On the study of XY_2 $(m_y \ll m_x)$ plane molecules

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Abstract

The 'expanded local mode approach' derived in Ref. [1] (Ulenikov et al., Spectrochim. Acta Part A, 52 (1996) 1829) is modified in an appropriate way for the analysis of XY_2 (C_{2v}) molecules having an arbitrary value of the equilibrium interbond angle $2\alpha_e$. It is shown that the conditions considered allow one to estimate with good enough accuracy the harmonic frequencies (quadratic force field parameters) of a molecule on the basis of experimental information on pure rotational spectra only. © 1997 Elsevier Science B.V.

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1. Introduction

In Ref. [1] we have shown that for XY_2 (C_{2v} symmetry) molecules with a value of the equilibrium interbond angle $2\alpha_e$ near to $\pi/2$ and $m_y/m_x \ll 1$ (we will further denote $m_y \equiv m$, $m_x \equiv M$), analysis of the properties of $l_{N\alpha\lambda}$ transformation

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[1] The first systematic study of the rotational energy level structure of XY_2 (C_{2v}) molecules in the strict local mode limit was made by Halonen and Robiette in Ref. [2]. They assumed (a) that mass M of the central nucleus X is far greater than the masses m of the nuclei Y, and in the limit $(m/M) = 0$, (b) that the equilibrium angle $2\alpha_e = \pi/2$, and (c) that deformational

motion is totally absent in a molecule, and in the potential function V only changes of valence bond lengths Δr_i ($i = 2,3$) are taken into account (in this case $f_{rr'} = f_{r\alpha} = f_{\alpha\alpha} = 0$). In Ref. [1] we have retained conditions (a) and (b), but rejected conditions (c).

coefficients and of the intramolecular potential function V provides the possibility to improve on results of the local mode approach formerly given in the spectroscopic literature[1] and to derive new relations, e.g., between centrifugal distortion parameters (for more details, see Ref. [1]). In this case, the main idea of Ref. [1] was an analytical determination and analyzing of the ambiguous parameter $\sin \gamma$, which the $l_{N\alpha\lambda}$ transformation coefficients depend on, in a simple form. In turn, that gave us the possibility to obtain simple relations between the $\zeta^\alpha_{\lambda\mu}$ and $a^{\chi\beta}_\lambda$ parameters and, as a consequence, between different spectroscopic parameters.

It should be mentioned here that the condition $2\alpha_e = \pi/2$ restricts the number of molecules to which the results of Ref. [1] can be applied. In this respect it would be interesting to apply the procedure used in Ref. [1] to a more general situation

with arbitrary value of the interbond angle $2\alpha_e$ and to look at the consequences of such a consideration for some spectroscopic problems.

Thus, in Section 2 an approach is considered that allows the possibility of determining the ambiguous parameter $\sin \gamma$ for any value of equilibrium interbond angle $2\alpha_e$ under the condition $m/M \ll 1$. Section 3 presents formulas obtained under the above conditions for the Coriolis $\zeta_{\lambda\mu}^{\alpha}$ and $a_{\lambda}^{\chi\beta}$ parameters. In Section 4 centrifugal distortion parameters, which are obtained as a result of the above approximation, are considered. And in Section 5 a procedure is discussed which allows one to estimate with good enough accuracy the harmonic frequencies (quadratic force field parameters) of a molecule on the basis of experimental information on pure rotational spectra only.

2. Potential function and determination of sin γ parameter

As was mentioned in Ref. [1], in the general case the Coriolis $\zeta_{\lambda\mu}^{\alpha}$ and vibration–rotation α_{λ}^{β} parameters of an XY_2 (C_{2v}) molecule have the following form:

$$\zeta_{13} = \zeta_{13}^{y} = -\zeta_{31}^{y} = -\sqrt{\frac{I_{xx}^{e}}{I_{yy}^{e}}}\sin \gamma + \sqrt{\frac{I_{zz}^{e}}{I_{yy}^{e}}}\cos \gamma,$$

