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Reinvestigation of The 2ν_4(A, E) Infrared Band of Phosphorus Trifluoride

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Abstract

The $v_4 = 2^0$ and $v_4 = 2^{-2}$ excited states of the oblate molecule PF$_3$, lying near 693 cm^{-1}, were reinvestigated by high-resolution FTIR spectroscopy. Assumed to be isolated, these levels were treated by applying different reduction forms of the effective rovibrational Hamiltonian recently developed for the $v_t(E) = 2$ vibrational state of a C_{3v} symmetric top molecule, with models taking into account ℓ- and k-type intravibrational resonances. Parameters up to sixth order have been accurately determined. The unitary equivalence of the derived parameter sets in different reductions was successfully verified.

Keywords: Phosphorus trifluoride PF$_3$, FTIR spectroscopy, Rovibration, Overtone band, Reductions

1. Introduction

Phosphorus trifluoride PF$_3$, a ligand in metal complexes of chemistry interest, is an oblate symmetric top molecule belonging to C_{3v} point group. Therefore, it has four normal modes of vibration: two totally symmetric, ν_1 and ν_2, and two doubly degenerate, ν_3 and ν_4.

The ν_2 [1] and ν_4 [2] fundamental bands have quite recently been studied by Fourier transform infrared (FTIR) spectroscopy. An accurate rotational ground state (GS) C_0 value, 0.159 970 436 (69) cm^{-1}, has been determined and used to derive an improved GS structure of PF$_3$, r_0(P-F) = 1.563 244 05 (11) Å and $\measuredangle$(FPF) = 97.752 232 (29) °. The $v_2 = 1$ state was assumed as an isolated level and treated by a classical model. However, the degenerate vibrational level $v_4 = 1$ was treated by applying the theory of reduction of the effective rovibrational Hamiltonian H_{vr}.

The present work extends the studies on the vibrationally excited states of symmetric top fluoride molecules, phosphorus trifluoride PF$_3$ [1-9], and nitrogen trifluoride NF$_3$ [10-14]. The main objective is to test, for the $v_4 = 2$ vibrational state of PF$_3$ around 693 cm^{-1}, the unitary equivalence of parameter sets obtained from different reduction forms of H_{vr}.

It has been demonstrated, for the $v_t = 1$ and $v_t = 2$ excited states of C_{3v} symmetric top molecules, that the molecular parameters of the effective rovibrational Hamiltonian cannot all be determined independently from the fitting of the experimental data, because they are strongly correlated. The number of parameters has to be reduced through a unitary transformation called reduction [15-21]. Many studies were performed [22-26] using this approach. The obtained results demonstrated that the procedure of reduction is an appropriate solution for the indeterminacy problems. Thus, the reduction method was successfully applied to the $v_3 = 1$ (E, ν_0 = 907.5413 cm^{-1}) [27], $v_4 = 2$ (A_1, ν_0 = 983.7017 cm^{-1}; E, ν_0 = 986.6223 cm^{-1}) [28], $v_1 = v_3 = 1$ (E, ν_0 = 1931.5775 cm^{-1}), and $v_3 = 2$ (A_1, ν_0 = 1803.1302 cm^{-1}; E, ν_0 = 1810.4239 cm^{-1}) [29] excited states of the nitrogen trifluoride ^{14}NF$_3$. More recently, the same method has been applied to the $v_4 = 1$ (E, ν_0 = 347.0861 cm^{-1}) degenerated state [2] of the phosphorus trifluoride PF$_3$.

2. Theory

The diagonal and off-diagonal matrix elements of the Hamiltonian operator H_{vr} that were considered for the ground and $v_4 = 2$ states of PF$_3$, which include contributions of higher order as well as K and J dependences of the interaction parameters, were taken as:

- The ground state energy:

$$E_0(J, K) = (C_0 - B_0)K^2 + B_0J(J + 1) - D_J^0J^2(J + 1)^2 - D_{JK}^0J(J + 1)K^2 - D_K^0K^4 \\ + H_{JJ}^0J^3(J + 1)^3 + H_{JK}^0J^2(J + 1)^2K^2 + H_{KJ}^0J(J + 1)K^4 + H_{KK}^0K^6$$

where $K = |k|$.

