lambda_1-\lambda_3)(4\lambda_1-\lambda_2)\hbar^{1/2} + (\pi c k_{112}(2\lambda_1-\lambda_2)/2I_xI_yI_z\lambda_2{}^{1/2}\times$$
$$\lambda_1{}^{3/4}(4\lambda_1-\lambda_2)\hbar^{3/2})[a_1^{zz}(I_x-I_y)/I_z + a_1^{yy}] + \pi c k_{122}\lambda_1{}^{1/4} \times$$
$$\lambda_2{}^{1/2}a_3^{xy}\zeta_{23}(\lambda_2-3\lambda_3)/3I_xI_yI_z\lambda_3(\lambda_2-\lambda_3)(4\lambda_2-\lambda_1)\hbar^{1/2} + (\pi c \times$$
$$k_{122}/2I_xI_yI_z\lambda_2{}^{1/4}(4\lambda_2-\lambda_1)\hbar^{3/2})[a_2^{zz}(I_x-I_y)/I_z + a_2^{yy}]$$

$$(zxy12) = (yxz12) = \pi c k_{122}a_3^{xy}\zeta_{23}(2\lambda_2-\lambda_1)(\lambda_2-3\lambda_3)/3I_xI_yI_z\lambda_1{}^{1/2}\lambda_3 \times$$
$$(\lambda_2-\lambda_3)(4\lambda_2-\lambda_1)\hbar^{1/2} + (\pi c k_{122}(2\lambda_2-\lambda_1)/2I_xI_yI_z\lambda_1{}^{1/2}\lambda_2{}^{3/4}\times$$
$$(4\lambda_2-\lambda_1)\hbar^{3/2})[a_2^{zz}(I_x-I_y)/I_z + a_2^{yy}] + \pi c k_{112}\lambda_1{}^{3/4}a_3^{xy}\zeta_{13}\times$$
$$(\lambda_1-3\lambda_3)/3I_xI_yI_z\lambda_3(\lambda_1-\lambda_3)(4\lambda_1-\lambda_2)\hbar^{1/2} + (\pi c k_{112}\lambda_1{}^{1/2}/$$
$$2I_xI_yI_z\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)\hbar^{3/2}[a_1^{zz}(I_x-I_y)/I_z + a_1^{yy}]$$

$$(xzy11) = (yzx11) = \pi c k_{111}(a_1^{yy} - a_1^{xx})/4I_xI_yI_z\lambda_1^{5/4}\hbar^{3/2} +$$

$$\pi c k_{112}\lambda_1^{1/2}(a_2^{yy} - a_2^{xx})/2I_xI_yI_z\lambda_2^{3/4}(4\lambda_1-\lambda_2)\hbar^{3/2}$$

$$(xzy22) = (yzx22) = \quad ck_{222}(a_2^{yy} - a_2^{xx})/4I_xI_yI_z\lambda_2^{5/4}\hbar^{3/2} +$$

$$\pi c k_{122}\lambda_2^{1/2}(a_1^{yy} - a_1^{xx})/2I_xI_yI_z\lambda_1^{3/4}(4\lambda_2-\lambda_1)\hbar^{3/2}$$

$$(xzy21) = (yzx21) = \pi c k_{112}(2\lambda_1-\lambda_2)(a_1^{yy} - a_1^{xx})/4I_xI_yI_z\lambda_2^{1/2}\lambda_1^{3/4} \times$$

$$(4\lambda_1-\lambda_2)\hbar^{3/2} + \pi c k_{122}(a_2^{yy} - a_2^{xx})/2I_xI_yI_z\lambda_2^{1/4}(4\lambda_2-\lambda_1)\hbar^{3/2}$$

$$(xzy12) = (yzx12) = \pi c k_{122}(2\lambda_2-\lambda_1)(a_2^{yy} - a_2^{xx})/4I_xI_yI_z\lambda_1^{1/2}\lambda_2^{3/4} \times$$

$$(4\lambda_2-\lambda_1)\hbar^{3/2} + \pi c k_{112}(a_1^{yy} - a_1^{xx})/2I_xI_yI_z\lambda_1^{1/4}(4\lambda_1-\lambda_2)\hbar^{3/2}$$

$$(xyz33) = (zyx33) = [\pi c k_{133}\lambda_3^{1/2}/\hbar^{1/2}I_xI_yI_z(4\lambda_3-\lambda_1)][a_3^{xy}\zeta_{13}\lambda_1^{1/4} \times$$

$$(\lambda_1-3\lambda_3)/3\lambda_3(\lambda_1-\lambda_3) + (a_1^{zz}(I_x-I_y)/I_z - a_1^{xx})/2\hbar\lambda_1^{3/4}] +$$

$$[\pi c k_{233}\lambda_3^{1/2}/\hbar^{1/2}I_xI_yI_z(4\lambda_3-\lambda_2)][a_3^{xy}\zeta_{23}\lambda_2^{1/4}(\lambda_2-3\lambda_3)/$$

$$3\lambda_3(\lambda_2-\lambda_3) + (a_2^{zz}(I_x-I_y)/I_z - a_2^{xx})/2\hbar\lambda_2^{3/4}]$$

$$(zyx33) = (yxz33) = [\pi c k_{133}\lambda_3^{1/2}/\hbar^{1/2}I_xI_yI_z(4\lambda_3-\lambda_1)][a_3^{xy}\zeta_{13}\lambda_1^{1/4} \times$$

$$(\lambda_1-3\lambda_3)/3\lambda_3(\lambda_1-\lambda_3) + (a_1^{zz}(I_x-I_y)/I_z + a_1^{yy})/2\hbar\lambda_1^{3/4}] +$$

$$[\pi c k_{233}\lambda_3^{1/2}/\hbar^{1/2}I_xI_yI_z(4\lambda_3-\lambda_2)][a_3^{xy}\zeta_{23}\lambda_2^{1/4}(\lambda_2-3\lambda_3)/$$

$$3\lambda_3(\lambda_2-\lambda_3) + (a_2^{zz}(I_x-I_y)/I_z + a_2^{yy})/2\hbar\lambda_2^{3/4}]$$

$$(xzy33) = (yzx33) = (\pi c\lambda_3^{1/2}/2I_xI_yI_z\hbar^{3/2})[(a_1^{yy} - a_1^{xx})k_{133}/\lambda_1^{3/4} \times$$

$$(4\lambda_3-\lambda_1) + (a_2^{yy} - a_2^{xx})k_{233}/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$$

(3) Auxiliary coefficients $(U;\alpha,\beta\gamma;b;a) \equiv (\alpha,\beta\gamma ba)$:

In the following, $\alpha = x, y$; $j = 1, 2$

$$(z,\ 13) = (-8\pi c\lambda_3^{1/4}/3I\ {}^2I_z\hbar^{5/2})[(\zeta_{13}\lambda_1^{1/4}/(\lambda_1-\lambda_3))[a_1^{\alpha\alpha}k_{111}/\lambda_1^{3/4}$$

$$+ a_2^{\alpha\alpha}k_{112}\lambda_1/\lambda_2^{3/4}(4\lambda_1-\lambda_2)] + (\zeta_{23}\lambda_2^{1/4}/(\lambda_2-\lambda_3))[a_2^{\alpha\alpha} \times$$

$$k_{122}\ {}_2{}^{3/4}/\ {}_1{}^{1/2}(4\ {}_2-\ {}_1) + a_1\ k_{112}\ {}_1{}^{3/4}/\ {}_2{}^{1/2}(4\ {}_1-\ {}_2)]]$$

$$(z,\ 23) = (-8\pi c\lambda_3^{1/4}/3I_\alpha^2I_z\hbar^{5/2})[(\zeta_{23}\lambda_2^{1/4}/(\lambda_2-\lambda_3))[a_2^{\alpha\alpha}k_{222}/\lambda_2^{3/4}$$

$$+ a_1^{\alpha\alpha}k_{122}\lambda_2/\lambda_1^{3/4}(4\lambda_2-\lambda_1)] + (\zeta_{13}\lambda_1^{1/4}/(\lambda_1-\lambda_3))[a_2^{\alpha\alpha} \times$$

$$k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]]$$

$$(z,zz13) = (-8\pi c\lambda_3^{1/4}/3I_z^3\hbar^{5/2})[(\zeta_{13}\lambda_1^{1/4}/(\lambda_1-\lambda_3))[a_1^{zz}k_{111}/\lambda_1^{3/4} + a_2^{zz}k_{112}\lambda_1/\lambda_2^{3/4}(4\lambda_1-\lambda_2)] + (\zeta_{23}\lambda_2^{1/4}/(\lambda_2-\lambda_3))[a_2^{zz} \times k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + a_1^{zz}k_{112}\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]] + (8\zeta_{13}\lambda_1^{1/4}\lambda_3^{1/4}/3I_z^3\hbar^2)[\lambda_1^{1/2}\zeta_{13}^2/(\lambda_1-\lambda_3)^2 + \lambda_2^{1/2} \times \zeta_{23}^2(\lambda_1+\lambda_2-2\lambda_3)/(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)^2]$$

$$(z,zz23) = (-8\pi c\lambda_3^{1/4}/3I_z^3\hbar^{5/2})[(\zeta_{23}\lambda_1^{1/4}/(\lambda_2-\lambda_3))[a_2^{zz}k_{222}/\lambda_2^{3/4} + a_1^{zz}k_{122}\lambda_2/\lambda_1^{3/4}(4\lambda_2-\lambda_1)] + (\zeta_{13}\lambda_1^{1/4}/(\lambda_1-\lambda_3))[a_1^{zz} \times k_{112}\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + a_2^{zz}k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1)]] + (8\zeta_{23}\lambda_2^{1/4}\lambda_3^{1/4}/3I_z^3\hbar^2)[\lambda_2^{1/2}\zeta_{23}^2/(\lambda_2-\lambda_3)^2 + \lambda_1^{1/2} \times \zeta_{13}^2(\lambda_1+\lambda_2-2\lambda_3)/(\lambda_2-\lambda_3)(\lambda_1-\lambda_3)^2]$$

$$(z,\alpha\alpha 3j) = (-8\pi c\zeta_{j3}\lambda_j^{1/4}\lambda_3^{5/4}/3I_\alpha^2 I_z(\lambda_j-\lambda_3)\hbar^{5/2})[a_1^{\alpha\alpha}k_{133}/\lambda_1^{3/4} \times (4\lambda_3-\lambda_1) + a_2^{\alpha\alpha}k_{233}/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$$

$$(z,zz3j) = (-8\pi c\zeta_{j3}\lambda_j^{1/4}\lambda_3^{1/4}/3I_z^3(\lambda_j-\lambda_3)\hbar^{5/2})[a_1^{zz}k_{133}/(4\lambda_3-\lambda_1) \times \lambda_1^{3/4} + a_2^{zz}k_{233}/(4\lambda_3-\lambda_2)\lambda_2^{3/4}] + (8\zeta_{j3}\lambda_j^{1/4}\lambda_3^{1/4}/3I_z^3 \times (\lambda_j-\lambda_3)\hbar^2)[\zeta_{13}^2/(\lambda_1-\lambda_3) + \zeta_{23}^2/(\lambda_2-\lambda_3)]$$

$$(z,xyij) = (z,yxij) = [-8\pi c a_3^{xy}k_{i33}\zeta_{j3}\lambda_j^{1/4}\lambda_3/3I_xI_yI_z\hbar^{5/2}\lambda_i^{1/2} \times (\lambda_j-\lambda_3)(4\lambda_3-\lambda_i) + \zeta_{i3}\zeta_{j3}(\lambda_i\lambda_j\lambda_3^2)^{1/4}(I_x-I_y)/2I_x^2I_y^2I_z \times \hbar(\lambda_i-\lambda_3)(\lambda_j-\lambda_3)] \quad , i = 1,\ 2\ ;\ j = 1,\ 2$$

$$(z,xy33) = (z,yx33) = (z,xy11) + (z,xy22)$$

(4) <u>Auxiliary coefficients $(N;\alpha,\beta\gamma;b;a) \equiv (\alpha,\beta\gamma ba)$:</u>

In the following, $\alpha = x,\ y\ ;\ j = 1,\ 2$

$$(z,\alpha\alpha j3) = 6\zeta_{j3}\lambda_j^{1/4}/(\lambda_j-\lambda_3)\lambda_3^{1/4}I_z^2I_\alpha + [4\pi\zeta_{j3}\lambda_j^{1/4}\lambda_3^{1/4}/3I_\alpha^2I_z \times \hbar^{1/2}(\lambda_j-\lambda_3)][a_1^{\alpha\alpha}k_{133}(3\lambda_3-\lambda_1)/\lambda_1^{3/4}(4\lambda_3-\lambda_1) + a_2^{\alpha\alpha}k_{233} \times (3\lambda_3-\lambda_2)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$$

$$(z,zzj3) = (8\pi c \zeta_{j3}\lambda_j^{1/4}\lambda_3^{1/4}/3I_z^{3}(\lambda_j-\lambda_3)\hbar^{1/2})[a_1^{zz}k_{133}(3\lambda_3-\lambda_1)/\lambda_1^{3/4}(4\lambda_3-\lambda_1) + a_2^{zz}k_{233}(3\lambda_3-\lambda_2)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)] + (\zeta_{j3} \times \lambda_j^{1/4}/(\lambda_j-\lambda_3)\lambda_3^{1/4}I_z^{3})[\zeta_{13}^{2}/(\lambda_1-\lambda_3) + \zeta_{23}^{2}/(\lambda_2-\lambda_3)]$$

$$(z,xx31) = 6\zeta_{13}\lambda_3^{1/4}\sin^2\gamma/(\lambda_1-\lambda_3)\lambda_1^{1/4}I_x^{2}I_z + (8\pi c\zeta_{13}\lambda_1^{1/4}\lambda_3^{1/4}/3(\lambda_1-\lambda_3)I_x^{2}I_z\hbar^{1/2})[2a_1^{xx}k_{111}/\lambda_1^{3/4} + a_2^{xx}k_{112}(3\lambda_1-\lambda_2)/(4\lambda_1-\lambda_2)\lambda_2^{3/4}] + (4\pi c\zeta_{23}\lambda_2^{1/4}\lambda_3^{1/4}/3(\lambda_2-\lambda_3)I_x^{2}I_z\hbar^{1/2}) \times [(5\lambda_1-\lambda_2)a_1^{xx}k_{112}/(4\lambda_1-\lambda_2)\lambda_1^{3/4} + (5\lambda_2-\lambda_1)a_2^{xx}k_{122}/\lambda_2^{3/4} \times (4\lambda_2-\lambda_1)] + 3\zeta_{13}\lambda_3^{1/4}\sin\gamma\cos\gamma/(\lambda_1-\lambda_3)\lambda_2^{1/4}I_x^{2}I_z$$

$$(z,xx32) = 6\zeta_{23}\lambda_3^{1/4}\cos^2\gamma/(\lambda_2-\lambda_3)\lambda_2^{1/4}I_x^{2}I_z + (8\pi c\zeta_{23}\lambda_2^{1/4}\lambda_3^{1/4}/3(\lambda_2-\lambda_3)I_x^{2}I_z\hbar^{1/2})[2a_2^{xx}k_{222}/\lambda_2^{3/4} + a_1^{xx}k_{122}(3\lambda_2-\lambda_1)/(4\lambda_2-\lambda_1)\lambda_1^{3/4}] + (4\pi c\zeta_{13}\lambda_1^{1/4}\lambda_3^{1/4}/3(\lambda_1-\lambda_3)I_x^{2}I_z\hbar^{1/2}) \times [(5\lambda_2-\lambda_1)a_2^{xx}k_{122}/(4\lambda_2-\lambda_1)\lambda_2^{3/4} + (5\lambda_1-\lambda_2)a_1^{xx}k_{112}/\lambda_1^{3/4} \times (4\lambda_1-\lambda_2)] + 3\zeta_{23}\lambda_3^{1/4}\sin\gamma\cos\gamma/(\lambda_2-\lambda_3)\lambda_1^{1/4}I_x^{2}I_z$$

$$(z,yy31) = 6\zeta_{13}\lambda_3^{1/4}\cos^2\gamma/(\lambda_1-\lambda_3)\lambda_1^{1/4}I_y^{2}I_z + (8\pi c\zeta_{13}\lambda_1^{1/4}\lambda_3^{1/4}/3(\lambda_1-\lambda_3)I_y^{2}I_z\hbar^{1/2})[2a_1^{yy}k_{111}/\lambda_1^{3/4} + a_2^{yy}k_{112}(3\lambda_1-\lambda_2)/(4\lambda_1-\lambda_2)\lambda_2^{3/4}] + (4\pi c\zeta_{23}\lambda_2^{1/4}\lambda_3^{1/4}/3(\lambda_2-\lambda_3)I_y^{2}I_z\hbar^{1/2}) \times [(5\lambda_1-\lambda_2)a_1^{yy}k_{112}/(4\lambda_1-\lambda_2)\lambda_1^{3/4} + (5\lambda_2-\lambda_1)a_2^{yy}k_{122}/\lambda_2^{3/4} \times (4\lambda_2-\lambda_1)] - 3\zeta_{13}\lambda_3^{1/4}\sin\gamma\cos\gamma/(\lambda_1-\lambda_3)\lambda_2^{1/4}I_y^{2}I_z$$

$$(z,yy32) = 6\zeta_{23}\lambda_3^{1/4}\sin^2\gamma/(\lambda_2-\lambda_3)\lambda_2^{1/4}I_y^{2}I_z + (8\pi c\zeta_{23}\lambda_2^{1/4}\lambda_3^{1/4}/3(\lambda_2-\lambda_3)I_y^{2}I_z\hbar^{1/2})[2a_2^{yy}k_{222}/\lambda_2^{3/4} + a_1^{yy}k_{122}(3\lambda_2-\lambda_1)/(4\lambda_2-\lambda_1)\lambda_1^{3/4}] + (4\pi c\zeta_{13}\lambda_1^{1/4}\lambda_3^{1/4}/3(\lambda_1-\lambda_3)I_y^{2}I_z\hbar^{1/2}) \times [(5\lambda_2-\lambda_1)a_2^{yy}k_{122}/(4\lambda_2-\lambda_1)\lambda_2^{3/4} + (5\lambda_1-\lambda_2)a_1^{yy}k_{112}/\lambda_1^{3/4} \times (4\lambda_1-\lambda_2)] - 3\zeta_{23}\lambda_3^{1/4}\sin\gamma\cos\gamma/(\lambda_2-\lambda_3)\lambda_1^{1/4}I_y^{2}I_z$$

$$(z,xy11) = (z,yx11) = [-3\zeta_{13}/2(\lambda_1-\lambda_3)I_x^{2}I_y^{2}I_z^{3/2}][I_x^{1/2}\cos\gamma + I_y^{1/2}\sin\gamma] + 4\pi c\zeta_{13}\lambda_1^{1/4}(5\lambda_3-\lambda_1)k_{133}/3(\lambda_1-\lambda_3)\lambda_3^{1/2} \times (4\lambda_3-\lambda_1)I_xI_yI_z\hbar^{1/2} - \zeta_{13}(\lambda_1+\lambda_3)(I_x-I_y)/2(\lambda_1-\lambda_3)^{2}I_x^{2}I_y^{2}I_z$$

$$(z,xy22) = (z,yx22) = [\zeta_{23}/2(\lambda_2-\lambda_3)I_x{}^2I_y{}^2I_z{}^{3/2}][5I_x{}^{1/2}\sin\gamma -$$
$$I_y{}^{1/2}\cos\gamma] + 4\pi c\zeta_{23}\lambda_2{}^{1/4}(5\lambda_3-\lambda_2)k_{233}/3(\lambda_2-\lambda_3)\lambda_3{}^{1/2} \times$$
$$(4\lambda_3-\lambda_2)I_xI_yI_z\hbar^{1/2} - \zeta_{23}^2(\lambda_2+\lambda_3)(I_x-I_y)/2(\lambda_2-\lambda_3)^2I_x{}^2I_y{}^2I_z$$

$$(z,xy12) = (z,yx12) = [\zeta_{13}\lambda_1{}^{1/4}/\lambda_2{}^{1/4}(\lambda_1-\lambda_3)I_x{}^2I_y{}^2I_z{}^{3/2}][5I_x{}^{1/2} \times$$
$$\sin\gamma - I_y{}^{1/2}\cos\gamma] + 4\pi c\zeta_{13}\lambda_1{}^{1/4}(5\lambda_3-\lambda_2)k_{233}/3(\lambda_1-\lambda_3) \times$$
$$(4\lambda_3-\lambda_2)\lambda_3{}^{1/2}I_xI_yI_z\hbar^{1/2} - \zeta_{13}\zeta_{23}\lambda_1{}^{1/4}(\lambda_2+\lambda_3)(I_x-I_y)/$$
$$2(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)\lambda_2{}^{1/4}I_x{}^2I_y{}^2I_z$$

$$(z,xy21) = (z,yx21) = [-3\zeta_{23}\lambda_2{}^{1/4}/2\lambda_1{}^{1/2}(\lambda_2-\lambda_3)I_x{}^2I_y{}^2I_z{}^{3/2}][I_x^{1/2} \times$$
$$\cos\gamma + I_y{}^{1/2}\sin\gamma] + 4\pi c\zeta_{23}\lambda_2{}^{1/4}(5\lambda_3-\lambda_1)k_{133}/3(\lambda_2-\lambda_3) \times$$
$$(4\lambda_3-\lambda_1)\lambda_3{}^{1/2}I_xI_yI_z\hbar^{1/2} - \zeta_{13}\zeta_{23}\lambda_2{}^{1/4}(\lambda_1+\lambda_3)(I_x-I_y)/$$
$$2(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)\lambda_1{}^{1/4}I_x{}^2I_y{}^2I_z$$

$$(z,zz31) = [8\pi c\zeta_{13}\lambda_1{}^{1/4}\lambda_3{}^{1/4}/3(\lambda_1-\lambda_3)I_z{}^3\hbar^{1/2}][2a_1^{zz}k_{111}/\lambda_1{}^{3/4} +$$
$$a_2^{zz}k_{112}(3\lambda_1-\lambda_2)/(4\lambda_1-\lambda_2)\lambda_2{}^{3/4}] + 4\zeta_{13}^3\lambda_3{}^{1/4}(\lambda_1+\lambda_3)/3I_z{}^3 \times$$
$$\lambda_1{}^{1/4}(\lambda_1-\lambda_3)^2 + [4\pi c\zeta_{23}\lambda_2{}^{1/4}\lambda_3{}^{1/4}/3(\lambda_2-\lambda_3)I_z{}^3\hbar^{1/2}] \times$$
$$[(5\lambda_1-\lambda_2)a_1^{zz}k_{112}/(4\lambda_1-\lambda_2)\lambda_1{}^{3/4} + (5\lambda_2-\lambda_1)a_2^{zz}k_{122}/\lambda_2{}^{3/4} \times$$
$$(4\lambda_2-\lambda_1)] + 4\zeta_{13}\zeta_{23}^2\lambda_3{}^{1/4}(\lambda_1+\lambda_3)(\lambda_1+\lambda_2-2\lambda_3)/3(\lambda_2-\lambda_3)^2 \times$$
$$\lambda_1{}^{1/4}(\lambda_1-\lambda_3)I_z{}^3 + 3\zeta_{13}\lambda_3{}^{1/4}(a_1^{zz})^2/2(\lambda_1-\lambda_3)\lambda_1{}^{1/4}I_z{}^4 +$$
$$3\zeta_{23}\lambda_3{}^{1/4}a_1^{zz}a_2^{zz}/4(\lambda_2-\lambda_3)\lambda_1{}^{1/4}I_z{}^4$$

$$(z,zz32) = [8\pi c\zeta_{23}\lambda_2{}^{1/4}\lambda_3{}^{1/4}/3(\lambda_2-\lambda_3)I_z{}^3\hbar^{1/2}][2a_2^{zz}k_{222}/\lambda_2{}^{3/4} +$$
$$a_1^{zz}k_{122}(3\lambda_2-\lambda_1)/(4\lambda_2-\lambda_1)\lambda_1{}^{3/4}] + 4\zeta_{23}^3\lambda_3{}^{1/4}(\lambda_2+\lambda_3)/3I_z{}^4 \times$$
$$\lambda_2{}^{1/4}(\lambda_2-\lambda_3)^2 + [4\pi c\zeta_{13}\lambda_1{}^{1/4}\lambda_3{}^{1/4}/3(\lambda_1-\lambda_3)I_z{}^3\hbar^{1/2}] \times$$
$$[(5\lambda_2-\lambda_1)a_2^{zz}k_{122}/(4\lambda_2-\lambda_1)\lambda_2{}^{3/4} + (5\lambda_1-\lambda_2)a_1^{zz}k_{112}/\lambda_1{}^{3/4} \times$$
$$(4\lambda_1-\lambda_2)] + 4\zeta_{23}\zeta_{13}^2\lambda_3{}^{1/4}(\lambda_2+\lambda_3)(\lambda_1+\lambda_2-2\lambda_3)/3(\lambda_1-\lambda_3)^2 \times$$
$$\lambda_2{}^{1/4}(\lambda_2-\lambda_3)I_z{}^3 + 3\zeta_{23}\lambda_3{}^{1/4}(a_2^{zz})^2/2(\lambda_2-\lambda_3)\lambda_2{}^{1/4}I_z{}^4 +$$
$$3\zeta_{13}\lambda_3{}^{1/4}a_1^{zz}a_2^{zz}/4(\lambda_1-\lambda_3)\lambda_2{}^{1/4}I_z{}^4$$

$$(z,xy33) = (z,yx33) = (z,xy11) + (z,xy22)$$

(5) Auxiliary coefficients $(X;\alpha\beta,\gamma;b;a) \equiv (\alpha\beta,\gamma ba)$:

