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Line Strengths for Rotational Spectrum of Asymmetric Rotors

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Abstract —— The first-rank tensor operator has been used to develop the relations between the direction cosines and the first-order rotational representations. These relations have been used to derive the explicit formulas in terms of 3j symbols for the line strengths of the asymmetric rotors. Some detail calculations and comparsions with CHK (1) have been discussed. The nonvanishing magnitudes of 3j symbols used specially for the rotational transitions for J up to 4 have also been tabulated.

I. Introduction

In the previous work performed by the same author (2), the formula in terms of 3j symbols for the line strengths of the symmetric tops has been established by the first-order rotational representations. It is found that this formula is easy and convenient to calculate the line strengths. It will be interesting and feasible to extend this work to include the case for the asymmetric rotors. Actually in calculating the line strengths of the asymmetric rotors, the direction cosine matrix elements and the wave functions for the energy levels play important roles.

There are usually two approaches to the calculations of the line strengths of the asymmetric rotors. The first one, using the tabulated direction cosine matrix elements, yields a complicated procedure involving the summation over the projection quantum numbers and space-fixed components. The second one, employing the direction cosine matrix elements in terms of Clebsch-Gordan coefficients (3), however still has the same tedious work as the first one. The formulas for the intensity factors in molecular spectra (4) are actually not explicit and simple enough for direct calculations. Thus the methods mentioned above, in fact, do not directly help too much for computing the line strengths.

The purpose of this paper is to present an alternate and convenient treatment for calculating the line strengths of the asymmetric rotors. The treatment shown here not only reduces much tedious work arisen in the conventional method, thus provides a convenient and direct calculation either by digital computers or by hand calculations, but is also able to be easily coupled to the other effects in molecular spectra. If we consider the transformation properties in both spherical and cartesian coordinates and the linear combination properties between the spherical coordinates and cartesian coordinates for both space-fixed and body-fixed frames, then we can obtain the relations of the linear combinations between the direction cosines and the first-order rotational representations. These relations and that the wave functions can be expressed by the rotational representations (5) indicate that the direction cosine matrix elements can be represented in terms of 3j symbols by integrating three D's (6, 7). The explicit form of this integration has been used widely (8-10). The wave functions of the asymmetric rotors are the linear combinations of those of the symmetric tops, so that the direction cosine matrix elements for the asymmetric rotors may also be expressed in terms of 3j symbols. Consequently the line strengths of the asymmetric rotors can be expressed explicitly in terms of 3j symbols. After detailed evaluation we found that it is simple to obtain the final forms of the line strengths by using Wang wave functions (11) and the Wang transformation factor $\sqrt{2}$. This procedure will be used here.

II. Derivations

1. The relations between the direction cosines and the first-order rotational representations.

In a spherical system, the transformation property of a k^{th}-rank tensor operator $T^{(k)}$ under a rotation of the coordinate system is given as (12)

$$T_q^{(k)} = \sum_{q'} D_{qq'}^{(k)} T_{q'}^{\prime(k)} ,$$

or

$$T^{(k)} = D^{(k)}\ T^{\prime(k)} \tag{1}$$

Where the symbol $D^{(k)}$ designates a (2k+1) dimensional matrix representation of the rotational group which depends upon the Euler's angles; $T^{(k)}$ and $T^{\prime(k)}$ represent the tensor operators respectively in space-fixed frame and body-fixed frame.

In a cartesian system, the transformation property between T and T' is that

$$T = \Phi T' . \tag{2}$$

Where the expression Φ represents the direction cosine matrix and it can be expressed as

$$\Phi = \begin{bmatrix} \Phi_{Xx} & \Phi_{Xy} & \Phi_{Xz} \\ \Phi_{Yx} & \Phi_{Yy} & \Phi_{Yz} \\ \Phi_{Zx} & \Phi_{Zy} & \Phi_{Zz} \end{bmatrix} ,$$

T and T' are the first-rank tensor operators respectively in the space-fixed frame and the body-fixed frame.

For a first-rank tensor operator, the linear combinations between the spherical components $T_q^{(1)}$ and the components T_x, T_y, and T_z are given as (13)

$$T_0^{(1)} = T_z,\ T_\pm^{(1)} = \mp(1/\sqrt{2})\,(T_X \pm iT_Y),$$

or

$$T^{(1)} = UT,$$

$$\text{where } U = \begin{bmatrix} -1/\sqrt{2} & -i/\sqrt{2} & 0 \\ 0 & 0 & 1 \\ 1/\sqrt{2} & -i/\sqrt{2} & 0 \end{bmatrix} .$$