- The excited state energy:

$$E(\mathrm{v}, \ell, J, K) = \nu_0 + (C - B)K^2 + BJ(J + 1) - D_JJ^2(J + 1)^2 - D_{JK}J(J + 1)K^2 - D_KK^4 \\ + H_{JJ}J^3(J + 1)^3 + H_{JK}J^2(J + 1)^2K^2 + H_{KJ}J(J + 1)K^4 + H_{KK}K^6 \\ + [-2C\zeta + \eta_JJ(J + 1) + \eta_KK^2 + \eta_{JJ}J^2(J + 1)^2 + \eta_{JK}J(J + 1)K^2 + \eta_{KK}K^4]k\ell$$

where $\ell = 0, \pm 2$.

- The $\ell(2, 2)$ interaction (q resonance) between $2\nu_4^0$ and $2\nu_4^{-2}$ components, employing the phase convention of Cartwright and Mills [30]:

$$\langle \mathrm{v}, \ell, J, k\, |H_{\mathrm{vr}}/hc|\, \mathrm{v}, \ell \pm 2, J, k \pm 2\rangle = \\ -1/4\{q + q_JJ(J + 1) + q_K[k^2 + (k \pm 2)^2] + q_{JJ}J^2(J + 1)^2 + q_{JK}J(J + 1)[k^2 + (k \pm 2)^2]\} \\ \mathrm{x}\ [(\mathrm{v} \pm \ell + 2)(\mathrm{v} \mp \ell)]^{1/2} F_{\pm}(J, k)\, F_{\pm}(J, k \pm 1)$$

with $F_{\pm}(J, k) = [J(J + 1) - k(k \pm 1)]^{1/2}$.

- The $\ell(2, -1)$ interaction (r resonance) between $2\nu_4^0$ and $2\nu_4^{-2}$ components:

$$\langle \mathrm{v}, \ell, J, k\, |H_{\mathrm{vr}}/hc|\, \mathrm{v}, \ell \mp 2, J, k \pm 1\rangle = r\,(2k \pm 1)\ \mathrm{x}\ [(\mathrm{v} \pm \ell + 2)(\mathrm{v} \mp \ell)]^{1/2} F_{\pm}(J, k)$$

- The k (0, 3) interaction (ℓ-dependent d resonance):

$$\langle \mathrm{v}, \ell = \pm 2, J, k\, |H_{\mathrm{vr}}/hc|\, \mathrm{v}, \ell = \pm 2, J, k \pm 3\rangle = \ell\, d\, F_{\pm}(J, k)\, F_{\pm}(J, k \pm 1)\, F_{\pm}(J, k \pm 2)$$

- The k (0, 3) interaction (ℓ-independent ε resonance):

$$\langle \mathrm{v}, J, k\, |H_{\mathrm{vr}}/hc|\, \mathrm{v}, J, k \pm 3\rangle = \varepsilon\,(2k \pm 3)\, F_{\pm}(J, k)\, F_{\pm}(J, k \pm 1)\, F_{\pm}(J, k \pm 2)$$

According to the theory of equivalent reductions, and in order to prevent correlations in the fitting experimental data, some of the molecular parameters have to be constrained. One of the off-diagonal parameters accounting for $\Delta(k - \ell) \neq 0$ interaction can be refined while the others are fixed, usually to zero value.

In the case of an isolated $\mathrm{v}_t = 2$ state of a symmetric top, five equivalent *D*-, *Q*-, *QD*-, *L*-, and *LD*-reduction schemes were proposed [15-19].

- In the *D*-reduction, the d and ε parameters of the (0, 3) k-type interaction are constrained to zero, while the r parameter of the (2, –1) ℓ-type resonance is refined.
- In the *Q*-reduction, the r and ε parameters are fixed to zero.
- In the *QD*-reduction, the ε parameter is refined.
- In the *L*- and *LD*-reductions, the constraints concern the two interaction constants ε and d respectively.

Furthermore, the condition $r_K = 0$ and $q_K = 0$, or $\eta_{JJ} = 0$, or $\eta_{JK} = 0$, or $\eta_{KK} = 0$ has to be imposed in all reductions in order to avoid collinearity problems [16,18].