In the following, α = x, y, z

$$(\alpha\alpha,z31) = a_1^{\alpha\alpha}a_1^{zz}\lambda_3^{1/4}\zeta_{13}/I_\alpha^2 I_z^2\lambda_1^{5/4} + a_2^{\alpha\alpha}(a_1^{zz}\zeta_{23} + a_2^{zz}\zeta_{13})\lambda_3^{1/4}/ 2I_\alpha^2 I_z^2\lambda_1^{1/4}\lambda_2 + (2\pi c a_1^{\alpha\alpha}\lambda_3^{1/4}/3I_\alpha^2 I_z\lambda_1^{3/4}\hbar^{1/2})[k_{111} \times \zeta_{13}(\lambda_3-7\lambda_1)/\lambda_1^{3/4}(\lambda_3-\lambda_1) + k_{112}\zeta_{23}((2\lambda_1-\lambda_2)/(4\lambda_1-\lambda_2) \times \lambda_2^{3/4} - 2\lambda_2^{1/4}/(\lambda_3-\lambda_2)) - 2k_{133}\zeta_{13}\lambda_3^{1/2}/(4\lambda_3-\lambda_1)\lambda_1^{1/4}] + (2\pi c a_2^{\alpha\alpha}\lambda_3^{1/4}/3I_\alpha^2 I_z\lambda_2^{3/4}\hbar^{1/2})[k_{112}\zeta_{13}\lambda_1^{1/4}(\lambda_3-9\lambda_1+ 2\lambda_2)/(4\lambda_1-\lambda_2)(\lambda_3-\lambda_1) + k_{122}\zeta_{23}\lambda_2^{1/4}(\lambda_3-9\lambda_2+2\lambda_1)/(4\lambda_2- \lambda_1)(\lambda_3-\lambda_2) - k_{133}\zeta_{23}\lambda_3^{1/2}/\lambda_2^{1/4}(4\lambda_3-\lambda_1) - k_{233}\zeta_{13}\lambda_3^{1/2}/ \lambda_1^{1/4}(4\lambda_3-\lambda_2)]$$

$$(\alpha\alpha,z32) = a_2^{\alpha\alpha}a_2^{zz}\lambda_3^{1/4}\zeta_{23}/I_\alpha^2 I_z^2\lambda_2^{5/4} + a_1^{\alpha\alpha}(a_2^{zz}\zeta_{13} + a_1^{zz}\zeta_{23})\lambda_3^{1/4}/ 2I_\alpha^2 I_z^2\lambda_2^{1/4}\lambda_1 + (2\pi c a_2^{\alpha\alpha}\lambda_3^{1/4}/3I_\alpha^2 I_z\lambda_2^{3/4}\hbar^{1/2})[k_{222} \times \zeta_{23}(\lambda_3-7\lambda_2)/\lambda_2^{3/4}(\lambda_3-\lambda_2) + k_{122}\zeta_{13}((2\lambda_2-\lambda_1)/(4\lambda_2-\lambda_1) \times \lambda_1^{3/4} - 2\lambda_1^{1/4}/(\lambda_3-\lambda_1)) - 2k_{233}\zeta_{23}\lambda_3^{1/2}/(4\lambda_3-\lambda_2)\lambda_2^{1/4}] + (2\pi c a_1^{\alpha\alpha}\lambda_3^{1/4}/3I_\alpha^2 I_z\lambda_1^{3/4}\hbar^{1/2})[k_{122}\zeta_{23}\lambda_2^{1/4}(\lambda_3-9\lambda_2+ 2\lambda_1)/(4\lambda_2-\lambda_1)(\lambda_3-\lambda_2) + k_{112}\zeta_{13}\lambda_1^{1/4}(\lambda_3-9\lambda_1+2\lambda_2)/(4\lambda_1- \lambda_2)(\lambda_3-\lambda_1) - k_{233}\zeta_{13}\lambda_3^{1/2}/\lambda_1^{1/4}(4\lambda_3-\lambda_2) - k_{133}\zeta_{23}\lambda_3^{1/2}/ \lambda_2^{1/4}(4\lambda_3-\lambda_1)]$$

$$(\alpha\alpha,z13) = (-a_1^{\alpha\alpha}/2I_\alpha^2\hbar^{1/2}\lambda_1^{3/4})[\hbar^{1/2}a_1^{zz}\zeta_{13}/I_z^2\lambda_3^{1/4} + (4\pi c/3I_z)\times [2\lambda_3^{5/4}(2\lambda_1+\lambda_3)\zeta_{13}k_{133}/(4\lambda_3-\lambda_1)(\lambda_3-\lambda_1)\lambda_1^{3/4} - \lambda_1^{1/2} \times \lambda_2^{1/4}\zeta_{23}k_{112}/(4\lambda_1-\lambda_2)\lambda_3^{1/4} - \zeta_{13}k_{111}/\lambda_1^{1/4}\lambda_3^{1/4}]] + (-a_2^{\alpha\alpha}/2I_\alpha^2\hbar^{1/2}\lambda_2^{3/4})[\hbar^{1/2}a_2^{zz}\zeta_{13}\lambda_1^{1/4}/I_z^2\lambda_2^{1/4}\lambda_3^{1/4} + (4\pi c/3I_z\ )[\lambda_1^{1/4}\lambda_3^{1/4}(\lambda_1+2\lambda_2-9\lambda_3)\zeta_{13}k_{233}/(4\lambda_3-\lambda_2)(\lambda_1- \lambda_3) + \lambda_3^{1/4}(2\lambda_3-\lambda_1)\zeta_{23}k_{133}/(4\lambda_3-\lambda_1)\lambda_1^{1/2}\lambda_2^{1/4} - \lambda_2^{1/4} \times (2\lambda_2-\lambda_1)\zeta_{23}k_{122}/(4\lambda_2-\lambda_1)\lambda_1^{1/2}\lambda_3^{1/4} - \lambda_1^{3/4}\zeta_{23}k_{112}/ (4\lambda_1-\lambda_2)\lambda_3^{1/4}$$

$$(\alpha\alpha,z23) = (-a_1^{\alpha\alpha}/2I_\alpha^2\hbar^{1/2}\lambda_1^{3/4})[\hbar^{1/2}a_1^{zz}\zeta_{23}\lambda_2^{1/4}/I_z^2\lambda_1^{1/4}\lambda_3^{1/4} + (4\pi c/3I_z)[\lambda_2^{1/4}\lambda_3^{1/4}(\lambda_2+2\lambda_1-9\lambda_3)\zeta_{23}k_{133}/(4\lambda_3-\lambda_1)(\lambda_2-\lambda_3) + \lambda_3^{1/4}(2\lambda_3-\lambda_2)\zeta_{13}k_{233}/(4\lambda_3-\lambda_2)\lambda_1^{1/4}\lambda_2^{1/4} - \lambda_1^{1/4} \times (2\lambda_1-\lambda_2)\zeta_{13}k_{112}/(4\lambda_1-\lambda_2)\lambda_3^{1/4}\lambda_2^{1/2} - \lambda_2^{3/4}\zeta_{13}k_{122}/(4\lambda_2-\lambda_1)\lambda_3^{1/4}]] + (-a_2^{\alpha\alpha}/2I_\alpha^2\hbar^{1/2}\lambda_2^{3/4})[\hbar^{1/2}a_2^{zz}\zeta_{23}/I_z^2\lambda_3^{1/4} + (4\pi c/3I_z)[2\lambda_3^{5/4}(2\lambda_2+\lambda_3)\zeta_{23}k_{233}/(4\lambda_3-\lambda_2)(\lambda_3-\lambda_2)\lambda_2^{3/4} - - \lambda_1^{1/4}\lambda_2^{1/2}\zeta_{13}k_{122}/(4\lambda_2-\lambda_1)\lambda_3^{1/4} - \zeta_{23}k_{222}/\lambda_2^{1/4}\lambda_3^{1/4}]]$$

$$(xy,z11) = (yx,z11) = -a_3^{xy}a_1^{zz}\zeta_{13}/2I_xI_yI_z^2\lambda_3 - (2\pi c a_3^{xy}/3I_xI_yI_z \times \lambda_3^{3/4}\hbar^{1/2})[2k_{133}\zeta_{13}\lambda_3^{5/4}(2\lambda_1+\lambda_3)/(4\lambda_3-\lambda_1)(\lambda_3-\lambda_1)\lambda_1^{3/4} - k_{112}\zeta_{23}\lambda_1^{1/2}\lambda_2^{1/4}/\lambda_3^{1/4}(4\lambda_1-\lambda_2) - k_{111}\zeta_{13}/\lambda_1^{1/4}\lambda_3^{1/4}]$$

$$(xy,z22) = (yx,z22) = -a_3^{xy}a_2^{zz}\zeta_{23}/2I_xI_yI_z^2\lambda_3 - (2\pi c a_3^{xy}/3I_xI_yI_z \times \lambda_3^{3/4}\hbar^{1/2})[2k_{233}\zeta_{23}\lambda_3^{5/4}(2\lambda_2+\lambda_3)/(4\lambda_3-\lambda_2)(\lambda_3-\lambda_2)\lambda_2^{3/4} - k_{122}\zeta_{13}\lambda_2^{1/2}\lambda_1^{1/4}/\lambda_3^{1/4}(4\lambda_2-\lambda_1) - k_{222}\zeta_{23}/\lambda_2^{1/4}\lambda_3^{1/4}]$$

$$(xy,z12) = (yx,z12) = -a_3^{xy}a_2^{zz}\zeta_{13}\lambda_1^{1/4}/2I_xI_yI_z^2\lambda_3\lambda_2^{1/4} - (2\pi c a_3^{xy}/3I_xI_yI_z\lambda_3^{3/4}\hbar^{1/2})[k_{233}\zeta_{13}\lambda_1^{1/4}\lambda_3^{1/4}(\lambda_1+2\lambda_2-9\lambda_3)/(4\lambda_3-\lambda_1)(\lambda_2-\lambda_3) + k_{133}\zeta_{23}\lambda_3^{1/4}(2\lambda_3-\lambda_1)\lambda_1^{1/2}\lambda_2^{1/4}(4\lambda_3-\lambda_1) - k_{122}\zeta_{23}\lambda_2^{1/4}(2\lambda_2-\lambda_1)/\lambda_1^{1/2}\lambda_3^{1/4}(4\lambda_2-\lambda_1) - k_{112}\zeta_{23} \times \lambda_1^{3/4}/\lambda_3^{1/4}(4\lambda_1-\lambda_2)]$$

$$(xy,z21) = (yx,z21) = -a_3^{xy}a_1^{zz}\zeta_{23}\lambda_2^{1/4}/2I_xI_yI_z^2\lambda_3\lambda_1^{1/4} - (2\pi c a_3^{xy}/3I_xI_yI_z\lambda_3^{3/4}\hbar^{1/2})[k_{133}\zeta_{23}\lambda_2^{1/4}\lambda_3^{1/4}(\lambda_2+2\lambda_1-9\lambda_3)/(4\lambda_3-\lambda_2)(\lambda_1-\lambda_3) + k_{233}\zeta_{13}\lambda_3^{1/4}(2\lambda_3-\lambda_2)\lambda_2^{1/2}\lambda_1^{1/4}(4\lambda_3-\lambda_2) - k_{112}\zeta_{13}\lambda_1^{1/4}(2\lambda_1-\lambda_2)/\lambda_2^{1/2}\lambda_3^{1/4}(4\lambda_1-\lambda_2) - k_{122}\zeta_{13} \times \lambda_2^{3/4}/\lambda_3^{1/4}(4\lambda_2-\lambda_1)]$$

(6) Auxiliary coefficients $(G;\alpha\beta;b;a) \equiv (\alpha\beta ba)$:

In the following, $\alpha = x, y$; $i = 1, 2$; $j = 1, 2$

$(\alpha\alpha zj3) = (z\alpha\alpha j3) = [(-)^{\delta_{\alpha x}} a_3^{xy}/8I_xI_y\lambda_j^{3/4}\lambda_3^{1/4}][a_j^{\alpha\alpha}/I_\alpha^2 - 2a_j^{zz}/I_z^2]$

$(\alpha\alpha z3j) = (z\alpha\alpha 3j) = [(-)^{\delta_{\alpha y}} a_3^{xy}/8I_xI_y\lambda_j^{1/4}\lambda_3^{3/4}][a_j^{\alpha\alpha}/I_\alpha^2 - a_j^{zz}/I_z^2]$

$(\alpha z\alpha j3) = (-)^{\delta_{\alpha x}} a_j^{\alpha\alpha} a_3^{xy}/4I_\alpha^2 I_xI_y\lambda_j^{3/4}\lambda_3^{1/4}$

$(\alpha z\alpha 3j) = [(-)^{\delta_{\alpha y}} a_3^{xy}/4I_xI_y\lambda_j^{1/4}\lambda_3^{3/4}][a_j^{\alpha\alpha}/I_\alpha^2 - a_j^{zz}/I_z^2]$

$(xyzij) = (zyxij) = (a_i^{zz}/8I_z^2\lambda_i^{3/4}\lambda_j^{1/4})[a_j^{yy}/I_y^2 - a_j^{xx}/I_x^2] +$
$(a_i^{xx}/8I_x^2\lambda_i^{3/4}\lambda_j^{1/4})[a_j^{zz}/I_z^2 - a_j^{yy}/I_y^2]$

$(xyz33) = (zyx33) = (a_3^{xy})^2/8I_x^2I_y^2\lambda_3$

$(zxyij) = (yxzij) = (a_i^{yy}/8I_y^2\lambda_i^{3/4}\lambda_j^{1/4})[a_j^{xx}/I_x^2 - a_j^{zz}/I_z^2] +$
$(a_i^{zz}/8I_z^2\lambda_i^{3/4}\lambda_j^{1/4})[a_j^{yy}/I_y^2 - a_j^{xx}/I_x^2]$

$(zxy33) = (yxz33) = -(xyz33)$

$(xzyij) = (yzxij) = (a_i^{xx}/8I_x^2\lambda_i^{3/4}\lambda_j^{1/4})[a_j^{zz}/I_z^2 - a_j^{yy}/I_y^2] +$
$(a_i^{yy}/8I_y^2\lambda_i^{3/4}\lambda_j^{1/4})[a_j^{xx}/I_x^2 - a_j^{zz}/I_z^2]$

APPENDIX XIII

Coefficients $(3;\alpha\beta;bc;a)$ in h_3'

The coefficients $(3;\alpha\beta;bc;a)$ appearing in the third sum of (4.5) have the general form

$$(3;\alpha\beta;bc;a) = (U;\alpha\beta;bc;a) + (X;\underline{\alpha},\underline{\beta};bc;a) + (P;\alpha\beta;bc;a) + (T;\alpha\beta;\underline{b},\underline{c};a) + (N;\underline{\alpha},\underline{\beta};\underline{b},\underline{c};a) + (G;\alpha\beta;bc;a)$$

where $(U;\alpha\beta;bc;a)$, $(X;\alpha,\beta;bc;a)$, etc., are auxiliary coefficients to be listed in details later in this appendix. The underlining of the alphabetical indices means that the corresponding coefficients must be constructed from the original ones as a consequence of the desymmetrization of the rotational operators in the terms to which those coefficients belong. The significance of the underlining of the numerical indices is best illustrated in the example below:

$$(T;\alpha\beta;\underline{b},\underline{c};a) = [(T;\alpha\beta;b,c;a) + (T;\alpha\beta;c,b;a)]/(1 + \delta_{bc})$$

List (1) of this appendix shows specifically which ones of the above auxiliary coefficients actually contribute to the nonzero $(3;\alpha\beta;bc;a)$-coefficients. In this list the symbol "3" and all separating semicolons are omitted from the coefficients, with the understanding that the alphabetical and numerical indices therein appear in their original orders. The auxiliary coefficients $(U;\alpha\beta;bc;a)$, $(X;\alpha,\beta;bc;a)$, etc., are listed separately in lists (2) to (7). In these lists the symbols "U", "X", etc., are omitted since it is only when the coefficients appear together that one really needs to keep these distinguishing symbols. Again, all separating semicolons are omitted.

(1) Coefficients (3;$\alpha\beta$;bc;a) ≡ ($\alpha\beta$bca) :

In the following, α = x, y ; i = 1, 2 ; j = 1, 2

($\alpha\alpha$iij) = (U$\alpha\alpha$iij) + (P$\alpha\alpha$iij) + (T$\alpha\alpha$i,ij)

($\alpha\alpha$12j) = ($\alpha\alpha$21j) = (U$\alpha\alpha$12j) + (P$\alpha\alpha$12j) + (T$\alpha\alpha$1,2j) + (T$\alpha\alpha$2,1j)

($\alpha\alpha$33j) = (U$\alpha\alpha$33j) + (P$\alpha\alpha$33j)

($\alpha\alpha$j33) = (U$\alpha\alpha$j33) + (P$\alpha\alpha$j33) + (G$\alpha\alpha$j33)

($\alpha\alpha$3j3) = (U$\alpha\alpha$j33) + (P$\alpha\alpha$j33) - (G$\alpha\alpha$j33)

(zziij) = (Uzziij) + (Xz,ziij) + (Pzziij) + (Tzzi,ij) + (Nzzi,ij)

(zz12j) = (Uzz12j) + (Xz,z12j) + (Pzz12j) +

(Tzz1,2j) + (Tzz2,1j) + (Nzz1,2j) + (Nzz2,1j)

(zz21j) = (zz12j)

(zz33j) = (Uzz33j) + (Pzz33j) + (Tzz3,3j)

(zzj33) = (Uzzj33) + (Xz,zj33) + (Pzzj33) + (Tzzj,33) + (Tzz3,j3)

(Nzzj,33) + (Nzz3,j3)

(zz3j3) = (zzj33)

(xyi3j) = (Uxyi3j) + (Pxyi3j) + (Txyi,3j) + (Txy3,ij) + (Gxyi3j)

(yxi3j) = (xyi3j)

(xy3ij) = (Uxyi3j) + (Pxyi3j) + (Txyi,3j) + (Txy3,ij) -(Gxyi3j)

(yx3ij) = (xy3ij)

(xy123) = (xy213) = (yx123) = (yx213) = (Uxy123) + (Pxy123) +

[(Xx,y123) + (xy,x123)]/2

(xyjj3) = (Uxyjj3) + (Pxyjj3)

(yxjj3) = (xyjj3)

(xy333) = (yx333) = (Uxy333) + (Pxy333)

(2) Auxiliary coefficients $(U;\alpha\beta;bc;a) \equiv (\alpha\beta bca)$:

In the following, $\alpha = x,\ y,\ z$

$$
\begin{aligned}
(\alpha\alpha 111) = {} & (-8\pi^2c^2k_{112}\lambda_1/3I_\alpha^{\,2}\hbar^{3/2}\lambda_2^{\,1/2}(4\lambda_1-\lambda_2))[a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/ \\
& \lambda_1^{\,3/4}(4\lambda_1-\lambda_2) + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{\,3/4}(4\lambda_2-\lambda_1)] - (16\pi^2c^2 \times \\
& k_{111}/3I_\alpha^{\,2}\hbar^{3/2}\lambda_1^{\,1/2})[2a_1^{\alpha\alpha}k_{111}/\lambda_1^{\,3/4} + a_2^{\alpha\alpha}k_{112}(3\lambda_1-\lambda_2)/ \\
& \lambda_2^{\,3/4}(4\lambda_1-\lambda_2)] - (12\pi ck_{111}/\hbar I_\alpha^{\,2}\lambda_1)[\delta_{\alpha x}\sin^2\gamma + \delta_{\alpha y}\cos^2\gamma] \\
& -(1-\delta_{\alpha z})(6\pi ck_{112}\lambda_1^{\,3/4}/\hbar I_\alpha^{\,2}\lambda_2^{\,3/4}(4\lambda_1-\lambda_2))[(-)^{1-\delta_{\alpha x}}\sin\gamma \times \\
& \cos\gamma] + \delta_{\alpha z}[-3\pi ck_{111}(a_1^{zz})/\hbar I_z^{\,3}\lambda_1 - 3\pi ck_{112}a_1^{zz}a_2^{zz}\lambda_1^{\,3/4}/ \\
& 2\hbar I_z^{\,3}\lambda_2^{\,3/4}(4\lambda_1-\lambda_2) - 8\pi ck_{111}\zeta_{13}^2(\lambda_1+\lambda_3)/3I_z^{\,2}\hbar\lambda_1(\lambda_1-\lambda_3) - \\
& -8\pi ck_{112}\lambda_1^{\,3/4}\zeta_{13}\zeta_{23}(\lambda_1+\lambda_3)(\lambda_1+\lambda_2-2\lambda_3)/3I_z^{\,2}\hbar\lambda_2^{\,3/4}(\lambda_1-\lambda_3) \times \\
& (\lambda_2-\lambda_3)(4\lambda_1-\lambda_2)]
\end{aligned}
$$

$$
\begin{aligned}
(\alpha\alpha 121) = {} & (\alpha\alpha 211) = (-32\pi^2c^2k_{112}\lambda_1/3I_\alpha^{\,2}\hbar^{3/2}\lambda_2^{\,1/2}(4\lambda_1-\lambda_2))[2a_1^{\alpha\alpha}k_{111}/ \\
& \lambda_1^{\,3/4} + a_2^{\alpha\alpha}k_{112}(3\lambda_1-\lambda_2)/\lambda_2^{\,3/4}(4\lambda_1-\lambda_2)] - (16\pi^2c^2k_{122}\lambda_2/ \\
& 3I_\alpha^{\,2}\hbar^{3/2}\lambda_1^{\,1/2}(4\lambda_2-\lambda_1))[a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/\lambda_1^{\,3/4}(4\lambda_1-\lambda_2) + \\
& a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{\,3/4}(4\lambda_2-\lambda_1)] - (24\pi ck_{112}\lambda_1^{\,1/2}/\hbar I_\alpha^{\,2} \times \\
& \lambda_2^{\,1/2}(4\lambda_1-\lambda_2))[\delta_{\alpha x}\sin^2\gamma + \delta_{\alpha y}\cos^2\gamma] - (1-\delta_{\alpha z})(12\pi ck_{122} \times \\
& \lambda_2^{\,3/4}/\hbar I_\alpha^{\,2}\lambda_1^{\,3/4}(4\lambda_2-\lambda_1))[(-)^{1-\delta_{\alpha x}}\sin\gamma\cos\gamma] - \delta_{\alpha z}[6\pi c \times \\
& k_{112}(a_1^{zz})\lambda_1^{\,1/2}/\hbar I_z^{\,3}\lambda_2^{\,1/2}(4\lambda_1-\lambda_2) + 3\pi ck_{122}a_1^{zz}a_2^{zz}\lambda_2^{\,3/4}/ \\
& \hbar I_z^{\,3}\lambda_1^{\,3/4}(4\lambda_2-\lambda_1) + 16\pi ck_{122}\lambda_2^{\,3/4}\zeta_{13}\zeta_{23}(\lambda_1+\lambda_3)(\lambda_1+\lambda_2- \\
& 2\lambda_3)/3I_z^{\,2}\hbar\lambda_1^{\,3/4}(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)(4\lambda_2-\lambda_1) + 16\pi ck_{112}\lambda_1^{\,1/2} \times \\
& \zeta_{13}^2(\lambda_1+\lambda_3)/3I_z^{\,2}\hbar\lambda_2^{\,1/2}(\lambda_1-\lambda_3)(4\lambda_1-\lambda_2)]
\end{aligned}
$$

$$
\begin{aligned}
(\alpha\alpha 221) = {} & (-8\pi^2c^2k_{222}/3I_\alpha^{\,2}\hbar^{3/2}\lambda_1^{\,1/2})[a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/\lambda_1^{\,3/4}(4\lambda_1-\lambda_2) \\
& + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{\,3/4}(4\lambda_2-\lambda_1)] - (16\pi^2c^2k_{122}\lambda_2/3I_\alpha^{\,2} \times \\
& \hbar^{3/2}\lambda_1^{\,1/2}(4\lambda_2-\lambda_1))[2a_1^{\alpha\alpha}k_{111}/\lambda_1^{\,3/4} + a_2^{\alpha\alpha}k_{112}(3\lambda_1-\lambda_2)/ \\
& \lambda_2^{\,3/4}(4\lambda_1-\lambda_2)] - (12\pi ck_{122}\lambda_2/\hbar I_\alpha^{\,2}\lambda_1(4\lambda_2-\lambda_1)[\delta_{\alpha x}\sin^2\gamma + \\
& \delta_{\alpha y}\cos^2\gamma] - (1-\delta_{\alpha z})(6\pi ck_{222}/\hbar I_\alpha^{\,2}\lambda_2^{\,3/4}\lambda_1^{\,1/4})[(-)^{1-\delta_{\alpha x}} \times \ldots
\end{aligned}
$$

