JOURNAL OF MOLECULAR SPECTROSCOPY 153, 145–166 (1992)

Vibration–Rotational Interactions in the States $v_2 = 1$ and $v_5 = 1$ of $H_3{}^{12}CF$

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The vibration–rotational bands ν_2 and ν_5 of gaseous fluoromethane $H_3{}^{12}CF$ have been measured in the region 1250–1600 cm^{-1} with resolution 0.0034 cm^{-1}; the 2046 lines that have been assigned include 85 lines of the $\Delta k = \pm 2$ perturbation-allowed transitions to the doubly degenerate vibrational state $v_5 = 1$. A variational approach has been applied to the analysis of both bands which are strongly perturbed by x–y Coriolis interaction and by "2, −1" l-type coupling. Simultaneously with 96 previously reported frequencies of pure rotational transitions in the ground vibrational state and 202 frequencies in the excited vibrational states $v_2 = 1$ and $v_5 = 1$ [Pracna, Papoušek, Belov, Tretyakov, and Sarka, *J. Mol. Spectrosc.* **146,** 120–126 (1991)], the wavenumbers of 2046 vibration–rotational transitions of the bands ν_2 and ν_5 have been fitted to determine 7 parameters of the ν_2 band and 21 parameters of the ν_5 band. The ground state parameters $A_0 = 5.1820107(12)$ cm^{-1} and $D_K^0/10^{-6} = 70.39(15)$ cm^{-1} are in excellent agreement with those determined previously [Graner, *Mol. Phys.* **31,** 1833–1843 (1976)]. A standard deviation of 8.0×10^{-4} cm^{-1} has been obtained in the simultaneous fit of the infrared data and 0.38 MHz of the rotational frequencies of the upper state, but in the ν_5 band inexplicable systematic differences up to 0.02 cm^{-1} between the experimental and calculated wavenumbers remain for certain values of the rotational quantum number K at $J > 25$. From the analysis of the absolute intensities of lines of the ν_2 and ν_5 bands, we found that $(\partial\mu_x/\partial q_{5a})/(\partial\mu_z/\partial q_2) = +1.75$, which indicates a negative perturbation of intensity $(\zeta^y_{2,5a} < 0)$. © 1992 Academic Press, Inc.

INTRODUCTION

As fluoromethane is a stable molecule having a large, permanent dipole moment it is of particular interest for its use in molecular lasers. Because coincidences between frequencies are sought in different spectral regions for optically pumped lasers, accurate values of the vibration–rotational energies are required for these applications. Among the candidates for such applications are the vibration–rotational bands ν_2 and ν_5, which are prototypical instances of parallel (ν_2) and perpendicular (ν_5) bands, the

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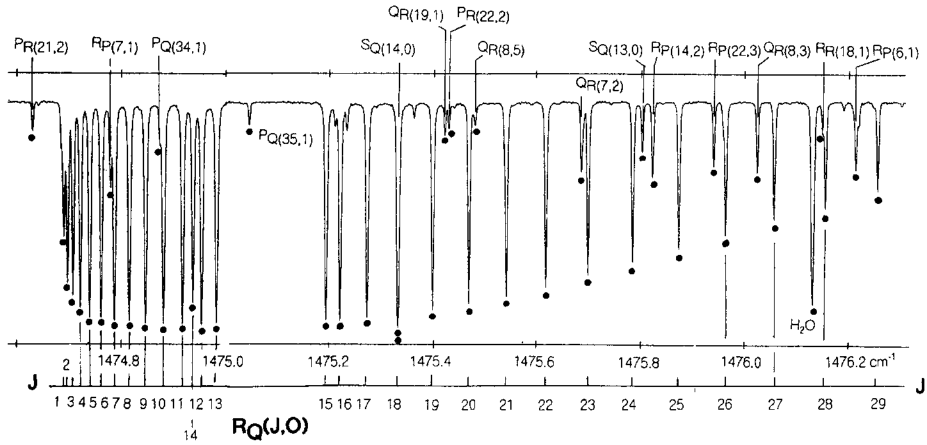

FIG. 1. Part of the spectrum of the bands ν_2 and ν_5 of $H_3{}^{12}CF$.

wavenumbers and intensities of which are strongly perturbed by the vibration–rotational interactions between and within the states $v_2 = 1$ (vibrational symmetry A) and $v_5 = 1$ (E).

In their paper on the Coriolis interactions caused by rotations about x, y molecular axes in symmetric top molecules, di Lauro and Mills (*1*) discussed qualitatively the intensity perturbations in the bands ν_2 and ν_5 of H_3CF. Wavenumber perturbations in the Raman bands ν_2 and ν_5 of H_3CF measured with a resolution about 0.3 cm^{-1} have been studied by Escribano, Mills, and Brodersen (*2*), and by Betrencourt, Morillon-Chapey, and Pinson (*3*) in the infrared bands ν_2 and ν_5 of $H_3{}^{12}CF$ measured with a resolution of 0.015–0.02 cm^{-1}.

The purely rotational transitions within the states $v_2 = 1$ and $v_5 = 1$ have been studied by both microwave spectroscopy (*4, 5*) and submillimeter-wave spectroscopy up to $J = 12$ (*6*).

In the present work, we have remeasured the vibration–rotational bands ν_2 and ν_5 of $H_3{}^{12}CF$ with resolution 0.0034 cm^{-1} and analyzed simultaneously the infrared data with the frequencies of pure rotational transitions in the excited vibrational states $v_2 = 1$ and $v_5 = 1$ (*4–6*) and in the ground vibrational state using the reduced Hamiltonian for the interacting vibrational states of C_{3v} molecules according to Lobodenko *et al.* (*7*). We assigned 85 lines to the $\Delta k = \pm 2$ perturbation-allowed transitions [cf., e.g., Ref. (*8*)] and determined the ground-state parameters A_0 and $D_0^{(K)}$, which agree well with those determined previously by Graner (*9*). Preliminary measurements of the absolute intensities of about 80 selected lines have confirmed the presence of a negative perturbation of intensity. Extension of this work to $H_3{}^{13}CF$ should aid the understanding of the recently observed difference in the rates of *ortho–para* conversions between $H_3{}^{12}CF$ and $H_3{}^{13}CF$ [cf. Ref. (*10*)].

EXPERIMENTAL PROCEDURE

The infrared spectra were measured in absorption in an optical path 2.84 m by means of an interferometric spectrometer (Bruker IFS 120 HR) at an unapodised resolution 0.0034 cm^{-1}. The spectrometer was calibrated as described previously (*11*). The sample pressure was 50 Pa at 298 K. A segment of the spectrum between 1474.6

TABLE I

Vibration–Rotational Parameters/cm^{-1} of the Bands ν_2 and ν_5 of $H_3{}^{12}CF$

Parameter	I[a]	II[b]	III[c]	IV[d]
E_2	1459.39161[e]	1459.39126(15)	1459.39165(8)	1459.3922(11)
B_2	0.84964490(148)	0.84964887(130)	0.84964621(59)	0.8496306(77)
A_2	5.2044380(2575)	5.2049873(165)	5.2049698(110)	5.204882(63)
$D_J^2/10^{-6}$	2.01910(909)	2.00299(153)	1.99955(121)	1.9665(96)
$D_{JK}^2/10^{-6}$	12.513(344)	13.523(116)	13.302(42)	13.83(21)
$D_K^2/10^{-6}$	74.556[e]	74.322(300)	74.678(307)	70.33[e]
$H_J^2/10^{-9}$	0.[e]	0.[e]	0.[e]	0.[e]
$H_{JK}^2/10^{-9}$	1.293(164)	1.346(130)	1.182(61)	0.0441[e]
$H_{KJ}^2/10^{-9}$	0.[e]	0.[e]	0.[e]	0.810[e]
$H_K^2/10^{-9}$	0.[e]	0.[e]	0.[e]	0.[e]
E_5	1467.81321(35)	1467.81396(7)	1467.81381(5)	1467.8129(5)
B_5	0.85372758(1045)	0.85369607(160)	0.85369991(106)	0.8536710(34)
A_5	5.13666944(33943)	5.13741027(452)	5.13741758(370)	5.137524(16)
$A\zeta_5^z$	-1.2962768(2928)	-1.2958922(87)	-1.2958669(70)	-1.295676(42)
$D_J^5/10^{-6}$	2.07149(461)	2.07079(75)	2.07174(91)	2.0916(45)
$D_{JK}^5/10^{-6}$	13.1363(1411)	12.8447(302)	12.9408(180)	12.752(46)
$D_K^5/10^{-6}$	70.5871[e]	70.646(50)	70.706(155)	70.33[e]
$H_J^5/10^{-9}$	0.[e]	-0.000691(307)	-0.000611(303)	0.0441[e]
$H_{JK}^5/10^{-9}$	0.[e]	-0.4625(184)	-0.4149(129)	0.810[e]
$H_{KJ}^5/10^{-9}$	0.[e]	4.578(126)	4.763(109)	0.[e]
$H_K^5/10^{-9}$	0.[e]	0.[e]	0.[e]	0.[e]
$\eta_J/10^{-4}$	-0.6582(1077)	-0.3604(186)	-0.3756(119)	0.[e]
$\eta_K/10^{-4}$	0.[e]	-0.8720(189)	-0.8524(134)	-0.904(17)
$\tau_J/10^{-6}$	0.[e]	-0.003788(98)	-0.004173(63)	0.[e]
$\tau_{JK}/10^{-6}$	0.08601(1005)	0.10773(166)	0.10581(140)	0.[e]
$\tau_K/10^{-6}$	0.[e]	-0.04717(331)	-0.04351(295)	0.[e]
$C_{11}^{(1)}$	0.5180705(384)	0.5181724(62)	0.5181645(43)	0.518374(26)
$C_{11}^{(3a)}/10^{-5}$	-0.30866(396)	-0.28971(70)	-0.29034(44)	-0.2907(41)
$C_{11}^{(3b)}/10^{-5}$	18.441(2987)	10.364(516)	10.923(331)	0.[e]
$C_{11}^{(2)}/10^{-3}$	1.83719(1324)	1.81082(321)	1.81424(185)	-1.7506(34)
$q_{12}/10^{-3}$	2.40106(469)	2.41351(106)	2.41342(90)	2.4079(22)
$f_{12}^K/10^{-6}$	0.[e]	0.7384(572)	0.7698(486)	0.[e]
B_0	-	0.851794269[e]	0.851795021(321)	0.85179425[e]
A_0	-	5.182009[e]	5.1820107(12)	5.182009[e]
$D_J^0/10^{-6}$	-	2.00877[e]	2.00875(87)	2.0090[e]
$D_{JK}^0/10^{-6}$	-	14.67037[e]	14.68468(403)	14.660[e]
$D_K^0/10^{-6}$	-	70.33[e]	70.39(15)	70.33[e]
$H_J^0/10^{-9}$	-	-0.001072[e]	-0.001072[e]	0.[e]
$H_{JK}^0/10^{-9}$	-	0.064946[e]	0.064946[e]	0.0441[e]
$H_{KJ}^0/10^{-9}$	-	0.745882[e]	0.745882[e]	0.810[e]
$H_K^0/10^{-9}$	-	0.[e]	0.[e]	0.[e]
Standard deviation				
GS rot/MHz	-	-	0.203	
US rot/MHz	0.742	-	0.367	
VR/cm^{-1}	-	7.94×10^{-4}	8.04×10^{-4}	3.7×10^{-3}

[a] Separate fit to the $v_2 = 1$ and $v_5 = 1$ pure rotational transition frequencies (*6*).

[b] Separate fit to the infrared data. The ground state parameters were constrained to the values obtained previously by fitting the purely rotational transition frequencies in the ground state (*11*); A_0 and D_K^0 were constrained to values obtained by Graner (*9*) [$A_0 = 5.182009(12)$, $D_K^0 = 70.33(25)$ cm^{-1}].

[c] Simultaneous fit of the wavenumbers of vibration–rotational transitions with the frequencies of rotational frequencies of the ground and upper states.

[d] Parameters obtained by Betrencourt *et al.* (*3*).

[e] Constrained value.

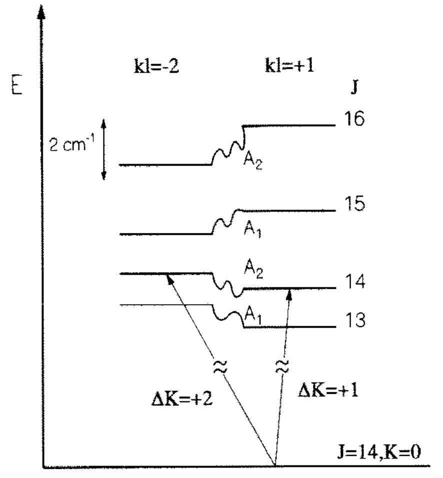

FIG. 2. Scheme of the energy level crossings in the states $kl = -2$ and $kl = +1$ of the level $v_5 = 1$ (positions of levels differing in J are not drawn to scale); A_1 and A_2 are the overall symmetry species.

and 1476.2 cm^{-1} is shown in Fig. 1. The bands ν_2 and ν_5 of H_3CF lie in the same region as the ν_2 band of water vapor. We have therefore recorded also the water spectrum at a pressure of 30 Pa using the same optical path 2.84 m, which made it possible to eliminate easily the H_2O lines from the H_3CF spectrum.

THEORY AND ANALYSIS

The difference of the energies of the vibrational states $v_2 = 1$ and $v_5 = 1$ is (in wavenumber units) only 8.42 cm^{-1}; hence one must use a variational approach to determine the molecular parameters in the excited states $v_2 = 1$ and $v_5 = 1$. According

TABLE II

Coefficients c_1 and c_2 in $c_1|0, 1^{\pm 1}; J, \mp 1\rangle + c_2|1, 0^0; J, \mp 2\rangle$

J'	E/cm^{-1}	c_1	c_2	Assignment[a]
16	1714.266	0.659	0.703	$^qX(J'',2)$
16	1691.272	0.749	-0.647	$^pX(J'',2)$
17	1743.565	0.668	0.688	$^qX(J'',2)$
17	1719.351	0.740	-0.656	$^pX(J'',2)$
18	1774.551	0.677	0.674	$^qX(J'',2)$
18	1749.115	0.731	-0.663	$^pX(J'',2)$
19	1807.221	0.684	0.661	$^qX(J'',2)$
19	1780.565	0.723	-0.670	$^pX(J'',2)$
20	1841.575	0.691	0.648	$^qX(J'',2)$
20	1813.701	0.715	-0.677	$^pX(J'',2)$
21	1877.613	0.697	0.635	$^qX(J'',2)$
21	1848.521	0.708	-0.682	$^pX(J'',2)$
22	1915.334	0.703	0.622	$^pX(J'',2)$
22	1885.026	0.701	-0.687	$^qX(J'',2)$
23	1954.738	0.708	0.610	$^pX(J'',2)$
23	1923.214	0.694	-0.692	$^qX(J'',2)$
24	1995.823	0.713	0.598	$^pX(J'',2)$
24	1963.086	0.688	-0.697	$^qX(J'',2)$
25	2038.589	0.717	0.586	$^pX(J'',2)$
25	2004.641	0.682	-0.701	$^qX(J'',2)$

Note. [a] X stands for P, Q, R; $J'' = J' + 1$ for P, $J'' = J'$ for Q, and $J'' = J' - 1$ for R.

to this method, a matrix representation of the expanded vibration–rotational Hamiltonian is formed; the corresponding vibration–rotational energies are obtained by the numerical diagonalization of this matrix during the least-squares fit to the parameters corresponding to the minimum of the sum of the weighted squares of the differences between the experimental and calculated transition frequencies and wavenumbers.

The order of approximation that we use in fitting the data is essentially a matter of experience combined with a method of trial and error. In contrast, the form of a reduced vibration–rotational Hamiltonian involving only determinable molecular parameters can be chosen in a less empirical manner (*7*). We used the following expression for the diagonal elements of the matrix representation of the reduced vibration–rotational Hamiltonian,

$$\begin{aligned} E_{vr}(J,K,l)/hc &= E_v/hc + B_vJ(J+1) + (A_v - B_v)K^2 - 2(A\zeta_5^z)Kl \\ &\quad + \eta_J^5 J(J+1)Kl + \eta_K^5 K^3 l + \tau_J^5 J^2(J+1)^2 Kl + \tau_{JK}^5 J(J+1)K^3 l + \tau_K^5 K^5 l \\ &\quad - D_J^{(v)} J^2(J+1)^2 - D_{JK}^{(v)} J(J+1)K^2 - D_K^{(v)} K^4 + H_J^{(v)} J^3(J+1)^3 \\ &\quad + H_{JK}^{(v)} J^2(J+1)^2 K^2 + H_{KJ}^{(v)} J(J+1)K^4 + H_K^{(v)} K^6 + \cdots, \end{aligned} \tag{1}$$

in which $l = 0$ for the nondegenerate vibrational state $v_2 = 1$ and $l = \pm 1$ for the $\pm l$ sublevels of the doubly degenerate state $v_5 = 1$.

