

SOME PECULIARITIES OF A TECHNIQUE DEVELOPED FOR CALCULATING THE BROADENING OF SPECTRAL LINES OF TETRAHEDRAL MOLECULES. ROTATIONAL TRANSITIONS OF THE *A* AND *E* TYPES

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It is shown that symmetrized wave functions of tetrahedral molecules can be used to derive the calculational formulae for the coefficients of broadening of the spectral lines corresponding to the transitions from the energy levels with symmetry of the A_1 , A_2 , and E types. The formulae for the wave-breaking function taking into account the octupole–octupole, octupole–quadrupole, and dispersion interactions are derived in the Anderson–Tsao–Curnutte approximation. For A and E -type transitions the coefficients of pressure broadening of spectral lines of the ν_4 band of methane by air and nitrogen have been calculated. Comparison between experimental and computational data shows their good qualitative agreement.

INTRODUCTION

Advances in laser and Fourier spectroscopy call for an improved accuracy of calculations of the parameters of spectral lines. In particular, this concerns the calculations of half-widths and shifts of lines of tetrahedral molecules, typical example of which is the methane molecule. The peculiarities of tetrahedral splitting of spectrum make it impossible to measure directly the above-indicated parameters, which is why it is necessary to perform an exact calculation of broadening and shift of lines of molecules of this type. The applicability of the Anderson–Tsao–Curnutte⁶ theory of spectral line broadening to the study of various gases has already been proved. Based on this theory, self-broadening and broadening of linear and symmetric and asymmetric top molecules by foreign gases can be calculated.

Tejwani and Varanasi,¹ Yamomoto and Hirono,² and others generalize this theory to the molecules having nonzero first octupole moment in a ground state. Such highly symmetric molecules as CH_4 , SiF_4 , GeH_4 , SF_6 , and so on fall into this group.

In the Anderson–Tsao–Curnutte (ATC) approximation a main contribution to broadening comes from the wave breaking function $S_2(b)$. Calculational formulae for $S_2(b)$ including octupole interactions were presented in Refs. 1–5 and 7. A limitation of the calculational formulae obtained in Refs. 1–3 is that they were derived in the assumption of axisymmetric charge distribution in the methane molecule, using the wave function of a symmetric top. The last-mentioned results in the fact that the "strict" selection rules of octupole transitions are violated.

Neglect of a tetrahedral character of splitting of the methane spectrum results in the fact that the calculated values of line broadening coefficients corresponding to the transitions from rotational levels with different degrees of symmetry are equal in magnitude.^{1–7} This is totally inconsistent with the experimental data.^{8,9} For example, in Refs. 1–7 the difference between the calculated values

of broadening coefficients for rotational transitions of the A , E , and F -types becomes pronounced only for $J \leq 8$ exclusively due to the fact that not all necessary types of rotational symmetry at small J are taken into account in the wave functions, i.e., at $J \leq 8$ the number of possible nonradiating transitions differs strongly (with regard to the selection rules for octupole transitions).

Varanasi⁴ took into complete account the symmetry of a molecule and the character of tetrahedral spectrum splitting. He took into consideration the spherical character of charge distribution in methane and applied symmetrized rotational wave function to derive $S_2(b)$. These wave functions transform according to the representation of the symmetry group of a molecule. In so doing, the nonzero hexadecahedron moment of molecule and dispersion interaction between colliding particles were taken into consideration. We note that for broadening and shift of methane lines which have no pronounced dipole and quadrupole moments in the ground vibrational state, dispersion and induction interactions may be essential. The result obtained in Refs. 4 and 5 can be used to calculate broadening of the $F_1 \leftrightarrow F_2$ rovibrational transitions, but it is inapplicable to the $A_1 \leftrightarrow A_2$ and $E \leftrightarrow E$ transitions.

Such a limitation is caused by the fact that only for z -components of the F_1 and F_2 three-dimensional irreducible representations of the T_d symmetry group to which the methane molecule belongs, the wave functions have a compact form. Thus, only for the $F_1 \leftrightarrow F_2$ transition one can obtain simple enough expressions for the function $S_2(b)$.

