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Degeneracies of Vibration-Rotation Levels in Certain Octahedral Molecules

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by

C. D. Cantrell

DEGENERACIES OF VIBRATION-ROTATION LEVELS IN CERTAIN OCTAHEDRAL MOLECULES

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ABSTRACT

The degeneracies of the vibration-rotation levels of octahedral AB_6 molecules are calculated for the case in which the B nuclei are identical fermions of spin 1/2.

I. INTRODUCTION

The intensity of an absorption line in a molecular spectrum is proportional to the product of an absorption cross section, the Boltzmann factor $\exp(-E/kT)$, and the degeneracy of the lower molecular energy level. The statistical weight of a molecular level is also proportional to the product of $\exp(-E/kT)$ and the degeneracy. In this report, the degeneracy will be calculated for the class of molecules which have the composition AB_6, where the six B atoms are arranged at the vertices of an octahedron, with A at the center. It is assumed that the B nuclei are identical, and have spin 1/2. There are no restrictions on the spin of the A nucleus.

The degeneracies calculated here are expected to be useful in two ways.

(a) In identifying experimentally observed molecular transitions by comparing the observed and calculated relative intensities.

(b) In calculating an improved molecular partition function.

In the Born-Oppenheimer approximation, the molecular wave function is written as a product of functions depending separately on electronic, vibrational, rotational, and nuclear-spin coordinates

$$\psi = \psi_E \psi_V \psi_R \psi_S \quad . \tag{1}$$

One might suppose that for a spherical-top molecule the degeneracy of a given level would be

$$W = W_E W_V \, (2J + 1)^2 \, (2S_B + 1) \, (2S_A + 1) \quad , \tag{2}$$

where W_E and W_V are the electronic and vibrational degeneracies, J is the rotational angular momentum of the molecule, S_B is the total nuclear spin of the B nuclei, and S_A is the spin of the A nucleus. Since the interaction between the nuclear spins and the rest of the world is weak, one might suppose that the factor $(2S_B + 1)(2S_A + 1)$ would be the same for all levels, and could be dropped from Eq. (2) for the purpose of calculating relative degeneracies.

However, the Pauli exclusion principle requires that the total molecular wave function be antisymmetric (change sign) when the labels on any pair of identical nuclei are interchanged. The separate functions ψ_E, ψ_V, ψ_R, are all functions of the space coordinates of the B nuclei. Thus interchanging the labels on two identical nuclei will, in general, change ψ_E, ψ_V, and ψ_R into different functions of the electronic, vibrational, and rotational coordinates, respectively. The same interchange will, in general, convert ψ_S into a different function of the nuclear spin coordinates (i.e., of the Z-components of the nuclear spins).

The requirement that the total wave function be antisymmetric under interchange of the labels on any pair of identical nuclei implies two changes in our ideas of the molecular wave function.

(a) The wave function is a sum (linear combination) of products such as Eq. (1), with coefficients chosen so that the total wave function satisfies the Pauli principle.

(b) The degeneracy of each energy level is not given by Eq. (2). Instead, the degeneracy is equal to the number of different linear combinations referred to in (a) (corresponding to one particular energy level of the molecule).

The energy levels will be assumed here to be completely determined by the rotational quantum number J and the type of the irreducible representation of the molecular point group to which the vibronic (vibrational and electronic) wave function belongs. For a spherical top the rotational energy is (in first approximation) independent of K and M. However, there are additional (Coriolis) terms in the rotational Hamiltonian which couple the rotational angular momentum J with either the angular momentum of a degenerate vibrational state, or the electronic angular momentum, or both. This coupling leads to further splitting of the vibration-rotation energy levels, and hence a partial lifting of the degeneracy calculated here. However, this calculation is still useful, because

(a) The first-order Coriolis splitting does not affect the Q-branch transition frequencies for transitions from the ground state.[1] Hence the theoretical Q-branch line intensities are proportional to the degeneracies in Table I. (There are other proportionality constants which depend on J, arising from the rotational matrix elements.)[2]

(b) The results obtained here include the case in which the second-order Coriolis splitting (which can affect the Q-branch frequencies) is significant. This will be shown in detail in another report.