($\alpha\alpha$221), cont'd :

$\sin\gamma\cos\gamma] - \delta_{\alpha z}[3\pi c k_{112}(a_1^{zz})^2\lambda_2/\hbar I_z{}^3\lambda_1(4\lambda_2-\lambda_1) + 3\pi c \times$
$k_{222}a_1^{zz}a_2^{zz}/2\hbar I_z{}^3\lambda_2{}^{3/4}\lambda_1{}^{1/4} + 8\pi c k_{222}\zeta_{13}\zeta_{23}(\lambda_1+\lambda_3)(\lambda_1+\lambda_2$
$-2\lambda_3)/3I_z{}^2\lambda_1{}^{1/4}\lambda_2{}^{3/4}(\lambda_1-\lambda_3)(\lambda_2-\lambda_3) - 8\pi c k_{122}\lambda_2\zeta_{13}^2(\lambda_1+$
$\lambda_3)/3I_z\lambda_1(\lambda_1-\lambda_3)(4\lambda_2-\lambda_1)]$

($\alpha\alpha$112) = $(-8\pi^2c^2k_{111}/3I_\alpha{}^2\hbar^{3/2}\lambda_1{}^{1/2})[a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-$
$\lambda_2) + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)] - (16\pi^2c^2k_{112}\lambda_1/$
$3I_\alpha{}^2\hbar^{3/2}\lambda_2{}^{1/2}(4\lambda_1-\lambda_2))[2a_2^{\alpha\alpha}k_{222}/\lambda_2{}^{3/4} + a_1^{\alpha\alpha}k_{122}(3\lambda_2-\lambda_1)/$
$\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] - (12\pi c k_{112}\lambda_1/\hbar I_\alpha{}^2\lambda_2(4\lambda_1-\lambda_2))[\delta_{\alpha x}\cos^2\gamma+$
$\delta_{\alpha y}\sin^2\gamma] - (1-\delta_{\alpha z})(6\pi c k_{111}/\hbar I_\alpha{}^2\lambda_1{}^{3/4}\lambda_2{}^{1/4})[(-)^{1-\delta_{\alpha x}} \times$
$\sin\gamma\cos\gamma] - \delta_{\alpha z}[3\pi c k_{112}(a_2^{zz})^2\lambda_1/\hbar I_z{}^3\lambda_2(4\lambda_1-\lambda_2) + 3\pi c k_{111}\times$
$a_1^{zz}a_2^{zz}/2\hbar I_z{}^3\lambda_1{}^{3/4}\lambda_2{}^{1/4} - 8\pi c k_{111}\zeta_{13}\zeta_{23}(\lambda_1+\lambda_3)(\lambda_1+\lambda_2-$
$2\lambda_3)/3I_z{}^2\lambda_1{}^{3/4}\lambda_2{}^{1/4}(\lambda_1-\lambda_3)(\lambda_2-\lambda_3) - 8\pi c k_{112}\lambda_1\zeta_{23}^2(\lambda_2+\lambda_3)/$
$3I_z{}^2\lambda_2(\lambda_2-\lambda_3)(4\lambda_1-\lambda_2)]$

($\alpha\alpha$222) = $(-16\pi^2c^2k_{222}/3I_\alpha{}^2\hbar^{3/2}\lambda_2{}^{1/2})[2a_2^{\alpha\alpha}k_{222}/\lambda_2{}^{3/4} + a_1^{\alpha\alpha}k_{122} \times$
$(3\lambda_2-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] - (8\pi^2c^2k_{122}\lambda_2/3I_\alpha{}^2\hbar^{3/2}\lambda_1{}^{1/2} \times$
$(4\lambda_2-\lambda_1))[a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}(5\lambda_1-$
$\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2)] - (12\pi c k_{222}/\hbar I_\alpha{}^2\lambda_2)[\delta_{\alpha x}\cos^2 + \delta_{\alpha y} \times$
$\sin^2\gamma] - (1-\delta_{\alpha z})(6\pi c k_{122}\lambda_2{}^{3/4}/\hbar I_\alpha{}^2\lambda_1{}^{3/4}(4\lambda_2-\lambda_1))[(-)^{1-\delta_{\alpha x}} \times$
$\sin\gamma\cos\gamma] - \delta_{\alpha z}[3\pi c k_{222}(a_2^{zz})^2/\hbar I_z{}^3\lambda_2 + 3\pi c k_{112}a_1^{zz}a_2^{zz} \times$
$\lambda_2{}^{3/4}/\hbar I_z{}^3\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + 8\pi c k_{222}\zeta_{23}^2(\lambda_2+\lambda_3)/3I_z{}^2\hbar\lambda_2(\lambda_2-$
$\lambda_3) + 8\pi c k_{122}\lambda_2{}^{3/4}(\lambda_2+\lambda_3)(\lambda_1+\lambda_2-2\lambda_3)\zeta_{23}\zeta_{13}/3I_z{}^2\hbar\lambda_1{}^{3/4} \times$
$(\lambda_2-\lambda_3)(\lambda_1-\lambda_3)(4\lambda_2-\lambda_1)]$

($\alpha\alpha$122) = ($\alpha\alpha$212) = $(-32\pi^2c^2k_{122}\lambda_2/3I_\alpha{}^2\hbar^{3/2}\lambda_1{}^{1/2}(4\lambda_2-\lambda_1))[2a_2^{\alpha\alpha} \times$
$k_{222}/\lambda_2{}^{3/4} + a_1^{\alpha\alpha}k_{122}(3\lambda_2-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] - (16\pi^2c^2 \times$
$k_{112}\lambda_1/3I_\alpha{}^2\hbar^{3/2}\lambda_2{}^{1/2}(4\lambda_1-\lambda_2))[a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4} \times$...

($\alpha\alpha$122), cont'd.

$(4\lambda_1-\lambda_2) + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{3/4}(4\lambda_2-\lambda_1)] -(24\pi ck_{122}\ X$

$\lambda_2^{1/2}/\hbar I_\alpha^2\lambda_1^{1/2}(4\lambda_2-\lambda_1))[\delta_{\alpha x}\cos^2\gamma + \delta_{\alpha y}\sin^2\gamma] -(1-\delta_{\alpha z})X$

$(12\pi ck_{112}\lambda_1^{3/4}/\hbar I_\alpha^2\lambda_2^{3/4}(4\lambda_1-\lambda_2))[(-)^{1-\delta_{\alpha x}}\sin\gamma\cos\gamma] -$

$\delta_{\alpha z}[6\pi ck_{122}(a_2^{zz})^2\lambda_2^{1/2}/\hbar I_z^3\lambda_1^{1/2}(4\lambda_1-\lambda_2) + 3\pi ck_{112}a_1^{zz}\ X$

$a_2^{zz}\lambda_1^{3/4}/\hbar I_z^3\lambda_2^{1/2}(4\lambda_1-\lambda_2) + 16\pi ck_{122}\lambda_2^{1/2}\zeta_{23}^2(\lambda_2+\lambda_3)/$

$3I_z^2(\lambda_2-\lambda_3)(4\lambda_2-\lambda_1)\lambda_1^{1/2} - 16\pi ck_{112}(\lambda_1+\lambda_3)(\lambda_1+\lambda_2-2\lambda_3)\ X$

$\lambda_1^{3/4}\zeta_{13}\zeta_{23}/3I_z^2\lambda_2^{3/4}(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)(4\lambda_1-\lambda_2)]$

$(\alpha\alpha331) = (-16\pi^2c^2k_{133}\lambda_3/3I_\alpha^2\hbar^{3/2}\lambda_1^{1/2}(4\lambda_3-\lambda_1))[2a_1^{\alpha\alpha}k_{111}/\lambda_1^{3/4} +$

$a_2^{\alpha\alpha}k_{112}(3\lambda_1-\lambda_2)/\lambda_2^{3/4}(4\lambda_1-\lambda_2)] - (8\pi^2c^2k_{233}\lambda_3/3I_\alpha^2\hbar^{3/2}X$

$\lambda_2^{1/2}(4\lambda_3-\lambda_2))[a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/\lambda_1^{3/4}(4\lambda_1-\lambda_2) + a_2^{\alpha\alpha}k_{122}X$

$(5\lambda_2-\lambda_1)/\lambda_2^{3/4}(4\lambda_2-\lambda_1)] - (12\pi ck_{133}\lambda_3/\hbar I_\alpha^2\lambda_1(4\lambda_3-\lambda_1))X$

$[\delta_{\alpha x}\sin^2\gamma + \delta_{\alpha y}\cos^2\gamma] - (1-\delta_{\alpha z})(6\pi ck_{233}\lambda_3/\hbar I_\alpha^2\lambda_2^{3/4}\ X$

$\lambda_1^{1/4}(4\lambda_3-\lambda_2))[(-)^{1-\delta_{\alpha x}}\sin\gamma\cos\gamma] - \delta_{\alpha z}[3\pi c\lambda_3a_1^{zz}/\hbar I_z^3\ X$

$\lambda_1^{1/4}][a_1^{zz}k_{133}/\lambda_1^{3/4}(4\lambda_3-\lambda_1) + a_2^{zz}k_{233}/2\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$

$(\alpha\alpha332) = (-8\pi^2c^2k_{133}\ 3/3I_\alpha^2\hbar^{3/2}\lambda_1^{1/2}(4\lambda_3-\lambda_1))[a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/$

$\lambda_1^{3/4}(4\lambda_1-\lambda_2) + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{3/4}(4\lambda_2-\lambda_1)] - (16\pi^2X$

$c^2k_{233}\lambda_3/3I_\alpha^2\hbar^{3/2}\lambda_2^{1/4}(4\lambda_3-\lambda_2))[2a_2^{\alpha\alpha}k_{222}/\lambda_2^{3/4} + a_1^{\alpha\alpha}k_{122}X$

$(3\lambda_2-\lambda_1)/\lambda_1^{3/4}(4\lambda_2-\lambda_1)] - (12\pi ck_{233}\lambda_3/\hbar I_\alpha^2\lambda_2(4\lambda_3-\lambda_2))X$

$[\delta_{\alpha x}\cos^2\gamma + \delta_{\alpha y}\sin^2\gamma] - (1-\delta_{\alpha z})(6\pi ck_{133}\lambda_3/\hbar I_\alpha^2\lambda_1^{3/4}\ X$

$\lambda_2^{1/4}(4\lambda_3-\lambda_1)[(-)^{1-\delta_{\alpha x}}\sin\gamma\cos\gamma] - \delta_{\alpha z}[3\pi ck_{233}\lambda_3(a_2^{zz})^2/$

$\hbar I_z^3\lambda_2(4\lambda_3-\lambda_2) + 3\pi ck_{133}\lambda_3a_1^{zz}a_2^{zz}/2\hbar I_z\lambda_1^{3/4}\lambda_2^{1/4}(4\lambda_3-\lambda_1)]$

$(\alpha\alpha133) = (\alpha\alpha313) = (-16\pi^2c^2k_{133}\lambda_3/3I_\alpha^2\hbar^{3/2}\lambda_1^{1/2}(4\lambda_3-\lambda_1))[a_1^{\alpha\alpha}k_{133}X$

$(3\lambda_3-\lambda_1)/\lambda_1^{3/4}(4\lambda_3-\lambda_1) + a_2^{\alpha\alpha}k_{233}(3\lambda_3-\lambda_2)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$

$-(24\pi ck_{133}\lambda_3^{1/2}/\hbar I_\alpha I_z\lambda_1^{1/2}(4\lambda_3-\lambda_1))(1-\delta_{\alpha z})- \delta_{\alpha z}[16\pi c\ X$

$k_{133}\lambda_3^{1/2}/3I_z^2\hbar\lambda_1^{1/2}(4\lambda_3-\lambda_1)][\zeta_{13}^2/(\lambda_1-\lambda_3) + \zeta_{23}^2/(\lambda_2-\lambda_3)]$

$(\alpha\alpha 233) = (\alpha\alpha 323) = (-16\pi^2c^2k_{233}\lambda_3/3I_\alpha{}^2\hbar^{3/2}\lambda_2{}^{1/2}(4\lambda_3-\lambda_2))[a_1^{\alpha\alpha}k_{133}\times$
$(3\lambda_3-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_3-\lambda_1) + a_2^{\alpha\alpha}k_{233}(3\lambda_3-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_3-\lambda_2)]$
$- (24\pi ck_{233}\lambda_3{}^{1/2}/\hbar I_\alpha I_z\lambda_2{}^{1/2}(4\lambda_3-\lambda_2))(1 - \delta_{\alpha z})-\delta_{\alpha z}[16\pi c\ \times$
$k_{233}\lambda_3^{1/2}/3I_z{}^2\hbar\lambda_2{}^{1/2}(4\lambda_3-\lambda_2)][\zeta_{13}^2/(\lambda_1-\lambda_3) + \zeta_{23}^2/(\lambda_2-\lambda_3)]$

$(xy113) = (yx113) = (-8\pi^2c^2(5\lambda_3-\lambda_1)/3I_xI_y\hbar^{3/2}\lambda_3{}^{3/4})[k_{111}k_{133}/(4\lambda_3-$
$\lambda_1)\lambda_1{}^{1/2} + k_{112}k_{233}\lambda_1{}^{1/2}/(4\lambda_1-\lambda_2)(4\lambda_3-\lambda_2)] - (\pi c(I_y-I_x)/$
$I_x{}^2I_y{}^2\hbar\lambda_3{}^{1/4})[k_{111}\zeta_{13}(\lambda_1+\lambda_3)/\lambda_1{}^{3/4}(\lambda_1-\lambda_3) + k_{112}\zeta_{23}\lambda_1\times$
$(\lambda_2+\lambda_3)/\lambda_2{}^{3/4}(\lambda_2-\lambda_3)] + (3\pi ck_{111}/\hbar I_x{}^2I_y{}^2\lambda_1)[(I_x/I_z)^{1/2}\times$
$\cos\gamma + (I_y/I_z)^{1/2}\sin\gamma] - (\pi ck_{112}\lambda_1/\hbar I_x{}^2I_y{}^2\lambda_2{}^{3/4}\lambda_3{}^{1/4}\ \times$
$(4\lambda_1-\lambda_2))[5(I_x/I_z)^{1/2}\sin\gamma - (I_y/I_z)^{1/2}\cos\gamma]$

$(xy223) = (yx223) = (-8\pi^2c^2(5\lambda_3-\lambda_2)/3I_xI_y\hbar^{3/2}\lambda_3{}^{3/4})[k_{222}k_{233}/(4\lambda_3-$
$\lambda_2)\lambda_2{}^{1/2} + k_{122}k_{133}\lambda_2{}^{1/2}/(4\lambda_2-\lambda_1)(4\lambda_3-\lambda_1)] - (\pi c(I_y-I_x)/$
$I_x{}^2I_y{}^2\hbar\lambda_3{}^{1/4})[k_{222}\zeta_{23}(\lambda_2+\lambda_3)/\lambda_2{}^{3/4}(\lambda_2-\lambda_3) + k_{122}\zeta_{13}\lambda_2\times$
$(\lambda_1+\lambda_3)/\lambda_1{}^{3/4}(\lambda_1-\lambda_3)] + (3\pi ck_{122}\lambda_2/\hbar I_x{}^2I_y{}^2\lambda_1{}^{3/4}\lambda_3{}^{1/4}\ \times$
$(4\lambda_2-\lambda_1))[(I_x/I_z)^{1/2}\cos\gamma + (I_y/I_z)^{1/2}\sin\gamma] - (\pi ck_{222}/$
$\hbar I_x{}^2I_y{}^2\lambda_2{}^{3/4}\lambda_3{}^{1/4})[5(I_x/I_z)^{1/2}\sin\gamma - (I_y/I_z)^{1/2}\cos\gamma]$

$(xy123) = (yx123) = (xy213) = (yx213) = (-16\pi^2c^2/3I_xI_y\lambda_3{}^{3/4})[k_{122}\times$
$k_{233}\lambda_2(5\lambda_3-\lambda_2)/\lambda_1{}^{1/2}(4\lambda_2-\lambda_1)(4\lambda_3-\lambda_2) + k_{112}k_{133}\lambda_1(5\lambda_3-$
$\lambda_1)/\lambda_2{}^{1/2}(4\lambda_1-\lambda_2)(4\lambda_3-\lambda_1)] - (2\pi c(I_x-I_y)/I_x{}^2I_y{}^2\hbar\lambda_3{}^{1/4})\times$
$[k_{122}\zeta_{23}\lambda_2{}^{3/4}(\lambda_2+\lambda_3)/\lambda_1{}^{1/2}(\lambda_2-\lambda_3) + k_{112}\zeta_{13}\lambda_1{}^{3/4}(\lambda_1+\lambda_3)/$
$\lambda_2{}^{1/2}(\lambda_1-\lambda_3)] + (6\pi ck_{112}\lambda_1{}^{3/4}/\hbar I_x{}^2I_y{}^2\lambda_2{}^{1/2}\lambda_3{}^{1/4}(4\lambda_1-$
$\lambda_2))[(I_x/I_z)^{1/2}\cos\gamma + (I_y/I_z)^{1/2}\sin\gamma] - (\pi ck_{122}\lambda_2{}^{3/4}/\hbar\ \times$
$I_x{}^2I_y{}^2\lambda_2{}^{3/4}\lambda_3{}^{1/4}(4\lambda_1-\lambda_2))[5(I_x/I_z)^{1/2}\sin\gamma - (I_y/I_z)^{1/2}\times$
$\cos\gamma]$

$(xy131) = (yx131) = (xy311) = (yx311) = -8\pi^2c^2k_{133}^2\lambda_3{}^{1/4}/3I_xI_y\hbar^{3/2}\times$
$\lambda_1{}^{1/2}(5\lambda_3-\lambda_1)(4\lambda_3-\lambda_1)^2 - \pi ck_{133}\zeta_{13}\lambda_3{}^{3/4}(\lambda_1+\lambda_3)(I_y-I_x)/\ldots$

(xy131), cont'd.

$$I_x^2 I_y^2 \lambda_1^{3/4}(\lambda_1-\lambda_3)(4\lambda_3-\lambda_1) + (6\pi c k_{133}\lambda_3^{3/4}/\hbar I_x^2 I_y^2(4\lambda_3-\lambda_1)\lambda_1^{3/4})[(I_x/I_z)^{1/2}\cos\gamma + (I_y/I_z)^{1/2}\sin\gamma]$$

$$(xy232) = (yx232) = (xy322) = (yx322) = -8\pi^2c^2k_{233}\lambda_3^{1/4}/3I_xI_y\hbar^{3/2}\times \lambda_2^{1/2}(5\lambda_3-\lambda_2)(4\lambda_3-\lambda_2)^2 - \pi c k_{233}\zeta_{23}\lambda_3^{3/4}(\lambda_2+\lambda_3)(I_y-I_x)/I_x^2I_y^2\lambda_2^{3/4}(\lambda_2-\lambda_3)(4\lambda_3-\lambda_2) - (2\pi c k_{233}\lambda_3^{3/4}/\hbar I_x^2I_y^2(4\lambda_3-\lambda_2)\lambda_2^{3/4})[5(I_x/I_z)^{1/2}\sin\gamma - (I_y/I_z)^{1/2}\cos\gamma]$$

$$(xy333) = (yx333) = (xy131) + (xy232)$$

$$(xy132) = (yx132) = (xy312) = (yx312) = -8\pi^2c^2k_{133}k_{233}\lambda_3^{1/4}/3I_x\times I_y\hbar^{3/2}\lambda_1^{1/2}(5\lambda_3-\lambda_2)^{-1}(4\lambda_3-\lambda_1)(4\lambda_3-\lambda_2) - ck_{133}\zeta_{23}\lambda_3^{3/4}(\lambda_2+\lambda_3)(I_y-I_x)/I_x^2I_y^2\lambda_1^{1/2}\lambda_2^{1/4}(\lambda_2-\lambda_3)(4\lambda_3-\lambda_1) - 2\pi c k_{133}\times\lambda_3^{3/4}/\hbar I_x^2I_y^2\lambda_1^{1/2}\lambda_2^{1/2}(4\lambda_3-\lambda_1))[5(I_x/I_z)^{1/2}\sin\gamma - (I_y/I_z)^{1/2}\cos\gamma]$$

$$(xy231) = (yx231) = (xy321) = (yx321) = -8\pi^2c^2k_{133}k_{233}\lambda_3^{1/4}/3I_x\times I_y\hbar^{3/2}\lambda_2^{1/2}(5\lambda_3-\lambda_2)^{-1}(4\lambda_3-\lambda_1)(4\lambda_3-\lambda_2) - \pi c k_{233}\zeta_{13}(\lambda_1+\lambda_3)\lambda_3^{3/4}(I_y-I_x)/I_x^2I_y^2\lambda_2^{1/2}\lambda_1^{1/4}(\lambda_1-\lambda_3)(4\lambda_3-\lambda_2) + (6\pi c\times k_{233}\lambda_3^{3/4}/\hbar I_x^2I_y^2\lambda_2^{1/2}\lambda_1^{1/4}(4\lambda_3-\lambda_2))[(I_x/I_z)^{1/2}\cos\gamma + (I_y/I_z)^{1/2}\sin\gamma]$$