In this paper, the formulae which can be used to calculate the coefficients of broadening of lines of molecules with the T_d symmetry corresponding to the transition from rovibrational energy levels with any types of symmetry A_1 , A_2 , E , F_1 , and F_2 are presented. We note that expressions for intermolecular interaction potential and octupole and hexadecahedron moments in tensor form were borrowed from Ref 4. The selection rule

for J on octupole transitions yields $\Delta J = 0, \pm 1, \pm 2, \pm 3$ rather than $\Delta J = \pm 1, \pm 3$ as was mentioned in Refs. 1, 2, and 7 for the model of axial charge distribution. The selection rules for the other quantum numbers on octupole transitions remain the same, that is, $A_1 \leftrightarrow A_2$, $E \leftrightarrow E$, $F_1 \leftrightarrow F_2$, and $\Delta n = 0$.

1. WAVE FUNCTIONS

As has already been mentioned, formulae derived in Ref. 4 can be used to calculate the broadening only on the $F_1 \leftrightarrow F_2$ transitions. This is connected with the fact that the author used the rotational wave functions derived by Ozier and Fox.¹⁰ These functions are transformed directly with the use of irreducible representation of the T_d group. But orthogonal functions were obtained only for symmetry levels F_1 and F_2 . The wave functions transforming with the use of irreducible representations A_1 , A_2 , and E required further numerical orthogonalization.

In our work we applied the wave functions obtained independently by Itano¹¹ and by Cheglov and Ulenikov.¹²

Owing to cumbersome form, the functions themselves are not presented here. For further calculations it is convenient to write down the rotational wave functions $|JK\Gamma M\rangle$ in more universal and compact form. As usually, here J and K are the rotational quantum numbers, M is the magnetic quantum number, and Γ is the number indicating the symmetry of the energy level.

After simple manipulation on account of the fact that for even M and M'

$$d_{MM'}^J\left(\frac{\pi}{2}\right) = (-1)^J d_{M-M'}^J\left(\frac{\pi}{2}\right),$$

the functions transforming according to representations $\Gamma = A_1, A_2, E, F_1$, and F_2 of the T_d group may be written in the compact form

$$|JK\Gamma M\rangle = A_K^{J\Gamma} \sum_{\tilde{K}} B_{KK}^{J\tilde{\Gamma}} (|J\tilde{K}M\rangle + \tau^\Gamma (-1)^J |J - \tilde{K}M\rangle). \quad (1)$$

Here $|JKM\rangle$ are the known functions of a symmetric top

$$|JKM\rangle = \left(\frac{2J+1}{8\pi^2}\right) D_{MK}^J(\alpha \beta \gamma)^*, \quad (2)$$

where α , β , and γ are Eulerian angles. The magnitudes of the coefficients $A_K^{J\Gamma}$, $B_{KK}^{J\tilde{\Gamma}}$, and τ^Γ for various degrees of symmetry Γ are listed in Table I. The necessary coefficients are given for both components of doubly degenerate state E (due to the fact that only the $E_1 \leftrightarrow E_2$ transitions occur) and only for the z -components of the triple degenerate states F_1 and F_2 (for calculation of line broadening and shift it is sufficient to consider the transitions between the components $F_1^z \leftrightarrow F_2^z$).

Hereinafter for brevity $d_{K\tilde{K}}^J \equiv d_{K\tilde{K}}^J\left(\frac{\pi}{2}\right)$ are the components of the Wigner function. In equations (1) the indices K take only positive values with a step being equal to 4. Summation over indices \tilde{K} is performed up to J inclusively, and the number of functions with different \tilde{K} must be equal to the number of symmetry sublevels Γ at the level with the given J (see Refs. 10–12).

TABLE I.