These combinations hold in the space-fixed system and the body-fixed frame. Setting k in Eq. (1) equal to 1, and considering the unitary transformation, we obtain the relations between the direction cosines and the first-order rotational representations as

$$\Phi_{Xx} = 1/2(D_{11}^{(1)} - D_{1-1}^{(1)} - D_{-11}^{(1)} + D_{-1-1}^{(1)}) ,$$

$$\Phi_{Xy} = i/2(D_{11}^{(1)} + D_{1-1}^{(1)} - D_{-11}^{(1)} - D_{-1-1}^{(1)}) ,$$

$$\begin{aligned}
\Phi_{Xz} &= 1/\sqrt{2}\,(D^{(1)}_{-10} - D^{(1)}_{10}), \\
\Phi_{Yx} &= i/2\,(D^{(1)}_{1-1} + D^{(1)}_{-1-1} - D^{(1)}_{11} - D^{(1)}_{-11}), \\
\Phi_{Yy} &= 1/2\,(D^{(1)}_{11} + D^{(1)}_{1-1} + D^{(1)}_{-11} + D^{(1)}_{-1-1}), \\
\Phi_{Yz} &= i/\sqrt{2}\,(D^{(1)}_{10} + D^{(1)}_{-10}), \\
\Phi_{Zx} &= 1/\sqrt{2}\,(D^{(1)}_{0-1} - D^{(1)}_{01}), \\
\Phi_{Zy} &= -i/\sqrt{2}\,(D^{(1)}_{01} + D^{(1)}_{0-1}), \\
\Phi_{Zz} &= D^{(1)}_{00}.
\end{aligned} \tag{3}$$

The symbols X, Y, and Z represent the axes in the space-fixed system, and those x, y, and z represent the axes in the body-fixed system, the superscript indicates the rank and the first and second subscripts respectively indicate the sub-ranks in the space-fixed system and body-fixed system. The reversed form of Eq. (3) have been derived in Ref. 3.

2. The line strengths along x-axis

In order to employ the Wang wave functions to find the integration of three D's such that the procedure to obtain the final results will be simplified, it is certainly necessary to understand the relation between the integration of three D's by the Wang wave functions and that by the symmetric top wave functions. The relations between the Wang wave functions and symmetric top wave funcitons are

$$|\,JKM>_w = 1/\sqrt{2}\,[\,|JKM> + (-1)^r|J\text{-}KM>]_s\,,$$

and

$$|\,JOM>_w = |\,JOM>_s\,,$$

where r is 1 for oddness and 0 for evenness, which can be decided by the odd energy submatrices and even energy submatrices. The integration of three D's for both kinds of wave functions is

$$<J'K'M'\,|D^{(1)}_{qq'}\,|JKM>_w = ½[<J'K'M'\,| + (-1)^r <J'\text{-}K'M'\,|\,]\,D^{(1)}_{qq'}[\,|JKM> + (-1)^r\,|J\text{-}KM>]\,.$$

Considering the property of 3j symbols, evenness and oddness of r, and magnitudes of q', we obtain the simple relation

$$<J'K'M'\,|D^{(1)}_{qq'}\,|JKM>_w = <J'K'M'\,|D^{(1)}_{qq'}\,|JKM>_s\,,$$

the magnitudes of K' and K are positive. For the case that either K' or K is zero this relation will be changed to

$$<J'K'M'\,|D^{(1)}_{qq'}\,|JKM>_w = \sqrt{2}<J'K'M'\,|D^{(1)}_{qq'}\,|JKM>_s\,.$$

In the cartesian system, the line strength between two energy levels for an asymmetric rotor is given in Ref. 1, it is

$$\lambda_g(J'\tau' \to J\tau) = \sum_{FMM'} |\langle J'\tau'M' | \Phi_{Fg} | J\tau M\rangle|^2 , \tag{4}$$

where g indicates one axis in the body-fixed frame, x will be for this case, F one axis in the space-fixed frame, $J'\tau'$ and $J\tau$ two energy levels, M and M' the sub-quantum numbers in the space-fixed frame respectively for J and J'. The summation in Eq. (4) extends over the three directions (X, Y, and Z) of the space-fixed system and over all values of M and M'. The wave function $|J\tau M\rangle$ is the linear combination of the Wang wave functions of the same J and M, it is

$$|J\tau M\rangle = \sum_i C_i |JK_iM\rangle , \tag{5}$$

C_i's here are the linear combination coefficients and K_i's the projection quantum numbers in the body-fixed system. The procedure to calculate C_i's has been shown by King et al (14). Combining Eqs. (4) and (5), we can write the line strength along x-axis as

$$\lambda_x(J'\tau' \to J\tau) = \sum_{ij} \sum_{FMM'} |C_iC_j\langle J'K_iM' | \Phi_{Fx} | JK_jM\rangle|^2 . \tag{6}$$

By use of the proper relations between the direction cosine Φ_{Fx} and its rotational representations shown in Eq. (3), Eq. (6) can be written as

$$\lambda_x(J'\tau' \to J\tau) = \sum_{ij} \sum_{MM'} |C_i C_j \langle J'K_iM' | 1/2 (D^{(1)}_{11} - D^{(1)}_{1-1} - D^{(1)}_{-11} - D^{(1)}_{-1-1})$$
$$+ i/2 (D^{(1)}_{1-1} + D^{(1)}_{-1-1} - D^{(1)}_{11} - D^{(1)}_{-11}) + 1/\sqrt{2} (D^{(1)}_{0-1} - D^{(1)}_{01}) | JK_jM\rangle|^2 . \tag{7}$$