(3) Auxiliary coefficients $(X;\alpha,\beta;bc;a) = (\alpha,\beta bca)$:

In the following, $i = 1, 2$; $j = 1, 2$; $\underline{k} = [j+(-)^{(j+1)}\delta_{ij}]$

$$(z,ziij) = [-4\pi c\zeta_{j3}(\lambda_j+\lambda_3)/3I_z^2\hbar\lambda_j^{1/4}(\lambda_j-\lambda_3)][\zeta_{i3}(k_{iii}/\lambda_i^{3/4} - 2k_{i33}\lambda_3^{1/2}/\lambda_i^{1/4}(4\lambda_3-\lambda_i)) + \zeta_{\underline{k}3}k_{ii\underline{k}}\lambda_i/\lambda_{\underline{k}}^{3/4}(4\lambda_i-\lambda_{\underline{k}})]$$

$$(z,z12j) = (z,z21j) = [-8\pi c\zeta_{j3}(\lambda_j+\lambda_3)/3I_z^2\hbar(\lambda_j-\lambda_3)\lambda_j^{1/4}\lambda_3^{1/4}]\times[\lambda_2^{3/4}\lambda_3^{1/4}\zeta_{23}k_{122}/\lambda_1^{1/2}(4\lambda_2-\lambda_1)-\lambda_2^{1/4}\lambda_3^{3/4}\zeta_{23}k_{133}/\lambda_1^{1/2}(4\lambda_3-\lambda_1)+\lambda_1^{3/4}\lambda_3^{1/4}\zeta_{13}k_{112}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)-\lambda_1^{1/4}\times\lambda_3^{3/4}\zeta_{13}k_{233}/\lambda_2^{1/2}(4\lambda_3-\lambda_2)]$$

(z,zj33) = (z,z3j3) = 2(z,zjjj) + (z,zj$\underline{kk}$)

(4) <u>Auxiliary coefficients (P;$\alpha\beta$;bc;a) ≡ ($\alpha\beta$bca) :</u>

In the following, α = x, y, z, and in general ($\alpha\beta$bca) = ($\beta\alpha$cba).

$$(\alpha\alpha 111) = (-8\pi^2c^2a_1^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_1^{3/4})[3k_{111}^2/\lambda_1^{1/2} + \lambda_1k_{112}^2/\lambda_2^{1/2} \times (4\lambda_1-\lambda_2)] - (8\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4})[k_{111}k_{112}/\lambda_1^{1/2} + \lambda_1k_{112}k_{122}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$$

$$(\alpha\alpha 112) = (-8\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4})[3\lambda_2k_{111}k_{122}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + k_{112}k_{222}/\lambda_2^{1/2}] - (8\pi^2c^2a_1^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_1^{3/4})[k_{111}k_{112}/\lambda_1^{1/2} + \lambda_1k_{112}k_{122}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$$

$$(\alpha\alpha 122) = (-16\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4})[\lambda_1k_{112}k_{122}/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + 3\lambda_2k_{122}k_{222}/\lambda_1^{1/2}(4\lambda_2-\lambda_1)] - (16\pi^2c^2a_1^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_1^{3/4}) \times [\lambda_1k_{112}^2/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + \lambda_2k_{122}^2/\lambda_1^{1/2}(4\lambda_2-\lambda_1)]$$

$$(\alpha\alpha 121) = (-16\pi^2c^2a_1^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_1^{3/4})[3\lambda_1k_{111}k_{112}/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + \lambda_2k_{112}k_{122}/\lambda_1^{1/2}(4\lambda_2-\lambda_1)] - (16\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4}) \times [\lambda_1k_{112}/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + \lambda_2k_{122}/\lambda_1^{1/2}(4\lambda_2-\lambda_1)]$$

$$(\alpha\alpha 221) = (-8\pi^2c^2a_1^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_1^{3/4})[3\lambda_2k_{111}k_{122}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + k_{112}k_{222}/\lambda_2^{1/2}] - (8\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4})[\lambda_2k_{112}k_{122}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + k_{122}k_{222}/\lambda_2^{1/2}]$$

$$(\alpha\alpha 222) = (-8\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4})[3k_{222}^2/\lambda_2^{1/2} + \lambda_2k_{122}^2/\lambda_1^{1/2} \times (4\lambda_2-\lambda_1)] - (8\pi^2c^2a_1^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_1^{3/4})[k_{222}k_{122}/\lambda_2^{1/2} + \lambda_2k_{122}k_{112}/\lambda_1^{1/2}(4\lambda_2-\lambda_1)]$$

$$(\alpha\alpha 331) = (-8\pi^2c^2a_1^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_1^{3/4})[3\lambda_3k_{111}k_{133}/\lambda_1^{1/2}(4\lambda_3-\lambda_1) + \lambda_3 \times k_{112}k_{233}/\lambda_2^{1/2}(4\lambda_3-\lambda_2)] - (8\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4})[\lambda_3 \times k_{112}k_{133}/\lambda_1^{1/2}(4\lambda_3-\lambda_1) + \lambda_3k_{122}k_{233}/\lambda_2^{1/2}(4\lambda_3-\lambda_2)] + (\lambda_3^{1/2}\zeta_{13}/2I_\alpha^2I_z\hbar^{1/2}\lambda_1^{1/4})[\zeta_{13}a_1^{\alpha\alpha}/\lambda_1 + \zeta_{23}a_2^{\alpha\alpha}/\lambda_2]$$

$$(\alpha\alpha 332) = (-8\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4})[\lambda_3k_{122}k_{133}/\lambda_1^{1/2}(4\lambda_3-\lambda_1) + 3\lambda_3k_{222}k_{233}/\lambda_2^{1/2}(4\lambda_3-\lambda_2)] - (8\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4}) \times [\lambda_3k_{112}k_{133}/\lambda_1^{1/2}(4\lambda_3-\lambda_1) + \lambda_3k_{122}k_{233}/\lambda_2^{1/2}(4\lambda_3-\lambda_2)] + (\lambda_3^{1/2}\zeta_{23}/2I_\alpha^2I_z\hbar^{1/2}\lambda_2^{1/4})[\zeta_{23}a_2^{\alpha\alpha}/\lambda_2 + \zeta_{13}a_1^{\alpha\alpha}/\lambda_1]$$

$$(\alpha\alpha 133) = (-16\pi^2c^2a_1^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_1^{3/4})[\lambda_3k_{133}^2/\lambda_1^{1/2}(4\lambda_3-\lambda_1)] - (16\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4})[\lambda_3k_{133}k_{233}/\lambda_1^{1/2}(4\lambda_3-\lambda_1)] - \zeta_{13}^2a_1^{\alpha\alpha}/2I_\alpha^2I_z\hbar^{1/2}\lambda_1^{3/4} - \lambda_1^{1/4}\zeta_{13}\zeta_{23}a_2^{\alpha\alpha}/2I_\alpha^2I_z\hbar^{1/2}\lambda_2$$

$$(\alpha\alpha 233) = (-16\pi^2c^2a_2^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_2^{3/4})[\lambda_3k_{233}/\lambda_2^{1/2}(4\lambda_3-\lambda_2)] - (16\pi^2c^2a_1^{\alpha\alpha}/3I_\alpha^2\hbar^{3/2}\lambda_1^{3/4})[\lambda_3k_{233}k_{133}/\lambda_2^{1/2}(4\lambda_3-\lambda_2)] - \zeta_{23}^2a_2^{\alpha\alpha}/2I_\alpha^2I_z\hbar^{1/2}\lambda_2^{3/4} - \lambda_2^{1/4}\zeta_{23}\zeta_{13}a_1^{\alpha\alpha}/2I_\alpha^2I_z\hbar^{1/2}\lambda_1$$

$$(xy113) = (-8\pi^2c^2a_3^{xy}/3I_xI_y\hbar^{3/2}\lambda_3^{3/4})[k_{111}k_{133}/\lambda_1^{1/2} + k_{112}k_{233} \times \lambda_1/\lambda_2^{1/2}(4\lambda_1-\lambda_2)] + \lambda_1^{1/2}\zeta_{13}^2a_3^{xy}/2I_xI_y\hbar^{1/2}\lambda_3^{5/4}$$

$$(xy223) = (-8\pi^2c^2a_3^{xy}/3I_xI_y\hbar^{3/2}\lambda_3^{3/4})[k_{222}k_{233}/\lambda_2^{1/2} + k_{122}k_{133} \times \lambda_2/\lambda_1^{1/2}(4\lambda_2-\lambda_1)] + \lambda_2^{1/2}\zeta_{23}^2a_3^{xy}/2I_xI_y\hbar^{1/2}\lambda_3^{5/4}$$

$$(xy123) = (-8\pi^2c^2a_3^{xy}/3I_xI_y\hbar^{3/2}\lambda_3^{3/4})[\lambda_1k_{112}k_{133}/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + \lambda_2k_{122}k_{233}/\lambda_1^{1/2}(4\lambda_2-\lambda_1)] + \lambda_1^{1/4}\lambda_2^{1/4}\zeta_{13}\zeta_{23}a_3^{xy}/2I_xI_y \times I_z\hbar^{1/2}\lambda_3^{5/4}$$

$$(xy333) = (-8\pi^2c^2a_3^{xy}/3I_xI_y\hbar^{3/2}\lambda_3^{3/4})[\lambda_3k_{133}k_{133}/\lambda_1^{1/2}(4\lambda_3-\lambda_1) + \lambda_3k_{233}k_{233}/\lambda_2^{1/2}(4\lambda_3-\lambda_2)]$$

$$(xyi3j) = (-16\pi^2c^2a_3^{xy}/3I_xI_y\hbar^{3/2}\lambda_3^{3/4})[\lambda_3k_{i33}k_{j33}/\lambda_i^{1/2}(4\lambda_3-\lambda_i)] - \lambda_i^{1/4}\zeta_{j3}\zeta_{i3}a_3^{xy}/2I_xI_yI_z\hbar^{1/2}\lambda_j^{1/4}\lambda_3^{3/4} \;;\; i = 1, 2 \;;\; j = 1,2$$

(5) <u>Auxiliary coefficients $(T;\alpha\beta;b,c;a) = (\alpha\beta b,ca)$:</u>

In the following, $\alpha = x, y,$; $i = 1, 2$; $j = 1, 2$

$$(xy3,ij) = (yx3,ij) = 16\pi^2c^2k_{i33}k_{j33}a_3^{xy}\lambda_3^{5/4}/3I_xI_y\hbar^{3/2}\lambda_i^{1/2}(4\lambda_3-\lambda_i)(4\lambda_3-\lambda_j) + 2\pi ck_{j33}\lambda_i^{1/4}\lambda_3^{3/4}\zeta_{i3}(I_y-I_x)/I_x^2I_y^2(4\lambda_3-\lambda_j)(\lambda_i-\lambda_3)$$

$$(xyi,j3) = (yxi,j3) = 16\pi^2c^2k_{i33}k_{j33}a_3^{xy}\lambda_3^{3/4}(2\lambda_3-\lambda_i)/3I_xI_y\hbar^{3/2} \times$$
$$\lambda_i^{1/2}\lambda_j^{1/2}(4\lambda_3-\lambda_i)(4\lambda_3-\lambda_j) + 2\pi ck_{i33}\zeta_{j3}(I_y-I_x)(2\lambda_3-$$
$$\lambda_i)\lambda_3^{1/4}\lambda_j^{1/4}/I_x^2I_y^2\lambda_i^{1/2}(4\lambda_3-\lambda_i)(\lambda_j-\lambda_3)$$

$$(xyi,3j) = (yxi,3j) = 16\pi^2c^2k_{ijj}k_{j33}a_3^{xy}\lambda_3^{3/4}(2\lambda_j-\lambda_i)/3I_xI_y\hbar^{3/2} \times$$
$$\lambda_i^{1/2}\lambda_j^{1/2}(4\lambda_j-\lambda_i)(4\lambda_3-\lambda_j) + 16\pi^2c^2k_{jji}k_{i33}a_3^{xy}\lambda_3^{3/4}/$$
$$3I_xI_y\hbar^{3/2}(4\lambda_i-\lambda_j)(4\lambda_3-\lambda_i) + 2\pi ck_{ijj}\zeta_{j3}\lambda_3^{1/4}\lambda_j^{1/4}(2\lambda_j-$$
$$\lambda_i)(I_y-I_x)/I_x^2I_y^2\lambda_j^{1/2}(4\lambda_j-\lambda_i)(\lambda_j-\lambda_3) + 2\pi ck_{jii}\zeta_{i3}(I_y-$$
$$I_x)\lambda_3^{1/4}\lambda_i^{3/4}/I_x^2I_y^2(4\lambda_i-\lambda_j)(\lambda_i-\lambda_3)\ ,\ j \neq i$$

$$(xy1,31) = (yx1,31) = 16\pi^2c^2k_{111}k_{133}a_3^{xy}\lambda_3^{3/4}/3I_xI_y\hbar^{3/2}\lambda_1(4\lambda_3-\lambda_1) +$$
$$16\pi^2c^2k_{112}k_{233}a_3^{xy}\lambda_3^{3/4}\lambda_1^{1/2}/3I_xI_y\hbar^{3/2}(4\lambda_1-\lambda_2)(4\lambda_3-\lambda_2)\times$$
$$\lambda_2^{1/2} + 2\pi ck_{111}\zeta_{13}\lambda_3^{1/4}(I_y-I_x)/I_x^2I_y^2\lambda_1^{1/4}(\lambda_1-\lambda_3) +$$
$$2\pi ck_{112}\zeta_{23}\lambda_1^{1/2}\lambda_2^{1/4}\lambda_3^{1/4}(I_y-I_x)/I_x^2I_y^2(4\lambda_1-\lambda_2)(\lambda_2-\lambda_3)$$

$$(xy2,32) = (yx2,32) = 16\pi^2c^2k_{222}k_{233}a_3^{xy}\lambda_3^{3/4}/3I_xI_y\hbar^{3/2}\lambda_1(4\lambda_3-\lambda_2) +$$
$$16\pi^2c^2k_{122}k_{133}a_3^{xy}\lambda_3^{3/4}\lambda_2^{1/2}/3I_xI_y\hbar^{3/2}(4\lambda_2-\lambda_1)(4\lambda_3-\lambda_1)\times$$
$$\lambda_1^{1/2} + 2\pi ck_{222}\zeta_{23}\lambda_3^{1/4}(I_y-I_x)/I_x^2I_y^2\lambda_2^{1/4}(\lambda_2-\lambda_3) +$$
$$2\pi ck_{122}\zeta_{13}\lambda_2^{1/2}\lambda_1^{1/4}\lambda_3^{1/4}(I_y-I_x)/I_x^2I_y^2(4\lambda_2-\lambda_1)(\lambda_1-\lambda_3)$$

$$(\alpha\alpha 1,11) = (16\pi^2c^2k_{111}/3I_\alpha^2\hbar^{3/2}\lambda_1^{1/2})[a_1^{\alpha\alpha}k_{111}/\lambda_1^{3/4} + a_2^{\alpha\alpha}k_{112}\lambda_1/$$
$$\lambda_2^{3/4}(4\lambda_1-\lambda_2)] + (16\pi^2c^2k_{112}\lambda_1^{1/2}/3I_\alpha^2\hbar^{3/2}(4\lambda_1-\lambda_2))[a_2^{\alpha\alpha}\times$$
$$k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$$

$$(\alpha\alpha 2,11) = (16\pi^2c^2k_{112}(2\lambda_1-\lambda_2)/3I_\alpha^2\hbar^{3/2}(4\lambda_1-\lambda_2)\lambda_2^{1/2})[a_1^{\alpha\alpha}k_{111}/$$
$$\lambda_1^{3/4} + a_2^{\alpha\alpha}k_{112}\lambda_1/\lambda_2^{3/4}(4\lambda_1-\lambda_2)] + (16\pi^2c^2k_{122}\lambda_1^{1/2}/$$
$$3I_\alpha^2\hbar^{3/2}(4\lambda_1-\lambda_2))[a_2^{\alpha\alpha}k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}\times$$
$$\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$$

$$(\alpha\alpha 1,12) = (16\pi^2c^2k_{122}(2\lambda_2-\lambda_1)/3I_\alpha^2\hbar^{3/2}\lambda_1^{1/2}(4\lambda_2-\lambda_1))[a_2^{\alpha\alpha}k_{122}\times$$
$$\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)] +$$
$$(16\pi^2c^2k_{112}\lambda_1^{1/2}/3I_\alpha^2\hbar^{3/2}(4\lambda_1-\lambda_2))[a_1^{\alpha\alpha}k_{111}/\lambda_1^{3/4} + \ldots$$

$(\alpha\alpha 1,12)$, cont'd.

$+\ a_2^{\alpha\alpha}k_{112}\lambda_1/\lambda_2^{3/4}(4\lambda_1-\lambda_2)]$

$(\alpha\alpha 2,12) = (16\pi^2c^2k_{222}/3I_\alpha^2\hbar^{3/2}\lambda_2^{1/2})[a_2^{\alpha\alpha}k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1)$
$+\ a_1^{\alpha\alpha}k_{112}\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)] + (16\pi^2c^2k_{122}\lambda_2^{1/2}/3I_\alpha^2 \times$
$\hbar^{3/2}(4\lambda_2-\lambda_1))[a_1^{\alpha\alpha}k_{111}/\lambda_1^{3/4} + a_2^{\alpha\alpha}k_{112}\lambda_1/\lambda_2^{3/4}(4\lambda_1-\lambda_2)]$

$(\alpha\alpha 1,21) = (16\pi^2c^2k_{112}\lambda_1^{1/2}/3I_\alpha^2\hbar^{3/2}(4\lambda_1-\lambda_2))[a_2^{\alpha\alpha}k_{222}/\lambda_2^{3/4} + a_1^{\alpha\alpha}\times$
$k_{122}\lambda_2/\lambda_1^{3/4}(4\lambda_2-\lambda_1)] + (16\pi^2c^2k_{111}/3I_\alpha^2\hbar^{3/2}\lambda_1^{1/2})[a_2^{\alpha\alpha}\times$
$k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$

$(\alpha\alpha 2,21) = (16\pi^2c^2k_{122}\lambda_2^{1/2}/3I_\alpha^2\hbar^{3/2}(4\lambda_2-\lambda_1))[a_2^{\alpha\alpha}k_{222}/\lambda_2^{3/4} + a_1^{\alpha\alpha}\times$
$k_{122}\lambda_2/\lambda_1^{3/4}(4\lambda_2-\lambda_1)] + (16\pi^2c^2k_{112}(2\lambda_1-\lambda_2)/3I_\alpha^2\hbar^{3/2}\times$
$\lambda_2^{1/2}(4\lambda_1-\lambda_2))[a_2^{\alpha\alpha}k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}\times$
$\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$

$(\alpha\alpha 1,22) = (16\pi^2c^2k_{122}(2\lambda_2-\lambda_1)/3I_\alpha^2\hbar^{3/2}\lambda_1^{1/2}(4\lambda_2-\lambda_1))[a_2^{\alpha\alpha}k_{222}/$
$\lambda_2^{3/4} + a_1^{\alpha\alpha}k_{122}\lambda_2/\lambda_1^{3/4}(4\lambda_2-\lambda_1)] + (16\pi^2c^2k_{112}\lambda_1^{1/2}/$
$3I_\alpha^2\hbar^{3/2}(4\lambda_1-\lambda_2))[a_2^{\alpha\alpha}k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}\times$
$\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-\lambda_2)]$

$(\alpha\alpha 2,22) = (16\pi^2c^2k_{222}/3I_\alpha^2\hbar^{3/2}\lambda_2^{1/2})[a_2^{\alpha\alpha}k_{222}/\lambda_2^{3/4} + a_1^{\alpha\alpha}k_{122}\lambda_2/$
$\lambda_1^{3/4}(4\lambda_2-\lambda_1)] + (16\pi^2c^2k_{122}\lambda_2^{1/2}/3I_\alpha^2\hbar^{3/2}(4\lambda_2-\lambda_1))\times$
$[a_2^{\alpha\alpha}k_{122}\lambda_2^{3/4}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}\lambda_1^{3/4}/\lambda_2^{1/2}(4\lambda_1-$
$\lambda_2)]$

$(\alpha\alpha 3,3j) = (16\pi^2c^2\lambda_3^{3/2}/3I_\alpha^2\hbar^{3/2}(4\lambda_3-\lambda_j))[a_1^{\alpha\alpha}k_{133}/\lambda_1^{3/4}(4\lambda_3-\lambda_1) +$
$a_2^{\alpha\alpha}k_{233}/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$

$(\alpha\alpha j,33) = (16\pi^2c^2k_{j33}(2\lambda_3-\lambda_j)/3I_\alpha^2\hbar^{3/2}\lambda_j^{1/2}(4\lambda_3-\lambda_j))[a_1^{\alpha\alpha}k_{133}/$
$\lambda_1^{3/4}(4\lambda_3-\lambda_1) + a_2^{\alpha\alpha}k_{233}/\lambda_2^{3/4}(4\lambda_3-\lambda_2)]$

In the following, (b,ca) will be used to denote the expression obtained when z is substituted for α in $(\alpha\alpha b,ca)$:

$$\begin{aligned}(zz1,11) = (1,11) &- (8\pi c\zeta_{13}/3I_z{}^2\hbar)[2k_{111}\zeta_{13}/(\lambda_1-\lambda_3) + k_{112}(2\lambda_1-\lambda_2) \times \\ &\zeta_{23}\lambda_1{}^{1/4}(\lambda_1+\lambda_2-2\lambda_3)/\lambda_2{}^{1/4}(4\lambda_1-\lambda_2)(\lambda_1-\lambda_3)(\lambda_2-\lambda_3)]\end{aligned}$$

$$\begin{aligned}(zz2,11) = (2,11) &- (8\pi c\zeta_{13}\lambda_1{}^{1/4}/3I_z{}^2\hbar(\lambda_1-\lambda_3))[2k_{112}(2\lambda_1-\lambda_2)\zeta_{13}\lambda_1{}^{1/4}/ \\ &\lambda_2{}^{1/2}(4\lambda_1-\lambda_2) + k_{122}\lambda_2{}^{3/4}\zeta_{23}(\lambda_1+\lambda_2-2\lambda_3)/(4\lambda_2-\lambda_1)(\lambda_2-\lambda_3)]\end{aligned}$$

$$\begin{aligned}(zz1,12) = (1,12) &- (8\pi c\zeta_{13}/3I_z{}^2\hbar(\lambda_1-\lambda_3))[k_{122}(2\lambda_2-\lambda_1)\lambda_2{}^{1/4}\zeta_{23}(\lambda_1+\lambda_2 \\ &-2\lambda)/\lambda_1{}^{1/4}(4\lambda_2-\lambda_1)(\lambda_2-\lambda_3) + 2k_{112}\lambda_1\zeta_{13}/(4\lambda_1-\lambda_2)]\end{aligned}$$

$$\begin{aligned}(zz2,12) = (2,12) &- (8\pi c\zeta_{13}\lambda_1{}^{1/4}/3I_z{}^2\hbar(\lambda_1-\lambda_3))[\zeta_{23}(\lambda_1+\lambda_2-2\lambda_3)k_{222}/(\lambda_2 \\ &-\lambda_1)\lambda_2{}^{1/4} + 2k_{122}\lambda_2{}^{1/2}\lambda_1{}^{1/4}\zeta_{13}/(4\lambda_2-\lambda_1)]\end{aligned}$$

$$\begin{aligned}(zz1,21) = (1,21) &- (8\pi c\lambda_2{}^{1/2}\zeta_{23}/3I_z{}^2\hbar(\lambda_2-\lambda_3))[2k_{112}\lambda_1{}^{1/2}\zeta_{23}/(4\lambda_1-\lambda_2) \\ &k_{111}\zeta_{13}(\lambda_1+\lambda_2-2\lambda_3)/\lambda_1{}^{1/4}(\lambda_1-\lambda_3)\lambda_2{}^{1/4}]\end{aligned}$$

$$\begin{aligned}(zz2,21) = (2,21) &- (8\pi c\zeta_{23}/3I_z{}^2\hbar(\lambda_2-\lambda_3))[2k_{122}\lambda_2\zeta_{23}/(4\lambda_2-\lambda_1) + k_{112}\times \\ &(2\lambda_1-\lambda_2)\lambda_1{}^{1/4}\zeta_{13}(\lambda_1+\lambda_2-2\lambda_3)/\lambda_2{}^{1/4}(4\lambda_1-\lambda_2)(\lambda_1-\lambda_3)]\end{aligned}$$

$$\begin{aligned}(zz2,22) = (2,22) &- (8\pi c\zeta_{23}/3I_z{}^2\hbar(\lambda_2-\lambda_3))[2k_{222}\zeta_{23} + k_{122}\lambda_1{}^{1/4}\lambda_2{}^{3/4} \times \\ &\zeta_{13}(\lambda_1+\lambda_2-2\lambda_3)/(4\lambda_2-\lambda_1)(\lambda_1-\lambda_3)]\end{aligned}$$

$$\begin{aligned}(zz3,31) = (3,31) &- (16\pi ck_{133}\lambda_3/3I_z{}^2\hbar(4\lambda_3-\lambda_1))[\zeta_{13}^2/(\lambda_1-\lambda_3) + \zeta_{23}^2/(\lambda_2- \\ &\lambda_3)]\end{aligned}$$

$$(zz3,32) = (3,32) - (16\pi ck_{233}\lambda_3/3I_z{}^2\hbar(4\lambda_3-\lambda_2))[\zeta_{13}^2/(\lambda_1-\lambda_3)+\zeta_{23}^2/(\lambda_2-\lambda_3)]$$

$$\begin{aligned}(zz1,33) = (1,33) &- (16\pi ck_{133}(2\lambda_3-\lambda_1)\lambda_3{}^{1/2}/3I_z{}^2\hbar(4\lambda_3-\lambda_1))[\zeta_{13}^2/(\lambda_1-\lambda_3) \\ &+ \zeta_{23}/(\lambda_2-\lambda_3)]\end{aligned}$$

$$\begin{aligned}(zz2,33) = (2,33) &- (16\pi ck_{233}(2\lambda_3-\lambda_2)\lambda_3{}^{1/2}/3I_z{}^2\hbar(4\lambda_3-\lambda_2))[\zeta_{13}^2/(\lambda_1-\lambda_3) \\ &+ \zeta_{13}/(\lambda_1-\lambda_3)]\end{aligned}$$