For convenience, the degeneracies (the final result of the calculation) are shown in Table I. The angular momentum is written modulo 12; that is, J = 12 p + k, where p is 0 or any positive integer, and k = 0, 1, 2, ..., 11. This is simply a compact way of presenting the results of any value of J. A numerical table presenting the same information for a useful range of J values would be much more lengthy.

II. THE OCTAHEDRAL GROUP[3]

The rotational symmetry operations of a regular octahedron are depicted in Fig. 1. There are five classes, hence five irreducible representations, the characters of which are given in Table III. Each symmetry operation corresponds to a permutation of the nuclear labels. The correlation between rotations and nuclear-label permutations is given in Table II, which may be verified by inspecting Fig. 1.

Since each of the six B nuclei has spin 1/2, hence, two possible eigenvalues of S_Z, there are $2^6 = 64$ different spin vectors of the form $| m_1 m_2 --- m_{\bar{3}} >$. The symmetry operations, which induce permutations of the nuclear labels, also induce permutations of the vectors $| m_1 m_2 --- m_{\bar{3}} >$. For example $(1 2 \bar{1} \bar{2}) (3) (\bar{3})$ transforms $| m_1 m_2 m_3 m_{\bar{1}} m_{\bar{2}} m_{\bar{3}} >$ into $| m_2 m_{\bar{1}} m_3 m_{\bar{2}} m_1 m_{\bar{3}} >$. Thus each symmetry operation corresponds to a 64 x 64 permutation matrix acting on the vectors $| m_1 --- m_{\bar{3}} >$. The set of matrices defined in this way is a reducible representation Γ_S of the group O. Whenever a vector $| m_1 --- m_{\bar{3}} >$

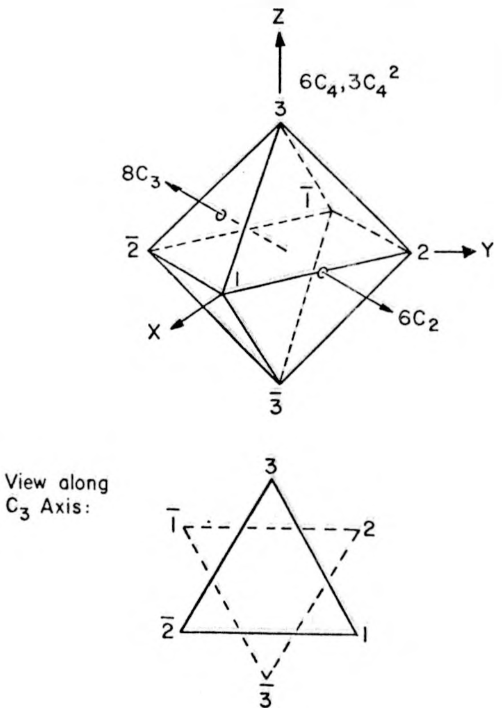

Fig. 1. Symmetries of a regular octahedron.

is left unchanged by a permutation P, there is a 1 on the main diagonal of the permutation matrix $\Gamma_S(P)$. Thus the character of $\Gamma_S(P)$ is equal to the number of vectors $| m_1 \text{ --- } m_{\bar{3}} >$ which are left unchanged by P. This number is equal to $2^{C(P)}$, where C(P) is the number of cycles in P. The spin characters χ_S are given in Table IV.

The character table for O, together with the group-theoretical orthogonality relations, enables one to express the spin representation Γ_S as a sum of irreducible representations of O (Table IV).

The Pauli exclusion principle requires that the total molecular wave function be unchanged by a permutation P which consists of an even number of interchanges of pairs of nuclear labels, and change sign under an odd number. Table II shows that the only rotations which induce permutations with an odd number of pair interchanges are $6C_2$ and $6C_4$, since a cyclic permutation of n objects (e.g., $(12\bar{1}\bar{2})$) can be expressed as a product of n-1 pair interchanges (e.g., $(1\bar{2})$ $(1\bar{1})$ (12)). Therefore the total molecular wave function must belong to a representation of O (under the operations of nuclear-label permutations) which is one-dimensional; is -1 on $6C_2$ and $6C_4$; and is +1 on all other elements of the group. There is one such representation, A_2 (Table III).