3. Results and Discussion

The set of the IR experimental data of the $2\nu_4$ overtone band of PF_3 used in this work is the same as in Ref. [7]. The body of data comprised 1046 NZW IR lines of the $2\nu_4^0$ parallel component and 198 NZW energies of the $\mathrm{v}_4 = 2^{-2}$ substate deduced from the observed lines of the hot band $2\nu_4^{-2} - \nu_4^{-1}$ by adding to the wavenumbers of these lines the energies of the $\mathrm{v}_4 = 1^{-1}$ level. The fit calculations were carried out with the nonlinear least-squares program SIMFIT [31], according to the same reduction schemes of the rovibrational Hamiltonian already performed for the $\mathrm{v}_4 = 2$ excited level of NF_3 [28]. A weight ascribed to the observed transitions was chosen as inverse of the square of the experimental precision (2×10^{-4} cm^{-1}). The GS constants were fixed to the values of Table 1. All experimental data were fitted with the five reduction forms of H_{rv} proposed by Sarka and Harder [18], using the option to simultaneously constraining to zero the q_K and r_K K-dependent interaction terms. The results obtained in different reductions for the $\mathrm{v}_4 = 2$ state are given in Table 2.

The sextic centrifugal distortion constants H could not be refined with significance and were constrained to the values calculated from the GS (Table 1) and $\mathrm{v}_4 = 1$ state values [2]. For the same reason, the η_{JJ}, η_{JK}, η_{KK}, q_J, q_{JJ} and q_{JK} terms were fixed.

As can be seen in Table 2, all parameters appear at the correct order of magnitude. The standard deviations of the fits are practically similar for the five reductions applied, and close to the quality of measurements (2×10^{-4} cm^{-1}).

Table 1: Ground state parameters constants (cm^{-1}) of PF_3

Parameter	Value	Reference
C_0	0.159 970 436 (69)	[2]
B_0	0.260 846 962 3 (36)	[32]
$D_J^0 \times 10^7$	2.619 095 (46)	[32]
$D_{JK}^0 \times 10^7$	−3.925 47 (18)	[32]
$D_K^0 \times 10^7$	1.73 [a]	[33]
$H_{JJ}^0 \times 10^{13}$	5.421 (26)	[32]
$H_{JJ}^0 \times 10^{12}$	−2.330 (23)	[32]
$H_{JK}^0 \times 10^{12}$	3.102 (46)	[32]
$H_{JK} \times 10^{12}$	0. [b]	-

[a] From harmonic force field calculations, uncertainty not given. [b] Fixed to zero because unknown.

Table 2: Parameters (cm^{-1}) in different reductions for the $v_4 = 2$ level of PF_3