Γ	K	\tilde{K}	$A_K^{J\Gamma}$	$B_{KK}^{J\tilde{\Gamma}}$	τ^Γ
A_1	0, 4, 8	0, 4, 8	$1/\sqrt{6}$	$4d_{K\tilde{K}}^J + \delta_{K\tilde{K}}$	1
A_2	2, 6, 10, 2, 6, 10	2, 6, 10	$1/\sqrt{6}$	$4d_{K\tilde{K}}^J - \delta_{K\tilde{K}}$	1
E_1	0, 4, 8	0, 4, 8	$1/2\sqrt{6}$	$4d_{K\tilde{K}}^J - 2\delta_{K\tilde{K}}$	1
E_2	0, 4, 8	2, 6, 10	-2	$d_{K\tilde{K}}^J$	1
F_1^z	0, 4, 8	0, 4, 8	$\frac{1 - (-1)^J \delta_{K0}}{\sqrt{2} (1 + \delta_{K0})^{3/2}}$	$\delta_{K\tilde{K}}$	-1
F_2^z	2, 6, 10, 2, 6, 10	2, 6, 10	$1/\sqrt{2}$	$\delta_{K\tilde{K}}$	-1

As was noted in Refs. 10–12, the vibrational functions of type (1) for the A_1 , A_2 , and E symmetry are not orthogonal. Numerical orthogonalization makes it impossible to obtain the equation for the wave breaking function $S_2(b)$. It was shown in Ref. 12 that it is possible to orthogonalize this function in analytical form. The orthogonalization of functions is carried out according to the formula

$$|JK\Gamma M\rangle_{\text{ort}} = \sum_{K=L}^K \alpha_{K\tilde{K}}^{J\Gamma} |\tilde{J}\tilde{K}\Gamma M\rangle, \quad (3)$$

where the coefficients are represented by the following equations:

$$\alpha_{KK}^{J\Gamma} = \left\{ 1 + \delta_{K0} (-1)^J + (4(-1)^J - 6\delta_{\Gamma E}) d_{KK}^J - \sum_{l=L}^{K-4} \sum_{\substack{i \leq l \\ j \leq l}} \alpha_{li}^{J\Gamma} \alpha_{ij}^{J\Gamma} [\delta_{Ki} + (4(-1)^\Gamma - 6\delta_{\Gamma E}) d_{Ki}^J] \times \right. \\ \left. \times [\delta_{Kj} + (4(-1)^\Gamma - 6\delta_{\Gamma E}) d_{Kj}^J] \right\}^{-1/2}, \quad (4)$$

$$\alpha_{Kl}^{J\Gamma} = -\alpha_{KK}^{J\Gamma} \sum_{i=l}^{K-4} \sum_{j=L}^i \alpha_{ij}^{J\Gamma} \alpha_{il}^{J\Gamma} [\delta_{Kj} + (4(-1)^\Gamma - 6\delta_{\Gamma E}) d_{Kj}^J]. \quad (5)$$

The term $(-1)^\Gamma$ in Eqs. (4) and (5) is equal to $(-1)^{A_2} = -1$; $(-1)^{A_1} = (-1)^E = 1$, and L is equal to the initial value of K from Table II.

Substituting Eq. (1) into Eq. (3), we derive the final compact expression for the orthogonal functions, transforming according to A_1 , A_2 , and E representations.

The possible values of the indices K , \tilde{K} , and K^* entering into the formula

$$|JK\Gamma M\rangle = \sum_{\tilde{K}=L}^K \alpha_{K\tilde{K}}^{J\Gamma} A_{\tilde{K}}^{J\Gamma} \sum_{K^*} B_{K\tilde{K}K^*}^{J\Gamma} \times \\ \times (|JK^*M\rangle + \tau^\Gamma (-1)^J |J - K^*M\rangle) \quad (6)$$

are listed in Table II.

TABLE II.

Γ	A_1	A_2	E	F_1	F_2
K, \tilde{K}	0, 4, 8	2, 6, 10	0, 4, 8, 12, 16	0, 4, 8	2, 6, 10
K^*	0, 4, 8	2, 6, 10	0, 4, 8, 2, 6, 10	0, 4, 8	2, 6, 10

2. THE FUNCTION $S_2(b)$ FOR OCTUPOLE INTERACTIONS

The salient points of the theory of spectral line pressure broadening were discussed at length in Refs. 1, 4, and 6; therefore, here we note only some moments and consider as an example the expression for the function $S_2(b)$ in some important cases of multipole interactions, being significant when calculating the spectral line broadening of methane.