We can now state the algorithm for calculating the rotational degeneracies.[4] If the spin, rotational, and vibrational wave functions belong to the (reducible) representations Γ_S, Γ_R, and Γ_V of O, then the total wave function must be one of the linear combinations of the functions transforming according to $\Gamma_S \times \Gamma_R \times \Gamma_V$ which belongs to the representation A_2. The number of such linear combinations - in other words, the number of times the representation A_2 occurs in the reduction of $\Gamma_S \times \Gamma_R \times \Gamma_V$ is the rotational degeneracy, taking the Pauli principle into account, but barring Coriolis interactions. Coriolis interactions will cause some of the levels (corresponding to irreducible representations of O) which belong to $\Gamma_R \times \Gamma_V$ to be separated (split) in energy. This will be discussed in detail in another report.

It would be reasonable to ask at this point why it is possible to calculate the degeneracies using only the group O, instead of O_h. The group O_h is the full octahedral symmetry group, including the inversion; O is the subgroup of O_h which consists of proper rotations. O_h is the direct product of O with ι, the group consisting of the identity E and the inversion I. Consequently the representations of O_h are the direct product of the representations of O and ι. The two representations of ι are both one-dimensional; one is the identity representation (1 for both E and I), and the other is +1 for E and -1 for I. It is conventional to call the former the g (gerade) representation and the latter the u (ungerade) representation. The g and u representations correspond to even and odd parity under inversion, respectively.

The representations $\Gamma_{j,p}$ of O_h therefore carry two labels: one (j) indicating a representation of O, the other (p) indicating g or u. The direct product of three such representations will be

$$
\begin{aligned}
&\Gamma_{j_1,p_1} \times \Gamma_{j_2,p_2} \times \Gamma_{j_3 p_3} \\
&= (\Gamma_{j_1} \times \Gamma_{j_2} \times \Gamma_{j_3}) \times \Gamma_{p_1} \times \Gamma_{p_2} \times \Gamma_{p_3} \qquad (3) \\
&= (\Gamma_{j_1} \times \Gamma_{j_2} \times \Gamma_{j_3}) \times (g \text{ or } u) \quad ,
\end{aligned}
$$

where the last line indicates that the direct product of three irreducible representations of ι simply g or u, which are one-dimensional. The weight of a given irreducible representation of O_h in Eq. (3) is equal to the weight of the corresponding representation of O in the reduction of $\Gamma_{j_1} \times \Gamma_{j_2} \times \Gamma_{j_3}$. Nothing except additional labor would be gained by calculating the degeneracies using O_h instead of O.

III. CHARACTERS OF THE ROTATIONAL WAVE FUNCTIONS

The rotational wave function ψ_{JKM} for the symmetric top is essentially the Wigner D-matrix (rotation matrix) $D^{(J)}_{MK}$ (Ω) where Ω stands for the three Euler angles.[5] The $D^{(J)}$ matrices are the matrices which describe the transformation of wave functions of angular momentum J under the rotation with Euler angles Ω. Under a rotation about the molecular Z-axis through an angle ϕ

$$D^{(J)}_{MK}(\Omega) \rightarrow e^{ik\phi} D^{(J)}_{MK}(\Omega)$$

and

$$\psi_{JKM} \to e^{ik\phi} \psi_{JKM} .$$

Since the trace (character) of a matrix is invariant under a similarity transformation, the character of a matrix describing the transformation of the symmetric-top functions ψ_{JKM} among themselves (for a given J) under rotation through an angle ϕ is

$$\sum_{K,M} e^{iK\phi} = (2J + 1) \frac{\sin (J + 1/2) \phi}{\sin 1/2 \phi} . \quad (4)$$

