

## THEORETICAL DETERMINATION OF THE SPECTROSCOPIC PARAMETERS OF THE AMMONIA MOLECULE

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*The spectroscopic parameters of the ammonia molecule have been calculated with inversion splitting taken into account of the inversion-vibrational energy levels  $E_n(v)$  lying within  $6000\text{ cm}^{-1}$  of the vibrational ground state.*

Ammonia is present in the Earth’s atmosphere as a minor component and is present in the atmospheres of other planets as well. Despite the fact that the ammonia molecule is one of the more thoroughly studied molecules with energy level inversion, a theoretical computation of the rotational structure of its excited vibrational states is complicated by elasticity effects. The latter fact stems from tunnelling of the nitrogen atom through the plane in which the three hydrogen atoms reside.

This paper presents a calculation of the spectroscopic parameters of the inversion- vibrational energy levels of the ammonia molecule lying within  $6000\text{ cm}^{-1}$  of the vibrational ground state. Their rotational structure has so far remained unexplored.

**Computational scheme.** First we solve the inverse spectroscopic problem of retrieving the potential function  $V$  from the available experimental values of the spectroscopic properties of the ammonia molecule. The ”optimal set” of force constants thus obtained is then used to calculate those specific constants whose experimental values remain unavailable. The computational scheme looks like this:

$$\begin{aligned}
 & V(K_u, k_1^1, F_{ij}^{(1)}, \vec{r}_p, a, \kappa, b, \dots) - \\
 & \quad \uparrow \\
 \rightarrow H_{cd}(E_n^{(v)}, B^{(n)}, C^{(n)}, q_\lambda^{(n)}, \Delta_3^{(n)}, J_x, J_y, J_z, \dots) \\
 & \quad \uparrow \quad (1)
 \end{aligned}$$

The effective rotational Hamiltonian  $H_{cd}$  is obtained via diagonalization of the initial Hamiltonian  $H$  for a nonrigid molecule in the basis of inversion-rotational wave functions  $\Psi_n(\rho) \cdot \Psi_v(q)$ .<sup>1-3</sup> The relationships describing the spectroscopic parameters obtained in this way account for elasticity effects in the molecule via the dependence of the inertia tensor on the inversion variable  $\rho$ , the dependence of the inversion wave functions  $\Psi_n(\rho)$  on the height of the inversion barrier  $h$ .<sup>1-3</sup> The wave functions  $\Psi_n(\rho)$  are

then found by numerical integration of the Schrodinger equation<sup>5,6</sup>:

$$H_0 \Psi_n(\rho) = \{T + V_0(\rho)\} \Psi_n(\rho) = E_n \Psi_n(\rho) \quad (2)$$

with a two-minima potential  $V_0(\rho)$ .

Such an approach differs from similar schemes developed for semi-rigid molecules. In addition, it differs from the approach developed in Ref. 5 to retrieve the molecular potential function. Spirko<sup>5</sup> operated with the effective inversion-rotational Hamiltonian  $\tilde{H}(\rho, f(\rho), J_\rho, J_x, J_y, J_z)$  obtained by diagonalization of the initial Hamiltonian  $H$  in the basis of the vibrational wave functions  $\Psi_v(q)$ . The variable parameters in  $\tilde{H}$  are the parameters of the potential function  $V$ , which are determined from the experimental energy levels or the transition frequencies. Employing the Hamiltonian  $H_{cd}$  in our scheme (1) makes it possible to use a large set of experimental data on the spectroscopic constants to determine the molecular potential field without, however, accounting for the experimental energy levels or the transition frequencies at which the energy levels were retrieved.