(6) Auxiliary coefficients $(N;\alpha,\beta;b,c;a) \equiv (\alpha,\beta b,ca)$:

In the following, $i = 1, 2$; $j = 1, 2$; $m = 1, 2$; $s = (-1)^{j+1}+j$

$$(z,zi,jj) = -2\zeta_{i3}\zeta_{j3}\lambda_i^{1/4}a_j^{zz}/I_z^{3}\hbar^{1/2}(\lambda_i-\lambda_3) - [8\pi c\,\zeta_{i3}\lambda_i^{1/4}\lambda_3^{1/4}/3I_z^{2}\hbar(\lambda_i-\lambda_3)][2k_{j33}\zeta_{j3}\lambda_3^{5/4}(2\lambda_j+\lambda_3)/(4\lambda_3-\lambda_j)(\lambda_3-\lambda_j) \times \lambda_j^{3/4} - k_{sjj}\zeta_{s3}\lambda_j^{1/2}\lambda_s^{1/4}/\lambda_3^{1/4}(4\lambda_j-\lambda_s) - k_{jjj}\zeta_{j3}/\lambda_3^{1/4}\lambda_j^{1/4}]$$

$$(z,zm,ij) = -2\zeta_{m3}^{2}\lambda_i^{1/4}a_j^{zz}/I_z^{3}\hbar^{1/2}(\lambda_m-\lambda_3) - [8\pi c\,\zeta_{m3}\lambda_m^{1/4}\lambda_3^{1/4}/3I_z^{2}\times\hbar(\lambda_m-\lambda_3)][\lambda_i^{1/4}\lambda_3^{1/4}\zeta_{i3}k_{j33}(\lambda_i+2\lambda_j-9\lambda_3)/(4\lambda_3-\lambda_j)(\lambda_i-\lambda_3) + \lambda_3^{1/4}\zeta_{j3}k_{i33}(2\lambda_3-\lambda_i)/\lambda_i^{1/2}\lambda_j^{1/4}(4\lambda_3-\lambda_i) - \lambda_j^{1/4}\times\zeta_{j3}k_{ijj}(2\lambda_j-\lambda_i)/\lambda_i^{1/4}\lambda_3^{1/4}(4\lambda_j-\lambda_i) - \lambda_i^{3/4}\zeta_{j3}k_{iij}/\lambda_3^{1/4}(4\lambda_i-\lambda_j)] \quad , i \neq j$$

$$(z,zj,33) = [8\pi c\,\zeta_{j3}\lambda_j^{1/4}\lambda_3^{1/2}/3I_z^{2}\hbar(\lambda_j-\lambda_3)][k_{133}\zeta_{13}(2\lambda_1^{2}+2\lambda_3^{2}-7\lambda_1\lambda_3)/\lambda_1^{3/4}(4\lambda_3-\lambda_1)(\lambda_3-\lambda_1) + k_{233}\zeta_{23}(2\lambda_2^{2}+2\lambda_3^{2}-7\lambda_2\lambda_3)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)(\lambda_3-\lambda_2)]$$

$$(z,z3,3j) = (2\lambda_3^{1/2}/I_z^{3}\hbar^{1/2}\lambda_j^{1/4})[2a_j^{zz}\zeta_{j3}^{2}/(\lambda_j-\lambda_3) + \zeta_{s3}(a_j^{zz}\zeta_{s3} + a_s^{zz}\zeta_{j3})/(\lambda_s-\lambda_3)] + [8\pi c\,\zeta_{j3}\lambda_j^{1/4}\lambda_3^{1/2}/3I_z^{2}\hbar(\lambda_j-\lambda_3)] \times [k_{jjj}\zeta_{j3}(\lambda_3-7\lambda_j)/\lambda_j^{3/4}(\lambda_3-\lambda_j) + k_{jjs}\zeta_{s3}((2\lambda_j-\lambda_s)/(4\lambda_j-\lambda_s)\lambda_s^{3/4} - 2\lambda_s^{1/4}/(\lambda_3-\lambda_s)) - 2k_{j33}\zeta_{j3}\lambda_3^{1/2}/\lambda_j^{1/4}(4\lambda_3-\lambda_j)] + [8\pi c\,\zeta_{s3}\lambda_s^{1/4}\lambda_3^{1/2}/3I_z^{2}\hbar(\lambda_s-\lambda_3)][k_{jjs}\zeta_{j3}\lambda_j^{1/4} \times (\lambda_3+2\lambda_s-9\lambda_j)/(4\lambda_j-\lambda_s)(\lambda_3-\lambda_j) + k_{jss}\zeta_{s3}\lambda_s^{1/4}(\lambda_3+2\lambda_j-9\lambda_s)/(4\lambda_s-\lambda_j)(\lambda_3-\lambda_s) - k_{j33}\zeta_{s3}\lambda_3^{1/2}/\lambda_s^{1/4}(4\lambda_3-\lambda_j) - k_{s33}\zeta_{j3}\lambda_3^{1/2}/\lambda_j^{1/4}(4\lambda_3-\lambda_s)]$$

$$(z,z3,j3) = (z,z1,j1) + (z,z2,j2)$$

(7) <u>Auxiliary coefficients $(G;\alpha\beta;bc;a) \equiv (\alpha\beta bca)$:</u>

In the following, $i = 1, 2$; $j = 1, 2$; $\alpha = x, y$:

$$(\alpha\alpha j33) = (\alpha\alpha 3j3) = (-)^{\delta_{\alpha y}} 2\zeta_{j3}\lambda_j^{1/4} a_3^{xy}/I_xI_yI_z^2\hbar^{1/2}(\lambda_j-\lambda_3)$$

$$(xyi3j) = (yxi3j) = -(xy3ij) = [\zeta_{i3}\lambda_i^{1/4}\lambda_3^{1/4}/I_z^2\hbar^{1/2}\lambda_j^{1/4}(\lambda_i-\lambda_3)]$$

$$\times\ [a_j^{yy}/I_y^2 - a_j^{xx}/I_x^2]$$

APPENDIX XIV

Coefficients $(3;\alpha\beta;-;abc)$ in h_3'

The coefficients $(3;\alpha\beta;-;abc)$ appearing in the fourth sum of (4.5) can be written in general as

$$(3;\alpha\beta;-;abc) = (\alpha\beta*-*abc) + (N;\alpha\beta;-;abc) + \sideset{^*}{}\sum_{(rst\equiv abc)}[(T;\alpha\beta;-;rs,t)+(U;\alpha,\beta;-;r,st)+(G;\alpha\beta;-;r,st)]$$

where $(\alpha\beta*-*abc)$ are the coefficients in H_3 as listed in Table X, $(N;\alpha\beta;-;abc)$, $(T;\alpha\beta;-;ab,c)$, $(U;\alpha,\beta;a,bc)$ and $(G;\alpha\beta;-;a,bc)$ are auxiliary coefficients to be listed in Lists (2), (3), (4) and (5) of this appendix, and $\sideset{^*}{}\sum_{(rst\equiv abc)}$ denotes the summation over all permutations of the indices r, s and t, subject to the restriction that the left of the two indices placed on the same side of the separating comma is less than, or equal to, the right index.

The nonzero $(3;\alpha\beta;-;abc)$-coefficients are listed in List (1), in which the separating asterisks and commas are omitted from the coefficients.

(1) <u>Coefficients $(3;\alpha\beta;-;abc) \equiv (3\alpha\beta abc)$:</u>

$(3\alpha\alpha111) = (\alpha\alpha111) + (N\alpha\alpha111) + (T\alpha\alpha11,1)$

$(3\alpha\alpha222) = (\alpha\alpha222) + (N\alpha\alpha222) + (T\alpha\alpha22,2)$

$(3\alpha\alpha112) = (3\alpha\alpha121) = (3\alpha\alpha211) = (\alpha\alpha112) + (N\alpha\alpha112) + (T\alpha\alpha11,2) + (T\alpha\alpha12,1)$

$(3\alpha\alpha122) = (3\alpha\alpha212) = (3\alpha\alpha221) = (\alpha\alpha122) + (N\alpha\alpha122) + (T\alpha\alpha12,2) + (T\alpha\alpha22,1)$

$(3\alpha\alpha 133) = (3\alpha\alpha 313) = (3\alpha\alpha 331) = (\alpha\alpha 133) + (T\alpha\alpha 13,3) + (T\alpha\alpha 33,1)$
$+ (G\alpha\alpha 3,13)$

$(3\alpha\alpha 233) = (3\alpha\alpha 323) = (3\alpha\alpha 332) = (\alpha\alpha 233) + (T\alpha\alpha 23,3) + (T\alpha\alpha 33,1)$
$+ (G\alpha\alpha 3,23)$

In the above $\alpha = x,\ y$

$(3zz111) = (zz111) + (Nzz111) + (Tzz11,1) + (Uz,z1,11)$

$(3zz222) = (zz222) + (Nzz222) + (Tzz22,2) + (Uz,z2,22)$

$(3zz112) = (zz112) + (Nzz112) + (Tzz11,2) + (Tzz12,1) +$
$(Uz,z1,12) + (Uz,z2,11)$
$= (3zz121) = (3zz211)$

$(3zz122) = (zz122) + (Nzz122) + (Tzz12,2) + (Tzz22,1) +$
$(Uz,z1,22) + (Uz,z2,12)$

$(3zz133) = (Tzz13,3) + (Tzz33,1) + (Uz,z1,33) + (Uz,z3,13)$
$= (3zz313) = (3zz331)$

$(3zz233) = (Tzz23,3) + (Tzz33,2) + (Uz,z2,33) + (Uz,z3,23)$
$= (3zz323) + (3zz332)$

$(3xy113) = (xy113) + (Nxy113) + (Txy11,3) + (Txy13,1) + (Gxy1,13)$
$= (3xy131) = (3xy311) = (3yx113) = (3yx131) = (3yx311)$

$(3xy223) = (xy223) + (Nxy223) + (Txy22,3) + (Txy23,2) + (Gxy2,23)$
$= (3xy232) = (3xy322) = (3yx223) = (3yx232) = (3yx322)$

$(3xy123) = (xy123) + (Nxy123) + (Txy12,3) + (Txy13,2) +$
$(Gxy1,23) + (Gxy2,13)$
$= (3xy132) = (3xy213) = (3xy231) = (3xy312) = (3xy321)$
$= (3yx123) =$ etc, ...

$(3xy333) = (xy333) + (Nxy333) + (Txy33,3)$

(2) <u>Auxiliary coefficients $(N;\alpha\beta;abc) \equiv (\alpha\beta abc)$ and all permutation:</u>

In the following, $\alpha = x, y, z$

$$(\alpha\alpha 111) = 4\pi c h^{1/2} a_1^{\alpha\alpha} k_{1111}/I_\alpha^2 \lambda_1^{3/4} - (8\pi^2 c^2 \hbar^{1/2} a_1^{\alpha\alpha}/3I_\alpha^2\lambda_1^{3/4})[3 \times k_{111}^2/\lambda_1^{1/2} + k_{112}^2(2\lambda_1-\lambda_2)/\lambda_2^{1/2}(4\lambda_1-\lambda_2)] + \pi c\hbar^{1/2}a_2^{\alpha\alpha} \times k_{1112}/I_\alpha^2\lambda_2^{3/4} - (2\pi^2c^2\hbar^{1/2}a_2^{\alpha\alpha}/3I_\alpha^2\lambda_2^{3/4})[k_{111}k_{112}(7\lambda_1-\lambda_2)/\lambda_1^{1/2}(4\lambda_1-\lambda_2) + k_{112}k_{122}(13\lambda_1\lambda_2-2\lambda_1^2-5\lambda_2^2)/\lambda_2^{1/2} \times (4\lambda_1-\lambda_2)(4\lambda_2-\lambda_1)]$$

$$(\alpha\alpha 112) = 2\pi c h^{1/2} a_2^{\alpha\alpha} k_{1122}/I_\alpha^2\lambda_2^{3/4} - (8\pi^2c^2\hbar^{1/2}a_2^{\alpha\alpha}/3I_\alpha^2\lambda_2^{3/4}) \times [k_{112}k_{222}(3\lambda_1-\lambda_2)/\lambda_2^{1/2}(4\lambda_1-\lambda_2) + k_{111}k_{122}(3\lambda_2-\lambda_1)/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + 2k_{112}^2\lambda_1^{1/2}/(4\lambda_1-\lambda_2) + 2k_{122}^2\lambda_2^{1/2}/(4\lambda_2-\lambda_1)] + 3\pi c h^{1/2}a_1^{\alpha\alpha}k_{1112}/I_\alpha^2\lambda_1^{3/4} - (2\pi^2c^2\hbar^{1/2}a_1^{\alpha\alpha}/I_\alpha^2 \times \lambda_1^{3/4})[k_{111}k_{112}(7\lambda_1-\lambda_2)/\lambda_1^{1/2}(4\lambda_1-\lambda_2) + k_{112}k_{122}(13\lambda_1 \times \lambda_2-2\lambda_1^2-5\lambda_2^2)/\lambda_2^{1/2}(4\lambda_1-\lambda_2)(4\lambda_2-\lambda_1)]$$

$$(\alpha\alpha 122) = 3\pi c h^{1/2}a_2^{\alpha\alpha}k_{1222}/I_\alpha^2\lambda_2^{3/4} - (2\pi^2c^2\hbar^{1/2}a_2^{\alpha\alpha}/I_\alpha^2\lambda_2^{3/4}) \times [k_{122}k_{222}(7\lambda_2-\lambda_1)/\lambda_2^{1/2}(4\lambda_2-\lambda_1) + k_{112}k_{122}(13\lambda_1\lambda_2-2\lambda_2^2-5\lambda_1^2)/\lambda_1^{1/2}(4\lambda_1-\lambda_2)(4\lambda_2-\lambda_1)] + 2\pi c\hbar^{1/2}a_1^{\alpha\alpha}k_{1122}/I_\alpha^2 \times \lambda_1^{3/4} - (8\pi^2c^2\hbar^{1/2}a_1^{\alpha\alpha}/3I_\alpha^2\lambda_1^{3/4})[k_{112}k_{222}(3\lambda_1-\lambda_2)/(4\lambda_1-\lambda_2)\lambda_2^{1/2} + k_{111}(3\lambda_2-\lambda_1)k_{122}/\lambda_1^{1/2}(4\lambda_2-\lambda_1) + 2k_{112}^2\lambda_1^{1/2}/(4\lambda_2-\lambda_1) + 2k_{122}^2\lambda_2^{1/2}/(4\lambda_1-\lambda_2)]$$

$$(\alpha\alpha 222) = 4\pi c h^{1/2}a_2^{\alpha\alpha}k_{2222}/I_\alpha^2\lambda_2^{3/4} - (8\pi^2c^2\hbar^{1/2}a_2^{\alpha\alpha}/3I_\alpha^2\lambda_2^{3/4})[3 \times k_{222}^2/\lambda_2^{1/2} + k_{122}^2(2\lambda_2-\lambda_1)/\lambda_1^{1/2}(4\lambda_2-\lambda_1)] + \pi c\hbar^{1/2}a_1^{\alpha\alpha} \times k_{1222}/I_\alpha^2\lambda_1^{3/4} - (2\pi^2c^2\hbar^{1/2}a_1^{\alpha\alpha}/3I_\alpha^2\lambda_1^{3/4})[k_{222}k_{122}(7\lambda_2-\lambda_1)/\lambda_2^{1/2}(4\lambda_2-\lambda_1) + k_{122}k_{112}(13\lambda_1\lambda_2-2\lambda_2^2-5\lambda_1^2)/\lambda_1^{1/2} \times (4\lambda_2-\lambda_1)(4\lambda_1-\lambda_2)]$$

$$(xy113) = (yx113) = 2\pi c h^{1/2}a_3^{xy}k_{1133}/I_xI_y\lambda_3^{3/4} - (4\pi^2c^2\hbar^{1/2}a_3^{xy}/3 \times I_xI_y\lambda_3^{3/4})[k_{111}k_{133}(5\lambda_3-2\lambda_1)/\lambda_1^{1/2}(4\lambda_3-\lambda_1) + k_{112}k_{233} \times \ldots$$

(xy113), cont'd.

$((2\lambda_1-\lambda_2)/2\lambda_2{}^{1/2}(4\lambda_1-\lambda_2) + (2\lambda_3-\lambda_2)/2\lambda_2{}^{1/2}(4\lambda_3-\lambda_2)) +$

$2k_{133}^2\lambda_3{}^{1/2}/(4\lambda_3-\lambda_1)]$

$(xy123) = (yx123) = 2\pi c\hbar^{1/2}a_3^{xy}k_{1233}/I_xI_y\lambda_3{}^{3/4} - (8\pi^2c^2\hbar^{1/2}a_3^{xy}/3 \text{ X}$

$I_xI_y\lambda_3{}^{3/4})[k_{122}k_{233}((2\lambda_3-\lambda_2)/\lambda_2{}^{1/2}(4\lambda_3-\lambda_2) + \lambda_2{}^{1/2}/(4\lambda_2-$

$\lambda_1)) + k_{112}k_{133}((2\lambda_3-\lambda_1)/\lambda_1{}^{1/2}(4\lambda_3-\lambda_1) + \lambda_1{}^{1/2}/(4\lambda_1-\lambda_2))$

$+ 2k_{133}k_{233}\lambda_3{}^{1/2}(8\lambda_3-\lambda_1-\lambda_2)/(4\lambda_3-\lambda_1)(4\lambda_3-\lambda_2)]$

$(xy223) = (yx223) = 2\pi c\hbar^{1/2}a_3^{xy}k_{2233}/I_xI_y\lambda_3{}^{3/4} - (4\pi^2c^2\hbar^{1/2}a_3^{xy}/3 \text{ X}$

$I_xI_y\lambda_3{}^{3/4})[k_{222}k_{233}(5\lambda_3-2\lambda_2)/\lambda_2{}^{1/2}(4\lambda_3-\lambda_2) + (k_{122}k_{133}/$

$\lambda_1{}^{1/2})((2\lambda_2-\lambda_1)/(4\lambda_2-\lambda_1) + (2\lambda_3-\lambda_1)/(4\lambda_3-\lambda_1)) + 2k_{233}^2 \text{ X}$

$\lambda_3{}^{1/2}/(4\lambda_3-\lambda_2)]$

$(xy333) = (yx333) = 4\pi c\hbar^{1/2}a_3^{xy}k_{3333}/I_xI_y\lambda_3{}^{3/4} - (8\pi^2c^2\hbar^{1/2}a_3^{xy}/3 \text{ X}$

$I_xI_y\lambda_3{}^{3/4})[k_{133}^2(2\lambda_3-\lambda_1)/\lambda_1{}^{1/2}(4\lambda_3-\lambda_1) + k_{233}^2(2\lambda_3-\lambda_2)/$

$\lambda_2{}^{1/2}(4\lambda_3-\lambda_2)]$

(3) Auxiliary coefficients $(T;\alpha\beta;ab,c) \equiv (\alpha\beta ab,c)$:

In the following, $\alpha = x, y, z$

$(\alpha\alpha 11,1) = (3\pi c\hbar/I_\alpha{}^2\lambda_1{}^{1/4})[2k_{111}(\delta_{\alpha y}\cos^2\gamma - \delta_{\alpha x}\sin^2\gamma)/\lambda_1{}^{3/4} +$

$(-)^{\delta_{\alpha x}}(1-\delta_{\alpha z})k_{112}(2\lambda_1-\lambda_2)\sin\gamma\cos\gamma/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] -$

$\delta_{\alpha z}(3\pi c\hbar a_1^{zz}/4I_z{}^3\lambda_1{}^{1/4})[2k_{111}a_1^{zz}/\lambda_1{}^{3/4} + k_{112}a_2^{zz}(2\lambda_1-$

$\lambda_2)/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] - (8\pi c\hbar^{1/2}k_{111}/3I_\alpha{}^2\lambda_1{}^{1/2})[2a_1^{\alpha\alpha}k_{111}/$

$\lambda_1{}^{3/4} + a_2^{\alpha\alpha}k_{112}(3\lambda_1-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] - [4\pi c\hbar^{1/2}k_{112}\text{X}$

$(2\lambda_1-\lambda_2)/3I_\alpha{}^2\lambda_2{}^{1/2}(4\lambda_1-\lambda_2)][a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-$

$\lambda_2) + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]$

$(\alpha\alpha 22,2) = (3\pi c\hbar/I_\alpha{}^2\lambda_2{}^{1/4})[2k_{222}(\delta_{\alpha y}\sin^2\gamma - \delta_{\alpha x}\cos^2\gamma)/\lambda_2{}^{3/4} +$

$(-)^{\delta_{\alpha x}}(1-\delta_{\alpha z})k_{122}(2\lambda_2-\lambda_1)\sin\gamma\cos\gamma/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] -$

$\delta_{\alpha z}(3\pi c h a_2^{zz}/4I_z{}^3\lambda_2{}^{1/4})[2k_{222}a_2^{zz}/\lambda_2{}^{3/4} + k_{122}a_1^{zz} \text{ X} \ldots$

$(\alpha\alpha 22,2)$, cont'd.