Since the trigonometric functions in Eq. (4) are periodic in J with period $2\pi/\phi$, and since $\phi = \pi$, $2\pi/3$, and $\pi/2$ all occur in O, the set of rotational characters [Eq. (4)] for all C_ϕ in O is periodic in J with a period equal to the least common multiple of 2, 3, and 4 - i.e., 12. Thus it is convenient to express J modulo 12, as $J = 12p + k$ (where p and k are integers, $p \geq 0$ and $0 \leq k \leq 11$). The characters [Eq. (4)] are presented in Table V in a form convenient for calculation. The reduction of the rotational representations corresponding to angular momentum J into irreducible representations of the group O are given in Table VI.

IV. CALCULATION OF THE ROTATIONAL DEGENERACIES

The number of times a given irreducible representation of O occurs in the reduction of $\Gamma_V \times \Gamma_R \times \Gamma_S$ can now be calculated (for each Γ_V) from the known Γ_S (Table IV) and Γ_R (Table VI), using the multiplication table for irreducible representations of O (Table VII). The latter table can be calculated quickly from the character table of O (Table III). The rotational degeneracy is equal to the weight of A_2 in the reduction of $\Gamma_V \times \Gamma_R \times \Gamma_S$; this is given in Tables VIII through XII and is summarized in Table I.

V. ACKNOWLEDGMENTS

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TABLE I

ROTATIONAL DEGENERACIES FOR AB_6 MOLECULES, WHERE SPIN (B) = 1/2

$\psi_E\psi_V$	A_1	A_2	E	F_1	F_2
J = 12p	64p + 2	64p + 10	128p + 8	192p + 6	192p + 6
J = 12p + 1	64p + 6	64P + 6	128p + 12	192p + 22	192p + 36
J = 12p + 2	64p + 14	64p + 14	128p + 32	192p + 42	192p + 34
J = 12p + 3	64p + 22	64p + 14	128p + 32	192p + 58	192p + 58
J = 12p + 4	64p + 22	64p + 30	128p + 52	192p + 70	192p + 70
J = 12p + 5	64p + 26	64p + 26	128p + 56	192p + 86	192p + 94
J = 12p + 6	64p + 38	64p + 38	128p + 72	192p + 96	192p + 68
J = 12p + 7	64p + 42	64p + 34	128p + 76	192p + 122	192p + 122
J = 12p + 8	64p + 42	64p + 50	128p + 96	192p + 134	192p + 134
J = 12p + 9	64p + 50	64p + 50	128p + 96	192p + 150	192p + 158
J = 12p + 10	64p + 58	64p + 58	128p + 116	192p + 170	192p + 162
J = 12p + 11	64p + 62	64p + 54	128p + 120	192p + 186	192p + 186

NOTES:
1. The integer p = 0, 1, 2, ...
2. Multiply all weights by (2J + 1).

TABLE II

CORRELATION BETWEEN ROTATIONS AND NUCLEAR-LABEL PERMUTATIONS

Class	Example of Label Permutation	Spin Character χ_s
E	$(1)\ (2)\ (3)\ (\overline{1})\ (\overline{2})\ (\overline{3})$	$2^6 = 64$
$6C_4$	$(12\overline{1}\overline{2})\ (3)\ (\overline{3})$	$2^3 = 8$
$3C_4{}^2$	$(1\overline{1})\ (2\overline{2})\ (3)\ (\overline{3})$	$2^4 = 16$
$8C_3$	$(13\overline{2})\ (2\overline{1}\overline{3})$	$2^2 = 4$
$6C_2$	$(12)\ (\overline{1}\overline{2})\ (3\overline{3})$	$2^3 = 8$

TABLE III

CHARACTER TABLE OF O

	Class	E	$6C_4$	$3C_4^2$	$8C_3$	$6C_2$
Representation	A_1	1	1	1	1	1
	A_2	1	-1	1	1	-1
	E	2	0	2	-1	0
	F_1	3	1	-1	0	-1
	F_2	3	-1	-1	0	1