**The potential field model.** The molecular potential function  $V$  was chosen in the form of a series expansion:

$$\begin{aligned}
 V(\rho, S) = & V_0 + \sum_i F_i(\rho) S_i + \\
 & + \frac{1}{2} \sum_{ij} F_{ij}(\rho) S_i S_j + \frac{1}{6} \sum_{ijkl} F_{ijkl}(\rho) S_i S_j S_l + \\
 & + \frac{1}{24} \sum_{ijklk} F_{ijklk}(\rho) S_i S_j S_l S_k \quad (3)
 \end{aligned}$$

over the symmetry coordinates  $S_i$ , corresponding to the low-amplitude vibrations of the molecule ( $i, j, l, k = 1, 3\lambda, 4\lambda, \lambda = a, b$ ). The expansion coeffi-

icients  $F$  in Eq. (3) are function of the inversion coordinate  $\rho$ , defined in Ref. 6. The symmetry coordinates  $S$  are expressed in terms of the normal coordinates  $Q$  as

$$S_i = \sum_k L_i^k(\rho) Q_k + \frac{1}{2} \sum_{kl} L_i^{kl}(\rho) Q_k Q_l + \frac{1}{6} \sum_{klj} L_i^{klj}(\rho) Q_k Q_l Q_j + \frac{1}{24} \sum_{kljlm} L_i^{kljlm}(\rho) Q_k Q_l Q_j Q_m, \quad (4)$$

in which the functions  $L(\rho)$  are calculated according to the scheme outlined in Refs. 7 and 8. Using the relation between the dimensional ( $Q$ ) and dimensionless normal coordinates ( $q$ ), the potential function  $V$  may be expressed in the form

$$V(\rho, q) = V_0(\rho) + \sum_i K_i(\rho) q_i + \frac{1}{2} \sum_{ij} \left\{ \omega_i(\rho) \delta_{ij} + K_{ij}(\rho) \right\} q_i q_j + \frac{1}{6} \sum_{ijkl} K_{ijkl}(\rho) q_i q_j q_l + \dots \quad (5)$$

TABLE I.

Inversion vibrational energy levels for the ammonia molecule ( $\text{cm}^{-1}$ ); experiment vs force field calculations (fragment)  $\Delta E = E_{exp} - E_{comp}$