An extremely useful result of the theoretical considerations of Lobodenko *et al.* (*7*) is that one must constrain four parameters of the transformed effective third-order Hamiltonian for the Coriolis interaction between the vibrational states $v_2 = 1$ and $v_5 = 1$ so as to eliminate the ambiguity of this Hamiltonian. We chose the following constraints

$$q_{22}^5 = \eta_K^5 = C_{21}^{(2)} = \alpha^5 = 0. \tag{2}$$

Thus we fitted the following parameters for the Coriolis interaction,

$$\begin{aligned} &\langle 0, 1^{+1}; J, k+1 | (H_{21} + H_{23})/hc | 1, 0^0; J, k\rangle \\ &\quad = -\langle 1, 0^0; J, k+1 | (H_{21} + H_{23})/hc | 0, 1^{-1}; J, k\rangle \\ &\qquad = 2^{1/2}\{C_{11}^{(1)} + C_{11}^{(3a)} J(J+1) + C_{11}^{(3b)}[k^2 + (k+1)^2]\}F(J,k), \end{aligned} \tag{3}$$

in which

$$F(J,k) = [J(J+1) - k(k+1)]^{1/2}. \tag{4}$$

The "2, −1" l-type interaction has the determinable parameters,

$$\begin{aligned} &\langle 0, 1^{-1}; J, k+1 | (H_{22} + H_{24})/hc | 0, 1^{+1}; J, k\rangle \\ &\qquad = 2\{q_{12}^5(2k+1) + f_{12}^{5,K}[k^3 + (k+1)^3]\}F(J,k), \end{aligned} \tag{5}$$

as well as the interaction described by the matrix element

$$\begin{aligned} &\langle 0, 1^{+1}; J, k+1 | H_{22}/hc | 1, 0^0; J, k\rangle \\ &\quad = \langle 1, 0^0; J, k+1 | H_{22}/hc | 0, 1^{-1}; J, k\rangle = 2^{1/2} C_{11}^{(2)}(2k+1)F(J,k). \end{aligned} \tag{6}$$

We use the notation and phase conventions for the off-diagonal matrix elements described in Ref. (*12*).

TABLE III

Wavenumbers/cm^{-1} of Lines in the Bands ν_2 and ν_5 of $H_3{}^{12}CF$

Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc	
qP(1, 0)	(1457.68806)			qP(26, 1)	1393.79405	(10)	25	qP(12, 4)	(1439.98412)		
qP(2, 0)	1455.83992	(10)	-21	qP(27, 1)	1391.11287	(20)	27	qP(13, 4)	(1438.39095)		
qP(3, 0)	1453.85539	(50)	-24	qP(28, 1)	1388.43013	(20)	24	qP(14, 4)	(1436.80519)		
qP(4, 0)	1451.74793	(10)	-21	qP(29, 1)	1385.74600	(30)	6	qP(15, 4)	(1435.22651)		
qP(5, 0)	1449.53411	(20)	-17	qP(30, 1)	1383.06098	(30)	1	qP(16, 4)	(1433.65459)		
qP(6, 0)	1447.23077	(10)	-29	qP(31, 1)	1380.37492	(30)	-30	qP(17, 4)	(1432.08912)		
qP(7, 0)	1444.85395	(10)	-26	qP(32, 1)	1377.68850	(30)	-42	qP(6, 5)	(1449.85918)		
qP(8, 0)	1442.41712	(10)	-22	qP(33, 1)	1375.00164	(30)	-60	qP(7, 5)	(1448.17477)		
qP(9, 0)	1439.93149	(20)	-25	qP(34, 1)	1372.31418	(50)	-122	qP(8, 5)	(1446.49368)		
qP(10, 0)	1437.40642	(10)	-19	qP(35, 1)	(1369.62855)			qP(9, 5)	(1444.81599)		
qP(11, 0)	1434.84919	(10)	-12	qP(3, 2)	(1454.64771)			qP(10, 5)	(1443.14180)		
qP(12, 0)	1432.26562	(10)	-13	qP(4, 2)	(1453.23395)			qP(11, 5)	(1441.47118)		
qP(13, 0)	1429.66049	(10)	-12	qP(5, 2)	(1451.87883)			qP(12, 5)	(1439.80424)		
qP(14, 0)	1427.03760	(10)	-8	qP(6, 2)	(1450.56434)			qP(13, 5)	(1438.14106)		
qP(15, 0)	1424.39997	(10)	-1	qP(7, 2)	(1449.27631)			qP(14, 5)	(1436.48174)		
qP(16, 0)	1421.75004	(10)	4	qP(8, 2)	(1448.00417)			qP(15, 5)	(1434.82638)		
qP(17, 0)	1419.08981	(10)	8	qP(9, 2)	(1446.74024)			qP(16, 5)	(1433.17507)		
qP(18, 0)	1416.42096	(10)	12	qP(10, 2)	(1445.47900)			qP(17, 5)	(1431.52790)		
qP(19, 0)	1413.74489	(10)	19	qP(11, 2)	(1444.21647)			qP(7, 6)	(1448.39991)		
qP(20, 0)	1411.06273	(10)	25	qP(12, 2)	(1442.94984)			qP(8, 6)	(1446.69469)		
qP(21, 0)	1408.37549	(50)	36	qP(13, 2)	(1441.67710)			qP(9, 6)	1444.98950	(60)	-8
qP(22, 0)	1405.68391	(30)	42	qP(14, 2)	(1440.39687)			qP(10, 6)	1443.28487	(60)	10
qP(23, 0)	1402.98876	(10)	49	qP(15, 2)	(1439.10821)			qP(11, 6)	1441.58111	(80)	70
qP(24, 0)	1400.29056	(10)	49	qP(16, 2)	(1437.81054)			qP(12, 6)	1439.87629	(100)	-39
qP(25, 0)	1397.58992	(20)	49	qP(17, 2)	(1436.50354)			qP(13, 6)	1438.17292	(100)	-89
qP(26, 0)	1394.88731	(10)	50	qP(18, 2)	(1435.18710)			qP(14, 6)	(1436.47199)		
qP(27, 0)	1392.18318	(20)	58	qP(19, 2)	(1433.86126)			qP(15, 6)	(1434.77143)		
qP(28, 0)	1389.47772	(40)	54	qP(20, 2)	(1432.52619)			qP(16, 6)	(1433.07235)		
qP(29, 0)	1386.77130	(20)	43	qP(21, 2)	(1431.18215)			qP(17, 6)	(1431.37498)		
qP(30, 0)	1384.06436	(30)	40	qP(22, 2)	(1429.82950)			qP(8, 7)	(1446.98961)		
qP(31, 0)	1381.35679	(20)	10	pP(23, 2)	(1428.46861) A			qP(9, 7)	(1445.26838)		
qP(32, 0)	1378.64916	(30)	-16	pP(24, 2)	(1427.09992) A			qP(10, 7)	(1443.54541)		
qP(33, 0)	1375.94189	(40)	-16	pP(25, 2)	(1425.72390) A			qP(11, 7)	(1441.82088)		
qP(34, 0)	1373.23475	(40)	-35	pP(26, 2)	(1424.34103) A			qP(12, 7)	(1440.09499)		
qP(35, 0)	1370.52764	(70)	-99	pP(27, 2)	(1422.95180) A			qP(13, 7)	(1438.36797)		
qP(36, 0)	(1367.81822)			pP(28, 2)	(1421.55669) A			qP(14, 7)	(1436.64004)		
qP(2, 1)	1455.75830	(10)	-23	pP(29, 2)	(1420.15621) A			qP(15, 7)	(1434.91143)		
qP(3, 1)	1453.55027	(10)	-12	pP(30, 2)	(1418.75081) A			qP(16, 7)	(1433.18240)		
qP(4, 1)	1451.21163	(10)	-18	pP(31, 2)	(1417.34107) A			qP(17, 7)	(1431.45319)		
qP(5, 1)	1448.79306	(50)	-15	qP(4, 3)	(1452.94401)			qP(9, 8)	(1445.62688)		
qP(6, 1)	1446.32210	(10)	-14	qP(5, 3)	(1451.34736)			qP(10, 8)	(1443.89239)		
qP(7, 1)	1443.81432	(10)	-9	qP(6, 3)	(1449.77421)			qP(11, 8)	(1442.15500)		
qP(8, 1)	1441.27883	(10)	-10	qP(7, 3)	(1448.22268)			qP(12, 8)	(1440.41490)		
qP(9, 1)	1438.72156	(10)	-12	qP(8, 3)	(1446.69077)			qP(13, 8)	(1438.67231)		
qP(10, 1)	1436.14657	(10)	-7	qP(9, 3)	(1445.17642)			qP(14, 8)	(1436.92744)		
qP(11, 1)	1433.55666	(10)	-7	qP(10, 3)	(1443.67756)			qP(15, 8)	(1435.18054)		
qP(12, 1)	1430.95408	(10)	-4	qP(11, 3)	(1442.19222)			qP(16, 8)	(1433.43184)		
qP(13, 1)	1428.34048	(50)	-4	qP(12, 3)	(1440.71852)			qP(17, 8)	(1431.68160)		
qP(14, 1)	1425.71733	(100)	-2	qP(13, 3)	(1439.25474)			qP(10, 9)	(1444.31089)		
qP(15, 1)	1423.08578	(10)	3	qP(14, 3)	(1437.79928)			qP(11, 9)	(1442.56491)		
qP(16, 1)	1420.44678	(10)	6	qP(15, 3)	(1436.35074)			qP(12, 9)	(1440.81527)		
qP(17, 1)	1417.80119	(10)	9	qP(16, 3)	(1434.90786)			qP(13, 9)	(1439.06218)		
qP(18, 1)	1415.14977	(10)	14	qP(17, 3)	(1433.46956)			qP(14, 9)	(1437.30585)		
qP(19, 1)	1412.49341	(30)	43	qP(5, 4)	(1451.37052)			qP(15, 9)	(1435.54652)		
qP(20, 1)	1409.83197	(20)	23	qP(6, 4)	(1449.71677)			qP(16, 9)	(1433.78440)		
qP(21, 1)	1407.16669	(10)	28	qP(7, 4)	(1448.07249)			qP(17, 9)	(1432.01976)		
qP(22, 1)	1404.49778	(10)	29	qP(8, 4)	(1446.43745)			qP(11,10)	(1443.04101)		
qP(23, 1)	1401.82569	(10)	30	qP(9, 4)	(1444.81139)			qP(12,10)	(1441.28475)		
qP(24, 1)	1399.15081	(20)	31	qP(10, 4)	(1443.19402)			qP(13,10)	(1439.52436)		
qP(25, 1)	1396.47350	(10)	30	qP(11, 4)	(1441.58503)			qP(14,10)	(1437.76003)		

Note. In case the experimental wavenumber is missing, a value calculated from parameters in Table I is given (enclosed in parentheses). The experimental uncertainties (in parentheses) and the difference between observed and calculated wavenumbers are given in units of the last wavenumber digit quoted. Wavenumbers denoted with (*) have not been taken in the fit, A—see Table II. If the A_1–A_2 splitting is indicated for the J'', K'' = 3 lines, the first wavenumber in the doublet corresponds to a transition to the larger block in the symmetry factorized matrix of the Hamiltonian, i.e., for J' even it is the $A_1 \leftarrow A_2$, for J' odd the $A_2 \leftarrow A_1$ transition.

TABLE III—*Continued*

Transition	Wavenumber	Obs-Calc		Transition	Wavenumber		Obs-Calc		Transition	Wavenumber		Obs-Calc	
qP(15,10)	(1435.99199)			qQ(14, 2)	1464.63313		(20)	-4	qQ(29, 3)	1465.79463	*		423
qP(16,10)	(1434.22046)			qQ(15, 2)	1465.03319		(30)	0	qQ(30, 3)	1466.05140	*		-73
qP(17,10)	(1432.44568)			qQ(16, 2)	1465.42315		(30)	6	qQ(30, 3)	1466.04653	*		207
qP(12,11)	(1441.81665)			qQ(17, 2)	1465.80280		(30)	6	qQ(31, 3)	1466.30638	*		-76
qP(13,11)	(1440.05106)			qQ(18, 2)	1466.17219		(30)	7	qQ(31, 3)	1466.29918	*		227
qP(14,11)	(1438.28102)			qQ(19, 2)	1466.53151		(20)	16	qQ(32, 3)	1466.56115	*		-61
qP(15,11)	(1436.50674)			qQ(20, 2)	1466.88083		(60)	18	qQ(32, 3)	1466.55021	*		249
qP(16,11)	(1434.72845)			qQ(21, 2)	1467.22051		(10)	20	qQ(33, 3)	1466.81670	*		-33
qP(17,11)	(1432.94638)			pQ(22, 2)	1467.55094	A	(30)	25	qQ(33, 3)	1466.79989	*		293
qP(13,12)	(1440.63727)			pQ(23, 2)	1467.87245	A	(20)	30	qQ(34, 3)	1467.07551	*		10
qP(14,12)	(1438.86309)			pQ(24, 2)	1468.18544	A	(20)	32	qQ(34, 3)	1467.04778	*		312
qP(15,12)	(1437.08428)			pQ(25, 2)	1468.49038	A	(30)	35	qQ(4, 4)	1459.88519		(10)	6
qP(16,12)	(1435.30107)			pQ(26, 2)	1468.78751	A	(100)	18	qQ(5, 4)	1459.93371		(10)	-4
qP(17,12)	(1433.51368)			pQ(27, 2)	1469.07783	A	(10)	38	qQ(6, 4)	1459.99217		(80)	59
qP(14,13)	(1439.50228)			pQ(28, 2)	1469.36126	A	(10)	43	qQ(7, 4)	1460.05830		(10)	0
qP(15,13)	(1437.72016)			pQ(29, 2)	1469.63834	A	(20)	44	qQ(8, 4)	1460.13447		(500)	86
qP(16,13)	(1435.93333)			pQ(30, 2)	1469.90971	A	(30)	53	qQ(9, 4)	1460.21769		(500)	50
qP(17,13)	(1434.14204)			pQ(31, 2)	1470.17538	A	(20)	49	qQ(10, 4)	1460.29939		(1000)	-927
qQ(1, 1)	(1459.16559)			pQ(32, 2)	1470.43612	A	(20)	57	qQ(11, 4)	1460.40764		(10)	-5
qQ(2, 1)	(1458.66086)			pQ(33, 2)	1470.69195	A	(40)	45	qQ(12, 4)	1460.51373		(500)	-13
qQ(3, 1)	1458.02533	(50)	-22	pQ(34, 2)	1470.94367	A	(30)	56	qQ(13, 4)	1460.62673		(20)	-10
qQ(4, 1)	1457.30989	(100)	-12	pQ(35, 2)	1471.19122	A	(60)	51	qQ(14, 4)	1460.74620		(100)	0
qQ(5, 1)	1456.54174	(50)	-14	qQ(3, 3)	1459.75710		(100)	30	qQ(15, 4)	1460.87171		(100)	9
qQ(6, 1)	1455.73646	(10)	-12	qQ(4, 3)	1459.86289		(10)	-9	qQ(16, 4)	1461.00275		(10)	4
qQ(7, 1)	1454.90318	(10)	-12	qQ(5, 3)	1459.99217		(30)	-26	qQ(17, 4)	1461.13953		(100)	41
qQ(8, 1)	1454.04769	(10)	-17	qQ(6, 3)	1460.14287		(10)	-33	qQ(18, 4)	1461.28067		(20)	14
qQ(9, 1)	1453.17411	(10)	-10	qQ(7, 3)	1460.31289		(1000)	-37	qQ(19, 4)	1461.42669		(10)	7
qQ(10, 1)	1452.28508	(10)	-12	qQ(8, 3)	1460.50038		(100)	-12	qQ(20, 4)	1461.57714		(10)	5
qQ(11, 1)	1451.38290	(10)	-6	qQ(9, 3)	1460.70263		(10)	-15	qQ(21, 4)	1461.73172		(50)	8
qQ(12, 1)	1450.46912	(10)	-3	qQ(10, 3)	1460.91897		(100)	85	qQ(22, 4)	1461.89008		(20)	5
qQ(13, 1)	1449.54514	(20)	0	qQ(11, 3)	1461.14448		(100)	-7	qQ(23, 4)	1462.05208		(50)	9
qQ(14, 1)	1448.61157	(40)	-45	qQ(12, 3)	1461.38025		(20)	-6	qQ(24, 4)	1462.21738		(20)	6
qQ(15, 1)	1447.67080	(10)	4	qQ(13, 3)	1461.62388		(80)	8	qQ(25, 4)	1462.38648		(60)	68
qQ(16, 1)	1446.72218	(10)	4	qQ(14, 3)	1461.87340		(10)	-11	qQ(26, 4)	1462.55725		(20)	0
qQ(17, 1)	1445.76687	(10)	2	qQ(15, 3)	1462.12810		(20)	-6	qQ(27, 4)	1462.73137		(10)	-11
qQ(18, 1)	1444.80565	(60)	14	qQ(16, 3)	1462.38648		(30)	-13	qQ(28, 4)	1462.91090		(300)	256
qQ(19, 1)	1443.83886	(20)	21	qQ(17, 3)	1462.64784		(10)	-4	qQ(29, 4)	1463.08736		(40)	-31
qQ(20, 1)	1442.86678	(10)	3	qQ(18, 3)	1462.91090		(50)	-19	qQ(30, 4)	1463.26890		(80)	-46
qQ(21, 1)	1441.89065	(20)	42	qQ(18, 3)	1462.91090		(50)	13	qQ(31, 4)	1463.45239		(30)	-88
qQ(22, 1)	1440.90958	(30)	10	qQ(19, 3)	1463.17542		(30)	-11	qQ(32, 4)	1463.63830		(40)	-101
qQ(23, 1)	(1439.92483)			qQ(19, 3)	1463.17542		(30)	32	qQ(33, 4)	1463.82615		(50)	-123
qQ(24, 1)	(1438.93660)			qQ(20, 3)	1463.44044		(50)	-15	qQ(34, 4)	1464.01597		(60)	-142
qQ(25, 1)	(1437.94507)			qQ(20, 3)	1463.44044		(50)	43	qQ(5, 5)	1460.07446		(500)	-12
qQ(26, 1)	(1436.95048)			qQ(21, 3)	1463.70562	*		-11	qQ(6, 5)	1460.09088		(100)	-112
qQ(27, 1)	(1435.95309)			qQ(21, 3)	1463.70562	*		65	qQ(7, 5)	1460.11305		(1000)	62
qQ(28, 1)	(1434.95309)			qQ(22, 3)	1463.97041	*		-17	qQ(8, 5)	1460.13447		(1000)	-137
qQ(29, 1)	(1433.95068)			qQ(22, 3)	1463.97041	*		82	qQ(9, 5)	1460.16254		(500)	20
qQ(30, 1)	(1432.94605)			qQ(23, 3)	1464.23446	*		-32	qQ(10, 5)	1460.19203		(10)	11
qQ(2, 2)	1459.75710	(100)	-81	qQ(23, 3)	1464.23446	*		96	qQ(11, 5)	1460.22466		(500)	1
qQ(3, 2)	1460.04722	(100)	-10	qQ(24, 3)	1464.49760	*		-46	qQ(12, 5)	1460.26059		(10)	3
qQ(4, 2)	1460.39520	(500)	0	qQ(24, 3)	1464.49760	*		119	qQ(13, 5)	1460.29196		(500)	-774
qQ(5, 2)	1460.78328	(50)	-15	qQ(25, 3)	1464.76029	*		3	qQ(14, 5)	1460.34189		(100)	-24
qQ(6, 2)	1461.19776	(500)	-9	qQ(25, 3)	1464.76029	*		215	qQ(15, 5)	1460.38807		(100)	17
qQ(7, 2)	1461.62388	(400)	-394	qQ(26, 3)	1465.02032	*		-89	qQ(16, 5)	1460.43697		(20)	-4
qQ(8, 2)	1462.06550	(30)	-13	qQ(26, 3)	1465.02032	*		182	qQ(17, 5)	1460.48954		(30)	-1
qQ(9, 2)	1462.50561	(10)	-7	qQ(27, 3)	1465.27964	*		-122	qQ(18, 5)	1460.54558		(30)	2
qQ(10, 2)	1462.94387	(10)	-10	qQ(27, 3)	1465.27964	*		227	qQ(19, 5)	1460.60442		(100)	-63
qQ(11, 2)	1463.37751	(10)	-11	qQ(28, 3)	1465.53743	*		-175	qQ(20, 5)	1460.66809		(90)	0
qQ(12, 2)	1463.80457	(10)	-2	qQ(28, 3)	1465.53743	*		274	qQ(6, 6)	1460.31289		(1000)	-201
qQ(13, 2)	1464.22338	(80)	-5	qQ(29, 3)	1465.79463	*		-160	qQ(7, 6)	(1460.31086)			