$$\zeta_{23} = \zeta_{23}^{y} = -\zeta_{32}^{y} = \sqrt{\frac{I_{xx}^{e}}{I_{yy}^{e}}}\cos \gamma + \sqrt{\frac{I_{zz}^{e}}{I_{yy}^{e}}}\sin \gamma, \quad (1)$$

and

$$a_1^{xx} = 2I_{xx}^{e1/2}\cos \gamma, \ a_1^{zz} = 2I_{zz}^{e1/2}\sin \gamma,$$

$$a_2^{xx} = 2I_{xx}^{e1/2}\sin \gamma, \ a_2^{zz} = -2I_{zz}^{e1/2}\cos \gamma,$$

$$a_1^{yy} = 2I_{yy}^{e1/2}\zeta_{23}, \ a_2^{yy} = -2I_{yy}^{e1/2}\zeta_{13},$$

$$a_3^{xz} = a_3^{zx} = -2\left(\frac{I_{xx}^{e}I_{zz}^{e}}{I_{yy}^{e}}\right)^{1/2}. \quad (2)$$

In this case, $\sin \gamma$ is an ambiguous parameter which can be obtained from the condition

$$W_{12} \equiv (\partial^2 V/\partial q_1 \partial q_2)_{q=0} = 0, \quad (3)$$

where the quadratic part $V_{(2)}$ of the potential function has the form

$$V_{(2)} = \tfrac{1}{2}f_{rr}(\Delta r_2^2 + \Delta r_3^2) + f_{rr'}\Delta r_2\Delta r_3 + \tfrac{1}{2}f_{\alpha\alpha}(r_e\Delta\alpha)^2$$

$$+ f_{r\alpha}(\Delta r_2 + \Delta r_3)r_e\Delta\alpha. \quad (4)$$

As was shown in Ref. [1], Eq. (3) can be exactly transformed to a form convenient for further analysis[2]:

$$A\cos 2\gamma = B\sin 2\gamma, \quad (5)$$

where

$$\left(\frac{M}{2m+M}\right)^{1/2}\left(\frac{A}{\sin 2\alpha_e}\right)$$

$$= f_{rr} + f_{rr'} - 2f_{\alpha\alpha} + 4f_{r\alpha}\frac{\cos 2\alpha_e}{\sin 2\alpha_e} \quad (6)$$

and

$$BM = (f_{rr} + f_{rr'})(M\sin^2\alpha_e - (2m+M)\cos^2\alpha_e)$$

$$+ \frac{2f_{\alpha\alpha}}{\sin^2 2\alpha_e}(M\sin^2\alpha_e(1+\cos 2\alpha_e)^2$$

$$- (2m+M)\cos^2\alpha_e(1-\cos 2\alpha_e)^2)$$

$$+ \frac{2f_{r\alpha}}{\sin 2\alpha_e}(M\sin^2\alpha_e(1+\cos 2\alpha_e)^2$$

$$+ (2m+M)\cos^2\alpha_e(1-\cos 2\alpha_e)^2). \quad (7)$$

It should be mentioned that Eq. (7) can be exactly transformed to a simpler form:

$$B = (-f_{rr} - f_{rr'} + 2f_{\alpha\alpha})\cos 2\alpha_e + 2f_{r\alpha}\sin 2\alpha_e$$

$$+ \frac{2m}{M}(-2f_{\alpha\alpha}\sin^2\alpha_e - (f_{rr}+f_{rr'})\cos^2\alpha_e$$

$$+ 2f_{r\alpha}\sin^2\alpha_e\sin 2\alpha_e). \quad (8)$$

Now, (1) if one assumes that all three conditions (a), (b) and (c) of footnote 1 are fulfilled, then the results of the Strict Local Mode Approach can be obtained at once; (2) if one assumes that conditions (a) and (b) are fulfilled (condition (c) is not fulfilled), then the results and relations of the Expanded Local Mode Approach will be obtained [1].