TABLE IV

SPIN CHARACTERS OF O
FOR SIX SPIN-1/2 NUCLEI

Class	E	$6C_4$	$3C_4^2$	$8C_3$	$6C_2$
χ_s	64	8	16	4	8

$\Gamma_s = 10A_1 + 2A_2 + 8E + 6F_1 + 6F_2$

TABLE V

CHARACTERS OF THE ROTATIONAL FUNCTIONS

Class	E	$6C_4$	$3C_4^2$	$8C_3$	$6C_2$
χ_R	$24p + 2k + 1$	$\sqrt{2} \cos \frac{\pi}{4} (1-2k)$	$(-1)^k$	$\frac{2}{\sqrt{3}} \sin \frac{2\pi}{3} (1-k)$	$(-1)^k$

NOTES: 1. The angular momentum $J = 12p + k$.

2. Multiply all characters by $(2J + 1)$.

TABLE VI

SYMMETRY OF THE ROTATIONAL FUNCTIONS

$J = 12p$	$(2J + 1)[(p + 1)A_1 + pA_2 + 2pE + 3pF_1 + 3pF_2]$
$J = 12p + 1$	$(2J + 1)[pA_1 + pA_2 + 2pE + (3p + 1)F_1 + 3pF_2]$
$J = 12p + 2$	$(2J + 1)[pA_1 + pA_2 + (2p + 1)E + 3pF_1 + (3p + 1)F_2]$
$J = 12p + 3$	$(2J + 1)[pA_1 + (p + 1)A_2 + 2pE + (3p + 1)F_1 + (3p + 1)F_2]$
$J = 12p + 4$	$(2J + 1)[(p + 1)A_1 + pA_2 + (2p + 1)E + (3p + 1)F_1 + (3p + 1)F_2]$
$J = 12p + 5$	$(2J + 1)[pA_1 + pA_2 + (2p + 1)E + (3p + 2)F_1 + (3p + 1)F_2]$
$J = 12p + 6$	$(2J + 1)[(p + 1)A_1 + (p + 1)A_2 + (2p + 1)E + (3p + 1)F_1 + (3p + 2)F_2]$
$J = 12p + 7$	$(2J + 1)[pA_1 + (p + 1)A_2 + (2p + 1)E + (3p + 2)F_1 + (3p + 2)F_2]$
$J = 12p + 8$	$(2J + 1)[(p + 1)A_1 + pA_2 + 2(p + 1)E + (3p + 2)F_1 + (3p + 2)F_2]$
$J = 12p + 9$	$(2J + 1)[(p + 1)A_1 + (p + 1)A_2 + (2p + 1)E + 3(p + 1)F_1 + (3p + 2)F_2]$
$J = 12p + 10$	$(2J + 1)[(p + 1)A_1 + (p + 1)A_2 + 2(p + 1)E + (3p + 2)F_1 + 3(p + 1)F_2]$
$J = 12p + 11$	$(2J + 1)[pA_1 + (p + 1)A_2 + 2(p + 1)E + 3(p + 1)F_1 + 3(p + 1)F_2]$

NOTE: The integer $p = 0, 1, 2, \ldots$.

TABLE VII

MULTIPLICATION TABLE FOR REPRESENTATIONS OF O

	A_1	A_2	E	F_1	F_2
A_2	A_2	A_1	E	F_1	F_2
E	E	E	$A_1 + A_2 + E$	$F_1 + F_2$	$F_1 + F_2$
F_1	F_1	F_2	$F_1 + F_2$	$A_1 + E$ $+ F_1 + F_2$	$A_2 + E$ $+ F_1 + F_2$
F_2	F_2	F_1	$F_1 + F_2$	$A_2 + E$ $+ F_1 + F_2$	$A_1 + E$ $+ F_1 + F_2$