$V_1$	$V_2^\pm$	$V_3^1$	$V_4^1$	$^{14}\text{NH}_3$		$^{14}\text{ND}_3$		$^{15}\text{NH}_3$		$^{15}\text{ND}_3$	
				$E_{calc}$	$\Delta E$	$E_{calc}$	$\Delta E^*$	$E_{calc}$	$\Delta E^*$	$E_{calc}$	$\Delta E^*$
0	0-	0 <sup>0</sup>	0 <sup>0</sup>	0.79	0.0	0.04	0.01	1.00	-0.24	0.05	0.0
0	1+	0 <sup>0</sup>	0 <sup>0</sup>	931.7	0.7	744.2	1.4	928.3	0.0	738.7	0.8
0	1-	0 <sup>0</sup>	0 <sup>0</sup>	969.0	-0.9	747.6	1.6	964.4	-1.5	741.7	1.1
0	2+	0 <sup>0</sup>	0 <sup>0</sup>	1598.3	0.3	1361.0	-2.5	1592.8	1.6	1353.7	1.1
0	2-	0 <sup>0</sup>	0 <sup>0</sup>	1881.1	1.1	1425.9	3.1	1871.0	0.1	1414.6	—
0	3+	0 <sup>0</sup>	0 <sup>0</sup>	2381.7	2.5	1831.9	-1.9	2368.6	0.7	1819.9	—
0	3-	0 <sup>0</sup>	0 <sup>0</sup>	2897.5	-1.9	2106.5	0.1	2880.0	-3.9	2087.6	—
1	0+	0 <sup>0</sup>	0 <sup>0</sup>	3321.8	14.4	2426.2	-6.1	3318.0	—	2421.9	—
1	0-	0 <sup>0</sup>	0 <sup>0</sup>	3320.6	16.5	2426.1	-5.5	3318.3	—	2421.9	—
0	0+	1 <sup>1</sup>	0 <sup>0</sup>	3449.7	-6.1	2576.8	-12.9	3441.2	—	2564.6	—
0	0-	1 <sup>1</sup>	0 <sup>0</sup>	3449.7	-5.7	2576.8	-12.9	3441.9	—	2564.6	—
0	0+	0 <sup>0</sup>	1 <sup>1</sup>	1617.8	8.5	1174.7	16.3	1615.2	—	1771.6	—
0	0-	0 <sup>0</sup>	1 <sup>1</sup>	1619.0	8.3	1174.7	16.3	1616.8	—	1171.6	—
1	1+	0 <sup>0</sup>	0 <sup>0</sup>	4306.9	-6.4	3175.2	3.3	4300.1	—	3165.6	—
1	1-	0 <sup>0</sup>	0 <sup>0</sup>	4303.1	-17.0	3174.8	1.1	4296.6	—	3165.3	—
0	1+	1 <sup>1</sup>	0 <sup>0</sup>	4114.5	2.4	3331.4	3.5	4401.5	—	3313.1	—
0	1-	1 <sup>1</sup>	0 <sup>0</sup>	4431.1	4.3	3332.2	-2.6	4418.2	—	3313.9	—
0	1+	0 <sup>0</sup>	1 <sup>1</sup>	2559.4	-19.0	—	—	2552.5	—	—	—
0	1-	0 <sup>0</sup>	1 <sup>1</sup>	2596.4	-10.4	—	—	2588.9	—	—	—
1	0+	1 <sup>1</sup>	0 <sup>0</sup>	6628.7	-20.0	4926.4	12.0	6617.1	—	—	—
1	0-	1 <sup>1</sup>	0 <sup>0</sup>	6627.1	-18.4	4926.2	12.2	6617.1	—	—	—
0	0+	2 <sup>2</sup>	0 <sup>0</sup>	6825.2	24.7	5113.6	-12.9	6808.6	—	5089.6	—
0	0-	2 <sup>2</sup>	0 <sup>0</sup>	6824.9	24.1	5113.5	-12.8	6809.1	—	5089.6	—
0	1+	1 <sup>1</sup>	1 <sup>1</sup>	6012.1	0.3	—	—	5996.3	—	—	—
0	1-	1 <sup>1</sup>	1 <sup>1</sup>	6037.5	-1.5	—	—	6021.9	—	—	—
0	1+	0 <sup>0</sup>	2 <sup>0</sup>	—	—	3092.2	2.8	—	—	3079.7	—
0	1-	0 <sup>0</sup>	2 <sup>0</sup>	—	—	3095.7	-3.8	—	—	3083.1	—
0	0+	1 <sup>1</sup>	2 <sup>0</sup>	—	—	4902.4	-15.0	—	—	—	—
0	0-	1 <sup>1</sup>	2 <sup>2</sup>	—	—	4902.5	-14.8	—	—	—	—

The following representation of the functions  $F_{ij}(\rho)$  is assumed in this paper<sup>3</sup>:

$$F_{ij}(\rho) = F_{ij}^{(1)} + F_{ij}^{(2)} \left[ \rho - \frac{\pi}{2} \right]^2 \times \exp \left[ F_{ij}^{(3)} \left[ \rho - \frac{\pi}{2} \right]^2 \right], \quad (6)$$

where

$$F_{11}^{(1)} = f_{rr} + 2f_{rr'}; \quad F_{33}^{(1)} = f_{rr} - f_{rr'};$$

$$F_{44}^{(1)} = f_{\alpha\alpha} - f_{\alpha\alpha'}; \quad \text{and} \quad F_{34}^{(1)} = f_{r\alpha} - f_{r\alpha'}.$$