Now let us analyze the situation where only the condition $m/M \ll 1$ is fulfilled. Moreover, in the further discussion let us keep only terms which

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[2] It should be mentioned that Eq. (18) of Ref. [1] is a simple consequence of Eq. (5) of the present paper.

are proportional to $(m/M)^1$, and omit terms which are proportional $(m/M)^n$ with $n > 1$. In this case, Eq. (5) can be transformed to the following form:

$$\frac{\cos 2\alpha_e}{\sin 2\alpha_e}\sin 2\gamma = -\cos 2\gamma + O(m/M), \quad (9)$$

where

$$O(m/M) = \frac{4f_{r\alpha}}{f_{rr}}\frac{\cos^4\alpha_e + \sin^4\alpha_e}{\sin 2\alpha_e} - \frac{m}{M}. \quad (10)$$

In fact, in obtaining Eq. (9) it was taken into account that for molecules of the considered type the conditions $f_{r\alpha}/f_{rr} \ll 1$, $f_{\alpha\alpha}/f_{rr} \ll 1$ and $f_{rr}/f_{rr} \ll 1$ are valid (at least, there are many molecules of the type with $m/M \ll 1$ which satisfy these conditions). In this case, after substituting Eqs. (6) and (8) into Eq. (5) and omitting terms proportional to $(m/M)^n$ ($n > 1$) or $(m/M)^l(f/f_{rr})$ ($l \geq 1$, $f = f_{\alpha\alpha}$, $f_{r\alpha}$, or f_{rr}) one will simply obtain Eq. (9).

If one now looks at Eq. (10), one can see that its two parts have opposite signs, because both $f_{r\alpha}$ and f_{rr}, and $\sin 2\alpha$ have positive values. Moreover, as the analysis of situations in the literature shows (see, e.g., Ref. [3]) the two parts of Eq. (10) partially compensate each other. At least, one can assume that the second part $O(m/M)$ of Eq. (9) is a small value of the order $(m/M)^n$ (with $n > 1$), and it can be omitted. After this assumption one will obtain a very simple relation for the ambiguous parameter γ, namely

$$\tan 2\gamma = -\tan 2\alpha_e. \quad (11)$$

Eq. (11) now gives the possibility of obtaining the value of angle γ, and, as a consequence, of parameter $\sin \gamma$ which the transformation coefficients, $l_{N\alpha\lambda}$, Coriolis $\zeta_{\lambda\mu}^\alpha$ and vibration–rotation $a_\lambda^{\chi\beta}$ parameters depend on:

$$(\gamma + \alpha_e) = 0, \pm \pi/2, \pi. \quad (12)$$

As can be seen from further analysis, the solutions $(\gamma + \alpha_e) = 0$ and $(\gamma + \alpha_e) = \pi$ are physically unreasonable, because values $(\gamma + \alpha_e) = 0$ or π lead to an absolute value of the ζ_{13}^γ parameter equal to 1. Solutions $\pi/2$ and $-\pi/2$ lead to one and the same result. For this reason we will further consider only $(\gamma + \alpha_e) = \pi/2$. The last leads to the following result:

$$\sin \gamma = \cos \alpha_e \text{ and } \cos \gamma = \sin \alpha_e. \quad (13)$$

To illustrate this deduction, Table 1 presents values of parameter $\sin \gamma$ calculated with formula (11) (Column 2) and corresponding values of $\sin \gamma$ for the molecules H_2O, H_2S and H_2Se taken from Ref. [3] (Column 3). One can see a satisfactory correspondence (about 2–4 per cent) of the pairs of values. The second part of Table 1 presents values of $\sin \gamma$ also for the PH_2, CH_2 and SiH_2 free radicals. The values of angles α_e necessary for the calculations have been taken from references marked in Column 4 of Table 1. It should be mentioned here that the value of parameter $\sin \gamma$ for a molecule can be obtained, in principle, from a known value of the Coriolis parameter $\zeta_{\lambda\mu}^\alpha$ (see, e.g., Eq. (1) of the present paper, or the discussion in Refs. [7,8]), or from isotopic relations between the harmonic frequencies w_1 and w_2 of initial YH_2 and deuterated YD_2 species (see, e.g., Eq. (81) of Ref. [9]). However, both these methods require additional experimental data about excited vibrational states. At the same time, Eq. (11) only requires knowledge of angle α_e.