TABLE VIII

ROTATIONAL DEGENERACIES FOR A_1 VIBRATIONS

ψ_s :	$10A_1$	$2A_2$	8E	$6F_1$	$6F_2$
J = 12p	10p	2(p + 1)	16p	18p	18p
J = 12p + 1	10p	2p	16p	18p	6(3p + 1)
J = 12p + 2	10p	2p	8(2p + 1)	6(3p + 1)	18p
J = 12p + 3	10(p + 1)	2p	16p	6(3p + 1)	6(3p + 1)
J = 12p + 4	10p	2(p + 1)	8(2p + 1)	6(3p + 1)	6(3p + 1)
J = 12p + 5	10p	2p	8(2p + 1)	6(3p + 1)	6(3p + 2)
J = 12p + 6	10(p + 1)	2(p + 1)	8(2p + 1)	6(3p + 2)	6(3p + 1)
J = 12p + 7	10(p + 1)	2p	8(2p + 1)	6(3p + 2)	6(3p + 2)
J = 12p + 8	10p	2(p + 1)	16(p + 1)	6(3p + 2)	6(3p + 2)
J = 12p + 9	10(p + 1)	2(p + 1)	8(2p + 1)	6(3p + 2)	6(3p + 3)
J = 12p + 10	10(p + 1)	2(p + 1)	16(p + 1)	18(p + 1)	6(3p + 2)
J = 12p + 11	10(p + 1)	2p	16(p + 1)	18(p + 1)	18(p + 1)

NOTE: The integer p = 0, 1, 2, ...

TABLE IX

ROTATIONAL DEGENERACIES FOR A_2 VIBRATIONS

ψ_s :	$10A_1$	$2A_2$	8E	$6F_1$	$6F_2$
J = 12p	10(p + 1)	2p	16p	18p	18p
J = 12p + 1	10p	2p	16p	6(3p + 1)	18p
J = 12p + 2	10p	2p	8(2p + 1)	18p	6(3p + 1)
J = 12p + 3	10p	2(p + 1)	16p	6(3p + 1)	6(3p + 1)
J = 12p + 4	10(p + 1)	2p	8(2p + 1)	6(3p + 1)	6(3p + 1)
J = 12p + 5	10p	2p	8(2p + 1)	6(3p + 2)	6(3p + 1)
J = 12p + 6	10(p + 1)	2(p + 1)	8(2p + 1)	6(3p + 1)	6(3p + 2)
J = 12p + 7	10p	2(p + 1)	8(2p + 1)	6(3p + 2)	6(3p + 2)
J = 12p + 8	10(p + 1)	2p	8(2p + 2)	6(3p + 2)	6(3p + 2)
J = 12p + 9	10(p + 1)	2(p + 1)	8(2p + 1)	18(p + 1)	6(3p + 2)
J = 12p + 10	10(p + 1)	2(p + 1)	16(p + 1)	6(3p + 2)	18(p + 1)
J = 12p + 11	10p	2(p + 1)	16(p + 1)	18(p + 1)	18(p + 1)

NOTE: The integer p = 0, 1, 2, ...

TABLE X

ROTATIONAL DEGENERACIES FOR E VIBRATIONS

ψ_s :	$10A_1$	$2A_2$	8E	$6F_1$	$6F_2$
J = 12p	20p	4p	8(4p + 1)	36p	36p
J = 12p + 1	20p	4p	32p	6(6p + 1)	6(6p + 1)
J = 12p + 2	10(2p + 1)	2(2p + 1)	8(4p + 1)	6(6p + 1)	6(6p + 1)
J = 12p + 3	20p	4p	8(4p + 1)	12(3p + 1)	12(3p + 1)
J = 12p + 4	10(2p + 1)	2(2p + 1)	16(2p + 1)	12(3p + 1)	12(3p + 1)
J = 12p + 5	10(2p + 1)	2(2p + 1)	8(4p + 1)	18(2p + 1)	18(2p + 1)
J = 12p + 6	10(2p + 1)	2(2p + 1)	8(4p + 3)	18(2p + 1)	18(2p + 1)
J = 12p + 7	10(2p + 1)	2(2p + 1)	16(2p + 1)	12(3p + 2)	12(3p + 2)
J = 12p + 8	20(p + 1)	4(p + 1)	8(4p + 3)	12(3p + 2)	12(3p + 2)
J = 12p + 9	10(2p + 1)	2(2p + 1)	8(4p + 3)	6(6p + 5)	6(6p + 5)
J = 12p + 10	20(p + 1)	4(p + 1)	32(p + 1)	6(6p + 5)	6(6p + 5)
J = 12p + 11	20(p + 1)	4(p + 1)	8(4p + 3)	36(p + 1)	36(p + 1)

NOTE: The integer p = 0, 1, 2, ...