We tested the consistency of the submillimeter-wave and infrared data by fitting these data separately and simultaneously (cf. Table I). The data were weighted according to the inverse square, $(\Delta\nu)^{-2}$, of the experimental uncertainty $\Delta\nu$ of the lines. The estimated uncertainties of the pure rotational transitions were stated previously (6); the uncertainties of the infrared data are indicated in Table III below. Each uncertainty stated in this paper represents one standard error.

TABLE III—*Continued*

Transition	Wavenumber		Obs-Calc	Transition	Wavenumber		Obs-Calc	Transition	Wavenumber			Obs-Calc
qQ(8, 6)	(1460.30655)			qQ(18,10)	(1461.14510)			qR(10, 2)	1482.10502		(10)	-10
qQ(9, 6)	(1460.30209)			qQ(19,10)	(1461.05360)			qR(11, 2)	1484.23232		(100)	-5
qQ(10, 6)	(1460.29760)			qQ(20,10)	(1460.95892)			qR(12, 2)	1486.35092		(20)	0
qQ(11, 6)	(1460.29323)			qQ(11,11)	(1462.20353)			qR(13, 2)	1488.45971		(20)	-3
qQ(12, 6)	(1460.28913)			qQ(12,11)	(1462.13424)			qR(14, 2)	1490.55819		(10)	3
qQ(13, 6)	(1460.28545)			qQ(13,11)	(1462.05988)			qR(15, 2)	1492.64576		(20)	1
qQ(14, 6)	(1460.28236)			qQ(14,11)	(1461.98061)			qR(16, 2)	1494.72266		(40)	37
qQ(15, 6)	(1460.28003)			qQ(15,11)	(1461.89660)			qR(17, 2)	1496.78786		(10)	10
qQ(16, 6)	(1460.27863)			qQ(16,11)	(1461.80805)			qR(18, 2)	1498.84229		(20)	8
qQ(17, 6)	(1460.27835)			qQ(17,11)	(1461.71514)			qR(19, 2)	1500.88604		(10)	24
qQ(18, 6)	(1460.27936)			qQ(18,11)	(1461.61806)			qR(20, 2)	1502.91902		(20)	21
qQ(19, 6)	(1460.28185)			qQ(19,11)	(1461.51704)			pR(21, 2)	1504.94171	A	(50)	21
qQ(20, 6)	(1460.28600)			qQ(20,11)	(1461.41229)			pR(22, 2)	1506.95448	A	(30)	26
qQ(7, 7)	1460.60442	(500)	168	qQ(12,12)	1462.70816	(200)	-363	pR(23, 2)	1508.95765	A	(30)	30
qQ(8, 7)	1460.58192	(200)	0	qQ(13,12)	1462.62925	(200)	-337	pR(24, 2)	1510.95165	A	(50)	40
qQ(9, 7)	1460.55939	(200)	46	qQ(14,12)	(1462.54817)			pR(25, 2)	1512.93689	A	(30)	56
qQ(10, 7)	1460.53404	(200)	13	qQ(15,12)	(1462.45859)			pR(26, 2)	1514.91334	A	(40)	36
qQ(11, 7)	1460.50695	(1000)	-3	qQ(16,12)	(1462.36406)			pR(27, 2)	1516.88220	A	(50)	61
qQ(12, 7)	1460.47845	(500)	9	qQ(17,12)	(1462.26477)			pR(28, 2)	1518.84317	A	(100)	64
qQ(13, 7)	1460.44838	(50)	19	qQ(18,12)	(1462.16093)			qR(3, 3)	1466.67573		(20)	-4
qQ(14, 7)	1460.41648	(50)	-19	qQ(19,12)	(1462.05273)			qR(4, 3)	1468.50787		(10)	-19
qQ(15, 7)	1460.38807	(500)	405	qQ(20,12)	(1461.94040)			qR(5, 3)	1470.36137		(10)	-5
qQ(16, 7)	1460.35408	(200)	368	qR(0, 0)	(1460.95083)			qR(6, 3)	1472.23371		(50)	-8
qQ(17, 7)	1460.31289	(200)	-316	qR(1, 0)	(1462.37330)			qR(7, 3)	1474.12290		(10)	-9
qQ(18, 7)	1460.27992	(150)	-128	qR(1, 1)	(1462.06792)			qR(8, 3)	1476.02681		(10)	-4
qQ(19, 7)	1460.24628	(150)	22	qR(2, 1)	(1463.13602)			qR(9, 3)	1477.94323		(10)	-9
qQ(20, 7)	1460.21130	(100)	44	qR(3, 1)	(1464.12374)			qR(10, 3)	1479.87036		(10)	-8
qQ(8, 8)	1460.93637	(200)	-11	qR(4, 1)	(1465.05868)			qR(11, 3)	1481.80626		(10)	-8
qQ(9, 8)	1460.90123	(200)	-31	qR(5, 1)	1465.95605	(100)	-17	qR(12, 3)	1483.74930		(10)	-7
qQ(10, 8)	1460.86321	(500)	0	qR(6, 1)	1466.82566	(100)	17	qR(13, 3)	1485.69796		(10)	-6
qQ(11, 8)	1460.82151	(500)	-14	qR(7, 1)	1467.67167	(100)	-56	qR(14, 3)	1487.65072		(30)	-21
qQ(12, 8)	1460.77721	(500)	20	qR(8, 1)	1468.50030	(100)	-11	qR(15, 3)	1489.60685		(10)	-8
qQ(13, 8)	1460.72957	(100)	9	qR(9, 1)	1469.31275	(50)	-3	qR(16, 3)	1491.56490		(10)	-4
qQ(14, 8)	1460.67892	(100)	-30	qR(10, 1)	1470.11141	(10)	-2	qR(17, 3)	1493.52404		(10)	-6
qQ(15, 8)	1460.62673	(100)	27	qR(11, 1)	1470.89779	(80)	-21	qR(17, 3)	1493.52404		(10)	26
qQ(16, 6)	1460.57138	(100)	0	qR(12, 1)	1471.67387	(200)	9	qR(18, 3)	1495.48350		(20)	-11
qQ(17, 8)	(1460.51421)			qR(13, 1)	1472.43985	(40)	2	qR(18, 3)	1495.48350		(20)	33
qQ(18, 8)	(1460.45516)			qR(14, 1)	1473.19702	(30)	-2	qR(19, 3)	1497.44277		(30)	-5
qQ(19, 8)	(1460.39446)			qR(15, 1)	1473.94624	(40)	5	qR(19, 3)	1497.44277		(30)	53
qQ(20, 8)	(1460.33234)			qR(16, 1)	1474.69288	(500)	498	qR(20, 3)	1499.40105	*		-10
qQ(9, 9)	1461.31490	(500)	-19	qR(17, 1)	1475.42285	(20)	12	qR(20, 3)	1499.40105	*		65
qQ(10, 9)	1461.26717	(500)	-50	qR(18, 1)	1476.15171	(100)	54	qR(21, 3)	1501.35798	*		-20
qQ(11, 9)	1461.21557	(500)	-49	qR(19, 1)	1476.87391	(20)	25	qR(21, 3)	1501.35798	*		79
qQ(12, 9)	1461.15986	(500)	-58	qR(20, 1)	1477.59080	(30)	23	qR(22, 3)	1503.31321	*		-27
qQ(13, 9)	1461.10053	(100)	-42	qR(21, 1)	1478.30259	(30)	36	qR(22, 3)	1503.31321	*		101
qQ(14, 9)	1461.03707	(100)	-71	qR(22, 1)	1479.01004	(150)	112	qR(23, 3)	1505.26638	*		-40
qQ(15, 9)	1460.97099	(100)	-12	qR(23, 1)	1479.71131	(30)	38	qR(23, 3)	1505.26638	*		125
qQ(16, 9)	1460.90123	(200)	8	qR(24, 1)	1480.40864	(40)	17	qR(24, 3)	1507.21719	*		-63
qQ(17, 9)	1460.82836	(150)	27	qR(25, 1)	1481.10186	(40)	10	qR(24, 3)	1507.21719	*		148
qQ(18, 9)	1460.75282	(100)	68	qR(26, 1)	1481.79122	(60)	24	qR(25, 3)	1509.16549	*		-92
qQ(19, 9)	(1460.67354)			qR(27, 1)	1482.47650	(60)	21	qR(25, 3)	1509.16549	*		179
qQ(20, 9)	(1460.59251)			qR(28, 1)	1483.15781	(100)	-2	qR(26, 3)	1511.11125	*		-120
qQ(10,10)	1461.73172	(700)	-598	qR(2, 2)	1465.15736	(100)	-16	qR(26, 3)	1511.11125	*		229
qQ(11,10)	1461.67747	(500)	-146	qR(3, 2)	1467.20852	(10)	-5	qR(27, 3)	1513.05401	*		-184
qQ(12,10)	1461.61432	(500)	-112	qR(4, 2)	1469.29972	(10)	-7	qR(27, 3)	1513.05401	*		265
qQ(13,10)	1461.54594	(200)	-146	qR(5, 2)	1471.41688	(50)	-8	qR(28, 3)	1514.98781	*		-882
qQ(14,10)	(1461.47498)			qR(6, 2)	1473.55025	(100)	86	qR(28, 3)	1514.98781	*		-298
qQ(15,10)	(1461.39834)			qR(7, 2)	1475.68937	(50)	6	qR(29, 3)	(1516.93486)			
qQ(16,10)	(1461.31768)			qR(8, 2)	1477.83096	(10)	-12	qR(29, 3)	(1516.92719)			
qQ(17,10)	(1461.23320)			qR(9, 2)	1479.97061	(10)	-5	qR(30, 3)	(1518.87075)			

We tested our computer program and the phase conventions by reproducing the calculated transition frequencies listed by Betrencourt *et al.* (*3*), using their parameters. In the entire range of their calculated transition frequencies, the differences between the corresponding calculated wavenumbers did not exceed 1×10^{-4} cm^{-1}, but to achieve this agreement we were obliged to change the sign given (*3*) for the parameter $C_{11}^{(2)}$.