3. Coriolis $\zeta_{\lambda\mu}^\alpha$ and $a_\lambda^{\chi\beta}$ parameters

Before speaking about the $\zeta_{\lambda\mu}^\alpha$ and $a_\lambda^{\chi\beta}$ parameters, let us mention that for XY_2 (C_{2v} symmetry) molecules the following exact relations between equilibrium moments of inertia and equilibrium rotational constants are fulfilled:

Table 1
Values of parameter $\sin \gamma$ for some XY_2 molecules

1 Molecule	2 $\sin \gamma$ (our)	3 $\sin \gamma$	4 Ref.
H_2O	0.6122	0.5913	[3]
H_2S	0.6934	0.6670	[3]
H_2Se	0.7014	0.6797	[3]
CH_2 ($\tilde{a}^1A_1$)	0.6266		[4]
CH_2 ($\tilde{b}^1B_1$)	0.3190		[4]
SiH_2 ($\tilde{x}^1X_1$)	0.6947		[5]
SiH_2 ($\tilde{a}^1B_1$)	0.4772		[5]
PH_2 ($\tilde{x}^1B_1$)	0.6972		[6]
PH_2 ($\tilde{a}^1A_1$)	0.4840		[6]

$$\frac{I^c_{xx}}{\sin^2\alpha_e} - I^e_{zz}\frac{M+2m}{M\cos^2\alpha_e} - I^e_{yy}\frac{M+2m}{M+2m\sin^2\alpha_e} = 2mr^2_e$$

$$\equiv I_e \tag{14}$$

and

$$B^e_x\sin^2\alpha_e = B^e_z\frac{M\cos^2\alpha_e}{M+2m} = B^e_y\frac{M+2m\sin^2\alpha_e}{M+2m} \equiv B_e/2, \tag{15}$$

where

$$B_e = \frac{\hbar}{4\pi c}(mr^2_e)^{-1}.$$

After this remark, by using Eq. (13) in Eq. (1) one can obtain

$$\zeta_{13} = \zeta^x_{13} = -\zeta^x_{31} = -\frac{m\sin 2\alpha_e}{2M}, \ \zeta_{23} = \zeta^y_{23} = -\zeta^y_{32}$$

$$= 1; \tag{16}$$

and

$$\frac{a^{xx}_1}{\sin^2\alpha_e} = \frac{a^{xx}_2}{\sin\alpha_e\cos\alpha_e} = \left(1 + \frac{m}{M}\right)\frac{a^{zz}_1}{\cos^2\alpha_e}$$

$$= -\left(1 - \frac{m}{M}\right)\frac{a^{zz}_2}{\sin\alpha_e\cos\alpha_e}$$

$$= \left(1 - \frac{m}{M}\cos^2\alpha_e\right)a^{yy}_1$$

$$= \left(1 + \frac{m}{M}\sin^2\alpha_e\right)\frac{a^{xz}_3}{\sin\alpha_e\cos\alpha_e} = 2\sqrt{I_e}.$$

$$a^{yy}_2 = \frac{m}{M}\sin 2\alpha_e\sqrt{I_e}. \tag{17}$$

In Eqs. (16) and (17), as in Eq. (9), we omitted terms proportional to $(m/M)^n$ $(n > 1)$.

4. Quartic centrifugal distortion constants

It is well known (see, e.g., Ref. [10]) that quartic centrifugal distortion coefficients $\tau_{\alpha\beta\gamma\delta}$ in the general case have the following form:

$$\tau_{\alpha\beta\gamma\delta} = -\sum_\lambda\frac{\mu^\lambda_{\alpha\beta}\mu^\lambda_{\gamma\delta}}{2\omega_\lambda}, \tag{18}$$

where

$$\mu^\lambda_{\alpha\beta} = -2\frac{B^e_\alpha B^e_\alpha}{\sqrt{\omega_\lambda}}\sqrt{\frac{8\pi c}{\hbar}}a^{\alpha\beta}_\lambda. \tag{19}$$