	Previous work [7]	*D*-Reduction	*Q*-Reduction	*QD*-Reduction	*L*-Reduction	*LD*-Reduction
	$v_4 = 2^0$ substate		1046 NZW lines			$K_{max}/J_{max} = 53/53$
$\sigma \times 10^3$	0.218	0.237	0.240	0.237	0.238	0.236
ν_0	692.846 944 (35)	692.846 847 (49)	692.846 864 (49)	692.846 900 (48)	692.846 850 (49)	692.846 892 (48)
C	0.159 549 8 (11)	0.159 302 74 (11)	0.159 302 55 (11)	0.159 302 31 (12)	0.159 302 73 (11)	0.159 302 37 (12)
B	0.261 053 39 (27)	0.261 053 86 (36)	0.261 053 92 (36)	0.261 053 61 (35)	0.261 053 87 (36)	0.261 053 62 (35)
$D_J \times 10^7$	2.635 2 (55)	2.378 (24)	2.380 (24)	2.407 (24)	2.392 (24)	2.413 (24)
$D_{JK} \times 10^7$	−4.156 (50)	−3.572 (48)	−3.576 (49)	−3.668 (49)	−3.600 (49)	−3.679 (49)
$D_K \times 10^7$	1.94	1.612 (23)	1.612 (24)	1.679 (25)	1.626 (24)	1.685 (25)
$H_{JJ} \times 10^{13}$	4.6 [a]	9.22 [c]	9.12 [c]	9.34 [c]	9.22 [c]	9.22 [c]
$H_{JK} \times 10^{12}$	−2.14 [a]	−3.107 [c]	−3.024 [c]	−3.073 [c]	−3.107 [c]	−3.107 [c]
$H_{KJ} \times 10^{12}$	3.31 [a]	3.412 [c]	3.262 [c]	3.340 [c]	3.412 [c]	3.412 [c]
$H_{KK} \times 10^{12}$	-	-	-	-	-	-
	$v_4 = 2^{-2}$ substate		198 NZW energies			$K_{max}/J_{max} = 18/28$
$\sigma \times 10^3$	0.523	0.581	0.580	0.565	0.578	0.564
ν_0	694.694 715 (55)	694.695 383 (84)	694.695 365 (85)	694.695 050 (97)	694.695 363 (85)	694.695 053 (96)
C	0.159 313 7 (37)	0.159 307 8 (33)	0.159 305 6 (35)	0.159 296 9 (36)	0.159 306 3 (35)	0.159 297 8 (37)
B	0.261 047 45 (36)	0.261 048 38 (51)	0.261 048 61 (53)	0.261 051 58 (69)	0.261 048 67 (53)	0.261 051 60 (69)
$D_J \times 10^7$	2.553 8 (77)	2.567 9 (68)	2.566 7 (68)	2.626 4 (10)	2.567 7 (68)	2.627 1 (10)
$D_{JK} \times 10^7$	−3.423 (42)	−3.507 (39)	−3.525 (40)	−4.115 (98)	−3.524 (40)	−4.116 (98)
$D_K \times 10^7$	1.373 (46)	1.511 (42)	1.528 (42)	2.067 (91)	1.530 (43)	2.065 (92)
$C\zeta$	−0.103 522 7 (32)	−0.103 566 90 (60)	−0.103 564 32 (61)	−0.103 536 83 (73)	−0.103 565 17 (61)	−0.103 538 29 (73)
$\eta_J \times 10^6$	−1.679 (18)	−1.741 (28)	−1.708 (29)	−1.438 (49)	−1.723 (30)	−1.456 (50)
$\eta_K \times 10^6$	1.268 (10)	0.511 (74)	0.412 (79)	0.175 (83)	0.448 (83)	0.219 (85)
$\eta_{JJ} \times 10^{10}$	-	−2.46 [c]	−2.47 [c]	−2.65 [c]	−2.46 [c]	−2.46 [c]
$\eta_{JK} \times 10^{10}$	-	5.92 [c]	6.01 [c]	6.29 [c]	5.92 [c]	5.92 [c]
$\eta_{KK} \times 10^{10}$	-	−3.584 [c]	−3.662 [c]	−3.785 [c]	−3.584 [c]	−3.584 [c]
$H_{JJ} \times 10^{13}$	4.6 [a]	9.22 [c]	9.12 [c]	9.34 [c]	9.22 [c]	9.22 [c]
$H_{JK} \times 10^{12}$	−2.14 [a]	−3.107 [c]	−3.024 [c]	−3.073 [c]	−3.107 [c]	−3.107 [c]
$H_{KJ} \times 10^{12}$	3.31 [a]	3.412 [c]	3.262 [c]	3.340 [c]	3.412 [c]	3.412 [c]
$H_{KK} \times 10^{12}$	-	-	-	-	-	-
			Interaction Terms			
$q \times 10^3$	0.503 94(14)	1.035 3 (33)	1.034 9 (33)	1.032 3 (32)	1.033 7 (33)	1.031 8 (32)
$q_J \times 10^9$	2.40 (20)	−3.03 [c]	−2.99 [c]	−3.08 [c]	−3.03 [c]	−3.03 [c]
$q_{JJ} \times 10^{13}$	-	−7.32 [c]	−8.50 [c]	−8.77 [c]	−7.32 [c]	−7.32 [c]
$q_{JK} \times 10^{12}$	-	1.020 [c]	1.091 [c]	1.106 [c]	1.020 [c]	1.020 [c]
$q_K \times 10^9$	6.59 (16)	0. [b]	0. [b]	0. [b]	0. [b]	0. [b]
$r \times 10^5$	-	1.71 (60)	0. [b]	0. [b]	1.19 (58)	1.17 (53)
$d \times 10^7$	-	0. [b]	5.05 (118)	0. [b]	4.88 (120)	0. [b]
$\varepsilon \times 10^7$	-	0. [b]	0. [b]	2.54 (19)	0. [b]	2.60 (18)

[a] Fixed to the ground state values [5]. [b] Imposed by the reduction. [c] Fixed from $v_4 = 1$ state [2].
Errors given in parentheses are one standard deviation expressed in units of the last digit quoted.