We determined the absolute intensities of selected lines in the bands ν_2 and ν_5 by

TABLE III—*Continued*

Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc	
qR(30, 3)	(1518.86050)			qR(22, 6)	1499.37048	(40)	-32	qR(17,11)	(1492.17243)		
qR(4, 4)	(1468.44836)			qR(23, 6)	1501.07179	(40)	-80	qR(18,11)	(1493.76325)		
qR(5, 4)	1470.20845	(10)	-11	qR(24, 6)	1502.77490	(40)	-85	qR(19,11)	(1495.34941)		
qR(6, 4)	1471.97740	(10)	1	qR(25, 6)	1504.47897	(40)	-144	qR(20,11)	(1496.93111)		
qR(7, 4)	1473.75469	(100)	22	qR(7, 7)	(1474.19506)			qR(12,12)	(1484.70716)		
qR(8, 4)	1475.54370	(500)	428	qR(8, 7)	(1475.87248)			qR(13,12)	(1486.31772)		
qR(9, 4)	1477.33187	(10)	2	qR(9, 7)	(1477.54742)			qR(14,12)	(1487.92248)		
qR(10, 4)	1479.13136	(10)	4	qR(10, 7)	(1479.22001)			qR(15,12)	(1489.52157)		
qR(11, 4)	1480.93738	(10)	-5	qR(11, 7)	(1480.89035)			qR(16,12)	(1491.11514)		
qR(12, 4)	1482.74982	(10)	6	qR(12, 7)	(1482.55857)			qR(17,12)	(1492.70334)		
qR(13, 4)	1484.56784	(10)	-1	qR(13, 7)	1484.22530	(90)	48	qR(18,12)	(1494.28632)		
qR(14, 4)	1486.39139	(10)	7	qR(14, 7)	1485.89434	(500)	508	qR(19,12)	(1495.86425)		
qR(15, 4)	1488.21970	(60)	-2	qR(15, 7)	1487.54852	(500)	-349	qR(20,12)	(1497.43731)		
qR(16, 4)	1490.05268	(20)	-1	qR(16, 7)	1489.21328	(100)	1	pP(1, 1)	1461.78019	(500)	8
qR(17, 4)	1491.88997	(20)	12	qR(17, 7)	1490.87810	(200)	490	pP(2, 1)	1460.32733	(10)	5
qR(18, 4)	1493.73085	(10)	4	qR(18, 7)	(1492.53196)			pP(3, 1)	1459.04431	(30)	17
qR(19, 4)	1495.57530	(10)	8	qR(19, 7)	1494.19028	(50)	53	pP(4, 1)	1457.85144	(10)	-2
qR(20, 4)	1497.42009	(250)	-267	qR(20, 7)	(1495.84674)			pP(5, 1)	1456.69426	(10)	0
qR(21, 4)	1499.27335	(20)	22	qR(8, 8)	1476.21541	*	425	pP(6, 1)	1455.54930	(10)	2
qR(22, 4)	1501.12600	(30)	0	qR(9, 8)	(1477.87236)			pP(7, 1)	1454.40039	(10)	5
qR(23, 4)	1502.98119	(30)	4	qR(10, 8)	(1479.52986)			pP(8, 1)	1453.23875	(10)	-2
qR(24, 4)	1504.83803	(150)	-23	qR(11, 8)	(1481.18375)			pP(9, 1)	1452.05941	(10)	-5
qR(25, 4)	1506.69709	(70)	-6	qR(12, 8)	(1482.83417)			pP(10, 1)	1450.85947	(10)	9
qR(5, 5)	(1470.30742)			qR(13, 8)	(1484.48125)			pP(11, 1)	1449.63689	(10)	4
qR(6, 5)	1472.02484	(500)	-482	qR(14, 8)	(1486.12514)			pP(12, 1)	1448.39112	(10)	1
qR(7, 5)	1473.75469	(50)	10	qR(15, 8)	(1487.76600)			pP(13, 1)	1447.12206	(10)	-2
qR(8, 5)	1475.48151	(500)	-68	qR(16, 8)	(1489.40399)			pP(14, 1)	1445.83029	(20)	7
qR(9, 5)	1477.21259	(30)	12	qR(17, 8)	(1491.03928)			pP(15, 1)	1444.51647	(60)	16
qR(10, 5)	1478.94532	(20)	-5	qR(18, 8)	(1492.67206)			pP(16, 1)	1443.18141	(40)	-4
qR(11, 5)	1480.68106	(20)	9	qR(19, 8)	(1494.30251)			pP(17, 1)	1441.82702	(60)	7
qR(12, 5)	1482.41947	(20)	26	qR(20, 8)	(1495.93082)			pP(18, 1)	(1440.45422)		
qR(13, 5)	1484.16071	(50)	61	qR(9, 9)	(1478.27187)			pP(19, 1)	1439.06444	(100)	-30
qR(14, 5)	1485.90366	(30)	2	qR(10, 9)	(1479.91884)			pP(20, 1)	1437.66036	(60)	32
qR(15, 5)	1487.65072	(100)	89	qR(11, 9)	(1481.56125)			pP(21, 1)	(1436.24159)		
qR(16, 5)	1489.39871	(40)	3	qR(12, 9)	(1483.19923)			pP(22, 1)	(1434.81085)		
qR(17, 5)	1491.14991	(40)	-22	qR(13, 9)	(1484.83289)			pP(23, 1)	(1433.36920)		
qR(18, 5)	1492.90428	(10)	2	qR(14, 9)	1486.46199	(200)	-39	pP(24, 1)	(1431.91793)		
qR(19, 5)	1494.66098	(20)	0	qR(15, 9)	(1488.08785)			pP(25, 1)	(1430.45827)		
qR(20, 5)	1496.42012	(30)	-19	qR(16, 9)	(1489.70946)			pP(26, 1)	(1428.99132)		
qR(21, 5)	1498.18210	(80)	-14	qR(17, 9)	(1491.32737)			pP(27, 1)	(1427.51811)		
qR(22, 5)	1499.94652	(50)	-22	qR(18, 9)	(1492.94176)			pP(28, 1)	(1426.03956)		
qR(23, 5)	1501.71358	(50)	-20	qR(19, 9)	(1494.55280)			pP(29, 1)	(1424.55648)		
qR(24, 5)	1503.48310	(60)	-23	qR(20, 9)	(1496.16069)			pP(30, 1)	(1423.06962)		
qR(25, 5)	1505.25470	(40)	-66	qR(10,10)	(1480.37563)			pP(2, 2)	1448.78327	(10)	7
qR(6, 6)	1472.21872	*	-712	qR(11,10)	(1482.00963)			pP(3, 2)	1446.80935	(10)	15
qR(7, 6)	1473.92272	(10)	0	qR(12,10)	(1483.63850)			pP(4, 2)	1444.72425	(10)	8
qR(8, 6)	1475.62118	(200)	212	qR(13,10)	(1485.26236)			pP(5, 2)	1442.55407	(10)	12
qR(9, 6)	1477.31511	(100)	19	qR(14,10)	(1486.88134)			pP(6, 2)	1440.31286	(10)	9
qR(10, 6)	1479.01004	(50)	-38	qR(15,10)	(1488.49557)			pP(7, 2)	1438.01646	(10)	8
qR(11, 6)	1480.70581	(10)	12	qR(16,10)	(1490.10521)			pP(8, 2)	1435.67596	(10)	7
qR(12, 6)	1482.40092	(20)	15	qR(17,10)	(1491.71041)			pP(9, 2)	1433.29970	(10)	12
qR(13, 6)	1484.09593	(40)	10	qR(18,10)	(1493.31135)			pP(10, 2)	1430.89371	(10)	9
qR(14, 6)	1485.79110	(10)	14	qR(19,10)	(1494.90820)			pP(11, 2)	1428.46276	(10)	7
qR(15, 6)	1487.48643	(10)	11	qR(20,10)	(1496.50113)			pP(12, 2)	1426.01048	(10)	10
qR(16, 6)	1489.18217	(20)	16	qR(11,11)	(1482.52111)			pP(13, 2)	1423.53957	(10)	8
qR(17, 6)	1490.87810	(80)	-7	qR(12,11)	(1484.14306)			pP(14, 2)	1421.05240	(10)	12
qR(18, 6)	1492.57491	(20)	-4	qR(13,11)	(1485.75947)			pP(15, 2)	1418.55073	(10)	14
qR(19, 6)	1494.27255	(20)	8	qR(14,11)	(1487.37047)			pP(16, 2)	1416.03610	(10)	16
qR(20, 6)	1495.97063	(20)	-22	qR(15,11)	(1488.97620)			pP(17, 2)	1413.50974	(10)	13
qR(21, 6)	1497.66991	(50)	-35	qR(16,11)	(1490.57681)			pP(18, 2)	1410.97283	(10)	10

means of the DECOMP program written by J. W. Brault. To the negative Napierian logarithm of the transmittance spectrum we fitted a Voigt profile within a small region about an isolated line, with the line amplitude, width, and a form parameter as fitting parameters. The line form is represented as a convolution of Dopplerian and Lorentzian profile functions with the corresponding parameter describing the relative contributions of these two functions. The intensity was estimated both as the product of height and width from the fit and as the area under the curve; the consistency of the two values was a criterion of the acceptability of the estimates. From these absolute intensities of

TABLE III—*Continued*

Transition	Wavenumber			Obs-Calc	Transition	Wavenumber			Obs-Calc	Transition	Wavenumber			Obs-Calc
pP(19, 2)	1408.42637		(10)	13	pP(24, 3)	1389.48866		(100)	132	pP(12, 5)	1396.29821		(10)	-7
pP(20, 2)	1405.87109		(10)	9	pP(25, 3)	1387.06196		(200)	-208	pP(13, 5)	1394.36946		(10)	-4
pP(21, 2)	1403.30782		(10)	6	pP(25, 3)	1387.05557		(200)	145	pP(14, 5)	1392.42376		(30)	-8
pP(22, 2)	1400.73719		(20)	-1	pP(26, 3)	1384.61661		(200)	-248	pP(15, 5)	1390.46183		(10)	-10
qP(23, 2)	1398.15993	A	(20)	-1	pP(26, 3)	1384.61106		(200)	145	pP(16, 5)	1388.48457		(10)	-9
qP(24, 2)	1395.57649	A	(20)	-6	pP(27, 3)	1382.16086		(200)	-289	pP(17, 5)	1386.49313		(10)	-19
qP(25, 2)	1392.98738	A	(20)	-14	pP(27, 3)	1382.15622		(200)	161	pP(18, 5)	1384.48985		(20)	-21
qP(26, 2)	1390.39316	A	(20)	-20	pP(28, 3)	1379.69512	*		-360	pP(19, 5)	1382.47879		(10)	-20
qP(27, 2)	1387.79417	A	(30)	-31	pP(28, 3)	1379.69169	*		182	pP(20, 5)	1380.46917		(40)	-26
qP(28, 2)	1385.19089	A	(30)	-41	pP(29, 3)	1377.21909	*		-562	pP(21, 5)	1378.48750		(20)	-27
qP(29, 2)	1382.58165	A	(200)	-256	pP(29, 3)	1377.21909	*		300	pP(22, 5)	1376.62462		(20)	-33
qP(30, 2)	1379.97273	A	(30)	-83	pP(30, 3)	1374.73681	*		-551	pP(23, 5)	1373.66564		(30)	-25
qP(31, 2)	1377.35863	A	(30)	-107	pP(30, 3)	1374.73681		(200)	292	pP(24, 5)	1371.73916		(100)	-17
qP(32, 2)	1374.73681	A	(300)	-612	pP(31, 3)	1372.24592	*		-625	pP(25, 5)	1369.68790		(20)	-48
qP(33, 2)	1372.12177	A	(40)	-179	pP(31, 3)	1372.24592	*		202	pP(26, 5)	1367.58601		(30)	-58
qP(34, 2)	1369.49951	A	(70)	-236	pP(32, 3)	1369.74859	*		-621	pP(27, 5)	1365.45530		(20)	-64
qP(35, 2)	1366.87524	A	(100)	-289	pP(32, 3)	1369.74859	*		193	pP(28, 5)	1363.30372		(20)	-85
pP(3, 3)	1435.70140		(10)	10	pP(33, 3)	1367.24415	*		-658	pP(29, 5)	1361.13527		(20)	-92
pP(3, 3)	1435.70140		(10)	11	pP(33, 3)	1367.24415	*		145	pP(30, 5)	1358.95130		(100)	-154
pP(4, 3)	1433.84583		(50)	5	pP(34, 3)	1364.73338	*		-707	pP(6, 6)	1395.97444		(10)	-6
pP(4, 3)	1433.84583		(50)	12	pP(34, 3)	1364.73338	*		87	pP(7, 6)	1394.18881		(10)	-10
pP(5, 3)	1431.94214		(50)	2	pP(35, 3)	1362.21687	*		-754	pP(8, 6)	1392.38966		(10)	-9
pP(5, 3)	1431.94214		(50)	26	pP(35, 3)	1362.21687	*		32	pP(9, 6)	1390.57702		(10)	-10
pP(6, 3)	1429.99224		(50)	-26	pP(4, 4)	1422.53732		(10)	5	pP(10, 6)	1388.75096		(10)	-17
pP(6, 3)	1429.99224		(50)	48	pP(5, 4)	1420.71697		(10)	4	pP(11, 6)	1386.91176		(10)	-14
pP(7, 3)	1427.99891		(150)	-114	pP(6, 4)	1418.86818		(10)	11	pP(12, 6)	1385.05943		(10)	-14
pP(7, 3)	1427.99891		(150)	136	pP(7, 4)	1416.99126		(10)	5	pP(13, 6)	1383.19412		(10)	-19
pP(8, 3)	1425.97599		(10)	11	pP(8, 4)	1415.08701		(10)	8	pP(14, 6)	1381.31617		(20)	-13
pP(8, 3)	1425.96184		(10)	12	pP(9, 4)	1413.15601		(10)	9	pP(15, 6)	1379.42556		(20)	-19
pP(9, 3)	1423.86586		(10)	10	pP(10, 4)	1411.19908		(10)	7	pP(16, 6)	1377.52272		(20)	-20
pP(9, 3)	1423.88700		(10)	16	pP(11, 4)	1409.21728		(10)	7	pP(17, 6)	1375.60791		(30)	-22
pP(10, 3)	1421.76290		(20)	9	pP(12, 4)	1407.21197		(10)	8	pP(18, 6)	1373.68159		(30)	-17
pP(10, 3)	1421.77576		(20)	15	pP(13, 4)	1405.18531		(10)	3	pP(19, 6)	1371.74413		(40)	-21
pP(11, 3)	1419.61777		(10)	3	pP(14, 4)	1403.14250		(20)	4	pP(20, 6)	1369.79637		(10)	-17
pP(11, 3)	1419.63096		(10)	12	pP(15, 4)	1401.10260		(10)	0	pP(21, 6)	1367.83920		(10)	-13
pP(12, 3)	1417.43946		(20)	1	pP(16, 4)	1399.22484		(30)	-5	pP(22, 6)	1365.87398		(10)	-12
pP(12, 3)	1417.45544		(20)	-25	pP(17, 4)	1396.69921		(70)	-6	pP(23, 6)	1363.90301		(10)	-5
pP(13, 3)	1415.23100		(10)	-6	pP(18, 4)	1394.59746		(20)	-9	pP(24, 6)	1361.92989		(10)	-2
pP(13, 3)	1415.25455		(10)	0	pP(19, 4)	1392.44916		(10)	-14	pP(25, 6)	1359.96134		(30)	5
pP(14, 3)	1412.99491		(20)	-5	pP(20, 4)	1390.27449		(20)	-25	pP(26, 6)	1358.01041		(30)	12
pP(14, 3)	1413.03766		(20)	-17	pP(21, 4)	1388.07880		(20)	-30	pP(27, 6)	1356.10508		(10)	22
pP(15, 3)	1410.73359		(20)	30	pP(22, 4)	1385.86424		(10)	-43	pP(28, 6)	1354.30434		(30)	11
pP(15, 3)	1410.87140		(30)	-101	pP(23, 4)	1383.63233		(10)	-56	pP(29, 6)	1350.55350		(20)	33
pP(16, 3)	1408.44773		(20)	-19	pP(24, 4)	1381.38418		(10)	-67	pP(30, 6)	(1348.81115)			
pP(16, 3)	1408.38482		(80)	133	pP(25, 4)	1379.12061		(20)	-84	pP(7, 7)	1382.58165		(30)	3
pP(17, 3)	1406.14034		(50)	-33	pP(26, 4)	1376.84251		(20)	-101	pP(8, 7)	1380.80838		(10)	-18
pP(17, 3)	1406.10827		(100)	97	pP(27, 4)	1374.55052		(20)	-131	pP(9, 7)	1379.02542		(10)	-19
pP(18, 3)	1403.81273		(30)	-41	pP(28, 4)	1372.24592		(20)	-119	pP(10, 7)	1377.23261		(10)	-19
pP(18, 3)	1403.79097		(100)	96	pP(29, 4)	1369.92818		(30)	-189	pP(11, 7)	1375.43002		(10)	-21
pP(19, 3)	1401.46630		(60)	-53	pP(30, 4)	1367.59923		(30)	-220	pP(12, 7)	1373.61777		(10)	-18
pP(19, 3)	1401.44968		(60)	103	pP(31, 4)	1365.25896		(30)	-284	pP(13, 7)	1371.79581		(10)	-24
pP(20, 3)	1399.10237		(50)	-73	pP(32, 4)	1362.90877		(60)	-330	pP(14, 7)	1369.96434		(10)	-29
pP(20, 3)	1399.08880		(80)	99	pP(33, 4)	1360.54900		(60)	-391	pP(15, 7)	1368.12355		(10)	-23
pP(21, 3)	1396.72230		(60)	-92	pP(5, 5)	1409.29403		(10)	0	pP(16, 7)	1366.27341		(10)	-22
pP(21, 3)	1396.71081		(80)	102	pP(6, 5)	1407.49362		(10)	-4	pP(17, 7)	1364.41410		(10)	-20
pP(22, 3)	1394.32720		(100)	-114	pP(7, 5)	1405.67420		(10)	0	pP(18, 7)	1362.54585		(10)	-11
pP(22, 3)	1394.31733		(100)	111	pP(8, 5)	1403.83579		(10)	-3	pP(19, 7)	1360.66874		(10)	-6
pP(23, 3)	1391.91816		(100)	-138	pP(9, 5)	1401.97871		(10)	-6	pP(20, 7)	1358.78311		(20)	5
pP(23, 3)	1391.90951		(100)	115	pP(10, 5)	1400.10331		(10)	1	pP(21, 7)	1356.88917		(10)	17
pP(24, 3)	1389.49611		(100)	-169	pP(11, 5)	1398.20963		(10)	-5	pP(22, 7)	1354.98737		(30)	37

vibration–rotational lines, we deduced the appropriate molecular parameters in the same manner that we described for PH_3 (*13*).