From Eq. (7), we find that there are two values for the second subscripts, they are 1 and -1, and that there are three values for the first one, they are 1, 0, and -1. Classifying these two subscripts, we may write Eq. (7) as

$$\lambda_x(J'\tau' \to J\tau) = \sum_{ijq'} \sum_{MM'} |C_i C_j \langle J'K_iM' | (1/2 + i/2) D_{1q'} +$$
$$(1/2 - i/2) D^{(1)}_{-1q'} - (1/\sqrt{2}) D^{(1)}_{oq'} | JK_jM\rangle|^2 ,$$

or

$$\lambda_x(J'\tau' \to J\tau) = \sum_{ijq'} \sum_{MM'} |(1/2 + i/2) C_i C_j \langle J'K_iM' | D^{(1)}_{1q'} | JK_jM\rangle$$
$$+ (1/2 - i/2) C_i C_j \langle J'K_iM' | D^{(1)}_{-1q'} | JK_jM\rangle$$
$$(-1/\sqrt{2}) C_i C_j \langle J'K_iM' | D^{(1)}_{oq'} | JK_jM\rangle|^2 , \tag{8}$$

where q' is 1 or -1. By means of the expression for integrating three D's that has been derived as

$$\langle J'K_iM' | D^{(1)}_{qq'} | JK_jM\rangle = (-1)^{M-K_j} [(2J'+1)(2J+1)]^{1/2}$$
$$\times \begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix} \times \begin{pmatrix} J & 1 & J' \\ M & -q & -M' \end{pmatrix} , \tag{9}$$

Eq. (8) may be written as

$$\lambda_x(J'\tau' \to J\tau) = (2J'+1)(2J+1)\,[\sum_{ijq'}(-1)^{-K_j} C_i C_j \begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}]^2$$
$$\times \left| \sum_{MM'}(-1)^M [(1/2 + i/2)\begin{pmatrix} J & 1 & J' \\ M & -1 & -M' \end{pmatrix} + (1/2 - i/2)\begin{pmatrix} J & 1 & J' \\ M & 1 & -M' \end{pmatrix}$$
$$- 1/\sqrt{2}\begin{pmatrix} J & 1 & J' \\ M & 0 & -M' \end{pmatrix}] \right|^2 . \tag{10}$$

Considering the orthogonality property of 3j symbols (15), we obtain the expression of the square of the absolute value in Eq. (10) as

$$\tfrac{1}{2} \sum_{MM'q(1,0,-1)} \begin{pmatrix} J & 1 & J' \\ M & -q & -M' \end{pmatrix}^2 ,$$

which gives value ½. Then we may reduce Eq. (10) to

$$\lambda_x(J'\tau' \to J\tau) = \tfrac{1}{2}(2J'+1)(2J+1)[\sum_{ijq'}(-1)^{-K_j} C_i C_j \begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}]^2 .$$

The values of K_j shown in the equation above will only be either even or odd, so that the power $(-1)^{-K_j}$ does not affect the phase of each magnitude but that of the summation. After being squared, the line strength shown above will be

$$\lambda_x(J'\tau' \to J\tau) = \tfrac{1}{2}(2J'+1)(2J+1)[\sum_{ijq'} C_i C_j \begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}]^2 . \tag{11}$$

3. The line strengths along y and z-axes

For the line strengths due to y-axis, considering the wave function shown in Eq. (5) with the definition showns in Eq. (4), using the linear combinations of the rotational representations for direction cosine Φ_{Fy} shown in Eq. (3), and classifying the values of two subscripts, we obtain the expression as

$$\lambda_y(J'\tau' \to J\tau) = \sum_{ij}\sum_{MM'} |C_i C_j \langle J'K_iM'|\,[(1/2 - i/2)D^{(1)}_{11} - (1/2 + i/2)D^{(1)}_{-11} - (1/\sqrt{2})D^{(1)}_{01}]$$
$$- [(1/2 - i/2)D^{(1)}_{1-1} - (1/2 + i/2)D^{(1)}_{-1-1} - (1/\sqrt{2})D^{(1)}_{0-1}]\,|JK_jM\rangle|^2 ,$$

or

$$\lambda_y(J'\tau' \to J\tau) = \sum_{ij}\sum_{\substack{MM' \\ q'(-1,1)}} |C_i C_j q' \langle J'K_iM'|(1/2 - i/2)D^{(1)}_{1q'} - (1/2 + i/2)D^{(1)}_{-1q'}$$
$$- (1/\sqrt{2})D^{(1)}_{0q'}|JK_jM\rangle|^2 . \tag{12}$$

Using the procedures from Eqs. (8) to (11), we may re-write Eq. (12) as

$$\lambda_y(J'\tau' \to J\tau) = \tfrac{1}{2}(2J'+1)(2J+1)[\sum_{jiq'} C_i C_j q' \begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}]^2 . \tag{13}$$

By use of the same procedures shown above, the line strength along the z-axis may be obtained as

$$\lambda_z(J'\tau' \to J\tau) = (2J'+1)(2J+1)[\sum_{ij} C_i C_j \begin{pmatrix} J & 1 & J' \\ K_j & 0 & -K_i \end{pmatrix}]^2 . \tag{14}$$

The expressions J and K_j shown in Eqs. (11), (13), and (14) are for the upper energy level and those J' and K_i are for the lower energy level. Since K_j or K_i in Eq. (11) and (13) may be zero, the expressions there will be respectively modified to

$$\lambda_x(J'\tau' \rightarrow J\tau) = \tfrac{1}{2}(2J'+1)(2J+1)[\Sigma C_i C_j \sqrt{2} \begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}]^2 , \qquad (15)$$

and

$$\lambda_y(J'\tau' \rightarrow J\tau) = \tfrac{1}{2}(2J'+1)(2J+1)[\Sigma C_i C_j \sqrt{2}\, q' \begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}]^2 . \qquad (16)$$

The magnitude $\sqrt{2}$ here will be multiplied when either K_j or K_i is zero, the magnitudes of K_j and K_i are decided by the energy submatrices as shown in Ref. 14.