TABLE XI

ROTATIONAL DEGENERACIES FOR F_1 VIBRATIONS

ψ_s :	$10A_1$	$2A_2$	8E	$6F_1$	$6F_2$
J = 12p	30p	6p	48p	54p	6(9p + 1)
J = 12p + 1	30p	2(3p + 1)	8(6p + 1)	6(9p + 1)	6(9p + 1)
J = 12p + 2	10(3p + 1)	6p	8(6p + 1)	6(9p + 2)	6(9p + 2)
J = 12p + 3	10(3p + 1)	2(3p + 1)	16(3p + 1)	18(3p + 1)	6(9p + 2)
J = 12p + 4	10(3p + 1)	2(3p + 1)	16(3p + 1)	18(3p + 1)	6(9p + 4)
J = 12p + 5	10(3p + 1)	2(3p + 2)	24(2p + 1)	6(9p + 4)	6(9p + 4)
J = 12p + 6	10(3p + 2)	2(3p + 1)	24(2p + 1)	6(9p + 5)	6(9p + 5)
J = 12p + 7	10(3p + 2)	2(3p + 2)	16(3p + 2)	18(3p + 2)	6(9p + 5)
J = 12p + 8	10(3p + 2)	2(3p + 2)	16(3p + 2)	18(3p + 2)	6(9p + 7)
J = 12p + 9	10(3p + 2)	6(p + 1)	8(6p + 5)	6(9p + 7)	6(9p + 7)
J = 12p + 10	30(p + 1)	2(3p + 2)	8(6p + 5)	6(9p + 8)	6(9p + 8)
J = 12p + 11	30(p + 1)	6(p + 1)	48(p + 1)	54(p + 1)	6(9P + 8)

NOTE: The integer p = 0, 1, 2, ...

TABLE XII

ROTATIONAL DEGENERACIES FOR F_2 VIBRATIONS

ψ_s :	$10A_1$	$2A_2$	8E	$6F_1$	$6F_2$
J = 12p	30p	6p	48p	6(9p + 1)	54p
J = 12p + 1	10(3p + 1)	6p	8(6p + 1)	6(9p + 2)	6(9p + 1)
J = 12p + 2	30p	2(3p + 1)	8(6p + 1)	6(9p + 2)	6(9p + 2)
J = 12p + 3	10(3p + 1)	2(3p + 1)	16(3p + 1)	6(9p + 2)	18(3p + 1)
J = 12p + 4	10(3p + 1)	2(3p + 1)	16(3p + 1)	6(9p + 4)	18(3p + 1)
J = 12p + 5	10(3p + 2)	2(3p + 1)	24(2p + 1)	6(9p + 4)	6(9p + 4)
J = 12p + 6	10(3p + 1)	2(3p + 2)	24(2p + 1)	6(9p + 5)	6(9p + 5)
J = 12p + 7	10(3p + 2)	2(3p + 2)	16(3p + 2)	6(9p + 5)	18(3p + 2)
J = 12p + 8	10(3p + 2)	2(3p + 2)	16(3p + 2)	6(9p + 7)	18(3p + 2)
J = 12p + 9	30(p + 1)	2(3p + 2)	8(6p + 5)	6(9p + 7)	6(9p + 7)
J = 12p + 10	10(3p + 2)	6(p + 1)	8(6p + 5)	6(9p + 8)	6(9p + 8)
J = 12p + 11	30(p + 1)	6(p + 1)	48(p + 1)	6(9p + 8)	54(p + 1)

NOTE: The integer p = 0, 1, 2, ...