Separate Fit to the Frequencies of the Pure Rotational Transitions in the Vibrational States $v_2 = 1$ and $v_5 = 1$

We reported previously (*6*) the measurement of the submillimeter-wave spectra of pure rotational transitions in the vibrational states $v_2 = 1$ and $v_5 = 1$ of $H_3{}^{12}CF$ and

TABLE III—*Continued*

Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc	
pP(23, 7)	1353.07815	(30)	65	pP(14,10)	1335.01170	(10)	-14	pP(18,13)	1292.31663	(20)	-57
pP(24, 7)	1351.16202	(20)	93	pP(15,10)	1333.25748	(10)	-9	pP(19,13)	1290.60850	(30)	-60
pP(25, 7)	1349.23979	(20)	123	pP(16,10)	1331.49963	(10)	-11	pP(20,13)	1288.90006	(30)	-66
pP(26, 7)	1347.31272	(30)	173	pP(17,10)	1329.73819	(10)	-19	pP(21,13)	1287.19149	(30)	-63
pP(27, 7)	1345.38207	(30)	219	pP(18,10)	1327.97343	(20)	-12	pP(22,13)	(1285.48331)		
pP(28, 7)	1343.45037	(40)	293	pP(19,10)	1326.20530	(10)	0	pP(23,13)	(1283.77430)		
pP(29, 7)	1341.52069	(40)	368	pP(20,10)	1324.43365	(10)	1	pP(24,13)	(1282.06514)		
pP(30, 7)	1339.59811	(100)	434	pP(21,10)	1322.65886	(20)	22	pP(25,13)	(1280.35585)		
pP(8, 8)	1369.11822	(10)	-10	pP(22,10)	1320.88063	(30)	28	pP(26,13)	(1278.64646)		
pP(9, 8)	1367.35660	(10)	-16	pP(23,10)	1319.09916	(20)	31	pP(27,13)	(1276.93701)		
pP(10, 8)	1365.58776	(10)	-17	pP(24,10)	1317.31484	(30)	64	pP(28,13)	(1275.22753)		
pP(11, 8)	1363.81167	(10)	-18	pP(25,10)	1315.52742	(40)	93	pP(29,13)	(1273.51807)		
pP(12, 8)	1362.02839	(10)	-23	pP(26,10)	1313.73656	(40)	75	pP(30,13)	(1271.80867)		
pP(13, 8)	1360.23800	(10)	-24	pP(27,10)	1311.94320	(40)	93	pP(14,14)	1287.03221	(20)	-27
pP(14, 8)	1358.44058	(20)	-21	pP(28,10)	(1310.14598)			pP(15,14)	1285.33705	(20)	-61
pP(15, 8)	1356.63616	(20)	-17	pP(29,10)	(1308.34711)			pP(16,14)	1283.64228	(50)	-100
pP(16, 8)	1354.82487	(20)	-6	pP(30,10)	(1306.54582)			pP(17,14)	1281.94808	(50)	-127
pP(17, 8)	1353.00673	(10)	6	pP(11,11)	1328.33681	(10)	38	pP(18,14)	1280.25417	(50)	-173
pP(18, 8)	1351.18188	(20)	26	pP(12,11)	1326.60795	(10)	33	pP(19,14)	(1278.56295)		
pP(19, 8)	1349.35051	(20)	63	pP(13,11)	1324.87658	(10)	16	pP(20,14)	(1276.87052)		
pP(20, 8)	1347.51262	(20)	105	pP(14,11)	1323.14290	(10)	6	pP(21,14)	(1275.17862)		
pP(21, 8)	1345.66844	(20)	162	pP(15,11)	1321.40693	(20)	1	pP(22,14)	(1273.48729)		
pP(22, 8)	1343.81820	(30)	240	pP(16,11)	1319.66865	(10)	-3	pP(23,14)	(1271.79652)		
pP(23, 8)	1341.96207	(30)	340	pP(17,11)	1317.92810	(10)	-8	pP(24,14)	(1270.10635)		
pP(24, 8)	1340.10032	(20)	465	pP(18,11)	1316.18547	(20)	4	pP(25,14)	(1268.41681)		
pP(25, 8)	1338.23313	(30)	605	pP(19,11)	1314.44062	(10)	16	pP(26,14)	(1266.72790)		
pP(26, 8)	1336.36102	(30)	779	pP(20,11)	1312.69351	(20)	19	pP(27,14)	(1265.03966)		
pP(27, 8)	1334.48462	(40)	1007	pP(21,11)	1310.94449	(30)	45	pP(28,14)	(1263.35211)		
pP(28, 8)	1332.60425	(30)	1268	pP(22,11)	1309.19335	(30)	70	pP(29,14)	(1261.66528)		
pP(29, 8)	1330.72071	(50)	1573	pP(23,11)	1307.44019	(40)	98	pP(30,14)	(1259.97921)		
pP(30, 8)	1328.83483	(50)	1918	pP(24,11)	1305.68520	(30)	143	pP(15,15)	1273.16244	(50)	-156
pP(9, 9)	1355.58763	(50)	-3	pP(25,11)	1303.92837	(40)	200	pP(16,15)	1271.47899	(50)	-221
pP(10, 9)	1353.83701	(10)	-10	pP(26,11)	1302.16946	(30)	237	pP(17,15)	1269.79675	(50)	-281
pP(11, 9)	1352.08117	(10)	-11	pP(27,11)	(1300.40598)			pP(18,15)	1268.11568	(50)	-343
pP(12, 9)	1350.32004	(10)	-17	pP(28,11)	(1298.64314)			pP(19,15)	(1266.43985)		
pP(13, 9)	1348.55371	(10)	-24	pP(29,11)	(1296.87865)			pP(20,15)	(1264.76179)		
pP(14, 9)	1346.78226	(40)	-27	pP(30,11)	(1295.11260)			pP(21,15)	(1263.08496)		
pP(15, 9)	1345.00572	(10)	-27	pP(12,12)	1314.62274	(10)	62	pP(22,15)	(1261.40937)		
pP(16, 9)	1343.22405	(20)	-32	pP(13,12)	1312.90479	(10)	42	pP(23,15)	(1259.73504)		
pP(17, 9)	1341.43739	(20)	-35	pP(14,12)	1311.18548	(10)	18	pP(24,15)	(1258.06197)		
pP(18, 9)	1339.64572	(20)	-42	pP(15,12)	1309.46497	(20)	2	pP(25,15)	(1256.39018)		
pP(19, 9)	1337.84911	(30)	-52	pP(16,12)	1307.74329	(10)	-4	pP(26,15)	(1254.71970)		
pP(20, 9)	1336.04772	(10)	-57	pP(17,12)	1306.02031	(10)	-17	pP(27,15)	(1253.05053)		
pP(21, 9)	1334.24141	(20)	-79	pP(18,12)	1304.29628	(10)	-15	pP(28,15)	(1251.38270)		
pP(22, 9)	1332.43039	(20)	-103	pP(19,12)	1302.57118	(20)	-2	pP(29,15)	(1249.71622)		
pP(23, 9)	1330.61479	(10)	-129	pP(20,12)	1300.84492	(40)	9	pP(30,15)	(1248.05111)		
pP(24, 9)	1328.79446	(20)	-181	pP(21,12)	1299.11758	(10)	24	pP(16,16)	(1259.25125)		
pP(25, 9)	1326.96965	(20)	-251	pP(22,12)	1297.38934	(30)	58	pP(17,16)	(1257.58093)		
pP(26, 9)	1325.14062	(30)	-326	pP(23,12)	1295.66034	(40)	121	pP(18,16)	(1255.91241)		
pP(27, 9)	1323.30734	(30)	-430	pP(24,12)	1293.93009	(40)	162	pP(19,16)	(1254.24572)		
pP(28, 9)	1321.46996	(30)	-571	pP(25,12)	1292.19907	(30)	222	pP(20,16)	(1252.58087)		
pP(29, 9)	1319.62875	(30)	-748	pP(26,12)	1290.46717	(30)	289	pP(21,16)	(1250.91786)		
pP(30, 9)	1317.78390	(30)	-977	pP(27,12)	(1288.73082)			pP(22,16)	(1249.25671)		
pP(31, 9)	1315.93606	(40)	-1231	pP(28,12)	(1286.99654)			pP(23,16)	(1247.59743)		
pP(32, 9)	1314.08558	(100)	-1527	pP(29,12)	(1285.26148)			pP(24,16)	(1245.94003)		
pP(33, 9)	(1312.25170)			pP(30,12)	(1283.52572)			pP(25,16)	(1244.28450)		
pP(10,10)	1341.99278	(30)	12	pP(14,13)	1299.14670	(10)	12	pP(26,16)	(1242.63087)		
pP(11,10)	1340.25304	(10)	7	pP(15,13)	1297.43951	(10)	-23	pP(27,16)	(1240.97915)		
pP(12,10)	1338.50962	(10)	4	pP(16,13)	1295.73224	(20)	-30	pP(28,16)	(1239.32933)		
pP(13,10)	1336.76242	(10)	-10	pP(17,13)	1294.02461	(20)	-42	pP(29,16)	(1237.68144)		

their analysis with the published microwave frequencies (*4, 5*). A simultaneous analysis of these data with the wavenumbers of the vibration–rotational transitions of the bands ν_2 and ν_5 revealed that the component of an A_1, A_2 doublet at lower frequency, namely the transition $J = 8 \leftarrow J = 7$, $kl = -2$ ($A_1 \leftarrow A_2$), cannot be assigned to the line 396176.71 MHz according to our paper (*6*), although the calculated frequency of that line was in perfect agreement with the experimental value. The reason is the

TABLE III—*Continued*

Transition	Wavenumber			Obs-Calc
pP(30,16)	(1236.03549)			
pQ(1, 1)	1463.73442		(10)	9
pQ(2, 1)	1464.15467		(10)	6
pQ(3, 1)	1464.66522		(10)	2
pQ(4, 1)	1465.21110		(10)	5
pQ(5, 1)	1465.76895		(10)	4
pQ(6, 1)	1466.32255		(10)	3
pQ(7, 1)	1466.86319		(10)	3
pQ(8, 1)	1467.38570		(10)	4
pQ(9, 1)	1467.88699		(10)	4
pQ(10, 1)	1468.36537		(10)	5
pQ(11, 1)	1468.81998		(10)	3
pQ(12, 1)	1469.25077		(10)	5
pQ(13, 1)	1469.65807		(40)	5
pQ(14, 1)	1470.04270		(20)	10
pQ(15, 1)	1470.40558		(20)	7
pQ(16, 1)	1470.74806		(80)	6
pQ(17, 1)	1471.07156		(20)	12
pQ(18, 1)	1471.37740		(20)	13
pQ(19, 1)	1471.66710		(80)	15
pQ(20, 1)	1471.94211		(10)	18
pQ(21, 1)	1472.20374		(30)	14
pQ(22, 1)	1472.45347		(30)	18
pQ(23, 1)	1472.69249		(20)	22
pQ(24, 1)	1472.92194		(20)	26
pQ(25, 1)	1473.14288		(10)	27
pQ(26, 1)	1473.35630		(10)	30
pQ(27, 1)	1473.56300		(30)	24
pQ(28, 1)	1473.76399		(30)	34
pQ(29, 1)	1473.95977		(100)	43
pQ(30, 1)	1474.15098		(20)	55
pQ(31, 1)	1474.33807		(20)	73
pQ(32, 1)	1474.52142		(30)	99
pQ(33, 1)	1474.70015		(600)	35
pQ(34, 1)	1474.87739		(200)	215
pQ(35, 1)	1475.04816		(30)	221
pQ(2, 2)	1451.91953		(10)	13
pQ(3, 2)	1451.53760		(10)	6
pQ(4, 2)	1451.07041		(10)	10
pQ(5, 2)	1450.53199		(10)	12
pQ(6, 2)	1449.93799		(10)	6
pQ(7, 2)	1449.29968		(20)	12
pQ(8, 2)	1448.62501		(10)	4
pQ(9, 2)	1447.92046		(10)	15
pQ(10, 2)	1447.19027		(10)	7
pQ(11, 2)	1446.43825		(10)	9
pQ(12, 2)	1445.66705		(10)	8
pQ(13, 2)	1444.87894		(20)	9
pQ(14, 2)	1444.07569		(20)	14
pQ(15, 2)	1443.25868		(10)	10
pQ(16, 2)	1442.42927		(10)	10
pQ(17, 2)	1441.58848		(10)	11
pQ(18, 2)	1440.73716		(10)	6
pQ(19, 2)	1439.87629		(20)	14
pQ(20, 2)	1439.00635		(10)	10
pQ(21, 2)	1438.12808		(20)	6
qQ(22, 2)	1437.24201	A	(20)	0
qQ(23, 2)	1436.34873	A	(20)	-4
qQ(24, 2)	1435.44855	A	(30)	-19
qQ(25, 2)	1434.54209	A	(30)	-26

Transition	Wavenumber			Obs-Calc
qQ(26, 2)	1433.62961	A	(20)	-39
qQ(27, 2)	1432.71164	A	(30)	-41
qQ(28, 2)	1431.78828	A	(30)	-55
qQ(29, 2)	1430.85937	A	(40)	-128
pQ(3, 3)	1440.65867		(20)	10
pQ(3, 3)	1440.65867		(20)	17
pQ(4, 3)	1440.45769		(20)	-4
pQ(4, 3)	1440.45769		(20)	18
pQ(5, 3)	1440.21046		(50)	-25
pQ(5, 3)	1440.21046		(50)	49
pQ(6, 3)	1439.91946		(800)	-111
pQ(6, 3)	1439.91946		(800)	139
pQ(7, 3)	1439.59851		(10)	13
pQ(7, 3)	1439.58435		(10)	14
pQ(8, 3)	1439.18990		(10)	7
pQ(8, 3)	1439.21106		(10)	14
pQ(9, 3)	1438.78814		(10)	10
pQ(9, 3)	1438.80100		(10)	17
pQ(10, 3)	1438.34367		(50)	5
pQ(10, 3)	1438.35691		(40)	18
pQ(11, 3)	1437.86549		(10)	2
pQ(11, 3)	1437.88182		(10)	10
pQ(12, 3)	1437.35666		(10)	1
pQ(12, 3)	1437.38020		(10)	6
pQ(13, 3)	1436.81871		(500)	-77
pQ(13, 3)	1436.86210		(10)	-25
pQ(14, 3)	1436.25596		(30)	-9
pQ(14, 3)	1436.39422		(10)	-95
pQ(15, 3)	1435.66802		(30)	-21
pQ(15, 3)	1435.60509		(10)	129
pQ(16, 3)	1435.05748		(20)	-26
pQ(16, 3)	1435.02539		(20)	104
pQ(17, 3)	1434.42572		(10)	-43
pQ(17, 3)	1434.40398		(20)	97
pQ(18, 3)	1433.77434		(20)	-57
pQ(18, 3)	1433.75771		(20)	98
pQ(19, 3)	1433.10459		(20)	-75
pQ(19, 3)	1433.09101		(20)	97
pQ(20, 3)	1432.41769		(30)	-95
pQ(20, 3)	1432.40637		(80)	116
pQ(21, 3)	1431.71491		(60)	-103
pQ(21, 3)	1431.70496		(60)	115
pQ(22, 3)	1430.99681		(100)	-144
pQ(22, 3)	1430.98824		(100)	116
pQ(23, 3)	1430.26482		(100)	-170
pQ(23, 3)	1430.25734		(100)	128
pQ(24, 3)	1429.51956		(200)	-205
pQ(24, 3)	1429.51309		(200)	140
pQ(25, 3)	1428.76177	*		-253
pQ(25, 3)	1428.75610	*		128
pQ(26, 3)	1427.99891	*		357
pQ(26, 3)	1427.98773	*		153
pQ(27, 3)	1427.21185	*		-354
pQ(27, 3)	1427.20853	*		198
pQ(28, 3)	1426.41963	*		-547
pQ(28, 3)	1426.41963	*		314
pQ(29, 3)	1425.61899	*		-606
pQ(29, 3)	1425.61284	*		-378
pQ(30, 3)	1424.80980	*		-597
pQ(30, 3)	1424.80980	*		230