In the ATC approximation (Ref. 6) $S_2(b)$ (more precisely $S_2(b)_0$) is calculated according to the following formula:

$$S_2(b)_0 = \frac{1}{2} \sum_{M_i M_2} \frac{(J_i K_i M_i J_2 K_2 M_2 | P^2 | J_i K_i M_i J_2 K_2 M_2)}{(2J_i + 1)(2J_2 + 1)} + \sum_{M_f M_2} \frac{(J_f K_f M_f J_2 K_2 M_2 | P^2 | J_f K_f M_f J_2 K_2 M_2)}{(2J_f + 1)(2J_2 + 1)}, \quad (7)$$

where

$$P = \int_{-\infty}^{\infty} U_0^{-1} H_c(t) U_0 dt, \quad (8)$$

$$(m | P | n) = \int_{-\infty}^{\infty} \exp(i \omega_{mn} t) (m | H_c(t) | n) dt. \quad (9)$$

Here $H_c(t)$ is a part of the intermolecular potential responsible for the concrete multipole interaction. The expressions for $H_c(t)$ (of CH_4) can be found in Refs. 2 and 4. The possible simplification

$$\begin{aligned} \sum_{M_i M_2} (J_i K_i M_i J_2 K_2 M_2 | P^2 | J_i K_i M_i J_2 K_2 M_2) &= \\ = \sum_{\substack{J'_i K'_i M'_i \\ J'_2 K'_2 M'_2}} |(J_i K_i M_i J_2 K_2 M_2 | P^2 | J'_i K'_i M'_i J'_2 K'_2 M'_2)|^2. \end{aligned} \quad (10)$$

is an important property of the operator P which can be used for calculation of the matrix elements in Eq. (7).

The matrix elements of Eqs. (7)–(10), in analogy with Ref. 6, are written on the basis of a symmetric top. We apply wave functions (6) and data listed in Tables I and II to calculate Eq. (7).

Introducing the designation

$$\begin{aligned} R_{J' C' K'}^{J \Gamma K} &= \left| \sum_{\tilde{K}=L}^{K, K'} \sum_{\tilde{K}^*=K^*, K^{**}} \alpha_{\tilde{K} \tilde{K}^*}^{J \Gamma} A_{\tilde{K}}^{J \Gamma} B_{\tilde{K} \tilde{K}^*}^{J \Gamma} \alpha_{\tilde{K} \tilde{K}^*}^{J' \Gamma'} A_{\tilde{K}'}^{J' \Gamma'} B_{\tilde{K}' \tilde{K}^{**}}^{J' \Gamma'} \times \right. \\ &\quad \left. \times [(-1)^{J'} (C_{JK3-2}^{J' K'} - C_{JK32}^{J' K'}) + \tau^\Gamma C_{JK3-2}^{J' -K'}] \right|^2, \end{aligned} \quad (11)$$

we can represent $S_2(b)_0$ in a very compact form. Dropping out cumbersome intermediate calculations, we note only that in the derivation of the resultant expressions the following symmetry relations for the Klebsch–Gordan coefficients¹³ were used:

$$\sum_{M, M'} (C_{J3M'm}^{JM})^2 = \frac{(2J+1)}{7}, \quad \sum_{K'} C_{JK32}^{J' K'} C_{JK3-2}^{J' K'} = 0,$$

$$C_{aab\beta}^{c\gamma} = (-1)^{b+\beta} \frac{2c+1}{2a+1} C_{c-\gamma b\beta}^{c-\alpha}.$$

a) Octupole – octupole interaction

$$S_2(b)_0 = \frac{16384}{1225} \left(\frac{\Omega_1 \Omega_2}{h \nu} \right)^2 \frac{1}{b^{12}} \sum_{\substack{J_i \Gamma_i K_i \\ J_2 \Gamma_2 K_2}} R_{J_i \Gamma_i K_i}^{J_i \Gamma_i K_i} R_{J_2 \Gamma_2 K_2}^{J_2 \Gamma_2 K_2} f_5(k) + [i \rightarrow f]. \quad (12)$$