$$(2\lambda_2-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] - (8\pi c\hbar^{1/2}k_{222}/3I_\alpha{}^2\lambda_2{}^{1/2})[2a_2^{\alpha\alpha} \times$$
$$k_{222}/\lambda_2{}^{3/4} + a_1^{\alpha\alpha}k_{122}(3\lambda_2-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1)] - [4\pi c\hbar^{1/2} \times$$
$$k_{122}(2\lambda_2-\lambda_1)/3I_\alpha{}^2\lambda_1{}^{1/2}(4\lambda_2-\lambda_1)][a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\ {}_2{}^{3/4} \times$$
$$(4\lambda_2-\lambda_1) + a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2)]$$

$$(\alpha\alpha 12,1) = (6\pi c\hbar/I_\alpha{}^2)[2k_{112}(\delta_{\alpha y}\cos^2\gamma-\delta_{\alpha x}\sin^2\gamma)/(4\lambda_1-\lambda_2) + (-)^{\delta_{\alpha x}} \times$$
$$(1-\delta_{\alpha z})k_{122}\sin\gamma\cos\gamma/(4\lambda_2-\lambda_1)] - \delta_{\alpha z}(3\pi cha_1^{zz}/2I_z{}^3)[2a_1^{zz} \times$$
$$k_{112}/(4\lambda_1-\lambda_2) + a_2^{zz}k_{122}/(4\lambda_2-\lambda_1)] - [16\pi c\hbar^{1/2}k_{112}\lambda_1{}^{1/2}/$$
$$3I_\alpha{}^2(4\lambda_1-\lambda_2)][2a_1^{\alpha\alpha}k_{111}/\lambda_1{}^{3/4} + a_2^{\alpha\alpha}k_{112}(3\lambda_1-\lambda_2)/\lambda_2{}^{3/4} \times$$
$$(4\lambda_1-\lambda_2)] - [8\pi c\hbar^{1/2}k_{122}\lambda_2{}^{1/2}/3I_\alpha{}^2(4\lambda_2-\lambda_1)][a_1^{\alpha\alpha}k_{112}(5\lambda_1$$
$$-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]$$

$$(\alpha\alpha 22,1) = (3\pi c\hbar/I_\alpha{}^2\lambda_1{}^{1/4})[2k_{122}(\delta_{\alpha y}\cos^2\gamma-\delta_{\alpha x}\sin^2\gamma)(2\lambda_2-\lambda_1)/(4\lambda_2-$$
$$\lambda_1)\lambda_1{}^{3/4} + (-)^{\delta_{\alpha x}}(1-\delta_{\alpha z})k_{222}\sin\gamma\cos\gamma/\lambda_2{}^{3/4}] - \delta_{\alpha z}(3\pi c \times$$
$$\hbar a_1^{zz}/4I_z{}^3\lambda_1{}^{1/4})[2k_{122}a_1^{zz}(2\lambda_2-\lambda_1)/\lambda_1{}^{3/4}(4\lambda_2-\lambda_1) + k_{222} \times$$
$$a_2^{zz}/\lambda_2{}^{3/4}] - (4\pi c\hbar^{1/2}k_{222}/3I_\alpha{}^2\lambda_2{}^{1/2})[a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/$$
$$\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)] - [8\pi c \times$$
$$\hbar^{1/2}k_{122}(2\lambda_2-\lambda_1)/3I_\alpha{}^2\lambda_1{}^{1/2}(4\lambda_2-\lambda_1)][2a_1^{\alpha\alpha}k_{111}/\lambda_1{}^{3/4} +$$
$$a_2^{\alpha\alpha}k_{112}(3\lambda_1-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)]$$

$$(\alpha\alpha 33,1) = (3\pi ch/I_\alpha{}^2\lambda_1{}^{1/4})[2k_{133}(\delta_{\alpha y}\cos^2\gamma-\delta_{\alpha x}\sin^2\gamma)(2\lambda_3-\lambda_1)/(4\lambda_3-$$
$$\lambda_1)\lambda_1{}^{3/4} + (-)^{\delta_{\alpha x}}(1-\delta_{\alpha z})k_{233}\sin\gamma\cos\gamma(2\lambda_3-\lambda_2)/(4\lambda_3-\lambda_2) \times$$
$$\lambda_2{}^{3/4}] -\delta_{\alpha z}(3\pi c\hbar a_1^{zz}/I_z{}^3\lambda_1{}^{1/4})[2k_{133}(2\lambda_3-\lambda_1)a_1^{zz}/\lambda_1{}^{3/4} \times$$
$$(4\lambda_3-\lambda_1) + k_{233}(2\lambda_3-\lambda_2)a_2^{zz}/\lambda_2{}^{3/4}(4\lambda_3-\lambda_2)] - [8\pi c\hbar^{1/2} \times$$
$$k_{133}(2\lambda_3-\lambda_1)/3I_\alpha{}^2\lambda_1{}^{1/2}(4\lambda_3-\lambda_1)][2a_1^{\alpha\alpha}k_{111}/\lambda_1{}^{3/4} + a_2^{\alpha\alpha} \times$$
$$k_{112}(3\lambda_1-\lambda_2)/\lambda_2{}^{3/4}(4\lambda_1-\lambda_2)] - [4\pi c\hbar^{1/2}k_{233}(2\lambda_3-\lambda_2)/3 \times$$
$$I_\alpha{}^2\lambda_2{}^{1/2}(4\lambda_3-\lambda_2)][a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/\lambda_1{}^{3/4}(4\lambda_1-\lambda_2) + a_2^{\alpha\alpha} \times$$
$$k_{122}(5\lambda_2-\lambda_1)/\lambda_2{}^{3/4}(4\lambda_2-\lambda_1)]$$

$$\begin{aligned}(\alpha\alpha 11,2) = {} & (3\pi c\hbar/I_\alpha^2\lambda_2^{1/4})[2k_{112}(\delta_{\alpha y}\sin^2\gamma-\delta_{\alpha x}\cos^2\gamma)(2\lambda_1-\lambda_2)/(4\lambda_1- \\ & \lambda_2)\lambda_2^{3/4} + k_{111}\sin\gamma\cos\gamma(-)^{\delta_{\alpha x}}(1-\delta_{\alpha z})/\lambda_1^{3/4}] - \delta_{\alpha z}[3\pi c \times \\ & \hbar a_2^{zz}/4I_z^3\lambda_2^{1/4}][2k_{112}(2\lambda_1-\lambda_2)a_2^{zz}/\lambda_2^{3/4}(4\lambda_1-\lambda_2) + k_{111}\times \\ & a_1^{zz}/\lambda_1^{3/4}] - [8\pi ch^{1/2}k_{112}(2\lambda_1-\lambda_2)/3I_\alpha^2\lambda_2^{1/2}(4\lambda_1-\lambda_2)] \times \\ & [2a_2^{\alpha\alpha}k_{222}/\lambda_2^{3/4} + a_1^{\alpha\alpha}k_{122}(3\lambda_2-\lambda_1)/\lambda_1^{3/4}(4\lambda_2-\lambda_1)] - [4\times \\ & \pi ch^{1/2}k_{111}/3I_\alpha^2\lambda_1^{1/2}][a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/\lambda_1^{3/4}(4\lambda_1-\lambda_2) + \\ & a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{3/4}(4\lambda_1-\lambda_2)]\end{aligned}$$

$$\begin{aligned}(\alpha\alpha 12,2) = {} & (6\pi c\hbar/I_\alpha^2)[2k_{122}(\delta_{\alpha y}\sin^2\gamma - \delta_{\alpha x}\cos^2\gamma)/(4\lambda_2-\lambda_1) + (-)^{\delta_{\alpha x}}\times \\ & (1-\delta_{\alpha z})k_{112}\lambda_1^{1/4}\sin\gamma\cos\gamma/\lambda_2^{1/2}(4\lambda_1-\lambda_2)] - \delta_{\alpha z}(3\pi c\hbar a_2^{zz}/ \\ & 2I_z^3)[2k_{122}a_2^{zz}/(4\lambda_2-\lambda_1) + k_{112}a_1^{zz}\lambda_1^{1/4}/\lambda_2^{1/4}(4\lambda_1-\lambda_2)] \\ & - [8\pi c\hbar^{1/2}k_{112}\lambda_1^{1/2}/3I_\alpha^2(4\lambda_1-\lambda_2)][a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/(4\lambda_1 \\ & -\lambda_2)\lambda_1^{3/4} + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{3/4}(4\lambda_1-\lambda_2)] - [16\pi c \times \\ & \hbar^{1/2}k_{122}/3I_\alpha^2(4\lambda_2-\lambda_1)][2a_2^{\alpha\alpha}k_{222}/\lambda_2^{3/4} + a_1^{\alpha\alpha}k_{122}(3\lambda_2- \\ & \lambda_1)/\lambda_1^{3/4}(4\lambda_2-\lambda_1)]\end{aligned}$$

$$\begin{aligned}(\alpha\alpha 33,2) = {} & (3\pi ch/I_\alpha^2\lambda_2^{1/4})[2k_{233}(\delta_{\alpha y}\sin^2\gamma - \delta_{\alpha x}\cos^2\gamma)(2\lambda_3-\lambda_2)/(4\lambda_3 \\ & -\lambda_2)\lambda_2^{3/4} + (-)^{\delta_{\alpha x}}(1-\delta_{\alpha z})k_{133}\sin\gamma\cos\gamma(2\lambda_3-\lambda_1)/\lambda_1^{3/4} \times \\ & (4\lambda_3-\lambda_1)] - \delta_{\alpha z}(3\pi c\hbar a_2^{zz}/4I_z^3\lambda_2^{1/4})[2a_2^{zz}k_{233}(2\lambda_3-\lambda_2)/ \\ & \lambda_2^{3/4}(4\lambda_3-\lambda_2) + a_1^{zz}k_{133}(2\lambda_3-\lambda_1)/\lambda_1^{3/4}(4\lambda_3-\lambda_1)] - [4\pi c \times \\ & \hbar^{1/2}k_{133}(2\lambda_3-\lambda_1)/3I_\alpha^2\lambda_1^{1/2}(4\lambda_3-\lambda_1)][a_1^{\alpha\alpha}k_{112}(5\lambda_1-\lambda_2)/ \\ & \lambda_1^{3/4}(4\lambda_1-\lambda_2) + a_2^{\alpha\alpha}k_{122}(5\lambda_2-\lambda_1)/\lambda_2^{3/4}(4\lambda_2-\lambda_1)] - [8\pi c \times \\ & \hbar^{1/2}k_{233}(2\lambda_3-\lambda_2)/3I_\alpha^2\lambda_2(4\lambda_3-\lambda_2)][2a_2^{\alpha\alpha}k_{222}/\lambda_2^{3/4} + a_1^{\alpha\alpha}\times \\ & k_{122}(3\lambda_2-\lambda_1)/\lambda_1^{3/4}(4\lambda_2-\lambda_1)]\end{aligned}$$

$$\begin{aligned}(\alpha\alpha j3,3) = {} & -(1-\delta_{\alpha z})[12\pi c\hbar k_{j33}/I_\alpha I_z(4\lambda_3-\lambda_j)] - \delta_{\alpha z}[8\pi chk_{j33}/3I_z^2 \times \\ & (4\lambda_3-\lambda_j)][\zeta_{13}/(\lambda_1-\lambda_3) + \zeta_{23}/(\lambda_2-\lambda_3)] - [16\pi c\hbar^{1/2}k_{j33}\times \\ & \lambda_3^{1/2}/3I_\alpha^2(4\lambda_3-\lambda_j)][a_1^{\alpha\alpha}k_{133}(3\lambda_3-\lambda_1)/\lambda_1^{3/4}(4\lambda_3-\lambda_1) + \\ & a_2^{\alpha\alpha}k_{233}(3\lambda_3-\lambda_2)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)] \;;\; j = 1,\ 2\end{aligned}$$

$(xy11,3) = (yx11,3) = (3\pi c\hbar k_{111}/2I_x^2 I_y^2 I_z^{1/2}\lambda_1^{3/4}\lambda_3^{1/4})[I_x^{1/2}\cos\gamma$
$I_y^{1/2}\sin\gamma] - \pi^2 c^2 \hbar^{1/2} k_{111} k_{133}(5\lambda_3-\lambda_1)/3I_x I_y \lambda_1^{1/2}\lambda_3^{3/4} X$
$(4\lambda_3-\lambda_1) + \pi c\hbar k_{111}\zeta_{13}(\lambda_1+\lambda_3)(I_x-I_y)/2I_x^2 I_y^2 \lambda_1^{3/4}\lambda_3^{1/4} X$
$(\lambda_1-\lambda_3) - [\pi c\hbar k_{112}(2\lambda_1-\lambda_2)/2I_x^2 I_y^2 I_z^{1/2}\lambda_2^{3/4}\lambda_3^{1/4}(4\lambda_1-$
$\lambda_2)][5I_x^{1/2}\sin\gamma - I_y^{1/2}\cos\gamma] - \pi^2 c^2 \hbar^{1/2} k_{112} k_{233}(2\lambda_1-$
$\lambda_2)(5\lambda_3-\lambda_2)/3I_x I_y \lambda_2^{1/2}\lambda_3^{3/4}(4\lambda_1-\lambda_2)(4\lambda_3-\lambda_2) + \pi c\hbar\zeta_{23}\ X$
$k_{112}(2\lambda_1-\lambda_2)(\lambda_2+\lambda_3)(I_x-I_y)/2I_x^2 I_y^2 \lambda_2^{3/4}(4\lambda_1-\lambda_2)(\lambda_2-\lambda_3) X$
$\lambda_3^{1/4}$

$(xy12,3) = (yx12,3) = [3\pi chk_{112}\lambda_1^{1/4}/I_x^2 I_y^2 I_z^{1/2}\lambda_3^{1/4}(4\lambda_1-\lambda_2)]\ X$
$[I_x^{1/2}\cos\gamma + I_y^{1/2}\sin\gamma] - 2\pi^2 c^2 \hbar^{1/2} k_{112} k_{133}\lambda_1^{1/2}(5\lambda_3-$
$\lambda_1)/3I_x I_y(4\lambda_1-\lambda_2)\lambda_3^{3/4}(4\lambda_3-\lambda_1) + \pi c\hbar k_{112}\zeta_{13}(\lambda_1+\lambda_3)(I_x-$
$I_y)\lambda_1^{1/4}/I_x^2 I_y^2 \lambda_3^{1/4}(\lambda_1-\lambda_3)(4\lambda_1-\lambda_2) - [\pi c\hbar k_{122}\lambda_2^{1/4}/$
$I_x^2 I_y^2 I_z^{1/2}\lambda_3^{1/4}(4\lambda_2-\lambda_1)][5I_x^{1/2}\sin\gamma - I_y^{1/2}\cos\gamma] - [2X$
$\pi^2 c^2 \hbar^{1/2} k_{122}\lambda_2^{1/2}/3I_x I_y(4\lambda_2-\lambda_1)][k_{233}(5\lambda_3-\lambda_2)/\lambda_3^{3/4}\ X$
$(4\lambda_3-\lambda_2)] + \pi c\hbar k_{122}\zeta_{23}\lambda_2^{1/4}(\lambda_2+\lambda_3)(I_x-I_y)/I_x^2 I_y^2 \lambda_3^{1/4} X$
$(4\lambda_2-\lambda_1)(\lambda_2-\lambda_3)$

$(xy22,3) = (yx22,3) = [3\pi\hbar k_{122}(2\lambda_2-\lambda_1)/2I_x^2 I_y^2 I_z^{1/2}\lambda_3^{1/4}\lambda_1^{3/4}(4\lambda_2$
$-\lambda_1)][I_x^{1/2}\cos\gamma + I_y^{1/2}\sin\gamma] - \pi^2 c^2 \hbar^{1/2} k_{122} k_{133}(2\lambda_2-$
$\lambda_1)(5\lambda_3-\lambda_1)/3I_x I_y \lambda_3^{3/4}\lambda_1^{1/2}(4\lambda_3-\lambda_1)(4\lambda_2-\lambda_1) + \pi c\hbar k_{122} X$
$\zeta_{13}(\lambda_1+\lambda_3)(2\lambda_2-\lambda_1)(I_x-I_y)/2I_x^2 I_y^2 \lambda_1^{3/4}\lambda_3^{1/4}(4\lambda_2-\lambda_1)(\lambda_1$
$-\lambda_3) - (\pi c\hbar k_{222}/2I_x^2 I_y^2 I_z^{1/2}\lambda_2^{3/4}\lambda_3^{1/4})[5I_x^{1/2}\sin\gamma -$
$I_y^{1/2}\cos\gamma] - \pi^2 c^2 \hbar^{1/2} k_{222} k_{233}(5\lambda_3-\lambda_2)/3I_x I_y \lambda_2^{1/2}\lambda_3^{3/4} X$
$(4\lambda_3-\lambda_2) + \pi chk_{222}\zeta_{23}(\lambda_2+\lambda_3)(I_x-I_y)/2I_x^2 I_y^2 \lambda_2^{3/4}\lambda_3^{1/4} X$
$(\lambda_2-\lambda_3)$

$(xy33,3) = (yx33,3) = [3\pi chk_{133}(2\lambda_3-\lambda_1)/2I_x^2 I_y^2 I_z^{1/2}\lambda_3^{1/4}\lambda_1^{3/4}\ X$
$(4\lambda_3-\lambda_1)][I_x^{1/2}\cos\gamma + I_y^{1/2}\sin\gamma] - \pi^2 c^2 \hbar^{1/2} k_{133} k_{133} X..$

(xy33,3), cont'd.

$(2\lambda_3-\lambda_1)(5\lambda_3-\lambda_1)/3I_xI_y\lambda_1^{1/2}\lambda_3^{3/4}(4\lambda_3-\lambda_1)(4\lambda_3-\lambda_1) + \pi c \times \hbar k_{133}\zeta_{13}(\lambda_1+\lambda_3)(2\lambda_3-\lambda_1)(I_x-I_y)/2I_x^2I_y^2\lambda_1^{3/4}\lambda_3^{1/4}(4\lambda_3-\lambda_1)(\lambda_1-\lambda_3) - [\pi c\hbar k_{233}(2\lambda_3-\lambda_2)/2I_x^2I_y^2I_z^{1/2}\lambda_2^{3/4}\lambda_3^{1/4} \times (4\lambda_3-\lambda_2)][5I_x^{1/2}\sin\gamma - I_y^{1/2}\cos\gamma] - \pi^2c^2\hbar^{1/2}k_{233}^2(2\lambda_3-\lambda_2)(5\lambda_3-\lambda_2)/3I_xI_y\lambda_2^{1/2}\lambda_3^{3/4}(4\lambda_3-\lambda_2)^2 + \pi c\hbar k_{233}\zeta_{23}(\lambda_2+\lambda_3)(2\lambda_3-\lambda_2)(I_x-I_y)/2I_x^2I_y^2\lambda_2^{3/4}\lambda_3^{1/4}(4\lambda_3-\lambda_2)(\lambda_2-\lambda_3)$

$(xyj3,1) = (yxj3,1) = [3\pi c\hbar k_{j33}\lambda_3^{1/4}/I_x^2I_y^2I_z^{1/2}(4\lambda_3-\lambda_j)\lambda_1^{1/4}] \times [I_x^{1/2}\cos\gamma + I_y^{1/2}\sin\gamma] - 8\pi^2c^2\hbar^{1/2}k_{133}k_{j33}(5\lambda_3-\lambda_1)/\lambda_3^{3/4}(4\lambda_3-\lambda_1)(4\lambda_3-\lambda_j) + \pi c\hbar k_{j33}\zeta_{13}\lambda_3^{1/4}(\lambda_1+\lambda_3)(I_x-I_y)/I_x^2I_y^2\lambda_1^{1/4}(4\lambda_3-\lambda_j)(\lambda_1-\lambda_3)$; $j = 1, 2$

$(xyj3,2) = (yxj3,2) = [-\pi c\hbar k_{j33}\lambda_3^{1/4}/I_x^2I_y^2I_z^{1/2}\lambda_2^{1/4}(4\lambda_3-\lambda_j)] \times [5I_x^{1/2}\sin\gamma - I_y^{1/2}\cos\gamma] - 8\pi^2c^2\hbar^{1/2}k_{233}k_{j33}(5\lambda_3-\lambda_2)/\lambda_3^{3/4}(4\lambda_3-\lambda_2) + \pi c\hbar k_{j33}\zeta_{23}\lambda_3^{1/4}(\lambda_2+\lambda_3)(I_x-I_y)/I_x^2I_y^2 \times \lambda_2^{1/4}(4\lambda_3-\lambda_j)(\lambda_2-\lambda_3)$

(4) Auxiliary coefficients $(U;\alpha,\beta;-;a,bc) \equiv (\alpha,\beta a,bc)$:

In the following, $i = 1, 2$; $j = 1, 2$

$(z,zi,jj) = -\hbar^{3/2}a_j^{zz}\zeta_{i3}\zeta_{j3}(\lambda_i+\lambda_3)/I_z^3\lambda_i^{1/4}\lambda_j^{1/2}(\lambda_i-\lambda_3) - [2\pi c\hbar \times \zeta_{i3}(\lambda_i+\lambda_3)/3\lambda_i^{1/4}(\lambda_i-\lambda_3)][k_{jjj}\zeta_{j3}(\lambda_3-7\lambda_j)/\lambda_j^{3/4}(\lambda_3-\lambda_j) + k_{ijj}\zeta_{i3}((2\lambda_j-\lambda_i)/\lambda_i^{3/4}(4\lambda_j-\lambda_i) - 2\lambda_i^{1/4}/(\lambda_3-\lambda_1)) - 2\lambda_3^{1/2}\zeta_{j3}k_{j33}/\lambda_j^{1/4}(4\lambda_3-\lambda_j)]$