Transition	Wavenumber			Obs-Calc
pQ(31, 3)	1423.99141	*		-638
pQ(31, 3)	1423.99141	*		176
pQ(32, 3)	1423.16490	*		-665
pQ(32, 3)	1423.16490	*		138
pQ(33, 3)	1422.33027	*		-724
pQ(33, 3)	1422.33027	*		70
pQ(4, 4)	1429.23162		(10)	9
pQ(5, 4)	1429.08513		(10)	7
pQ(6, 4)	1428.91033		(10)	4
pQ(7, 4)	1428.70785		(10)	7
pQ(8, 4)	1428.47820		(10)	5
pQ(9, 4)	1428.22227		(10)	9
pQ(10, 4)	1427.94094		(10)	9
pQ(11, 4)	1427.63551		(10)	6
pQ(12, 4)	1427.30822		(10)	2
pQ(13, 4)	1426.96411		(10)	1
pQ(14, 4)	1426.62233		(20)	3
pQ(15, 4)	1426.44195		(10)	3
pQ(16, 4)	1425.61284		(30)	-2
pQ(17, 4)	1425.20677		(10)	-9
pQ(18, 4)	1424.75333		(10)	-17
pQ(19, 4)	1424.27267		(10)	-22
pQ(20, 4)	1423.76986		(10)	-36
pQ(21, 4)	1423.24733		(20)	-44
pQ(22, 4)	1422.70635		(20)	-56
pQ(23, 4)	1422.14795		(20)	-72
pQ(24, 4)	1421.57307		(20)	-84
pQ(25, 4)	1420.98237		(10)	-105
pQ(26, 4)	1420.37666		(50)	-124
pQ(27, 4)	1419.75657		(20)	-150
pQ(28, 4)	1419.12267		(30)	-189
pQ(29, 4)	1418.47594		(30)	-211
pQ(30, 4)	1417.81619		(200)	-291
pQ(31, 4)	1417.14517		(40)	-338
pQ(32, 4)	1416.46313		(100)	-388
pQ(33, 4)	1415.77090		(300)	-446
pQ(5, 5)	1417.70908		(10)	0
pQ(6, 5)	1417.59151		(10)	6
pQ(7, 5)	1417.45544		(100)	86
pQ(8, 5)	1417.29863		(10)	0
pQ(9, 5)	1417.12381		(10)	-2
pQ(10, 5)	1416.93037		(10)	-5
pQ(11, 5)	1416.71860		(10)	-8
pQ(12, 5)	1416.48890		(10)	-9
pQ(13, 5)	1416.24175		(10)	-5
pQ(14, 5)	1415.97761		(10)	-7
pQ(15, 5)	1415.69736		(10)	-11
pQ(16, 5)	1415.40225		(10)	-18
pQ(17, 5)	1415.09442		(40)	-22
pQ(18, 5)	1414.77803		(20)	-15
pQ(19, 5)	1414.46210		(10)	-21
pQ(20, 5)	1414.17304		(20)	-35
pQ(21, 5)	1414.00191		(20)	-36
pQ(22, 5)	1412.73359		(30)	-28
pQ(23, 5)	1412.49341		(300)	-344
pQ(24, 5)	1412.13392		(30)	-36
pQ(25, 5)	1411.71911		(20)	-55
pQ(26, 5)	1411.27424		(30)	-71
pQ(27, 5)	1410.80739		(30)	-80
pQ(28, 5)	1410.32213		(20)	-95

accidental coincidence of the energy level $J = 7$, $kl = -2$ (larger A block, A_2 symmetry) with the level $J = 7$, $kl = +1$ (A_2) ($\Delta E = 0.552$ cm^{-1}) and the "2, −1" l-type interaction between them. The frequency 396176.71 MHz of this line is too large by about 32 MHz, which was compensated by the slightly modified values of the parameters A_5, $A\zeta_5^z$ and q_{12}, with respect to which the frequencies of the pure rotational transitions are less sensitive because of the selection rules $\Delta k = 0$, $\Delta l = 0$.

TABLE III—*Continued*

Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc	
pQ(29, 5)	1409.82066	(30)	-95	pQ(9, 8)	1382.59695	(10)	-13	pQ(24,10)	1357.91880	(20)	80
pQ(30, 5)	1409.30390	(80)	-114	pQ(10, 8)	1382.51988	(10)	-19	pQ(25,10)	1357.81326	(20)	91
pQ(31, 5)	1408.77273	(50)	-153	pQ(11, 8)	1382.43517	(10)	-19	pQ(26,10)	1357.70347	(30)	89
pQ(32, 5)	1408.22828	(80)	-165	pQ(12, 8)	1382.34274	(10)	-19	pQ(27,10)	1357.58996	(30)	119
pQ(33, 5)	1407.67053	(100)	-211	pQ(13, 8)	1382.24264	(10)	-18	pQ(28,10)	(1357.47103)		
pQ(6, 6)	1406.10433	(100)	42	pQ(14, 8)	1382.13488	(10)	-13	pQ(29,10)	(1357.34947)		
pQ(7, 6)	1406.00583	(10)	-9	pQ(15, 8)	1382.01952	(10)	-3	pQ(30,10)	(1357.22424)		
pQ(8, 6)	1405.89399	(10)	-9	pQ(16, 8)	1381.89653	(10)	8	pQ(11,11)	(1346.99449)		
pQ(9, 6)	1405.76834	(10)	-11	pQ(17, 8)	1381.76602	(10)	28	pQ(12,11)	1346.95991	(10)	31
pQ(10, 6)	1405.62898	(10)	-12	pQ(18, 8)	1381.62817	(10)	69	pQ(13,11)	1346.92181	(10)	11
pQ(11, 6)	1405.47602	(10)	-10	pQ(19, 8)	1381.48282	(10)	108	pQ(14,11)	1346.88080	(10)	2
pQ(12, 6)	1405.30951	(10)	-12	pQ(20, 8)	1381.33027	(20)	168	pQ(15,11)	1346.83675	(10)	-9
pQ(13, 6)	1405.12958	(20)	-18	pQ(21, 8)	1381.17068	(10)	253	pQ(16,11)	1346.78968	(1000)	-16
pQ(14, 6)	1404.93649	(10)	-19	pQ(22, 8)	1381.00399	(20)	344	pQ(17,11)	1346.73996	(20)	15
pQ(15, 6)	1404.73039	(10)	-20	pQ(23, 8)	1380.83061	(20)	464	pQ(18,11)	1346.68681	(20)	14
pQ(16, 6)	1404.51159	(30)	-19	pQ(24, 8)	1380.65079	(20)	615	pQ(19,11)	1346.63059	(20)	14
pQ(17, 6)	1404.28044	(10)	-13	pQ(25, 8)	1380.46917	(300)	1231	pQ(20,11)	1346.57156	(20)	44
pQ(18, 6)	1404.03728	(10)	-16	pQ(26, 8)	1380.27322	(20)	1024	pQ(21,11)	1346.50958	(20)	89
pQ(19, 6)	1403.78287	(50)	-14	pQ(27, 8)	1380.07627	(20)	1276	pQ(22,11)	1346.44409	(20)	95
pQ(20, 6)	1403.51804	(10)	-17	pQ(28, 8)	1379.87492	(20)	1586	pQ(23,11)	1346.37594	(30)	146
pQ(21, 6)	1403.24426	(10)	-11	pQ(29, 8)	1379.66985	(40)	1936	pQ(24,11)	1346.30453	(30)	181
pQ(22, 6)	1402.96369	(20)	0	pQ(30, 8)	1379.46231	(40)	2342	pQ(25,11)	1346.23026	(30)	240
pQ(23, 6)	1402.67979	(10)	4	pQ(9, 9)	1370.84138	(10)	6	pQ(26,11)	(1346.14994)		
pQ(24, 6)	1402.39923	(20)	4	pQ(10, 9)	1370.78398	(10)	-7	pQ(27,11)	(1346.06898)		
pQ(25, 6)	1402.13517	(20)	11	pQ(11, 9)	1370.72091	(10)	-12	pQ(28,11)	(1345.98501)		
pQ(26, 6)	1401.91537	(20)	13	pQ(12, 9)	1370.65207	(10)	-14	pQ(29,11)	(1345.89811)		
pQ(27, 6)	1401.79901	(20)	10	pQ(13, 9)	1370.57743	(10)	-20	pQ(30,11)	(1345.80833)		
pQ(28, 6)	1399.73121	(30)	41	pQ(14, 9)	1370.49703	(10)	-22	pQ(12,12)	(1334.97890)		
pQ(29, 6)	1399.67114	(20)	81	pQ(15, 9)	1370.41083	(10)	-25	pQ(13,12)	1334.95507	(20)	22
pQ(30, 6)	1399.44611	(20)	123	pQ(16, 9)	1370.31879	(10)	-33	pQ(14,12)	1334.92883	(20)	0
pQ(31, 6)	1399.12972	(30)	152	pQ(17, 9)	1370.22100	(10)	-37	pQ(15,12)	1334.90068	(20)	-17
pQ(32, 6)	1398.76163	(30)	175	pQ(18, 9)	1370.11738	(20)	-48	pQ(16,12)	1334.87070	(20)	-16
pQ(33, 6)	1398.36059	(30)	217	pQ(19, 9)	1370.00801	(20)	-58	pQ(17,12)	1334.83876	(30)	-8
pQ(34, 6)	1397.93547	(50)	255	pQ(20, 9)	1369.89287	(20)	-73	pQ(18,12)	1334.80482	(20)	2
pQ(7, 7)	1394.42161	(10)	-8	pQ(21, 9)	1369.77198	(10)	-94	pQ(19,12)	1334.76883	(30)	15
pQ(8, 7)	1394.33899	(10)	-15	pQ(22, 9)	1369.64530	(20)	-132	pQ(20,12)	1334.73095	(30)	46
pQ(9, 7)	1394.24618	(10)	-15	pQ(23, 9)	1369.51296	(20)	-179	pQ(21,12)	1334.69084	(20)	63
pQ(10, 7)	1394.14306	(10)	-19	pQ(24, 9)	1369.37503	(20)	-237	pQ(22,12)	1334.64886	(20)	106
pQ(11, 7)	1394.02974	(10)	-21	pQ(25, 9)	1369.23144	(20)	-326	pQ(23,12)	1334.60499	(30)	171
pQ(12, 7)	1393.90621	(10)	-23	pQ(26, 9)	1369.08245	(20)	-433	pQ(24,12)	1334.55888	(30)	225
pQ(13, 7)	1393.77256	(10)	-22	pQ(27, 9)	1368.92807	(20)	-575	pQ(25,12)	1334.51095	(30)	311
pQ(14, 7)	1393.62882	(10)	-20	pQ(28, 9)	1368.76854	(20)	-752	pQ(26,12)	1334.46103	(30)	412
pQ(15, 7)	1393.47504	(10)	-19	pQ(29, 9)	1368.60402	(20)	-974	pQ(27,12)	(1334.40385)		
pQ(16, 7)	1393.31134	(10)	-16	pQ(30, 9)	1368.43522	(20)	-1208	pQ(28,12)	(1334.34867)		
pQ(17, 7)	1393.13783	(10)	-11	pQ(31, 9)	1368.26176	(30)	-1534	pR(1, 1)	1467.56167	(100)	1
pQ(18, 7)	1392.95467	(10)	-2	pQ(32, 9)	1368.08463	(50)	-1910	pR(2, 1)	1469.77576	(10)	10
pQ(19, 7)	1392.76202	(10)	7	pQ(10,10)	1358.95130	(500)	164	pR(3, 1)	1472.02484	(50)	6
pQ(20, 7)	1392.56015	(10)	21	pQ(11,10)	1358.90379	(10)	2	pR(4, 1)	1474.28578	(10)	7
pQ(21, 7)	1392.34940	(10)	45	pQ(12,10)	1358.85351	(10)	-11	pR(5, 1)	1476.54206	(100)	-7
pQ(22, 7)	1392.13011	(10)	71	pQ(13,10)	1358.79919	(10)	-3	pR(6, 1)	1478.78540	(100)	7
pQ(23, 7)	1391.90293	(100)	108	pQ(14,10)	1358.74046	(10)	-10	pR(7, 1)	1481.01009	(10)	6
pQ(24, 7)	1391.66833	(20)	131	pQ(15,10)	1358.67746	(20)	-16	pR(8, 1)	1483.21319	(10)	5
pQ(25, 7)	1391.42763	(20)	170	pQ(16,10)	1358.61020	(20)	-19	pR(9, 1)	1485.39291	(10)	2
pQ(26, 7)	1391.18223	(20)	218	pQ(17,10)	1358.53876	(10)	-11	pR(10, 1)	1487.54852	(20)	10
pQ(27, 7)	1390.93457	(20)	302	pQ(18,10)	1358.46308	(10)	3	pR(11, 1)	1489.67960	(10)	4
pQ(28, 7)	1390.68728	(20)	359	pQ(19,10)	1358.38296	(10)	5	pR(12, 1)	1491.78672	(20)	7
pQ(29, 7)	1390.44593	(40)	429	pQ(20,10)	1358.29869	(10)	22	pR(13, 1)	1493.87046	(10)	7
pQ(30, 7)	1390.21887	(50)	506	pQ(21,10)	1358.21000	(20)	26	pR(14, 1)	1495.93185	(20)	6
pQ(31, 7)	1390.01995	(50)	564	pQ(22,10)	1358.11714	(30)	40	pR(15, 1)	1497.97258	(50)	53
pQ(8, 8)	1382.66623	(10)	-13	pQ(23,10)	1358.02011	(100)	64	pR(16, 1)	1499.99260	(20)	11

The results of the new fit to the 202 pure rotational transition frequencies ($J < 13$) which did not involve the frequency of the $J = 8 \leftarrow 7$, $kl = -2$ ($A_1 \leftarrow A_2$) line are given in Table I. The frequency of this line is predicted to be 396144.26 MHz.

Separate Fit to the Infrared Data

We have assigned 2046 lines in the region 1250–1600 cm^{-1} in which the bands ν_2 and ν_5 of $H_3{}^{12}CF$ appear, including 85 lines of the $\Delta k = \pm 2$ forbidden transitions