The two-minima function  $V_0(\rho)$ , which determines (in the zeroth approximation) the cross section of the potential surface along the inversion variable  $\rho$ , and the functions  $F_i(\rho)$ ,  $F_{ijl}(\rho)$ , and  $F_{ijkl}(\rho)$  are given by formulas from Ref. 5; in the same reference the constants  $K_u$ ,  $k_l^1$ ,  $a$ ,  $b$ ,  $\kappa$  ..., are assigned, which parametrize these functions. In particular we have

$$V_0(\rho) = \sum_u K_u [r_p \cos \rho]^{2u}, \quad (7)$$

where  $r_p$  is the N-H bond length for the flat configuration of the molecule. The formulas for the rotational ( $B$ ,  $C$ ) and centrifugal ( $D_j$ ,  $D_{jk}$ ,  $D_k$ ) constants and  $k$ - and  $l$ -doubling constants  $\Delta_3$  and  $q_\lambda^{1-4}$  include the integrals  $\langle \Psi_n(\rho) | f(\rho), df(\rho) / d\rho | \Psi_m(\rho) \rangle$  of the functions  $f(\rho)$  which define expansion (5) and the expansion of the inverse inertia tensor  $\mu_{\alpha\beta}(p, q)$  in a series in  $q$ :  $f(\rho) \equiv \{K_1(\rho), \omega_1(\rho), \dots, K_{ijl}(\rho), B_\alpha(\rho), B_k^{\alpha\beta}(\rho)\}$ . A technique for retrieving the wave functions  $\Psi_n(\rho)$  and the inversion vibrational energy levels  $E_n(v)$  is described in Ref. (9) ( $n, m = 0^\pm, 1^\pm, \dots$  where plus and minus serve to distinguish the two components of the doubly degenerate energy levels).

**Retrieval of the potential function.** In scheme (1) we employed 60 separate experimental values of the inversion vibrational energy levels, 14 values for the rotational constants  $B^{(n)}$ ,  $C^{(n)}$  (with  $n = 0^\pm, 1^\pm, 2^-$ ) of the  $^{14}\text{NH}_3$  and  $^{14}\text{ND}_3$  molecules, and also the  $k$ - and  $l$ -doubling constants values averaged over the inversion states taken from Refs. 10 and 11. The majority of the experimental data is given in Ref. 5. Additional experimental data are taken from Refs. 12-15. The optimal set of force parameters obtained by solving the inverse problem (1) is presented below.

$$f_{rr} = 7.6321 \text{ mdyn} \cdot \text{\AA}^{-1}$$

$$f_{rr'} = 0.2738 \text{ mdyn} \cdot \text{\AA}^{-1}$$

$$F_{11}^{(2)} = -7.1366 \text{ mdyn} \cdot \text{\AA}^{-1} \cdot \text{rad}^{-2}$$

$$F_{33}^{(2)} = -0.023 \text{ mdyn} \cdot \text{\AA}^{-1}$$

$$f_{\alpha\alpha} = 0.1918 \text{ mdyn} \cdot \text{\AA}^{-1}$$

$$f_{\alpha\alpha'} = 0.2752 \text{ mdyn} \cdot \text{\AA}^{-1}$$

$$F_{41}^{(2)} = 0.7665 \text{ mdyn} \cdot \text{\AA}^{-2} \cdot \text{rad}^{-2}$$