III. Comparisons and Discussions

From Eq. (9) we realize that the matrix elements of the first-order rotational representations contain three parts, J part, JK part, and JM part. Which is similar to those of the direction cosines. The summation over q(-1, 0, 1) in spherical coordinates is physically similar to that over X, Y, and Z axes in cartesian coordinates.

The expressions explicitly in terms of 3j symbols in Eqs. (14),(15),and (16) represent the line strengths respectively along the x-, y- and z-axes. From these three equations we realized the real line strengths are independent of the space fixed orientations. It is similar to that the energy levels are independent of the space-fixed orientations. The reason for the latter is that the energies are functions of the molecular structures, and that for the former is that the sum over the space-fixed quantities F, M, and M' have been taken into account as shown in Eq. (4). The line strengths of the symmetric tops shown in Ref. 2.

$$\lambda_s(J'K' \rightarrow JK) = (2J'+1)(2J+1) \begin{pmatrix} J & 1 & J' \\ K & 0 & -K' \end{pmatrix}^2 \qquad (17)$$

is a special case of that in Eq. (14). Some line strengths of propyne (16) have been calculated and shown in Table 1, we find that the magnitudes agree with those shown in Table 2 in Ref. 15.

In order to check whether or not the line strengths shown in Eqs. (14), (15), and (16) are reliable, some line strengths of the asymmetric parameter k= -0.5 have been calculated and tabulated. Table 2 gives the energy levels for J=2 and 3. Table 3 shows the transition lines for Q-branch ($\Delta J=0$) and Table 4 for those of R-branch ($\Delta J=1$). Table 5 gives the line strengths for a-type, Table 6 for b-type, and Table 7 for c-type. The magnitudes for λ_g^* are the line strengths shown in Table VI in Ref. 1. The energy levels shown in Table 2 were calculated by means of representation I^r(a $\rightarrow$z, b$\rightarrow$x, and c$\rightarrow$y) mentioned in Ref. 14. For instance the procedure for calculating the line strengths of $2_{21} \rightarrow 3_{12}$ (b-type) and $3_{12} \rightarrow 3_{22}$ (c-type) are shown as follows:

The wave functions for energy levels 2_{21} and 3_{12} are

$$2_{21} \Longrightarrow |22>$$

and

$$3_{12} \Longrightarrow 0.9970486\,|31> + 0.0767731\,|33> .$$

Using Eq. (11) with the wave functions shown above and expanding them, we have

$$\lambda_b(2_{21} \rightarrow 3_{12}) = \tfrac{1}{2}[(2x2+1)x(2x3+1)]\,[0.9970486 \begin{pmatrix} 3 & 1 & 2 \\ 1 & 1 & -2 \end{pmatrix}$$

$$+ 0.9970486 \begin{pmatrix} 3 & 1 & 2 \\ 1 & -1 & -2 \end{pmatrix} + 0.0767731 \begin{pmatrix} 3 & 1 & 2 \\ 3 & 1 & -2 \end{pmatrix} + 0.0767331 \begin{pmatrix} 3 & .1 & 2 \\ 3 & -1 & -2 \end{pmatrix}]^2 .$$

By use of the requirement that $K_j+(-q')+(-K_i)=0$ for the non-vanishing magnitudes of 3j symbols, we can reduce the equation above as

$$\lambda_b(2_{21}\rightarrow 3_{12})=17.5[0.9770486\begin{pmatrix}3 & 1 & 2\\ 1 & 1 & -2\end{pmatrix}+0.0767331\begin{pmatrix}3 & 1 & 2\\ 3 & -1 & -2\end{pmatrix}]^2,$$

and by use of the values $\begin{pmatrix}3 & 1 & 2\\ 1 & 1 & -2\end{pmatrix}=0.0975900$ and $\begin{pmatrix}3 & 1 & 2\\ 3 & -1 & -2\end{pmatrix}=0.3779645$, the line strength will be $\lambda_b(2_{21}\ 3_{12})=0.279241$, which agrees with 0.2792 calculated in Ref. 1.

The wave functions for energy levels 3_{12} and 3_{22} are $3_{12}\Rightarrow 0.9970486\,|31>+0.0767731\,|33>$, and $3_{22}\Rightarrow|32>$. Same procedure as above is **employed**, and the phase due to q' is considered, the line strength for $3_{12}\rightarrow 3_{22}$ is obtained as

$$\lambda_c(3_{12}\rightarrow 3_{22})=\tfrac{1}{2}[(2\text{x}3+1)\text{x}(2\text{x}3+1)]\,[0.9970486(1)\begin{pmatrix}3 & 1 & 3\\ 2 & -1 & -1\end{pmatrix}+0.0767731\,(-1)\begin{pmatrix}3 & 1 & 3\\ 2 & 1 & -3\end{pmatrix}]^2,$$

which yields

$\lambda_c(3_{12}\rightarrow 3_{22})=1.627832$. This is in agreement with the value of 1.6278 as obtained by Cross et al.