$(z,zj,12) = (z,zj,21) = -\hbar^{3/2}\zeta_{j3}(\lambda_j+\lambda_3)(a_1^{zz}\zeta_{23} + a_2^{zz}\zeta_{13})/I_z^3(\lambda_j-\lambda_3)\lambda_j^{1/4}\lambda_1^{1/4}\lambda_2^{1/4} - [4\pi c\hbar\zeta_{j3}(\lambda_j+\lambda_3)/3\lambda_j^{1/4}(\lambda_j-\lambda_3)] \times [(\lambda_3+2\lambda_2-9\lambda_1)\lambda_1^{1/4}\zeta_{13}k_{112}/(4\lambda_1-\lambda_2)(\lambda_3-\lambda_1) + (\lambda_3+2\lambda_1-9\lambda_2)\lambda_2^{1/4}\zeta_{23}k_{122}/(4\lambda_2-\lambda_1)(\lambda_3-\lambda_2) - \lambda_3^{1/2}\zeta_{23}k_{133}/(4\lambda_3-\lambda_1)\lambda_2^{1/4} - \lambda_3^{1/2}\zeta_{13}k_{233}/\lambda_1^{1/4}(4\lambda_3-\lambda_2)]$

$$\begin{aligned}(z,zj,33) = {} & [-2\pi c\hbar\,\zeta_{j3}(\lambda_j+\lambda_3)/3\lambda_j^{1/4}(\lambda_j-\lambda_3)][\zeta_{13}k_{133}(2\lambda_1^2 + 2\lambda_3^2 - \\ & 7\lambda_1\lambda_3)/\lambda_1^{3/4}(4\lambda_3-\lambda_1)(\lambda_3-\lambda_1) + \zeta_{23}k_{233}(2\lambda_2^2 + 2\lambda_3^2 - \\ & 7\lambda_2\lambda_3)/\lambda_2^{3/4}(4\lambda_3-\lambda_2)(\lambda_3-\lambda_2)]\end{aligned}$$

$$\begin{aligned}(z,z3,13) = (z,z3,31) = {} & \hbar^{3/2}a_1^{zz}\zeta_{13}^2(\lambda_1+\lambda_3)/I_z^3\lambda_3^{1/2}\lambda_1^{1/4}(\lambda_1-\lambda_3) + \\ & [4\pi c\hbar\,\zeta_{13}(\lambda_1+\lambda_3)/3I_z^2\lambda_1^{1/4}\lambda_3^{1/4}(\lambda_1-\lambda_3)][2\lambda_3^{5/4}(2\lambda_1+\lambda_3)\times \\ & \zeta_{13}k_{133}/(4\lambda_3-\lambda_1)(\lambda_3-\lambda_1)\lambda_1^{3/4} - \lambda_1^{1/2}\lambda_2^{1/4}\zeta_{23}k_{112}/(4\lambda_1- \\ & \lambda_2)\lambda_3^{1/4} - \zeta_{13}k_{111}/\lambda_1^{1/4}\lambda_3^{1/4}] + \hbar^{3/2}a_1^{zz}\zeta_{23}^2(\lambda_2+\lambda_3)/ \\ & I_z^3\lambda_3^{1/2}(\lambda_2-\lambda_3) + [4\pi c\hbar\,\zeta_{23}(\lambda_2+\lambda_3)/3I_z^2\lambda_2^{1/4}\lambda_3^{1/4}(\lambda_2- \\ & \lambda_3)][\lambda_2^{1/4}\lambda_3^{1/4}\zeta_{23}k_{133}(\lambda_2+2\lambda_1-9\lambda_3)/(4\lambda_3-\lambda_1)(\lambda_2-\lambda_3) + \\ & \lambda_3^{1/4}(2\lambda_3-\lambda_2)\zeta_{13}k_{233}/\lambda_1^{1/4}\lambda_2^{1/2}(4\lambda_3-\lambda_2) - \lambda_1^{1/4}\zeta_{13}\times \\ & k_{112}(2\lambda_1-\lambda_2)/\lambda_2^{1/2}\lambda_3^{1/4}(4\lambda_1-\lambda_2) - \lambda_2^{3/4}\zeta_{13}k_{122}/\lambda_3^{1/4}\times \\ & (4\lambda_2-\lambda_1)]\end{aligned}$$

$$\begin{aligned}(z,z3,23) = (z,z3,32) = {} & \hbar^{3/2}a_2^{zz}\zeta_{13}^2(\lambda_1+\lambda_3)/I_z^3\lambda_3^{1/2}\lambda_2^{1/4}(\lambda_1-\lambda_3) + \\ & [4\pi c\hbar\,\zeta_{13}(\lambda_1+\lambda_3)/3I_z^2\lambda_1^{1/4}\lambda_3^{1/4}(\lambda_1-\lambda_3)][\lambda_1^{1/4}\lambda_3^{1/4}\zeta_{13}\times \\ & k_{233}(\lambda_1+2\lambda_2-9\lambda_3)/(4\lambda_3-\lambda_2)(\lambda_1-\lambda_3) + \lambda_3^{1/4}(2\lambda_3-\lambda_1)\zeta_{23}\times \\ & k_{133}/\lambda_1^{1/2}\lambda_2^{1/4}(4\lambda_3-\lambda_1) - \lambda_2^{1/4}\zeta_{23}k_{122}(2\lambda_2-\lambda_1)/\lambda_1^{1/2}\times \\ & \lambda_3^{1/4}(4\lambda_2-\lambda_1) - \lambda_1^{3/4}\zeta_{23}k_{112}/\lambda_3^{1/4}(4\lambda_1-\lambda_2)] + \hbar^{3/2}a_2^{zz}\times \\ & \zeta_{23}^2(\lambda_2+\lambda_3)/I_z^3\lambda_2^{1/4}\lambda_3^{1/2}(\lambda_2-\lambda_3) + [4\pi c\hbar\,\zeta_{23}(\lambda_2+\lambda_3)/3\times \\ & I_z^2\lambda_2^{1/4}\lambda_3^{1/4}(\lambda_2-\lambda_3)][2\lambda_3^{5/4}\zeta_{23}k_{233}(2\lambda_2+\lambda_3)/(4\lambda_3-\lambda_2)\times \\ & (\lambda_3-\lambda_2)\lambda_2^{3/4} - \lambda_1^{1/4}\lambda_2^{1/2}\zeta_{13}k_{122}/\lambda_3^{1/4}(4\lambda_2-\lambda_1) - \zeta_{23}\times \\ & k_{222}/\lambda_2^{1/4}\lambda_3^{1/4}]\end{aligned}$$

(5) <u>Auxiliary coefficients $(G;\alpha\beta;-;a,bc) \equiv (\alpha\beta a,bc)$:</u>

$$\begin{aligned}(xyi,j3) = (yxi,j3) = {} & [\hbar^{3/2}\zeta_{j3}(\lambda_j+\lambda_3)/2I_z\lambda_j^{1/4}\lambda_3^{1/4}(\lambda_j-\lambda_3)][a_i^{yy}/ \\ & I_y^2\lambda_i^{1/4} - a_i^{xx}/I_x^2\lambda_i^{1/4}] \quad ; i = 1,\ 2 \quad ; j = 1,\ 2\end{aligned}$$

$$\begin{aligned}(xx3,j3) = -\ (yy3,j3) = {} & [-\hbar^{3/2}\zeta_{j3}(\lambda_j+\lambda_3)a_3^{xy}/I_xI_yI_z\lambda_j^{1/4}\lambda_3^{1/2}(\lambda_j \\ & -\lambda_3) \quad ; j = 1,2\end{aligned}$$

APPENDIX XV

Coefficients $(4;\alpha\beta,\gamma\delta\varepsilon\rho;-;-)$

The coefficients $(4;\alpha\beta;\gamma\delta\varepsilon\rho;-;-)$ appearing in the first sum of (4.6) can be written in the general form

$$(4\alpha\beta,\gamma\delta\varepsilon\rho;-;-) = (2\hbar/3)\sum_m [S;\alpha\beta;m;-](3;\gamma\delta\varepsilon\rho;-;m)$$

where $[S;\alpha\beta;m;-]$ are the coefficients of the first contact transformation S, and $(3;\gamma\delta\varepsilon\rho;-;m)$ are the coefficients in h_3'; they have been listed in Table XIII and Appendix XI, respectively. Written in the condensed form $(\alpha\beta,\gamma\delta\varepsilon\rho)$, the coefficients $(4;\alpha\beta;\gamma\delta\varepsilon\rho;-;-)$ are listed in List A and List B below.

A. For $\alpha = \beta =$ x, y, or z,

$$(\alpha\alpha,\gamma\delta\varepsilon\rho) = (2\hbar/3)([S;\alpha\alpha;1;-](3;\gamma\delta\varepsilon\rho;-;1) + [S;\alpha\alpha;2;-](3;\gamma\delta\varepsilon\rho;-;2))$$

The nonzero ones are:

(xx,xxxx), (yy,yyyy), (zz,zzzz), (xx,yyyy), (xx,zzzz), (yy,zzzz),

(yy,xxxx), (zz,xxxx), (zz,yyyy), (xx,xxyy)=(xx,yyxx),

(xx,xxzz)=(xx,zzxx), (yy,yyxx)=(yy,xxyy), (yy,yyzz)=(yy,zzyy)

(zz,zzxx)=(zz,xxzz), (zz,zzyy)=(zz,yyzz), (xx,yyzz)=(xx,zzyy)

(yy,zzxx)=(yy,xxzz), (zz,xxyy)=(zz,yyxx), (xx,xzxz)=(xx,zxzx)

(yy,xzxz)=(yy,zxzx), (zz,xzxz)=(zz,zxzx), (xx,yzyz)=(xx,zyzy)

(yy,yzyz)=(yy,zyzy), (zz,yzyz)=(zz,zyzy),

(xx,xyxy)=(xx,xyyx)=(xx,yxxy)=(xx,yxyx)

(yy,xyxy)=(yy,xyyx)=(yy,yxxy)=(yy,yxyx)

(zz,xyxy)=(zz,xyyx)=(zz,yxxy)=(zz,yxyx)

B. For $z \neq \alpha \neq \beta \neq z$,

$$(\alpha\beta,\gamma\delta\varepsilon\rho) \doteq (2\hbar/3)[S;\alpha\beta;3;-](3;\gamma\delta\varepsilon\rho;-;3)$$

The nonzero ones are:

List B, cont'd.

(xy,xxxy) = (yx,xxxy) = (xy,xxyx) = (yx,xxyx) = (xy,xyxx) =

(yx,xyxx) = (xy,yxxx) = (yx,yxxx)

(xy,yyxy) = (yx,yyxy) = (xy,yyyx) = (yx,yyyx) = (xy,xyyy) =

(yx,xyyy) = (xy,yxyy) = (yx,yxyy)

(xy,zxzy) = (yx,zxzy) = (xy,xzyz) = (yx,xzyz) = (xy,zyzx) =

(yx,zyzx) = (xy,yzxz) = (yx,yzxz)

(xy,zzxy) = (yx,zzxy) = (xy,zzyx) = (yx,zzyx)

(xy,xyzz) = (yx,xyzz) = (xy,zzyx) = (yx,zzyx)

(xy,zxxz) = (yx,zxxz)

(xy,zyyz) = (yx,zyyz)

APPENDIX XVI

Coefficients $(4;\alpha\beta\gamma\delta;-;ab)$

The coefficients $(4;\alpha\beta\gamma\delta;-;ab)$ appearing in the second sum of (4.6) can be written in general form

$$(4;\alpha\beta\gamma\delta;-;ab) = (0;\alpha\beta\gamma\delta;-;ab) + (R;\underline{\alpha},\underline{\beta\gamma\delta};-;\underline{a},\underline{b}) + (S;\underline{\alpha\beta},\underline{\gamma\delta};-;ab)$$

where $(0;\alpha\beta\gamma\delta;-;ab)$, $(R;\underline{\alpha},\underline{\beta\gamma\delta};-;ab)$ and $(S;\underline{\alpha\beta},\underline{\gamma\delta};-;ab)$ are auxiliary coefficients to be listed in Lists (2) to (4) of this appendix. In the condensed form $(\alpha\beta\gamma\delta ab)$, the coefficients $(4;\alpha\beta\gamma\delta;-;ab)$ are listed in List (1). Only those with a = b actually contribute to h_4.

(1) Coefficients $(4;\alpha\beta\gamma\delta;-;ab) \equiv (\alpha\beta\gamma\delta ab)$:

In the following, α = x, y, z ; β = x, y, z ; $\alpha \neq \beta$; i & j= 1, 2

$$(z\alpha\alpha zij) = (z\alpha\alpha zji) = [(1-\delta_{\alpha z})/2(1+\delta_{ij})][(Rz,z\alpha\alpha i,j)+(Rz,z\alpha\alpha j,i)]$$

$$(\alpha\alpha\alpha\alpha ij) = (\alpha\alpha\alpha\alpha ji) = (0\alpha\alpha\alpha\alpha ij) + (S\alpha\alpha,\alpha\alpha ij) + \delta_{\alpha z}[(Rz,zzzi,j) + (Rz,zzzj,i)]/(1+\delta_{ij})$$

$$(\alpha\alpha\alpha\alpha 33) = (0\alpha\alpha\alpha\alpha 33) + \delta_{\alpha z}(Rz,zzzz3,3)$$

$$(\alpha\alpha\beta\beta ij) = (\alpha\alpha\beta\beta ji) = (\beta\beta\alpha\alpha ij) = (\beta\beta\alpha\alpha ji) = (0\alpha\alpha\beta\beta ij) + (1/2)\times [(S\alpha\alpha,\beta\beta ij) + (S\beta\beta,\alpha\alpha ij)] + [\delta_{\alpha z}/2(1+\delta_{ij})][(Rz,\beta\beta zi,j) + (Rz,\beta\beta zj,i)]$$

$$(\alpha\alpha\beta\beta 33) = (\beta\beta\alpha\alpha 33) = (0\alpha\alpha\beta\beta 33) + (\delta_{\alpha z}/2)(Rz,z\beta\beta 3,3)$$

(2) Auxiliary coefficients $(0;\alpha\beta\gamma\delta;-;ab) \equiv (\alpha\beta\gamma\delta ab)$:

In general,

$$(0;\alpha\beta\gamma\delta;-;ab) = (2\hbar/3)\sum_m [S;-;m;ab](3;\alpha\beta\gamma\delta;-;m)$$

where [S;-;m;ab] are the coefficients of the first contact transformation S, listed in Table XVI, and $(3;\alpha\beta\gamma\delta;-;m)$ are the coefficients in h_3', listed in Appendix XI.

A. For a = b = 1, 2 or 3, and for $3 \neq a \neq b \neq 3$,

$$(0;\alpha\beta\gamma\delta;-;ab) = (2\hbar/3)[[S;-;1;ab](3;\alpha\beta\gamma\delta;-;1) + [S;-;2;ab](3;\alpha\beta\gamma\delta;-;2)]$$

and the nonzero ones are:

$(\alpha\alpha\alpha\alpha aa)$, $(\alpha\alpha\alpha\alpha 12) = (\alpha\alpha\alpha\alpha 21)$, $(\alpha\alpha\beta\beta aa)$, $(\alpha\alpha\beta\beta 12) = (\alpha\alpha\beta\beta 21)$,

(xyxyaa) = (xyyxaa) = (yxxyaa) = (yxyxaa)

(xyxy12) = (xyxy21) = (xyyx12) = (xyyx21) =

(yxxy12) = (yxxy21) = (yxyx12) = (yxyx21)

B. For (ab) = (13), (31), (23) Or (32),

$$(0;\alpha\beta\gamma\delta;-;ab) = (2\hbar/3)[S;-;3;ab](3;\alpha\beta\gamma\delta;-;3)$$

There are a total of forty eight nonzero coefficients of this type, seven of which are independent. They do not contribute to the final Hamiltonian, and therefore are not listed here.

(3) <u>Auxiliary coefficients $(R;\alpha,\beta\gamma\delta;-;a,b) \equiv (\alpha,\beta\gamma\delta a,b)$:</u>

The form in which these auxiliary coefficients relate to the coefficients $(4;\alpha\beta\gamma\delta;-;ab)$ is $(R;\underline{\alpha},\underline{\beta\gamma\delta};\underline{a},\underline{b})$, with the underlining having the significance as explained in Appendix XIII.

In general,

$$(R;\alpha,\beta\gamma\delta;-;a,b) = (-2\hbar/3)\sum_m [S;\alpha;-;am](3;\beta\gamma\delta;m;b)$$

where $[S;\alpha;-;am]$ are the coefficients of the first contact transformation S, as listed in Table XIV, and $(3;\beta\gamma\delta;m;b)$ are the coefficients in h_3', already given in Appendix XII.

The nonzero $(R;\alpha,\beta\gamma\delta;-;a,b)$ that contribute to the final Hamiltonian are:

$$(z,z\alpha\alpha i,j) = (z,\alpha\alpha zi,j) = (-2\hbar/3)[S;z;-;i3](3;z\alpha\alpha;3;j)$$

$(z,\alpha z\alpha i,j) = -(2\hbar/3)[S;z;-;i3](3;\alpha z\alpha;3;j)$

$(z,z\alpha\alpha 3,3) = -(2\hbar/3)[[S;z;-;13](3;z\alpha\alpha;1;3) + [S;z;-;23](3;z\alpha\alpha;2;3)]$

$(z,\alpha z\alpha 3,3) = -(2\hbar/3)[[S;z;-;13](3;\alpha z\alpha;1;3) + [S;\alpha z\alpha;23](3;\alpha z\alpha;2;3)]$

In the expressions for the $(\alpha,\beta\gamma\delta a,b)$'s above, α = x, y, z

i = 1, 2 and j = 1, 2

(4) <u>Auxiliary coefficients $(S;\alpha\beta,\gamma\delta;-;ab) \equiv (\alpha\beta,\gamma\delta ab)$:</u>

In general,

$$(S;\alpha\beta,\gamma\delta;-;ab) = (2\hbar/3)\sum_m [S;\alpha\beta;m;-](3;\gamma\delta;-;abm)(1+\delta_{am}+\delta_{bm})$$

where $[S;\alpha\beta;m;-]$ are the coefficients of the first contact transformation S, as listed in Table XIII, and $(3;\gamma\delta;-;abm)$ are the coefficients in h_3' , as given in Appendix XIV.

In the following, α = x, y, z ; β = x, y, z ; $\alpha = \beta$ and $\alpha \neq \beta$

$(\alpha\alpha,\beta\beta 11) = (2\hbar/3)[3[S;\alpha\alpha;1;-](3;\beta\beta;-;111)+[S;\alpha\alpha;2;-](3;\beta\beta;-;112)]$

$(\alpha\alpha,\beta\beta 12) = (4\hbar/3)[[S;\alpha\alpha;1;-](3;\beta\beta;-;121)+[S;\alpha\alpha;2;-](3;\beta\beta;-;122)]$

$(\alpha\alpha,\beta\beta 21) = (\alpha\alpha,\beta\beta 12)$

$(\alpha\alpha,\beta\beta 22) = [[S;\alpha\alpha;1;-](3;\beta\beta;-;221)+[S;\alpha\alpha;2;-](3;\beta\beta;-;222)](2\hbar/3)$

In addition to the above, there are:

$(xy,xyjj) = (xy,yxjj) = (yx,xyjj) = (yx,yxjj) =$

$(2\hbar/3)[S;xy;3;-](3;xy;-;jj3)$

$(xy,xy12) = (xy,xy21) = (xy,yx12) = (xy,yx21) = (yx,xy12) =$

$(yx,xy21) = (yx,yx12) = (yx,yx21) =$

$(2\hbar/3)[S;xy;3;-](3;xy;-;123)$

where j = 1, 2, 3

APPENDIX XVII

Coefficients $(4;\alpha\beta\gamma\delta;ab;-)$

The coefficients $(4;\alpha\beta\gamma\delta;ab;-)$ appearing in the third sum of (4.6) have the general form

$$(4;\alpha\beta\gamma\delta;ab;-) = (0;\alpha\beta\gamma\delta;ab;-) + (R;\underline{\alpha},\underline{\beta\gamma\delta};\underline{a},\underline{b};-) +$$
$$(S;\underline{\alpha\beta},\underline{\gamma\delta};ab;-) + (U;\alpha\beta\gamma\delta;\underline{a},\underline{b};-)$$

where $(0;\alpha\beta\gamma\delta;ab;-)$, $(R;\alpha,\beta\gamma\delta;a,b;-)$, etc., are auxiliary coefficients whose detailed expressions will be given later in this appendix. In condensed notations, the nonvanishing $(4;\alpha\beta\gamma\delta;ab;-)$'s that contribute to the final Hamiltonian are listed in List (1), while Lists (2) to (5) give the auxiliary coefficients appearing therein.

(1) Coefficients $(4;\alpha\beta\gamma\delta;ab;-) \equiv (ab\alpha\beta\gamma\delta)$:

In the following, $\alpha = x, y, z$; $\beta = x, y$; $i = j = 1, 2$

$$(ij\alpha\alpha\alpha\alpha) = (ji\alpha\alpha\alpha\alpha) = (0\alpha\alpha\alpha\alpha ij) + (S\alpha\alpha,\alpha\alpha ij) + [\delta_{\alpha z}/(1+\delta_{ij})] \times [(Rz,zzzi,j) + (Rz,zzzj,i)]$$

$$(33\alpha\alpha\alpha\alpha) = (0\alpha\alpha\alpha\alpha 33) + (\delta_{\alpha x} + \delta_{\alpha y})(U\alpha\alpha\alpha\alpha 3,3) + \delta_{\alpha z}(Rz,zzzz3,3)$$

$$(ijxxyy) = (ijyyxx) = (jixxyy) = (jiyyxx) = (0xxyyij) + (1/2) \times [(Sxx,yyij) + (Syy,xxij)] + [(Uxxyyi,j) + (Uxxyyj,i)]/(1+\delta_{ij})$$

$$(33xxyy) = (33yyxx) = (0xxyy33) + (Uxxyy3,3)$$

$$(ij\beta\beta zz) = (ji\beta\beta zz) = (0\beta\beta zzij) + [1/2(1+\delta_{ij})][(Rz,z\beta\beta i,j) + (Rz,z\beta\beta j,i)] + (1/2)[(S\beta\beta,zzij) + (Szz,\beta\beta ij)] + [(U\beta\beta zzi,j) + (U\beta\beta zzj,i)]/(1+\delta_{ij})$$

$$(33\beta\beta zz) = (0\beta\beta zz33) + (1/2)(Rz,z\beta\beta 3,3) + (U\beta\beta zz3,3)$$

$$(33zz\beta\beta) = (0zz\beta\beta 33) + (1/2)(Rz,z\beta\beta 3,3) + (Uzz\beta\beta 3,3)$$

$(ijzz\beta\beta) = (jizz\beta\beta) = (Ozz\beta\beta ij) + [1/2(1+\delta_{ij})][(Rz,z\beta\beta i,j) + (Rz,z\beta\beta j,i)] + (1/2)[(Szz,\beta\beta ij) + (S\beta\beta,zzij)] + [(Uzz\beta\beta i,j) + (Uzz\beta\beta j,i)]/(1+\delta_{ij})$

$(ijxyxy) = (ijxyyx) = (ijyxxy) = (ijyxyx) = (jixyxy) = (jixyyx) = (jiyxxy) = (jiyxyx) = (Oxyxyij) + (Sxy,xyij) + [(Uxyxyi,j) + (Uxyxyj,i)]/(1+\delta_{ij})$

$(33xyxy) = (33xyyx) = (33yxxy) = (33yxyx) = (Oxyxy33) + (Sxy,xy33) + (Uxyxy3,3)$

$(ijz\beta z\beta) = (jiz\beta z\beta) = (oz\beta z\beta ij) + [1/2(1+\delta_{ij})][(Rz,\beta z\beta i,j) + (Rz,\beta z\beta j,i)] + [(Uz\beta z\beta i,j) + (Uz\beta z\beta j,i)]/(1+\delta_{ij})$

$(33z\beta z\beta) = (Oz\beta z\beta 33) + (1/2)(Rz,\ z\ 3,3) + (Uz\ z\ 3,3)$

$(ijz\beta\beta z) = (jiz\beta\beta z) = (1/2(1+\delta_{ij})][(Rz,z\beta\beta i,j) + (Rz,z\beta\beta j,i)] + [(Uz\beta\beta zi,j) + (Uz\beta\beta zj,i)]/(1+\delta_{ij})$

$(33z\beta\beta z) = (1/2)(Rz,z\beta\beta 3,3) + (Uz\beta\beta z3,3)$

$(ij\beta zz\beta) = (ji\beta zz\beta) = [(U\beta zz\beta i,j) + (U\beta zz\beta j,i)]/(1+\delta_{ij})$

$(33\beta zz\beta) = (U\beta zz\beta 3,3)$

(2) <u>Auxiliary coefficients $(0;\alpha\beta\gamma\delta;ab;-) \equiv (\alpha\beta\gamma\delta ab)$:</u>

In general,

$$(0;\alpha\beta\gamma\delta;ab;-) = (2\hbar/3)\sum_m [S;-;abm;-](3;\alpha\beta\gamma\delta;-;m)(1+\delta_{am}+\delta_{bm})$$

where [S;-;abm;-] are the coefficients of the first contact transformation S, listed in Table XV, and $(3;\alpha\beta\gamma\delta;-;m)$ the coefficients in h_3', listed in Appendix XI.

Listed herein are only those $(0;\alpha\beta\gamma\delta;ab;-)$'s that contribute to the final Hamiltonian. They can be obtained from the general formula above, with m running from 1 to 2 only.