Substitution of relations Eqs. (14)–(16) into Eqs. (18) and (19) leads to the following expressions for τ-parameters:

$$\tau_{xxxx} = -\frac{2B^3_e}{\sin^6\alpha_e}\left(\frac{\sin^2\alpha_e}{\omega^2_1} + \frac{\cos^2\alpha_e}{\omega^2_2}\right),$$

$$\tau_{zzzz} = -\frac{2B^3_e}{\cos^6\alpha_e}\left(\frac{\cos^2\alpha_e}{\omega^2_1} + \frac{\sin^2\alpha_e}{\omega^2_2}\right)\left(1 + \frac{6m}{M}\right),$$

$$\tau_{yyyy} = -\frac{2B^3_e}{\omega^2_1}\left(1 + \frac{6m}{M}\cos^2\alpha_e\right),$$

$$\tau_{xxzz} = -\frac{2B^3_e}{\sin^2\alpha_e\cos^2\alpha_e}\left(\frac{1}{\omega^2_1} - \frac{1}{\omega^2_2}\right)\left(1 + \frac{3m}{M}\right),$$

$$\tau_{xxyy} = -\frac{2B^3_e}{\sin^2\alpha_e}\left(\frac{1}{\omega^2_1}\left[1 + \frac{3m}{M}\cos^2\alpha_e\right]\right.$$
$$\left. + \frac{1}{\omega^2_2}\frac{m}{M}\cos^2\alpha_e\right),$$

$$\tau_{zzyy} = -\frac{2B^3_e}{\cos^2\alpha_e}\left(\frac{1}{\omega^2_1}\left[1 + \frac{3m}{M}(1 + \cos^2\alpha_e)\right]\right.$$
$$\left. - \frac{1}{\omega^2_2}\frac{m}{M}\sin^2\alpha_e\right),$$

$$\tau_{xzxz} = -\frac{2B^3_e}{w^2_3\sin^2\alpha_e\cos^2\alpha_e}\left(1 + \frac{2m}{M}(1 + \cos^2\alpha_e)\right). \tag{20}$$

In turn, the well-known relations (51) from Ref. [11] allow one to connect the $\tau_{\alpha\beta\gamma\delta}$ parameters from Eq. (20) with Δ_K, Δ_{JK}, Δ_J, δ_K and δ_J parameters determined from experimental data. As a consequence, any experimentally determined Δ_K, Δ_{JK}, Δ_J, δ_K or δ_J parameter can be expressed as a simple function of the harmonic frequencies ω_1, ω_2, ω_3, of B_e and $\sin\alpha_e$. To illustrate this, Table 2 presents results of calculations of centrifugal distortion parameters for one of the most inconvenient molecules from the viewpoint of theoretical predictions, H_2O, on the basis of Eq. (20) and, for comparison, values of the same parameters obtained from experimental data (when we speak of the inconvenience of the H_2O molecule for theoretical predictions we mean the presence of such effects as strong resonance interactions and anomalously large bending effects which can strongly perturb both the picture of the spectrum

Table 2
Centrifugal distortion parameters of H_2O, D_2O, H_2S and H_2Se molecules (in 10^4 cm^{-1})

Parameter	Calc.	Exp.	Ref.
H_2O			
Δ_{JK}	−53.79	−57.66	[12]
Δ_J	12.158	12.489	
δ_J	4.900	5.084	
Δ_K	257.27	325.20	
δ_K	4.70	13.01	
D_2O			
Δ_{JK}	−13.426	−15.359	[16]
Δ_J	2.915	3.096	
δ_J	1.137	1.221	
Δ_K	73.691	92.457	
δ_K	1.724	3.658	
H_2S			
Δ_{JK}	−21.285	−22.803	[17]
Δ_J	6.239	6.526	
δ_J	2.816	2.955	
Δ_K	32.670	37.033	
δ_K	−1.812	−1.326	
H_2Se			
Δ_{JK}	−17.328	−18.491	[18]
Δ_J	5.041	5.283	
δ_J	2.392	2.425	
Δ_K	23.084	26.368	
δ_K	−2.092	−1.833	