TABLE III—*Continued*

Transition	Wavenumber		Obs-Calc	Transition	Wavenumber		Obs-Calc	Transition	Wavenumber		Obs-Calc
pR(17, 1)	1501.99470	(10)	21	pR(11, 3)	1457.80928	(300)	312	pR(29, 4)	(1469.00311)		
pR(18, 1)	1503.97960	(20)	12	pR(12, 3)	1458.94497	(30)	-10	pR(5, 5)	(1427.80685)		
pR(19, 1)	1505.94897	(10)	13	pR(12, 3)	1458.98772	(10)	-21	pR(6, 5)	1429.37194	(20)	12
pR(20, 1)	1507.90429	(80)	36	pR(13, 3)	1460.08045	(50)	-12	pR(7, 5)	1430.91738	(20)	0
pR(21, 1)	1509.84620	(30)	16	pR(13, 3)	1460.21769	(90)	-200	pR(8, 5)	1432.44370	(20)	0
pR(22, 1)	1511.77673	(20)	38	pR(14, 3)	1461.19090	(50)	-11	pR(9, 5)	1433.95084	(10)	-12
pR(23, 1)	1513.69621	(20)	21	pR(14, 3)	1461.12780	(60)	123	pR(10, 5)	1435.43931	(20)	-11
pR(24, 1)	1515.60632	(30)	32	pR(15, 3)	1462.27783	(20)	-21	pR(11, 5)	1436.90935	(10)	-5
pR(25, 1)	1517.50797	(100)	69	pR(15, 3)	1462.24678	(200)	211	pR(12, 5)	1438.35691	(500)	-438
pR(26, 1)	1519.40094	(50)	29	pR(16, 3)	1463.34273	(20)	-48	pR(13, 5)	1439.79543	(20)	-21
pR(27, 1)	1521.28711	(80)	27	pR(16, 3)	1463.32101	(20)	94	pR(14, 5)	1441.21308	(10)	-15
pR(28, 1)	(1523.16649)			pR(17, 3)	1464.38732	(40)	-59	pR(15, 5)	1442.61518	(10)	-7
pR(29, 1)	(1525.04013)			pR(17, 3)	1464.37076	(30)	103	pR(16, 5)	1444.00354	(20)	-21
pR(30, 1)	(1526.90816)			pR(18, 3)	1465.41272	(50)	-69	pR(17, 5)	1445.38262	(20)	-14
pR(2, 2)	1456.64799	(50)	25	pR(18, 3)	1465.39917	(30)	106	pR(18, 5)	1446.76127	(10)	-24
pR(3, 2)	1457.88383	(50)	14	pR(19, 3)	1466.41993	(50)	-94	pR(19, 5)	1448.16597	(20)	-30
pR(4, 2)	1459.04431	(500)	-390	pR(19, 3)	1466.40836	(70)	91	pR(20, 5)	1449.68765	(20)	-23
pR(5, 2)	1460.15722	(1000)	19	pR(20, 3)	1467.41014	(40)	-122	pR(21, 5)	1450.11088	(20)	-32
pR(6, 2)	1461.22153	(1000)	42	pR(20, 3)	1467.40026	(30)	102	pR(22, 5)	1451.56432	(20)	-51
pR(7, 2)	1462.24678	(200)	-185	pR(21, 3)	1468.38440	(40)	-145	pR(23, 5)	1452.89123	(30)	-57
pR(8, 2)	1463.24573	(10)	2	pR(21, 3)	1468.37575	(40)	108	pR(24, 5)	1454.16998	(300)	439
pR(9, 2)	1464.21724	(1000)	35	pR(22, 3)	1469.34353	(30)	-171	pR(25, 5)	1455.40738	(30)	-66
pR(10, 2)	1465.16583	(10)	17	pR(22, 3)	1469.33607	(30)	130	pR(26, 5)	1456.62643	(30)	-77
pR(11, 2)	1466.09485	(10)	9	pR(23, 3)	1470.28809	(30)	-223	pR(27, 5)	1457.82580	(70)	-92
pR(12, 2)	1467.00649	(10)	15	pR(23, 3)	1470.28181	(30)	140	pR(28, 5)	1459.00722	(30)	-130
pR(13, 2)	1467.90216	(20)	4	pR(24, 3)	1471.21937	(40)	-249	pR(29, 5)	(1460.17382)		
pR(14, 2)	1468.78751	(500)	396	pR(24, 3)	1471.21388	(40)	150	pR(30, 5)	1461.32122	(400)	-222
pR(15, 2)	1469.65807	(500)	626	pR(25, 3)	1472.13769	(40)	-285	pR(6, 6)	(1417.92092)		
pR(16, 2)	1470.50805	(10)	14	pR(25, 3)	1472.13305	(50)	165	pR(7, 6)	1419.50845	(200)	-180
pR(17, 2)	1471.35274	(10)	1	pR(26, 3)	1473.04323	(50)	-375	pR(8, 6)	1421.08536	(10)	-6
pR(18, 2)	1472.18715	(20)	14	pR(26, 3)	1473.04018	(50)	204	pR(9, 6)	1422.64632	(10)	-10
pR(19, 2)	1473.01152	(20)	11	pR(27, 3)	1473.93666 *		-512	pR(10, 6)	1424.19314	(10)	-18
pR(20, 2)	1473.82647	(20)	-3	pR(27, 3)	1473.93666 *		350	pR(11, 6)	1425.72591	(100)	-26
qR(21, 2)	1474.63279 A	(30)	-4	pR(28, 3)	(1474.82545)			pR(12, 6)	1427.24491	(10)	-17
qR(22, 2)	1475.43067 A	(60)	-17	pR(28, 3)	(1474.81702)			pR(13, 6)	1428.75002	(100)	-12
qR(23, 2)	1476.22061 A	(100)	-36	pR(4, 4)	(1437.59965)			pR(14, 6)	1430.24134	(10)	-18
qR(24, 2)	1477.00328 A	(30)	-29	pR(5, 4)	1439.12735	(20)	7	pR(15, 6)	1431.71901	(200)	-44
qR(25, 2)	1477.77872 A	(30)	-28	pR(6, 4)	1440.62699	(20)	12	pR(16, 6)	1433.18399	(20)	-23
qR(26, 2)	1478.54710 A	(100)	-48	pR(7, 4)	1442.09898	(10)	-1	pR(17, 6)	1434.63608	(10)	-17
qR(27, 2)	1479.30881 A	(30)	-77	pR(8, 4)	1443.54456	(10)	15	pR(18, 6)	1436.07599	(10)	-12
qR(28, 2)	1480.06408 A	(30)	-120	pR(9, 4)	1444.96410	(10)	9	pR(19, 6)	1437.50463	(20)	-4
qR(29, 2)	(1480.81491) A			pR(10, 4)	1446.35908	(10)	0	pR(20, 6)	1438.92321	(10)	-4
qR(30, 2)	(1481.55868) A			pR(11, 4)	1447.73183	(10)	6	pR(21, 6)	1440.33390	(10)	-4
pR(3, 3)	1447.27059	(20)	5	pR(12, 4)	1449.08702	(10)	0	pR(22, 6)	1441.74038	(10)	2
pR(3, 3)	1447.27059	(0)	29	pR(13, 4)	1450.44396	(10)	1	pR(23, 6)	1443.14900	(50)	-1
pR(4, 3)	1448.72611	(20)	-22	pR(14, 4)	1451.96217	(50)	55	pR(24, 6)	1444.57313	(20)	16
pR(4, 3)	1448.72611	(0)	52	pR(15, 4)	1452.83046	(90)	57	pR(25, 6)	1446.04010	(30)	10
pR(5, 3)	1450.13772	(100)	-107	pR(16, 4)	1454.12049	(80)	4	pR(26, 6)	1447.60932	(30)	4
pR(5, 3)	1450.13772	(0)	143	pR(17, 4)	1455.36271	(40)	-10	pR(27, 6)	1447.23077	(500)	530
pR(6, 3)	1451.51904	(10)	14	pR(18, 4)	1456.57693	(10)	-15	pR(28, 6)	1448.84906	(70)	109
pR(6, 3)	1451.50482	(10)	8	pR(19, 4)	1457.76805	(20)	-32	pR(29, 6)	1450.30530	(70)	124
pR(7, 3)	1452.81240	(10)	8	pR(20, 4)	1458.93848	(50)	-43	pR(30, 6)	1451.66884	(70)	135
pR(7, 3)	1452.83282	(500)	-58	pR(21, 4)	1460.09088	(100)	86	pR(7, 7)	(1407.95228)		
pR(8, 3)	1454.11216	(50)	4	pR(22, 4)	1461.22153	(200)	-115	pR(8, 7)	(1409.55987)		
pR(8, 3)	1454.12491	(500)	0	pR(23, 4)	1462.33700	(20)	-73	pR(9, 7)	1411.15639	(10)	-39
pR(9, 3)	1455.36884	(10)	0	pR(24, 4)	1463.44044	(400)	455	pR(10, 7)	1412.74253	(500)	-44
pR(9, 3)	1455.38206	(10)	10	pR(25, 4)	1464.51658	(30)	-123	pR(11, 7)	1414.31821	(20)	-22
pR(10, 3)	1456.59138	(10)	1	pR(26, 4)	1465.58257	(20)	-158	pR(12, 7)	1415.88294	(20)	-23
pR(10, 3)	1456.60776	(10)	14	pR(27, 4)	1466.63373	(30)	-179	pR(13, 7)	1417.43946	(200)	228
pR(11, 3)	1457.78267	(10)	0	pR(28, 4)	1467.67167	(100)	-87	pR(14, 7)	1418.98035	(20)	-12

induced by the "2, −1" l-type interaction between the $+l$, K and $-l$, $K+1$ levels in the $v_5 = 1$ vibrational state. As illustrated by Fig. 2, there are close coincidences and level crossings between the $+l$, K and $-l$, $K+1$ levels that give rise to the $\Delta k = \pm 2$ forbidden transitions. As can be seen in Fig. 1, the "2, −1" l-type interaction in such cases strongly perturbs the otherwise regular subbranches of the ν_5 band and leads to the transitions allowed by perturbations.

TABLE III—*Continued*

Transition	Wavenumber		Obs-Calc	Transition	Wavenumber		Obs-Calc	Transition	Wavenumber		Obs-Calc
pR(15, 7)	1420.51302	(20)	-9	rP(10, 0)	1462.59860	(10)	17	rP(11, 2)	1479.79218	(10)	5
pR(16, 7)	1422.03513	(10)	-2	rP(11, 0)	1461.74562	(100)	14	rP(12, 2)	1478.44114	(10)	6
pR(17, 7)	1423.54629	(40)	-39	rP(12, 0)	1460.91897	(200)	-142	rP(13, 2)	1477.11879	(10)	13
pR(18, 7)	1425.04797	(10)	12	rP(13, 0)	1460.11791	(200)	13	rP(14, 2)	1475.82397	(10)	10
pR(19, 7)	1426.53917	(20)	34	rP(14, 0)	1459.33380	(20)	10	rP(15, 2)	1474.55562	(20)	6
pR(20, 7)	1428.02039	(30)	51	rP(15, 0)	1458.56523	(20)	13	rP(16, 2)	1473.31243	(10)	12
pR(21, 7)	1429.49193	(30)	58	rP(16, 0)	1457.80928	(50)	-25	rP(17, 2)	1472.09225	(10)	1
pR(22, 7)	1430.95408	(50)	32	rP(17, 0)	1457.06529	(200)	21	rP(18, 2)	1470.89270	(20)	8
pR(23, 7)	1432.40637	(200)	-139	rP(18, 0)	1456.33019	(10)	8	rP(19, 2)	1469.70880	(20)	5
pR(24, 7)	1433.85612	(250)	174	rP(19, 0)	1455.60333	(20)	4	rP(20, 2)	1468.53074	(10)	3
pR(25, 7)	1435.29758	(70)	259	rP(20, 0)	1454.88357	(20)	1	rP(21, 2)	1467.33154	(20)	1
pR(26, 7)	1436.73469	(40)	296	rP(21, 0)	1454.16998	(200)	-1	rP(22, 2)	1466.01954	(20)	-14
pR(27, 7)	1438.17292	(200)	511	rP(22, 0)	1453.46182	(20)	-2	rP(23, 2)	1465.80913	(100)	-56
pR(28, 7)	(1439.60833)			rP(23, 0)	1452.75841	(10)	-2	rP(24, 2)	1464.57214	(20)	-10
pR(29, 7)	(1441.06168)			rP(24, 0)	1452.05941	(30)	17	rP(25, 2)	1463.46273	(100)	-99
pR(30, 7)	(1442.54192)			rP(25, 0)	1451.36366	(30)	-8	rP(26, 2)	1462.40985	(30)	-21
pR(8, 8)	(1397.90669)			rP(26, 0)	1450.67146	(20)	-9	rP(27, 2)	1461.38859	(70)	-20
pR(9, 8)	(1399.52923)			rP(27, 0)	1449.98217	(20)	-13	rP(28, 2)	1460.38807	(400)	-327
pR(10, 8)	(1401.14357)			rP(28, 0)	1449.29968	(400)	406	rP(29, 2)	1459.41350	(40)	-5
pR(11, 8)	1402.74921	(10)	-47	rP(29, 0)	1448.61157	(100)	37	rP(30, 2)	1458.45299	(70)	-1
pR(12, 8)	1404.34737	(30)	-14	rP(30, 0)	1447.92827	(100)	-45	rP(31, 2)	1457.50850	(60)	47
pR(13, 8)	1405.93700	(20)	-5	rP(31, 0)	1447.24731	(70)	-52	rP(32, 2)	(1456.57735)		
pR(14, 8)	1407.51809	(20)	-15	rP(32, 0)	1446.56742	(70)	-66	rP(5, 3)	1499.34301	(20)	-1
pR(15, 8)	1409.09112	(10)	4	rP(3, 1)	1480.78382	(20)	-7	rP(6, 3)	1497.77364	(100)	-15
pR(16, 8)	1410.65606	(30)	53	rP(4, 1)	1479.21606	(10)	4	rP(7, 3)	1496.23106	(10)	11
pR(17, 8)	1412.21240	(30)	79	rP(5, 1)	1477.69321	(10)	-3	rP(8, 3)	1494.71415	(100)	-4
pR(18, 8)	1413.76019	(20)	84	rP(6, 1)	1476.21541	(100)	0	rP(9, 3)	1493.22317	(10)	-3
pR(19, 8)	1415.30055	(20)	179	rP(7, 1)	1474.78238	(100)	23	rP(10, 3)	1491.75763	(10)	0
pR(20, 8)	1416.83219	(50)	227	rP(8, 1)	1473.39299	(10)	4	rP(11, 3)	1490.31704	(10)	0
pR(21, 8)	1418.35634	(60)	344	rP(9, 1)	1472.05153	(500)	447	rP(12, 3)	1488.90096	(10)	0
pR(22, 8)	1419.87236	(80)	451	rP(10, 1)	1470.74806	(500)	463	rP(13, 3)	1487.50746	(200)	-141
pR(23, 8)	1421.38092	(80)	597	rP(11, 1)	1469.48073	(10)	8	rP(14, 3)	1486.14026	(10)	2
pR(24, 8)	(1422.87442)			rP(12, 1)	1468.25683	(10)	11	rP(15, 3)	1484.79446	(10)	5
pR(25, 8)	(1424.36660)			rP(13, 1)	1467.06874	(10)	12	rP(16, 3)	1483.47069	(10)	-1
pR(9, 9)	(1387.78826)			rP(14, 1)	1465.91049	(20)	14	rP(17, 3)	1482.16840	(20)	0
pR(10, 9)	(1389.42380)			rP(15, 1)	1464.76029	(200)	-136	rP(18, 3)	1480.88662	(10)	0
pR(11, 9)	(1391.05303)			rP(16, 1)	1463.46273	(70)	59	rP(19, 3)	1479.62436	(20)	-6
pR(12, 9)	1392.67568	(20)	-22	rP(17, 1)	1462.82076	(10)	11	rP(20, 3)	1478.38061	(20)	-5
pR(13, 9)	1394.29208	(20)	-28	rP(18, 1)	1461.76415	(10)	4	rP(21, 3)	1477.15387	(20)	-3
pR(14, 9)	1395.90230	(20)	-5	rP(19, 1)	1460.76172	(60)	5	rP(22, 3)	1475.94217	(20)	-10
pR(15, 9)	1397.50553	(20)	-29	rP(20, 1)	1459.79193	(30)	1	rP(23, 3)	(1474.74313)		
pR(16, 9)	1399.10237	(80)	-39	rP(21, 1)	1458.84848	(10)	1	rP(24, 3)	1473.55025	(200)	-208
pR(17, 9)	1400.69276	(20)	-34	rP(22, 1)	1457.92791	(20)	-3	rP(25, 3)	1472.36252	(30)	-25
pR(18, 9)	1402.27623	(20)	-58	rP(23, 1)	1457.02800	(20)	4	rP(26, 3)	1471.16083	(20)	-10
pR(19, 9)	1403.85324	(20)	-65	rP(24, 1)	1456.14648	(10)	-3	rP(27, 3)	1469.91849	(50)	2
pR(20, 9)	1405.42339	(30)	-94	rP(25, 1)	1455.28193	(20)	-2	rP(6, 4)	1508.47574	(50)	-20
pR(21, 9)	1406.98689	(20)	-123	rP(26, 1)	1454.43269	(20)	-5	rP(7, 4)	1506.90956	(20)	-10
pR(22, 9)	1408.54344	(30)	-185	rP(27, 1)	1453.59751	(20)	-2	rP(8, 4)	1505.36562	(30)	-14
pR(23, 9)	1410.09376	(50)	-212	rP(28, 1)	1452.77525	(50)	13	rP(9, 4)	1503.84398	(10)	-5
pR(24, 9)	1411.63674	(30)	-321	rP(29, 1)	1451.96217	(200)	-222	rP(10, 4)	1502.34416	(10)	-6
pR(25, 9)	1413.17342	(40)	-418	rP(30, 1)	1451.16445	(50)	8	rP(11, 4)	1500.86613	(10)	7
pR(26, 9)	(1414.70897)			rP(31, 1)	1450.37406	(50)	-5	rP(12, 4)	1499.40914	(50)	-5
rP(2, 0)	1471.42545	(50)	-34	rP(32, 1)	(1449.59285)			rP(13, 4)	1497.97258	(80)	-71
rP(3, 0)	1470.00209	(10)	3	rP(4, 2)	1490.11188	(20)	-7	rP(14, 4)	1496.55793	(10)	-5
rP(4, 0)	1468.70094	(100)	5	rP(5, 2)	1488.54138	(20)	-8	rP(15, 4)	1495.16273	(10)	-9
rP(5, 0)	1467.50566	(10)	3	rP(6, 2)	1487.00368	(50)	-7	rP(16, 4)	1493.78732	(20)	-5
rP(6, 0)	1466.39921	(50)	7	rP(7, 2)	1485.49843	(10)	-5	rP(17, 4)	1492.43116	(20)	0
rP(7, 0)	1465.36494	(10)	10	rP(8, 2)	1484.02523	(10)	0	rP(18, 4)	1491.09351	(20)	-15
rP(8, 0)	1464.38058	(100)	7	rP(9, 2)	1482.58348	(10)	0	rP(19, 4)	1489.77406	(20)	-24
rP(9, 0)	1463.49174	(10)	12	rP(10, 2)	1481.17273	(10)	5	rP(20, 4)	1488.47232	(40)	-17