In the following list, α & β = x,y,z $\alpha\neq\beta$; γ = x,y ; i&j = 1,2

$(\alpha\alpha\alpha\alpha ij) = (\alpha\alpha\alpha\alpha ji)$, $(\alpha\alpha\alpha\alpha 33)$, $(z\gamma z\gamma ij) = (z\gamma z\gamma ji)$, $(z\gamma z\gamma 33)$,

$(\alpha\alpha\beta\beta\, ij) = (\alpha\alpha\beta\beta ji) = (\beta\beta\alpha\alpha ij) = (\beta\beta\alpha\alpha ji)$, $(\beta\beta\alpha\alpha 33) = (\beta\beta\alpha\alpha 33)$,

$(xyxyij) = (xyyxij) = (yxxyij) = (yxyxij) = (xyxyji) = (xyyxji) =$

$(yxxyji) = (yxyxji)$, $(xyxy33) = (xyyx33) = (yxxy33) = (yxyx33)$

(3) Auxiliary coefficients $(R;\alpha,\beta\gamma\delta;a,b;-) \equiv (\alpha,\beta\gamma\delta a,b)$:

In general,

$$(R;\alpha,\beta\gamma\delta;a,b;-) = (2\hbar/3)\sum_m [S;\alpha;am;-](3;\beta\gamma\delta;b;m)$$

where $[S;\alpha;am;-]$ are the coefficients of the first contact transformation S, listed in Table XV, and $(3;\alpha\beta\gamma\delta;b;m)$ the coefficients in h_3, listed in Appendix XII. Of the possible combinations of the vibrational operators' indices, a and b, only the following ones yield contributing auxiliary coefficients $(\alpha,\beta\gamma\delta a,b)$:

A. $b \equiv j = 1, 2$; $a \equiv i = 1, 2$, for which the general formula above reduces to

$$(R;\alpha,\beta\gamma\delta;i,j;-) = (2\hbar/3)[S;\alpha;i3;-](3;\beta\gamma\delta;j;3)$$

B. $a = b = 3$, for which the above formula reduces to

$$(R;\alpha,\beta\gamma\delta;3,3;-) = (2\hbar/3)[[S;\alpha;13;-](3;\beta\gamma\delta;3;1)+ [S;\alpha;23;-] \times (3\beta\gamma\delta;3;2)]$$

For these two cases, Table XIV and Appendix XII yield:

$(z,z\alpha\alpha i,j) = (z,\alpha\alpha zi,j)$, $(z,z\alpha\alpha 3,3) = (z,\alpha\alpha z3,3)$,

$(z,\alpha z\alpha i,j)$, $(z,\alpha z\alpha 3,3)$,

where $\alpha = x, y, z$; i & $j = 1, 2$

(4) Auxiliary coefficients $(S;\alpha\beta,\gamma\delta;ab;-) \equiv (\alpha\beta,\gamma\delta ab)$:

In general,

$$(S;\alpha\beta,\gamma\delta;ab;-) = (2\hbar/3)\sum_m [S;\alpha\beta;m;-](3;\gamma\delta;ab;m)$$

where $[S;\alpha\beta;m;-]$ are the coefficients of the first contact

transformation, listed in Table XIII, and $(3;\gamma\delta;ab;m)$ the coefficients in h_3', listed in Appendix XIII. Of the nonvanishing $(S;\alpha\beta,\gamma\delta;ab;-)$'s, only the following ones contribute to the final Hamiltonian:

A. $(S;\alpha\alpha,\beta\beta;ij;-) = (S;\alpha\alpha,\beta\beta;ji;-) = (2h/3)[[S;\alpha\alpha;1;-](3;\beta\beta;ij;1) + [S;\alpha\alpha;2;-](3;\beta\beta;ij;2)]$

$(S;\alpha\alpha,\beta\beta;33;-) = (2\hbar/3)[[S;\alpha\alpha;1;-](3;\beta\beta;3;1) + [S;\alpha\alpha;2;-] \times (3;\beta\beta;33;2)]$; $\alpha\,\&\,\beta = x,y,z$; $i\,\&\,j = 1,2$

B. $(S;xy,xy;ij;-)=(S;xy,yx;ij;-)=(S;yx,xy;ij;-)=(S;yx,yx;ij;-) = (S;xy,xy;ji;-)=(S;xy,yx;ji;-)=(S;yx,xy;ji;-) = (S;yx,yx;ji;-)= (2\hbar/3)[S;xy;3;-](3;xy;ij;3)$

$(S;xy,xy;33;-)=(S;xy,yx;33;-)=(S;yx,xy;33;-)=(S;yx;yx;33;-) = (2\hbar/3)[S;xy;3;-](3;xy;33;3)$; $i\,\&\,j = 1,2$

(5) Auxiliary coefficients $(U;\alpha\beta\gamma\delta;a,b;-) \equiv (\alpha\beta\gamma\delta a,b)$:

In terms of the coefficients $[S;\alpha\beta;a;-]$ in Table XIII and the coefficients $(2';\alpha\beta\gamma;b;-)$ to be given at the end of this appendix, the nonzero contributing $(U;\alpha\beta\gamma\delta;a,b;-)$'s are listed below. In this list symbols and separating semicolons are omitted from the corresponding coefficients, i. e., $[S;\alpha\beta;a;-]$ and $(2';\alpha\beta\gamma;b;-)$ are written in the condensed notations $(\alpha\beta a)$ and $(\alpha\beta\gamma b)$, respectively.

$(xxxx3,3) = 2\hbar(xy3)[2(zxx3) + (xzx3)]$

$(yyyy3,3) = -2\hbar(xy3)[2(zyy3) + (yzy3)]$

$(xxyy3,3) = (yyxx3,3) = -\hbar(xy3)[(xxz3) - (yyz3)]$

$(xxyyi,j) = (yyxxi,j) = \hbar(yyi)[(zxyj) + (xzyj)] - \hbar(xxi)[(xyzj) + (xzyj)]$

$(xxzz3,3) = (zzxx3,3) = \hbar(xy3)[(xzx3) + (zxx3) - (zzz3)]$

$(xxzzi,j) = (zzxxi,j) = \hbar(xxi)[(xzyj) + (xyzj)] -$

$\hbar(zzi)[(yxzj) + (xyzj)]$

$(yyzz3,3) = (zzyy3,3) = \hbar(xy3)[(yyz3) + (yzy3) - (zzz3)]$

$(yyzzi,j) = (zzyyi,j) = \hbar(zzi)[(xyzj) + (yxzj)] -$

$\hbar(yyi)[(yxzj) + (yzxj)]$

$(xyxy3,3) = (yxyx3,3) = \hbar(xy3)[(yzy3) - (xzx3)]$

$(xyxyi,j) = (yxyxi,j) = 2\hbar[(yyi)(xyzj) - (xxi)(zxyj)]$

$(zxzx3,3) = (xzxz3,3) = \hbar(xy3)[(zzz3) - 2(zxx3)]$

$(zxzxi,j) = (xzxzi,j) = 2\hbar[(xxi)(zxyj) - (zzi)(xzyj)]$

$(zyzy3,3) = (yzyz3,3) = \hbar(xy3)[2(zyy3) - (zzz3)]$

$(zyzyi,j) = (yzyzi,j) = 2\hbar[(zzi)(xzyj) - (yyi)(xyzj)]$

$(yxxy3,3) = -2\hbar(xy3)(zxx3)$

$(yxxyi,j) = 2\hbar(yyi)[(xzyj) + (zxyj)]$

$(xyyx3,3) = 2\hbar(xy3)(zyy3)$

$(xyyxi,j) = -\hbar(xxi)[(xzyj) + (xyzj)]$

$(xzzx3,3) = 2(xxzz3,3)$

$(xzzxi,j) = 2\hbar(xxi)[(xyzj) + (zyxj)]$

$(yzzy3,3) = 2\hbar(xy3)[(zyy3) + (yzy3) - (zzz3)]$

$(yzzyi,j) = 2(yyzz3,3)$

$(zxxzi,j) = -2\hbar(zzi)[(xyzj) + (zxyj)]$

$(z{-}yzi,j) = 2\hbar(zzi)[(xyzj) + (zxyj)]$

In the above list i & j = 1, 2 ; not every one of the coefficients is independent of the others.

The coefficients $(2';\alpha\beta\gamma;b;-)$ appearing in the preceding list are closely related to the coefficients $(2;\alpha\beta\gamma;b;-)$ in Appendix IV. They are as follows:

$$(2';zzz;3;-) = (2/3)(2;zzz;3;-)$$

$$(2';zxx;3;-) = (2';xxz;3;-) = (2/3)(2;zxx;3;-)$$

$$(2';zyy;3;-) = (2';yyz;3;-) = (2/3)(2;zyy;3;-)$$

$$(2';xzx;3;-) = (1/2)(2;xzx;3;-)$$

$$(2';yzy;3;-) = (1/2)(2;yzy;3;-)$$

$$(2';xzy;j;-) = (2';yzx;j;-) = (1/2)(2;xzy;j;-);\ j = 1,\ 2$$

$$(2';xyz;j;-) = (2';zyx;j;-) = (2/3)(2;xyz;j;-) - [a_j^{zz}(I_x-I_y) - a_j^{xx}I_z]/24I_xI_yI_z{}^2\lambda_j{}^{3/4}\hbar^{3/2}\ ;\ j = 1,\ 2$$

$$(2';yxz;j;-) = (2';zxy;j;-) = (2/3)(2;yxz;j;-) - [a_j^{zz}(I_x-I_y) + a_j^{yy}I_z]/24I_xI_yI_z{}^2\lambda_j{}^{3/4}\hbar^{3/2}\ ;\ j = 1,\ 2$$

APPENDIX XVIII

Coefficients $(4!\alpha\beta\gamma,\delta\varepsilon\rho!-!-)$ in $h_4^{@}$

The coefficients $(4!\alpha\beta\gamma,\delta\varepsilon\rho!-!-)$ in the second term of the first equation in (5.7) can be written in general as

$$(4!\alpha\beta\gamma,\delta\varepsilon\rho!-!-) = (-\hbar/2)\sum_m [\sigma;\alpha\beta\gamma;-;m](2;\delta\varepsilon\rho;m;-)$$

where $[\sigma;\alpha\beta\gamma;-;m]$ are the coefficients of the second contact transformation σ, listed in Table XVIII, and $(2;\delta\varepsilon\rho;m;-)$ the coefficients in $h_2^!$, listed in Appendix IV. The nonzero $(4!\alpha\beta\gamma,\delta\varepsilon\rho!-!-)$'s all contribute to the final Hamiltonian; they are listed below in the condensed notation $(\alpha\beta\gamma*\delta\varepsilon\rho)$ adopted in Chapter 5. Use has been made of Table XVIII to express $[\sigma;\alpha\beta\gamma;-;m]$ in terms of $(2;\alpha\beta\gamma;m;-)$.

A. In the following, α & β = x, y ; $\alpha \neq \beta$

$$(zzz*zzz) = (-\hbar/2\lambda_3^{1/2})(2;zzz;3;-)^2$$

$$(zzz*\alpha\alpha z) = (zzz*z\alpha\alpha) = (\alpha\alpha z*zzz) = (z\alpha\alpha*zzz) = (-\hbar/2\lambda_3^{1/2})(2;zzz;3;-)(2;z\alpha\alpha;3;-)$$

$$(zzz*\alpha z\alpha) = (\alpha z\alpha*zzz) = (-\hbar/2\lambda_3^{1/2})(2;zzz;3;-)(2;\alpha z\alpha;3;-)$$

$$(\alpha\alpha z*\alpha\alpha z) = (\alpha\alpha z*z\alpha\alpha) = (z\alpha\alpha*\alpha\alpha z) = (z\alpha\alpha*z\alpha\alpha) = (-\hbar/2\lambda_3^{1/2})(2;z\alpha\alpha;3;-)^2$$

$$(\alpha\alpha z*\beta\beta z) = (\alpha\alpha z*z\beta\beta) = (z\alpha\alpha*\beta\beta z) = (z\alpha\alpha*z\beta\beta) = (\beta\beta z*\alpha\alpha z) = (\beta\beta z*z\alpha\alpha) = (z\beta\beta*\alpha\alpha z) = (z\beta\beta*z\alpha\alpha) = (-\hbar/2\lambda_3^{1/2})(2;z\alpha\alpha;3;-)(2;z\beta\beta;3;-)$$

$$(\alpha\alpha z*\alpha z\alpha) = (z\alpha\alpha*\alpha z\alpha) = (\alpha z\alpha*\alpha\alpha z) = (\alpha z\alpha*z\alpha\alpha) = (-\hbar/2\lambda_3^{1/2})(2;z\alpha\alpha;3;-)(2;\alpha z\alpha;3;-)$$

$$(\alpha\alpha z*\beta z\beta) = (z\alpha\alpha*\beta z\beta) = (\beta z\beta*\alpha\alpha z) = (\beta z\beta*z\alpha\alpha) = (-\hbar/2\lambda_3^{1/2})(2;z\alpha\alpha;3;-)(2;\beta z\beta;3;-)$$

$$(\alpha z\alpha^*\alpha z\alpha) = (-\hbar/2\lambda_3^{1/2})(2;\alpha z\alpha;3;-)^2$$

$$(\alpha z\alpha^*\beta z\beta) = (\beta z\beta^*\alpha z\alpha) = (-\hbar/2\lambda_3^{1/2})(2;\alpha z\alpha;3;-)(2;\beta z\beta;3;-)$$

B. $(xyz^*xyz) = (xyz^*zyx) = (zyx^*xyz) = (zyx^*zyx) = (-\hbar/2)\ X$
$[(2;xyz;1;-)^2/\lambda_1^{1/2} + (2;xyz;2;-)^2/\lambda_2^{1/2}]$

$(xzy^*xzy) = (xzy^*yzx) = (yzx^*xzy) = (yzx^*yzx) = (-\hbar/2)\ X$
$[(2;xzy;1;-)^2/\lambda_1^{1/2} + (2;xzy;2;-)^2/\lambda_2^{1/2}]$

$(zxy^*zxy) = (zxy^*yxz) = (yxz^*zxy) = (yxz^*yxz) = (-\hbar/2)X$
$[(2;zxy;1;-)^2/\lambda_1^{1/2} + (2;zxy;2;-)^2/\lambda_2^{1/2}]$

$(xyz^*xzy) = (xyz^*yzx) = (zyx^*xzy) = (zyx^*yzx) = (xzy^*xyz) =$
$(xzy^*zyx) = (yzx^*xyz) = (yzx^*zyx) = (-\hbar/2)\ X$
$[(2;xyz;1;-)(2;xzy;1;-)/\lambda_1^{1/2} + (2;xyz;2;-)\ X$
$(2;xzy;2;-)/\lambda_2^{1/2}]$

$(xyz^*zxy) = (xyz^*yxz) = (zyx^*zxy) = (zyx^*yxz) = (zxy^*xyz) =$
$(zxy^*zyx) = (yxz^*xyz) = (yxz^*zyx) = (-\hbar/2)\ X$
$[(2;xyz;1;-)(2;zxy;1;-)/\lambda_1^{1/2} + (2;xyz;2;-)\ X$
$(2;zxy;2;-)/\lambda_2^{1/2}]$

$(xzy^*zxy) = (xzy^*yxz) = (yzx^*zxy) = (yzx^*yxz) = (zxy^*xzy) =$
$(zxy^*yzx) = (yxz^*xzy) = (yxz^*yzx) = (-\hbar/2)\ X$
$[(2;xzy;1;-)(2;zxy;1;-)/\lambda_1^{1/2} + (2;xzy;2;-)\ X$
$(2;zxy;2;-)/\lambda_2^{1/2}]$

APPENDIX XIX

Coefficients $(4!\alpha\beta\gamma,\delta!-!ab)$ in $h_4^{@}$

The coefficients $(4!\alpha\beta\gamma,\delta!-!ab)$ appearing in the second term of the second equation in (5.7) are of the following general form:

$$(4!\alpha\beta\gamma,\delta!-!ab) = (-\hbar/2)\sum_m [\sigma;\alpha\beta\gamma;-;m](2;\delta;m;ab)$$

where $[\sigma;\alpha\beta\gamma;-;m]$ are the coefficients of the second contact transformation, and $(2;\delta;m;ab)$ the coefficients in $h_2^{\frac{1}{2}}$: they are listed in Table XVIII and Appendix VIII, respectively. It was mentioned in Appendix XVI, that , of the coefficients listed therein, only those with equal indices of vibrational operator, a = b, actually contribute to the final Hamiltonian. This holds true also of the coefficients listed in Appendix XVII, which is why the condition i = j was imposed in the beginning of the listing. As a matter of fact, this condition of vibrational diagonality covers all quartic coefficients in the fourth-order, twice transformed Hamiltonian $h_4^{@}$. Therefore, the coefficients with $a \neq b$ will not be included in the list below. Again, the condensed notation adopted in Chapter 5 will be used here.

$$(zzz{*}zjj) = (-\hbar/2)[\sigma;zzz;-;3](2;z;3;jj)$$

$$(z\alpha\alpha{*}zjj) = (\alpha\alpha z{*}zjj) = (-\hbar/2)[\sigma;z\alpha\alpha;-;3](2;z;3;jj)$$

$$(\alpha z\alpha{*}zjj) = (-\hbar/2)[\sigma;\alpha z\alpha;-;3](2;z;3;jj)$$

In all the coefficients listed above, j = 1, 2 and α = x, y

APPENDIX XX

Coefficients $(4!\alpha\beta,\gamma\delta!-!ab)$ in $h_4^{@}$

The coefficients $(4!\alpha\beta,\gamma\delta!-!ab)$ appearing in the third term of the second equation in (5.7) has the following general form:

$$(4!\alpha\beta,\gamma\delta!-!ab) = (\hbar/2)\sum_m [\sigma;\alpha\beta;m;a](2;\gamma\delta;mb;-)(1+\delta_{bm})$$

where $[\sigma;\alpha\beta;a;m]$ are the coefficients of the second contact transformation, and $(2;\gamma\delta;mb;-)$ the coefficients in $h_2^{\prime}$; they are given in Table XIX and Appendix V, respectively. Of the nonvanishing coefficients $(4!\alpha\beta,\gamma\delta!-!ab)$, only those that really contribute to the final Hamiltonian are given in the following list:

$$(\alpha\alpha*\beta\beta 11) = (\hbar/2)[2[\sigma;\alpha\alpha;1;1](2;\beta\beta;-;11) + [\sigma;\alpha\alpha;2;1](2;\beta\beta;-;12)]$$

$$(\alpha\alpha*\beta\beta 22) = (\hbar/2)[[\sigma;\alpha\alpha;1;2](2;\beta\beta;-;12) + 2[\sigma;\alpha\alpha;2;2](2;\beta\beta;-;22)]$$

$$(\alpha\alpha*\beta\beta 33) = \hbar[\sigma;\alpha\alpha;3;3](2;\beta\beta;-;33)$$

$$(xy*xyjj) = (xy*yxjj) = (yx*xyjj) = (yx*yxjj) = (\hbar/2)[\sigma;xy;3;j](2;xy;-;3j)$$

$$(xy*xy33) = (xy*yx33) = (yx*xy33) = (yx*yx33) = (\hbar/2)[[\sigma;xy;1;3](2;xy;-;13) + [\sigma;xy;2;3](2;xy;-;23)]$$

APPENDIX XXI

Coefficients $(4!\alpha,\beta\gamma\delta!-!ab)$ in $h_4^{@}$

The coefficients $(4!\alpha,\beta\gamma\delta!-!ab)$ in the fourth term of the second equation in (5.7) can be expressed in general as:

$$(4!\alpha,\beta\gamma\delta!-!ab) = (-\hbar/2)\,{}^{*}\!\sum_{m}[\sigma;\alpha;-;mab](2;\beta\gamma\delta;m;-)(1+\delta_{am}+\delta_{bm})$$

where $[\sigma;\alpha;-;mab]$ are the coefficients of the second contact transformation, and $(2;\beta\gamma\delta;m;-)$ the coefficients in h_2'; they are listed in Table XXI and Appendix IV, respectively. The symbol ${}^{*}\!\sum_{m}$ denotes the summation over m and over all permutations of (mab), subject to the restriction: left index $\leqslant$ middle index $\leqslant$ right index.

Listed below are the coefficients $(4!\alpha,\beta\gamma\delta!-!ab)$, written in the condensed notation $(\alpha{*}\beta\gamma\delta ab)$ introduced in Chapter 5, that actually contribute to the final Hamiltonian.

$$
\begin{aligned}
(z{*}zzzjj) &= (-\hbar/2)[\sigma;z;-;jj3](2;zzz;3;-)(1+2\delta_{j3}) \\
(z{*}\alpha\alpha zjj) &= (z{*}z\alpha\alpha jj) \\
&= (-\hbar/2)[\sigma;z;-;jj3](2;\alpha\alpha z;3;-)(1+2\delta_{j3}) \\
(z{*}\alpha z\alpha jj) &= (-\hbar/2)[\sigma;z;-;jj3](2;\alpha z\alpha;3;-)(1+2\delta_{j3})
\end{aligned}
$$

In the coefficients listed above, α = x, y and j = 1, 2

APPENDIX XXIII

Coefficients $(4!\alpha\beta,\gamma\delta!ab!-)$ in $h_4^{@}$

The coefficients $(4!\alpha\beta,\gamma\delta!ab!-)$ appearing in the third term of the third equation in (5.7) are of the following general form:

$$(4!\alpha\beta,\gamma\delta!ab!-) = (-\hbar/2)\sum_{m} [\sigma;\alpha\beta;a;m](2;\gamma\delta;mb;-)(1+\delta_{bm})$$

where $[\sigma;\alpha\beta;a;m]$ are the coefficients of the second contact transformation, and $(2;\gamma\delta;mb;-)$ the coefficients in h_2'; they are given in Table XIX and Appendix V, respectively. Of the nonzero $(4!\alpha\beta,\gamma\delta!ab!-)$ coefficients, only those that actually contribute to the final Hamiltonian are included in the following list. The condensed notation $(ab\alpha\beta*\gamma\delta)$ of Chapter 5 is used here.

$$(11\alpha\alpha*\beta\beta) = (-\hbar/2)[2[\sigma;\alpha\alpha;1;1](2;\beta\beta;11;-) + [\sigma;\alpha\alpha;1;2](2;\beta\beta;12;-)]$$

$$(22\alpha\alpha*\beta\beta) = (-\hbar/2)[[\sigma;\alpha\alpha;2;1](2;\beta\beta;12;-) + 2[\sigma;\alpha\alpha;2;2](2;\beta\beta;22;-)]$$

$$(33\alpha\alpha*\beta\beta) = -\hbar[\sigma;\alpha\alpha;3;3](2;\beta\beta;33;-)$$

$$\begin{aligned}(jjxy*xy) &= (jjxy*yx) = (jjyx*xy) = (jjyx*yx)\\ &= (-\hbar/2)[[\sigma;xy;3;1](2;xy;13;-) + [\sigma;xy;3;2](2;xy;23;-)]\end{aligned}$$

In the coefficients listed above, α & β = x, y, z , j = 1, 2

APPENDIX XXIV

Coefficients $(4!\alpha,\beta\gamma\delta!ab{-}{-})$ in $h_4^{@}$

The coefficients $(4!\alpha,\beta\gamma\delta!ab!-)$ in the fourth term of the third equation in (5.7) can be written in general as follows:

$$(4!\alpha,\beta\gamma\delta!ab!-) = (-\hbar/2)\sum_m [\sigma;\alpha;ab;m](2;\beta\gamma\delta;m;-)$$

where $[\sigma;\alpha;ab;m]$ are the coefficients of the second contact transformation, and $(2;\beta\gamma\delta;m;-)$ the coefficients in h_2'; they are listed in Table XX and Appendix IV, respectively. Here are the nonzero, contributing $(4!\alpha,\beta\gamma\delta!ab!-)$'s, written in the condensed notation $(ab\alpha*\beta\gamma\delta)$ adopted in Chapter 5:

$$(jjz*zzz) = (-\hbar/2)[\ ;z;jj;3](2;zzz;3;-)$$

$$(jjz*\alpha z\alpha) = (-\hbar/2)[\ ;z;jj;3](2;\alpha z\alpha;3;-)$$

$$(jjz*\alpha\alpha z) = (jjz*z\alpha\alpha) = (-\hbar/2)[\sigma;z;jj;3](2;\alpha\alpha z;3;-)$$

In the coefficients listed above, $\alpha = x, y$ and $j = 1, 2, 3$

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