b) Octupole – quadrupole interaction

$$S_2(b)_0 = \frac{2048}{875} \left(\frac{\Omega_1 \Omega_2}{h \nu} \right) \frac{1}{b^{10}} \sum_{J_2} R_{J_i \Gamma_i K_i}^{J_i \Gamma_i K_i} (C_{J_2 0 2 0}^{J_2 0})^2 f_4(k) + [i \rightarrow f]. \quad (13)$$

c) Dispersion contributions

$$S_2(b)_0 = \frac{510p^2}{57344} \left(\frac{U_1 U_2}{U_1 + U_2} \frac{\alpha_2 A_1}{h \nu} \right)^2 \frac{1}{b^{12}} \sum_{J_i \Gamma_i K_i} R_{J_i \Gamma_i K_i}^{J_i \Gamma_i K_i} g_4(k) + [i \rightarrow f]. \quad (14)$$

In expressions (12)–(14), as usually, index 1 refers to an absorbing molecule and 2 – to a buffer molecule, i and f denote the lower and upper states of transitions. Ω is the octupole moment and Θ is the quadrupole moment. Designations of the rest quantities and concrete expressions for resonance functions $f_4(k)$, $f_5(k)$, and $g_4(k)$ can be found in Refs. 1–6.

For the cases of pressure broadening the part of the function $S_2(b)_m$, responsible for elastic collisions, is equal to zero, which is why the expressions for $S_2(b)_m$ are not presented here.

3. CALCULATION OF THE BROADENING OF LINES OF THE ν_4 BAND OF CH_4

As an example, let us calculate by the obtained formulae the line broadening of the P and R –branches of the ν_4 band of methane corresponding to the transitions from the energy levels with symmetry of the A_1 , A_2 , and E types. We also compare the obtained results with those reported in Ref. 9 and with the results of earlier calculations. Let us consider the case of pressure broadening of spectral lines of CH_4 by nitrogen and air. In so doing, the largest contribution to the broadening comes from octupole – quadrupole interaction. The constant dipole moment, arising in the ground state due to rovibrational interaction, is too small to make considerable contribution to broadening.

As usually, the coefficient of pressure broadening by air is equal to

$$\gamma_{\text{air}} = 0.79\gamma_{\text{N}_2} + 0.21\gamma_{\text{O}_2}.$$

For the ATC model^{1,2,4,6}

$$\nu_{J_i \Gamma_i K_i}^0 = \frac{n \nu}{2\pi c} \sum_{J_2} \rho_{J_2} \sigma_{J_2}, \tag{15}$$

$$\sigma_{J_2} = \pi b_0^2 [1 + S_2(b)_0],$$

where b_0 is the impact parameter, n is the molecular density at a pressure of 1 atm, ν is the rate of collision of molecules, ρ_{J_2} is the Boltzmann population of the level J_2 of a buffer molecule, σ_{J_2} is the collision cross section. The calculations were performed at a pressure of 1 atm and $T = 296$ K. The energy levels of ground and excited states were calculated with the use of rotational constants and constants of tetrahedral splitting reported in Ref. 14. In so doing, only diagonal matrix elements of Hamiltonian were taken into account.

The results of calculations for the cases of pressure broadening of lines with symmetry of A and E types by nitrogen and air are listed in Tables III and IV. The results for small values of J are absent, because the pressure broadening of lines with small J by nitrogen was not experimentally observed in Ref. 9.

TABLE III. Coefficients of pressure broadening of lines of the ν_4 band by N_2 ($\text{cm}^{-1}\cdot\text{atm}^{-1}$).