IV. Conclusions

The relations between the direction cosine and the first-order rotational representations has been obtained by considering the transformation properties in both spherical and cartesian coordinates. The direction cosine matrix elements has been proved to be able to expressed in terms of 3j symbols by integrating three D's. The expressions of the line strengths along x-, y- and z-axes have been derived. Some line strengths of water (17) and vinyle cyanide (18) have been checked and found they agree very well. The line strengths in terms of 3j symbols can also be extended to calculate the energy levels and line strengths of the Stark effects for both symmetric and asymmetric rotors. The expressions in carteisan forms are equivalent to those in spherical forms, but the latter is much easier not only in calculations but also in derivations. In addition, the expressions in terms of spherical forms can be easily extended to include coupling angular momenta by means of the spherical tensor method, and the explicit forms are in terms of nj symbols. Consequently a direct compulation can be immediately followed.

In conclusion, the treatment presented in this work suggests a more convenient and alternate method which can reduce much calculation work for the line strengths. The magnitudes of 3j symbols listed in Table VIII will be useful for calculating line strengths for both symmetric and asymmetric rotors.

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Table I. Line strengths of propyne.

Transition: lower state J',K'	upper state J,K	(2J'+1) x(2J+1)	$\begin{pmatrix} J & 1 & J' \\ K & 0 & -K' \end{pmatrix}$	$\begin{pmatrix} J & 1 & J' \\ K & 0 & -K' \end{pmatrix}^2$	Line strength
0, 0	1,0	3	-0.5773503	0.3333333	1.0000
1, 1	2,1	15	-0.3162278	0.10	1.5000
2, 2	3,2	35	-0.2182179	0.0476190	1.6667
3, 3	4,3	63	-0.1666667	0.0277778	1.7500
4, 0	5,0	99	-0.2247333	0.0505051	5.0000
4, 4	5,4	99	-0.1348400	0.0181818	1.8000
7, 0	8,0	255	0.1771230	0.0313725	8.0000
7, 2	8,2	255	0.1714986	0.0294118	7.5000
7, 5	8,5	255	-0.1382666	0.0191176	4.8750
8, 0	9,0	323	-0.1669245	0.0278638	9.0000
8, 4	9,4	323	-0.1495320	0.0223598	7.2222
8, 8	9,8	323	-0.0764719	0.0058480	1.8889

Table II. Energy levels for J=2, 3 and k = -0.5.

J	Energy level	Reduced energy	Wave function	Submatrix
2	2_{20}	2.6055512	$-0.1209848\vert 20\rangle+0.9926544\vert 22\rangle$	E^+
	2_{21}	2.5	$\vert 22\rangle$	E^-
	2_{11}	-2.0	$\vert 21\rangle$	0^-
	2_{12}	-3.5	$\vert 21\rangle$	0^+
	2_{02}	-4.6055512	$0.9926544\vert 20\rangle+0.1209848\vert 22\rangle$	E^-
3	3_{30}	6.8245553	$-0.0767731\vert 31\rangle+0.9970486\vert 33\rangle$	0^-
	3_{31}	6.8102497	$-0.0621055\vert 31\rangle+0.9980696\vert 33\rangle$	0^+
	3_{21}	-1.5	$-0.25\vert 30\rangle+0.9682458\vert 32\rangle$	E^+
	3_{22}	-2.0	$\vert 32\rangle$	E^-
	3_{12}	-5.8245553	$0.9970486\vert 31\rangle+0.0767731\vert 33\rangle$	0^-
	3_{13}	-8.8102497	$0.9980696\vert 31\rangle+0.0621055\vert 33\rangle$	0^+
	3_{03}	-9.5	$0.9682458\vert 30\rangle+0.25\vert 32\rangle$	E^+

Table III. Transition lines of Q-branch for J=3 and k = -0.5.

Transition	Type	Wave function of lower energy level	Wave function of upper energy level	Sub-matrices
$3_{31} \rightarrow 3_{30}$	a	$-0.0621055\vert 31\rangle$ $+0.9980696\vert 33\rangle$	$-0.0767731\vert 31\rangle$ $+0.9970486\vert 33\rangle$	$0^+ \rightarrow 0^-$
$3_{21} \rightarrow 3_{30}$	b	$-0.25\vert 30\rangle$ $+0.9682458\vert 32\rangle$	$-0.0767731\vert 31\rangle$ $+0.9970486\vert 33\rangle$	$E^+ \rightarrow 0^-$
$3_{12} \rightarrow 3_{22}$	c	$0.9970486\vert 31\rangle$ $+0.0767731\vert 33\rangle$	$\vert 32\rangle$	$0^- \rightarrow 0^+$

Table IV. Transition lines of R-branch for J=2, 3 and k = -0.5.

Transition	Type	Wave function of lower energy level	Wave function of upper energy level	Sub-matrices
$2_{11} \rightarrow 3_{30}$	a	$\vert 21\rangle$	$-0.0767731\vert 31\rangle$ $+0.9970486\vert 33\rangle$	$0^- \rightarrow 0^-$
$2_{21} \rightarrow 3_{12}$	b	$\vert 22\rangle$	$0.9970486\vert 31\rangle$ $+0.0767731\vert 33\rangle$	$E^- \rightarrow 0^-$
$2_{21} \rightarrow 3_{31}$	c	$\vert 22\rangle$	$-0.0621055\vert 31\rangle$ $+0.9980696\vert 33\rangle$	$E^- \rightarrow 0^+$

Table V. Line strengths of transitions for a-type.