$$F_{34}^{(2)} = -1.367 \text{ mdyn}$$

$$f_{r\alpha} = -0.3251 \text{ mdyn}$$

$$f_{r\alpha'} = -0.2357 \text{ mdyn}$$

$$K_1 = -0.5453 \text{ mdyn} \cdot \text{\AA}^{-1}$$

$$K_2 = 2.0519 \text{ mdyn} \cdot \text{\AA}^{-1}$$

$$K_3 = -0.7091 \text{ mdyn} \cdot \text{\AA}^{-1}$$

$$k_1^1 = 0.1409 \text{ mdyn} \cdot \text{\AA}^{-2}$$

$$k_2^1 = 0.9518 \text{ mdyn} \cdot \text{\AA}^{-4}$$

$$a = 0.9942 \quad b = 0.0 \quad \kappa = 0.1835$$

$$\gamma = -1.512 \quad \gamma_m = -0.5504 \quad r_p = 1.01482 \text{ \AA}$$

This set differs somewhat from that given in Ref. 5 since we have employed representation (4) for  $F_{ij}(\rho)$ , which then enters the formulas for the functions  $F_{ijl}(\rho)$  and  $F_{ijkl}(\rho)$  from Ref. 5. The parameter  $F_{11}^{(1)}$  in our calculations is, unfortunately, poorly determined. However, the values of  $K_u$ , which parameterize the two-minima potential function  $V_0(\rho)$ , are rather close. One can get an idea of the quality of retrieval of the experimental data from Tables I – III, which compare the experimental values of the inversion vibrational energy levels, the rotational constants, and the  $k$ - and  $l$ -doubling constants with those computed from the force field (see above). The data marked by an asterisk were not used in the solution of the inverse problem (6) (from Refs. 12-15). The maximum error in retrieving the inversion energy levels reaches roughly  $3 \text{ cm}^{-1}$ , and for the inversion vibrational energy levels it is on the order of  $25 \text{ cm}^{-1}$ . Such a level of accuracy is comparable to that obtained in Ref. 5. The maximum error in retrieving the rotational constants is  $0.1 \text{ cm}^{-1}$  for the  $(0, 2^-, 0, 0)$  state which is in resonance interaction with other states (see Table 2). The retrieved  $k$ -doubling constant  $\Delta_3$  is practically exact (Table III).

**Calculation of the molecule spectroscopic constants.** The obtained molecule force field makes possible direct calculations of the spectroscopic parameters that were not involved in the retrieval of the field for various inversion vibrational states. Partial results of such calculations are presented in Table. <sup>1-3</sup> To retrieve the rotational structure of the molecular energy levels we first need the values of the rotational constants  $B$  and  $C$ . These constants, according to Table II for the experimental data available from Refs. 12–15, are predicted to within an accuracy of  $0.1 \text{ cm}^{-1}$  (except for the two cases of states which participate in resonance interactions). Tables IV and V give an idea of the quality of the predictions for the quadratic ( $D$ ) and sextic ( $H$ ) constants of the centrifugal distortions. The sextic constants were computed from the formulas given

in Ref. 16, and these computations have, for the first time, theoretically demonstrated a difference between the values of the constants  $H$  for the symmetric (+) and antisymmetric (-) components. In addition, the ro-

tational constants of the centrifugal distortion  $D$  and  $H$ , and the  $k$ - and  $l$ -doubling constants for the isotopes  $^{15}\text{NH}_3$ ,  $^{15}\text{ND}_3$ ,  $^{15}\text{NT}_3$  were computed from the obtained force field. These results will be presented elsewhere.

TABLE II.

Experiment<sup>5,12-15</sup> and force-field calculations: rotational components of the ammonia molecule.

$V_1$	$V_2^+$	$V_3$	$V_4$	$^{14}\text{NH}_3$				$^{14}\text{ND}_3$			
				B		C		B		C	
				exp.	calc.	exp.	calc.	exp.	calc.	exp.	calc.
0	0+	0	0	9.95	9.99	6.23	6.19	5.14	5.15	3.12*	3.12
0	0-	0	0	9.94	9.98	6.23	6.19	5.14	5.15	3.12*	3.12
0	1+	0	0	10.07	10.08	6.09	6.00	5.12	5.13	—	3.08
0	1-	0	0	9.89	9.92	6.16	6.12	5.11	5.12	—	3.09
0	2+	0	0	10.30*	10.15	—	5.82	—	5.20	—	2.95
0	2-	0	0	9.63	9.73	6.17	6.15	—	5.09	—	3.06
0	0+	1	0	9.76*	9.88	6.23*	6.15	—	5.11	—	3.11
0	0-	1	0	9.76*	9.87	6.23*	6.16	—	5.11	—	3.11
0	0+	0	1	10.18*	10.23	—	6.15	—	5.24	—	3.11
0	0-	0	1	10.18*	10.25	—	6.15	—	5.24	—	3.11
0	1+	0	1	10.39*	10.35	—	5.94	5.23*	5.21	3.09*	3.07
0	1-	0	1	9.97*	10.18	—	6.08	5.22*	5.21	3.09*	3.08
0	2+	0	1	—	10.40	—	5.79	—	5.29	—	2.92
0	2-	0	1	—	10.18	—	6.12	—	5.19	—	3.05
0	1+	1	0	—	9.97	—	5.97	—	5.08	—	3.07
0	1-	1	0	—	9.80	—	6.08	—	5.07	—	3.08