and, as a consequence, the values of some parameters). In this case, the experimental values of the centrifugal parameters and the value of the B_e parameter necessary for the calculations were taken from Ref. [12], harmonic frequencies ω_λ from Ref. [13], and the value of equilibrium angle α_e from Ref. [3]. One can see a satisfactory enough correspondence between the experimental and predicted values of the Δ_{JK}, Δ_J and δ_J parameters. Some discrepancies between predicted and expected values of the Δ_K and δ_K parameters can be explained by the presence in the H_2O molecule of bending effects, which were not taken into account in Eq. (20).

The same Table 2 also presents results of estimates of the centrifugal parameters for the H_2S, H_2Se and D_2O molecules (harmonic frequencies necessary for the calculations were taken from Refs. [3], [13–15]). It is seen that even for the D_2O molecule (ratio $m/M = 1/8$) the results of predictions are correct enough.

5. Estimation of harmonic frequencies ω_λ from parameters of the ground vibrational state

What has been mentioned in the above sections allows one to consider such an important problem for applications as an estimate of the harmonic frequencies of a molecule on the basis of experimental data on parameters of the ground vibrational state alone. It can be especially important for molecular objects of which the experimental recording of spectra in excited vibrational states is complicated for one or other reason. Really, if one knows the experimental values of three rotational (A, B, and C) and five centrifugal distortion (Δ_K, Δ_{JK}, Δ_J, δ_K, and δ_J) parameters of the ground vibrational state, then it is possible (1) to use the A, B, and C parameters for estimation of the values of the B_e constant and equilibrium interbond angle α_e, at least in the first approximation, and then (2) to use experimental values of the centrifugal parameters and Eq. (20) of Section 4 for estimation of the three ω_λ harmonic frequencies. As was mentioned above, in this case it is important that the parameter sin γ, which cannot be determined without a number of experimental data about excited vibrational states, is not present in the formulas used.

Table 3
Results of estimation of harmonic frequencies of the H_2O, D_2O, H_2S and H_2Se molecules

Parameter	Calc. (cm^{-1})	Exp. (cm^{-1})	Diff. (%)	Ref.
H_2O				
ω_1	3880.49	3834.44	1.2	[13]
ω_2	1606.87	1646.99	2.4	[13]
ω_3	3882.92	3940.73	1.5	[13]
D_2O				
ω_1	2736.51	2763.80	1.0	[3]
ω_2	1159.37	1206.39	3.9	[3]
ω_3	2943.26	2888.78	1.9	[3]
H_2S				
ω_1	2699.35	2719.18	0.8	[14]
ω_2	1181.25	1212.84	2.6	[14]
ω_3	2756.06	2735.82	0.7	[14]
H_2Se				
ω_1	2407.94	2422.65	0.6	[15]
ω_2	1032.78	1060.94	2.6	[15]
ω_3	2464.88	2468.66	0.2	[15]

To illustrate the validity of this, Table 3 presents values of harmonic frequencies ω_λ for the molecules H_2O, D_2O, H_2S and H_2Se estimated by Eq. (20) and, for comparison, experimentally determined values of the same parameters from Refs. [3,13–15] (experimental values of the rotational and centrifugal distortion constants of the ground vibrational states of H_2O, D_2O, H_2S and H_2Se molecules were taken from Refs. [12,16–18]). In this case, since some XY_2 (C_{2v}) molecules possess peculiarities connected with a large amplitude bending motion, and these peculiarities first of all appear in the Δ_K and δ_K parameters, we used in our calculations experimental values of the Δ_{JK}, Δ_J and δ_J parameters. If one remembers that only the parameters of the ground vibrational states were used as the initial information, one can see a more than satisfactory correspondence between predicted and experimental values of the harmonic frequencies. This allows one to expect that the results of predictions for more exotic molecules, such as H_2Te, H_2Po, SiH_2, PH_2, CH_2, AsH_2, NH_2, H_2Cl and others, will be correct enough too.

Acknowledgements

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