Transition	Branch	$(2J'+1) \times (2J+1)$	Non-vanishing 3j symbols $\begin{pmatrix} J & 1 & J' \\ K_j & 0 & -K_i \end{pmatrix}$	$C_i C_j \begin{pmatrix} J & 1 & J' \\ K_j & 0 & -K_i \end{pmatrix}$
$3_{31} \rightarrow 3_{30}$	Q	49	$\begin{pmatrix} 3 & 1 & 3 \\ 1 & 0 & -1 \end{pmatrix} = -0.1091089$	$(-0.0621055) \times (-0.00767731) \times (-0.1091089) = -0.0005202$
			$\begin{pmatrix} 3 & 1 & 3 \\ 3 & 0 & -3 \end{pmatrix} = -0.3273268$	$0.9980696 \times 0.9970486 \times (-0.3273268) = -0.3257307$
			SUM / $\lvert SUM \rvert^2$	-0.3262509 / 0.1064397
			λ_a / λ_a^*	5.215543 / 5.2155
$2_{11} \rightarrow 3_{30}$	R	17.5	$\begin{pmatrix} 3 & 1 & 2 \\ 1 & 0 & -1 \end{pmatrix} = 0.2760262$	$-0.0767731 \times 1 \times (0.2760262) = -0.0211914$
			SUM / $\lvert SUM \rvert^2$	-0.0211914 / 0.0004491
			λ_a / λ_a^*	0.015718 / 0.0157

$SUM = \sum_{ij} C_i C_j \begin{pmatrix} J & 1 & J' \\ K_j & 0 & -K_i \end{pmatrix}$. λ_g^* is the line strength calculated in Ref. 1.

Table VI. Line strengths of transitions for b-type.

Transition	Branch	$\frac{1}{2}(2J'+1) \times (2J+1)$	Non-vanishing 3j symbols $\begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}$	$C_i C_j \begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}$
$3_{21} \rightarrow 3_{30}$	Q	24.5	$\begin{pmatrix} 3 & 1 & 3 \\ 1 & -1 & 0 \end{pmatrix}=0.2672612$	$(-0.25)\times(-0.0767731)\sqrt{2}$ $\times 0.2672612=0.0072544$
			$\begin{pmatrix} 3 & 1 & 3 \\ 1 & 1 & -2 \end{pmatrix}=-0.2439750$	$(0.9682458)\times(-0.0767731)$ $\times(-0.2439750)=0.0181359$
			$\begin{pmatrix} 3 & 1 & 3 \\ 3 & -1 & -2 \end{pmatrix}=0.1889822$	$0.9682458\times 0.9970486$ $\times 0.1889822=0.1824412$
			SUM / $\lvert SUM \rvert^2$	0.2078315 / 0.0431939
			λ_b / λ_b^*	1.058251 / 1.0583
$2_{21} \rightarrow 3_{12}$	R	17.5	$\begin{pmatrix} 3 & 1 & 2 \\ 1 & 1 & -2 \end{pmatrix}=0.0975900$	$0.9970486\times 1\times 0.09759$ $=0.0973020$
			$\begin{pmatrix} 3 & 1 & 2 \\ 3 & -1 & -2 \end{pmatrix}=0.3779645$	$0.0767731\times 1\times 0.3779645$ $=0.0290175$
			SUM / $\lvert SUM \rvert^2$	0.1263195 / 0.0159566
			λ_b / λ_b^*	0.279241 / 0.2792

Table VII. Line strengths of transitions for c-type.

Transition	Branch	$\frac{1}{2}(2J'+1) \times (2J+1)$	Non-vanishing 3j symbols $\begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}$	$q'C_iC_j \begin{pmatrix} J & 1 & J' \\ K_j & -q' & -K_i \end{pmatrix}$
$3_{12} \rightarrow 3_{22}$	Q	24.5	$\begin{pmatrix} 3 & 1 & 3 \\ 2 & -1 & -1 \end{pmatrix}$=-0.2439750	(1)x(0.9970486)x1 x(-0.2439750)=-0.2432549
			$\begin{pmatrix} 3 & 1 & 3 \\ 2 & 1 & -3 \end{pmatrix}$=0.1889822	(-1)x(0.0767731)x1 x(0.1889822)≑-0.0145087
			SUM / $\lvert SUM \rvert^2$	-0.2577637 / 0.0664421
			λ_c / λ^*_c	1.627832 / 1.6278
$2_{20} \rightarrow 3_{30}$	R	17.5	$\begin{pmatrix} 3 & 1 & 3 \\ 1 & -1 & 0 \end{pmatrix}$=0.2390457	(1)x(-0.1209848)x(-0.0767731) $\sqrt{2}$ x(0.2390457)=0.0031401
			$\begin{pmatrix} 3 & 1 & 2 \\ 1 & 1 & -2 \end{pmatrix}$=0.0975900	(-1)x(-0.0767731)x(0.9926544) x(0.0975900)=0.0074373
			$\begin{pmatrix} 3 & 1 & 2 \\ 3 & -1 & -2 \end{pmatrix}$=0.3779654	(1)x(0.9926544)x(0.9970486) x0.3779645=0.3740808
			SUM / $\lvert SUM \rvert^2$	0.3846582 / 0.1479619
			λ_c / λ^*_c	2.589354 / 2.5893

Table VIII. The non-vanishing magnitudes of symbols used specially for rotational transitions.