The unitary equivalence of the obtained parameter sets corresponding to the *D*-, *Q*-, *QD*-, *L*-, and *LD*-reductions can be checked with relations deduced from the theory reduction of H_{rv}. The relations used to test this equivalence are gathered in Table 3. It is worth noting that all five sets of expressions are satisfied within their error limits. However, the verification of the unitary equivalence is less accurate than in the $v_4 = 1$ state of PF_3

[2]. Obviously, the fits were based only on IR transitions with a small body of data and low values of the rotational quantum numbers J and K.

Equation (2), linking the two coupling terms d and ε is verified within 2.4 %. Equation (3), directly comparing the L- and LD-reductions is fulfilled within 7.4 %. This margin is conditioned by the limited significance of the small d^L coupling term. The fulfilment is particularly appreciable for the sum $\eta_J + \eta_K$ (Eq. (5)).

There are a few more equations which may be used to test the equivalence of parameters in different reductions applied to the $v_4 = 2$ state of PF_3. However, they involve parameters and their differences which could not be determined with sufficiently high significance to be used for comparison, and were therefore omitted. To summarize, the tried relations of equivalence seem to semi-quantitatively support the validity of the theory for the $v_4 = 2$ state of PF_3, but the invariance relations are less satisfactorily fulfilled for the $v_4 = 2$ state than for the $v_4 = 1$ state of the PF_3 oblate molecule. The principal reason is the smaller amount of data which did not allow us to determine the H sextic terms, and did not give any information about the small $t(2, -4)$ and $h_3(0, 6)$ splittings [4], which had to be neglected in the fits.

Table 3: Verification of unitary equivalence for PF_3 in the $v_4 = 2$ excited state

Equation	Quantity *	Value (cm^{-1})
(1)	$-2r^D/F$ $d^Q/2q$	$1.11\ (39) \times 10^{-4}$ $2.44\ (57) \times 10^{-4}$
(2)	$\varepsilon^{QD}/(C-B)$ $d^Q/2C\xi$	$-2.49\ (19) \times 10^{-6}$ $-2.44\ (56) \times 10^{-6}$
(3)	$\varepsilon^{LD}/(C-B)$ $d^L/2C\xi$	$-2.55\ (17) \times 10^{-6}$ $-2.36\ (57) \times 10^{--6}$
(4)	$8(r^D)^2/F$ $(d^Q)^2F/2q^2$ $\eta_J^D - \eta_J^Q$ $-(\eta_K^D - \eta_K^Q)$	$-0.075\ (52) \times 10^{-6}$ $-0.036\ (16) \times 10^{-6}$ $-0.033\ (57) \times 10^{-6}$ $-0.099\ (15) \times 10^{-6}$
(5)	$\eta_J^D + \eta_K^D$ $\eta_J^Q + \eta_K^Q$ $\eta_J^L + \eta_K^L$ $\eta_J^{QD} + \eta_K^{QD}$ $\eta_J^{LD} + \eta_K^{LD}$	$-1.23\ (10) \times 10^{-6}$ $-1.29\ (11) \times 10^{-6}$ $-1.27\ (11) \times 10^{-6}$ $-1.26\ (13) \times 10^{-6}$ $-1.24\ (14) \times 10^{-6}$

$^*F = C - B + 2C\zeta_4 = -0.308\ 88$ cm^{-1}

Conclusion

In the present study, the $2\nu_4$ overtone band of the oblate symmetric top molecule PF_3, lying near 693 cm^{-1}, was reinvestigated by high-resolution FTIR spectroscopy.

The experimental data of the $2\nu_4^0$ parallel and the $2\nu_4^2$ perpendicular components were fitted using different reduction forms of the rovibrational Hamiltonian. The standard deviations of the fits are comparable and the theoretical relations between parameters of different reductions are quite fulfilled.

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