TABLE III.

Experiment<sup>10,11</sup> and force-field calculations:  $l$ - ( $q_4$ ) and  $k$ -doubling ( $\Delta_3$ ) constants.

$V_2^\pm$	$q_4$				$\Delta_3$			
	$^{14}\text{ND}_3 \cdot 10^1 \text{cm}^{-1}$		$^{14}\text{ND}_3 \cdot 10^2 \text{cm}^{-1}$		$^{14}\text{ND}_3 \cdot 10^8 \text{cm}^{-1}$		$^{14}\text{ND}_3 \cdot 10^9 \text{cm}^{-1}$	
	exp.	calc.	exp.	calc.	exp.	calc.	exp.	calc.
0+	3.4	2.3	—	7.8	1.2	1.0	—	1.4
0-	3.4	2.7	—	7.6	1.2	1.2	—	1.4
1+	2.7	2.2	—	6.5	—	—	—	—
1-	2.7	2.6	—	8.9	—	—	—	—

TABLE IV.

Quadratic constants for the distortions (in  $10^{-4} \text{cm}^{-1}$ ) directly the molecular force field.

$V_2^\pm$	$^{14}\text{NH}_4$						$^{14}\text{ND}_3$					
	$D_j$		$-D_{jk}$		$D_k$		$D_j$		$-D_{jk}$		$D_k$	
	ex.	c.	ex.	c.	ex.	c.	ex.	c.	ex.	c.	ex.	c.
0+	8.5	7.5	15.8	13.9	10.1	8.7	2.0	1.9	3.5	3.3	—	2.0
0-	8.3	7.5	15.3	13.8	3.8	8.5	2.0	1.9	3.5	3.3	—	2.0
1+	11.3	8.4	24.2	17.3	—	12.3	1.9	1.9	3.7	3.6	—	2.3
1-	7.0	7.8	12.3	14.4	—	8.8	1.8	1.9	3.7	3.5	—	2.1

TABLE V.

Sixtic constants for the centrifugal distortions directly computed from the molecular force field.

$^{14}\text{NH}_3 \cdot 10^7 \text{ cm}^{-1}$	$0^+$		$0^-$		$1^+$		$1^-$	
	exp.	calc.	exp.	calc.	exp.	calc.	exp.	calc.
$H_j$	2.3	2.2	2.1	2.2	1.5	3.1	0.4	1.9
$H_{jk}$	-8.5	-5.8	-7.6	-5.7	-7.1	-8.6	-2.0	-5.1
$H_{kj}$	11.5	4.9	10.5	5.0	8.6	7.5	3.9	4.8
$H_k$	—	-0.8	—	-1.0	—	-0.9	—	-1.0
$^{14}\text{ND}_3 \cdot 10^8 \text{ cm}^{-1}$								
$H_j$	2.1	2.4	2.1	2.4	2.9	2.7	2.0	2.5
$H_{jk}$	-6.8	-7.2	-6.8	-7.2	-9.2	-8.2	-5.1	-7.5
$H_{kj}$	7.8	7.6	7.8	7.6	10.8	8.7	7.6	8.1
$H_k$	—	-2.2	—	-2.3	—	-2.1	—	-2.3

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