J	1	J	K_j	-q'	$-K_i$	3j symbols	square of 3j symbols
0	1	1	0	-1	1	0.5773503	0.3333333
0	1	1	0	0	0	-0.5773503	0.3333333
0	1	1	0	1	-1	0.5773053	0.3333333
1	1	0	-1	1	0	0.5773053	0.3333333
1	1	0	0	0	0	-0.5773053	0.3333333
1	1	0	1	-1	0	0.5773053	0.3333333
1	1	1	-1	0	1	0.4082483	0.1666667
1	1	1	-1	1	0	-0.4082483	0.1666667
1	1	1	0	-1	1	-0.4082483	0.1666667
1	1	1	0	1	-1	0.4082483	0.1666667
1	1	1	1	-1	0	0.4082483	0.1666667
1	1	1	1	0	-1	-0.4082483	0.1666667
1	1	2	-1	-1	2	0.4472136	0.2000000
1	1	2	-1	0	1	-0.3162278	0.1000000
1	1	2	-1	1	0	0.1825742	0.0333333
1	1	2	0	-1	1	-0.3162278	0.1000000
1	1	2	0	0	0	0.3651484	0.1333333
1	1	2	0	1	-1	-0.3162278	0.1000000
1	1	2	1	-1	0	0.1825742	0.0333333
1	1	2	1	0	-1	-0.3162278	0.1000000
1	1	2	1	1	-2	0.4472136	0.2000000
2	1	1	-2	1	1	0.4472136	0.2000000
2	1	1	-1	0	1	-0.3162278	0.1000000
2	1	1	-1	1	0	-0.3162278	0.1000000
2	1	1	0	-1	1	0.1825742	0.0333333
2	1	1	0	0	0	0.3651484	0.1333333
2	1	1	0	1	-1	0.1825742	0.0333333
2	1	1	1	-1	0	-0.3162278	0.1000000
2	1	1	1	0	-1	-0.3162278	0.1000000
2	1	1	2	-1	-1	0.4472136	0.2000000
2	1	2	-2	0	2	0.3651484	0.1333333
2	1	2	-2	1	1	-0.2581989	0.0666667
2	1	2	-1	-1	2	-0.2581989	0.0666667
2	1	2	-1	0	1	-0.1825742	0.0333333
2	1	2	-1	1	0	0.3162278	0.1000000
2	1	2	0	-1	1	0.3162278	0.1000000
2	1	2	0	1	-1	-0.3162278	0.1000000

2	1	2	1	-1	0	-0.3162278	0.1000000
2	1	2	1	0	-1	0.1825742	0.0333333
2	1	2	1	1	-2	0.2581989	0.0666667
2	1	2	2	-1	-1	0.2581989	0.0666667
2	1	2	2	0	-2	-0.3651481	0.1333333
2	1	3	-2	-1	3	0.3779645	0.1428571
2	1	3	-2	0	2	-0.2182179	0.0476190
2	1	3	-2	1	1	0.0975900	0.0095238
2	1	3	-1	-1	2	-0.3086067	0.0952381
2	1	3	-1	0	1	0.2760262	0.0761905
2	1	3	-1	1	0	-0.1690309	0.0285714
2	1	3	0	-1	1	0.2390457	0.0571429
2	1	3	0	0	0	-0.2927700	0.0857143
2	1	3	0	1	-1	0.2390457	0.0571429
2	1	3	1	-1	0	-0.1690309	0.0285714
2	1	3	1	0	-1	0.2760262	0.0761905
2	1	3	1	1	-2	-0.3086067	0.0952381
2	1	3	2	-1	-1	0.0975900	0.0095238
2	1	3	2	0	-2	-0.2182179	0.0476190
2	1	3	2	1	-3	0.3779645	0.1428571
3	1	2	-3	1	2	0.3779645	0.1428571
3	1	2	-2	0	2	-0.2182179	0.0476190
3	1	2	-2	1	1	-0.3086067	0.0952381
3	1	2	-1	-1	2	0.0975900	0.0095238
3	1	2	-1	0	1	0.2760262	0.0761905
3	1	2	-1	1	0	0.2390457	0.0571429
3	1	2	0	-1	1	-0.1690309	0.0285714
3	1	2	0	0	0	-0.2927700	0.0857143
3	1	2	0	1	-1	-0.1690309	0.0285714
3	1	2	1	-1	0	0.2390457	0.0571429
3	1	2	1	0	-1	0.2760262	0.0761905
3	1	2	1	1	-2	0.0975900	0.0095238
3	1	2	2	-1	-1	-0.3086067	0.0952381
3	1	2	2	0	-2	-0.2182179	0.0476190
3	1	2	3	-1	-2	0.3779645	0.1428571
3	1	3	-3	0	3	0.3273268	0.1071429
3	1	3	-3	1	2	-0.1889822	0.0357143
3	1	3	-2	-1	3	-0.1889822	0.0357143
3	1	3	-2	0	2	-0.2182179	0.0476190
3	1	3	-2	1	1	0.2439750	0.0595238
3	1	3	-1	-1	2	0.2439750	0.0595238
3	1	3	-1	0	1	0.1091089	0.0119048
3	1	3	-1	1	0	-0.2672612	0.0714286
3	1	3	0	-1	1	-0.2672612	0.0714286
3	1	3	0	1	-1	0.2672612	0.0714286