J	Γ	n	Experiment, Ref. 9	AFGL, Ref. 9	Calculation, Ref. 7	Our calculation
P_6	A_1	1	0.0580	0.0510	0.0527	0.0565
P_6	A_2	1	0.0599	0.0510	0.0527	0.0618
P_6	E	1	0.0586	0.0570	0.0601	0.0607
P_7	A_2	1	0.0574	0.0570	0.0600	0.0600
P_7	E	1	0.0461	0.0570	0.0600	0.0592
P_8	A_1	1	0.0515	0.0550	0.0576	0.0523
P_8	E	1	0.0465	0.0550	0.0581	0.0491
P_9	A_2	1	0.0570	0.0540	0.0567	0.0625
P_9	E	1	0.0505	0.0540	0.0567	0.0560
P_{10}	A_1	1	0.0544	0.0530	0.0555	0.0602
P_{10}	A_2	1	0.0448	0.0520	0.0555	0.0587
R_8	A_1	1	0.0481	0.0540	0.0576	0.0572
R_8	E	1	0.0521	0.0540	0.0581	0.0670
R_9	A_1	1	0.0539	0.0530	0.0567	0.0682
R_9	A_2	1	0.0481	0.0540	0.0567	0.0572

TABLE IV. Coefficients of pressure broadening of lines with symmetry of the A and E types by air.

J	Γ	n	Experiment, Ref. 9	Experiment, Ref. 8	AFGL, Ref. 9	Calculation, Ref. 7	Our calculation
P_2	E	1	0.0654		0.0530	0.0531	0.0632
P_3	A_2	1	0.0618		0.0580	0.0582	0.0622
P_4	A_1	1	0.0635		0.0470	0.0466	0.0632
P_4	E	1	0.0579		0.0550	0.0547	0.0603
P_5	E	1	0.0556		0.0610	0.0612	0.0584
P_6	A_1	1	0.0586		0.0510	0.0508	0.0625
P_6	A_2	1	0.0607		0.0510	0.0508	0.0558
P_6	E	1	0.0603		0.0570	0.0569	0.0647
P_7	A_2	1	0.0575		0.0570	0.0569	0.0622
P_7	E	1	0.0466		0.0570	0.0569	0.0543
P_8	A_1	1	0.0521		0.0550	0.0547	0.0523
P_8	E	1	0.0477		0.0550	0.0552	0.0543
R_0	A_1	1	0.0556		0.0610		0.0550
R_2	E	1	0.0571	0.0534	0.0490		0.0632
R_3	A_2	1	0.0576		0.0550		0.0678
R_4	A_1	1	0.0608	0.0586	0.0450		0.0632
R_4	E	1	0.0567	0.0547	0.0530		0.0603
R_5	E	1	0.0553		0.0590		0.0584
R_6	A_1	1	0.0584		0.0500		0.0624
R_6	A_2	1	0.0591		0.0500		0.0701
R_6	E	1	0.0556		0.0560		0.0572
R_7	A_2	1	0.0555		0.0550		0.0549
R_7	E	1	0.0461		0.0550		0.0543
R_8	A_1	1	0.0497		0.0540		0.0520
R_8	E	1	0.0519		0.0540		0.0616

CONCLUSIONS

These results are preliminary and must be refined. First, we took into consideration only octupole–quadrupole and fundamental dispersion interactions and ignored finer effects. Second, we did not adjust the parameters Ω , Θ , and b_{\min} . The

matter is that the values of Ω and Θ in various experiments differ strongly, resulting in large variation of $S_2(b)$. The values of Ω and Θ were borrowed by us from Ref. 5.

At present, there are a great number of experimental results on line broadening, but only some of them can be compared with the calculational results, because in the most

papers the data are reported for individual lines or they are represented in graphical form. Our data from Tables III and IV show the pronounced differences between the calculated values of the broadening coefficients corresponding to the transitions from the energy level with symmetry of the A_1 , A_2 , and E types. Such a dependence was not observed in the results of calculations of the other authors.

In conclusion it should be noted that the obtained formulae can be used to calculate the broadening of lines with the symmetry of the A , E , and F types.

Expressions (11) and (12) seem to be cumbersome, but in concrete calculations they simplify because in accordance with the selection rules the summation over certain indices is cancelled (for example, over Γ'_i and K'_i).

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