3	1	3	1	-1	0	0.2672612	0.0714286
3	1	3	1	0	-1	-0.1091089	0.0119048
3	1	3	1	1	-2	-0.2439750	0.0595238
3	1	3	2	-1	-1	-0.2439750	0.0595238
3	1	3	2	0	-2	0.2182179	0.0476190
3	1	3	2	1	-3	0.1889822	0.0357143
3	1	3	3	-1	-2	0.1889822	0.0357143
3	1	3	3	0	-3	-0.3273268	0.1071429
3	1	4	-3	-1	4	0.3333333	0.1111111
3	1	4	-3	0	3	-0.1666667	0.0277778
3	1	4	-3	1	2	0.0629941	0.0039683
3	1	4	-2	-1	3	-0.2886751	0.0833333
3	1	4	-2	0	2	0.2182179	0.0476190
3	1	4	-2	1	1	-0.1091089	0.0119048
3	1	4	-1	-1	2	0.2439750	0.0595238
3	1	4	-1	0	1	-0.2439750	0.0595238
3	1	4	-1	1	0	0.1543034	0.0238095
3	1	4	0	-1	1	-0.1992048	0.0396825
3	1	4	0	0	0	0.2519763	0.0634921
3	1	4	0	1	-1	-0.1992048	0.0396825
3	1	4	1	-1	0	0.1543034	0.0238095
3	1	4	1	0	-1	-0.2439750	0.0595238
3	1	4	1	1	-2	0.2439750	0.0595238
3	1	4	2	-1	-1	-0.1091089	0.0119048
3	1	4	2	0	-2	0.2182179	0.0476190
3	1	4	2	1	-3	-0.2886751	0.0833333
3	1	4	3	-1	-2	0.0629941	0.0039683
3	1	4	3	0	-3	-0.1666667	0.0277778
3	1	4	3	1	-4	0.3333333	0.1111111
4	1	3	-4	1	3	0.3333333	0.1111111
4	1	3	-3	0	3	-0.1666667	0.0277778
4	1	3	-3	1	2	-0.2886751	0.0833333
4	1	3	-2	-1	3	0.0629941	0.0039683
4	1	3	-2	0	2	0.2182179	0.0476190
4	1	3	-2	1	1	0.2439750	0.0595238
4	1	3	-1	-1	2	-0.1091089	0.0119048
4	1	3	-1	0	1	-0.2439750	0.0595238
4	1	3	-1	1	0	-0.1992048	0.0396825
4	1	3	0	-1	1	0.1543034	0.0238095
4	1	3	0	0	0	0.2519763	0.0634921
4	1	3	0	1	-1	0.1543034	0.0238095
4	1	3	1	-1	0	-0.1992048	0.0396825
4	1	3	1	0	-1	-0.2439750	0.0595238
4	1	3	1	1	-2	-0.1091089	0.0119048

4	1	3	2	-1	-1	0.2439750	0.0595238
4	1	3	2	0	-2	0.2182179	0.0476190
4	1	3	2	1	-3	0.0629941	0.0039683
4	1	3	3	-1	-2	-0.2886751	0.8333333
4	1	3	3	0	-3	-0.1666667	0.0277778
4	1	3	4	-1	-3	0.3333333	0.1111111
4	1	4	-4	0	4	0.2981424	0.0888889
4	1	4	-4	1	3	-0.1490712	0.0222222
4	1	4	-3	-1	4	-0.1490712	0.0222222
4	1	4	-3	0	3	-0.2236068	0.0500000
4	1	4	-3	1	2	0.1972027	0.0388889
4	1	4	-2	-1	3	0.1972027	0.0388889
4	1	4	-2	0	2	0.1490712	0.0222222
4	1	4	-2	1	1	-0.2236068	0.0500000
4	1	4	-1	-1	2	-0.2236068	0.0500000
4	1	4	-1	0	1	-0.0745356	0.0055556
4	1	4	-1	1	0	0.2357023	0.0555556
4	1	4	0	-1	1	0.2357023	0.0555556
4	1	4	0	1	-1	-0.2357023	0.0555556
4	1	4	1	-1	0	-0.2357023	0.0555556
4	1	4	1	0	-1	0.0745356	0.0055556
4	1	4	1	1	-2	0.2236068	0.0500000
4	1	4	2	-1	-1	0.2236068	0.0500000
4	1	4	2	0	-2	-0.1490712	0.0222222
4	1	4	2	1	-3	-0.1972027	0.0388889
4	1	4	3	-1	-2	-0.1972027	0.0388889
4	1	4	3	0	-3	0.2236068	0.0500000
4	1	4	3	1	-4	0.1490712	0.0222222
4	1	4	4	-1	-3	0.1490712	0.0222222
4	1	4	4	0	-1	-0.2981424	0.0888889