Because of the strong mixing of the wavefunctions mainly by the x–y Coriolis interaction and in some cases also by the "2, −1" l-type interactions, one has to take care to assign to the spectral lines the standard labels ${}^xP$, ${}^xQ$, ${}^xR$ ($x = p, q, r$) for the conventional transitions $\Delta K = -1, 0, +1$ and the labels ${}^yP$, ${}^yQ$, ${}^yR$ ($y = o, s$) for the perturbation-allowed transitions $\Delta K = -2, +2$. We based our assignments on the comparison of the absolute values of the coefficients of mixing of the wavefunctions

TABLE III—*Continued*

Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc	
rP(21, 4)	1487.18732	(20)	-22	rP(12, 7)	1530.65979	(100)	69	rQ(9, 1)	1487.77110	(10)	9
rP(22, 4)	1485.91861	(20)	-10	rP(13, 7)	1529.15463	(100)	-4	rQ(10, 1)	1488.20919	(50)	8
rP(23, 4)	1484.66494	(20)	-21	rP(14, 7)	1527.66697	(90)	98	rQ(11, 1)	1488.68570	(10)	15
rP(24, 4)	1483.42574	(20)	-16	rP(15, 7)	1526.19294	(30)	8	rQ(12, 1)	1489.19741	(10)	15
rP(25, 4)	1482.19949	(30)	-27	rP(16, 7)	1524.73543	(50)	36	rQ(13, 1)	1489.73826	(20)	11
rP(26, 4)	1480.98508	(30)	-20	rP(17, 7)	1523.29255	(50)	17	rQ(14, 1)	1490.28809	(20)	15
rP(27, 4)	1479.78043	(50)	-11	rP(18, 7)	1521.86456	(20)	0	rQ(15, 1)	1490.68630	(10)	10
rP(28, 4)	1478.58309	(30)	9	rP(19, 7)	1520.45113	(30)	-23	rQ(16, 1)	1491.74182	(10)	12
rP(29, 4)	1477.38925	(80)	31	rP(20, 7)	1519.05196	(30)	-54	rQ(17, 1)	1492.38139	(10)	6
rP(30, 4)	(1476.19279)			rP(21, 7)	1517.66716	(40)	-53	rQ(18, 1)	1493.07428	(20)	9
rP(7, 5)	1517.50797	(100)	-105	rP(22, 7)	1516.29375	(300)	-289	rQ(19, 1)	1493.79881	(20)	0
rP(8, 5)	(1515.94664)			rP(23, 7)	1514.93847	(30)	-54	rQ(20, 1)	1494.54882	(30)	2
rP(9, 5)	1514.40403	(50)	10	rP(24, 7)	(1513.59449)			rQ(21, 1)	1495.32069	(20)	0
rP(10, 5)	1512.88068	(20)	-2	rP(25, 7)	1512.26288	(30)	15	rQ(22, 1)	1496.11206	(10)	1
rP(11, 5)	1511.37684	(20)	7	rP(26, 7)	(1510.94333)			rQ(23, 1)	1496.92414	(500)	329
rP(12, 5)	1509.89189	(20)	2	rP(27, 7)	(1509.63593)			rQ(24, 1)	1497.74534	(20)	-1
rP(13, 5)	1508.42576	(20)	-1	rP(28, 7)	(1508.34012)			rQ(25, 1)	1498.58406	(20)	5
rP(14, 5)	1506.97824	(20)	4	rQ(1, 0)	1474.69288	(50)	6	rQ(26, 1)	1499.43534	(20)	-8
rP(15, 5)	1505.54870	(20)	-12	rQ(2, 0)	1474.70015	(50)	8	rQ(27, 1)	1500.29828	(20)	-4
rP(16, 5)	1504.13726	(20)	-5	rQ(3, 0)	1474.71095	(10)	3	rQ(28, 1)	1501.17167	(50)	11
rP(17, 5)	1502.74316	(20)	-18	rQ(4, 0)	1474.72539	(20)	2	rQ(29, 1)	1502.05429	(60)	21
rP(18, 5)	1501.36639	(30)	-12	rQ(5, 0)	1474.74341	(10)	2	rQ(30, 1)	1502.94516	(70)	21
rP(19, 5)	1500.00622	(20)	-21	rQ(6, 0)	1474.76496	(10)	4	rQ(3, 2)	1496.92414	(150)	-119
rP(20, 5)	1498.66250	(20)	-17	rQ(7, 0)	1474.78994	(50)	5	rQ(4, 2)	1497.05774	(10)	-8
rP(21, 5)	1497.33445	(50)	-31	rQ(8, 0)	1474.81827	(10)	7	rQ(5, 2)	1497.22278	(10)	-7
rP(22, 5)	1496.02193	(20)	-31	rQ(9, 0)	1474.84974	(10)	9	rQ(6, 2)	1497.42009	(30)	5
rP(23, 5)	1494.72266	(200)	-190	rQ(10, 0)	1474.88402	(100)	13	rQ(7, 2)	1497.64887	(10)	-2
rP(24, 5)	1493.44058	(20)	-59	rQ(11, 0)	1474.92033	(100)	17	rQ(8, 2)	1497.90889	(10)	0
rP(25, 5)	1492.17073	(40)	-72	rQ(12, 0)	1474.95655	(50)	24	rQ(9, 2)	1498.19940	(10)	3
rP(26, 5)	1490.91326	(30)	-145	rQ(13, 0)	1474.98466	(20)	55	rQ(10, 2)	1498.51968	(10)	5
rP(27, 5)	1489.66200	*	-818	rQ(14, 0)	1474.94012	(40)	144	rQ(11, 2)	1498.86902	(100)	16
rP(28, 5)	1488.44011	(50)	310	rQ(15, 0)	1475.19587	(10)	-79	rQ(12, 2)	1499.24623	(10)	9
rP(29, 5)	(1487.21414)			rQ(16, 0)	1475.22305	(30)	-52	rQ(13, 2)	1499.65048	(20)	5
rP(30, 5)	(1486.00037)			rQ(17, 0)	1475.27444	(10)	-35	rQ(14, 2)	1500.07914	(150)	-138
rP(8, 6)	(1526.44048)			rQ(18, 0)	1475.33394	(100)	-83	rQ(15, 2)	1500.53505	(10)	9
rP(9, 6)	1524.88294	(20)	26	rQ(19, 0)	1475.39998	(10)	-29	rQ(16, 2)	1501.01186	(10)	7
rP(10, 6)	1523.34263	(10)	7	rQ(20, 0)	1475.46988	(20)	-30	rQ(17, 2)	1501.50829	(10)	4
rP(11, 6)	1521.82019	(10)	18	rQ(21, 0)	1475.54370	(80)	-32	rQ(18, 2)	1502.01963	(10)	3
rP(12, 6)	1520.31491	(20)	9	rQ(22, 0)	1475.62118	(100)	-38	rQ(19, 2)	1502.53590	(20)	3
rP(13, 6)	1518.82839	(500)	158	rQ(23, 0)	1475.70225	(30)	-38	rQ(20, 2)	1503.03000	(20)	-1
rP(14, 6)	1517.35577	(50)	2	rQ(24, 0)	1475.78670	(50)	-41	rQ(21, 2)	1503.41043	(10)	-7
rP(15, 6)	1515.90150	(30)	10	rQ(25, 0)	1475.87445	(10)	-48	rQ(22, 2)	1504.89164	(10)	-12
rP(16, 6)	1514.46366	(20)	15	rQ(26, 0)	1475.96548	(60)	-53	rQ(23, 2)	1505.34428	(10)	-18
rP(17, 6)	1513.04172	(20)	-7	rQ(27, 0)	1476.05971	(20)	-60	rQ(24, 2)	1505.92482	(20)	-12
rP(18, 6)	1511.63584	(10)	-13	rQ(28, 0)	1476.15707	(60)	-68	rQ(25, 2)	1506.55892	(10)	-14
rP(19, 6)	1510.24565	(20)	-7	rQ(29, 0)	1476.25752	(30)	-76	rQ(26, 2)	1507.22409	(70)	-23
rP(20, 6)	1508.87030	(50)	-41	rQ(30, 0)	1476.36099	(20)	-86	rQ(27, 2)	1507.91225	(100)	16
rP(21, 6)	1507.51031	(30)	-28	rQ(31, 0)	1476.46750	(20)	-90	rQ(28, 2)	1508.61808	(20)	-9
rP(22, 6)	1506.16464	(30)	-36	rQ(32, 0)	1476.57691	(10)	-98	rQ(29, 2)	1509.33992	(70)	-17
rP(23, 6)	1504.83321	(50)	-33	rQ(33, 0)	1476.68927	(20)	-98	rQ(30, 2)	1510.07609	(50)	-4
rP(24, 6)	1503.51529	(20)	-50	rQ(34, 0)	1476.80447	(20)	-97	rQ(4, 3)	1507.85854	(40)	-10
rP(25, 6)	1502.21086	(20)	-46	rQ(35, 0)	1476.92231	(20)	-109	rQ(5, 3)	1507.99194	(10)	-7
rP(26, 6)	1500.91917	(20)	-50	rQ(36, 0)	1477.04304	(30)	91	rQ(6, 3)	1508.15137	(10)	-10
rP(27, 6)	1499.63996	(50)	-37	rQ(2, 1)	1485.89434	(50)	-1	rQ(7, 3)	1508.33661	(20)	-7
rP(28, 6)	1498.37244	(40)	-31	rQ(3, 1)	1486.02972	(10)	-1	rQ(8, 3)	1508.54730	(100)	1
rP(29, 6)	1497.11617	(30)	-20	rQ(4, 1)	1486.21004	(10)	0	rQ(9, 3)	1508.78283	(10)	-2
rP(30, 6)	(1495.87053)			rQ(5, 1)	1486.43503	(10)	0	rQ(10, 3)	1509.04294	(10)	1
rP(9, 7)	(1535.26854)			rQ(6, 1)	1486.70431	(10)	0	rQ(11, 3)	1509.32700	(10)	1
rP(10, 7)	1533.71486	(100)	-102	rQ(7, 1)	1487.01736	(10)	4	rQ(12, 3)	1509.63442	(200)	-3
rP(11, 7)	(1532.17945)			rQ(8, 1)	1487.37329	(20)	4	rQ(13, 3)	1509.96475	(10)	0

for a given vibration–rotational level. This method leads to unambiguous assignments except for the lines ${}^{q}X(J'', K = 2)$ and ${}^{p}X(J'', K = 2)$ $(X = P, Q, R)$ for which for $J' = 18$–23 the wavefunction $|0, 1^{\pm1}; J, k = \mp1\rangle$ has the largest contribution simultaneously to two perturbed wavefunctions. In this case (cf. Table II) assignments obviously cannot be unambiguous; we have used a convention that is obvious from

TABLE III—*Continued*

Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc	
rQ(14, 3)	1510.31718	(10)	1	rQ(17, 5)	1531.97096	(10)	-14	rQ(25, 7)	1555.05769	(30)	-57
rQ(15, 3)	1510.69102	(10)	1	rQ(18, 5)	1532.30543	(10)	-19	rQ(26, 7)	1555.43551	(20)	-59
rQ(16, 3)	1511.08544	(10)	-1	rQ(19, 5)	1532.65537	(20)	-18	rQ(27, 7)	1555.82365	(20)	-57
rQ(17, 3)	1511.49960	(10)	-2	rQ(20, 5)	1533.02007	(10)	-31	rQ(28, 7)	1556.22192	(20)	-24
rQ(18, 3)	1511.93247	(10)	-3	rQ(21, 5)	1533.39920	(10)	-37	rQ(29, 7)	1556.62915	(20)	-24
rQ(19, 3)	1512.38284	(10)	-4	rQ(22, 5)	1533.79210	(10)	-44	rQ(30, 7)	1557.04554	(20)	13
rQ(20, 3)	1512.84924	(10)	-8	rQ(23, 5)	1534.19823	(10)	-47	rQ(31, 7)	1557.46953	(50)	-8
rQ(21, 3)	1513.32977	(10)	-11	rQ(24, 5)	1534.61683	(30)	-52	rQ(9, 8)	1561.00085	(50)	13
rQ(22, 3)	1513.82178	(10)	-6	rQ(25, 5)	1535.04643	(10)	-136	rQ(10, 8)	1561.15298	(20)	14
rQ(23, 3)	1514.32090	(10)	-15	rQ(26, 5)	1535.48016	(800)	-904	rQ(11, 8)	1561.31981	(20)	30
rQ(24, 3)	1514.82025	(10)	-9	rQ(27, 5)	1535.94380	(20)	316	rQ(12, 8)	1561.50087	(10)	33
rQ(25, 3)	1515.30609	(10)	-5	rQ(28, 5)	1536.40334	(100)	230	rQ(13, 8)	1561.69603	(30)	28
rQ(26, 3)	1515.75012	(10)	6	rQ(29, 5)	1536.87149	(100)	235	rQ(14, 8)	1561.90515	(20)	25
rQ(27, 3)	1516.09270	(10)	31	rQ(30, 5)	1537.34621	(30)	281	rQ(15, 8)	1562.12803	(10)	25
rQ(28, 3)	1518.38811	(40)	17	rQ(7, 6)	1540.05692	(10)	27	rQ(16, 8)	1562.36436	(20)	20
rQ(29, 3)	1518.67689	(10)	10	rQ(8, 6)	1540.19987	(10)	24	rQ(17, 8)	1562.61399	(20)	22
rQ(30, 3)	1519.13137	(20)	20	rQ(9, 6)	1540.36006	(10)	18	rQ(18, 8)	1562.87630	(10)	-1
rQ(31, 3)	1519.67407	(200)	-277	rQ(10, 6)	1540.53741	(10)	20	rQ(19, 8)	1563.15149	(20)	-6
rQ(32, 3)	1520.27428	(30)	44	rQ(11, 6)	1540.73153	(10)	15	rQ(20, 8)	1563.43916	(20)	-2
rQ(33, 3)	1520.90412	(20)	87	rQ(12, 6)	1540.94226	(10)	13	rQ(21, 8)	1563.73874	(20)	-14
rQ(34, 3)	1521.55653	(40)	90	rQ(13, 6)	1541.16935	(10)	14	rQ(22, 8)	1564.05014	(30)	-19
rQ(5, 4)	1518.69286	(10)	-7	rQ(14, 6)	1541.41281	(50)	48	rQ(23, 8)	1564.37295	(30)	-25
rQ(6, 4)	1518.82839	(50)	-35	rQ(15, 6)	1541.67119	(20)	0	rQ(24, 8)	1564.70677	(30)	-39
rQ(7, 4)	1518.98660	(10)	-1	rQ(16, 6)	1541.94560	(40)	15	rQ(25, 8)	1565.05141	(30)	-43
rQ(8, 4)	1519.16626	(10)	0	rQ(17, 6)	1542.23466	(10)	-11	rQ(26, 8)	1565.40645	(60)	-41
rQ(9, 4)	1519.36743	(10)	2	rQ(18, 6)	1542.53876	(20)	-6	rQ(27, 8)	1565.77134	(30)	-49
rQ(10, 4)	1519.58971	(10)	1	rQ(19, 6)	1542.85692	(20)	-26	rQ(28, 8)	1566.14586	(30)	-50
rQ(11, 4)	1519.83276	(10)	0	rQ(20, 6)	1543.18922	(10)	-25	rQ(29, 8)	1566.52974	(20)	-30
rQ(12, 4)	1520.09620	(10)	-2	rQ(21, 6)	1543.53487	(20)	-41	rQ(30, 8)	1566.92236	(30)	-7
rQ(13, 4)	1520.37961	(20)	-1	rQ(22, 6)	1543.89371	(10)	-43	rQ(10, 9)	1571.31046	(50)	-38
rQ(14, 4)	1520.68250	(20)	-2	rQ(23, 6)	1544.26513	(20)	-49	rQ(11, 9)	1571.46803	(20)	-21
rQ(15, 4)	1521.00436	(20)	-4	rQ(24, 6)	1544.64873	(10)	-49	rQ(12, 9)	1571.63913	(20)	-10
rQ(16, 4)	1521.34461	(10)	-14	rQ(25, 6)	1545.04392	(30)	-52	rQ(13, 9)	1571.82351	(10)	-14
rQ(17, 4)	1521.70285	(10)	-12	rQ(26, 6)	1545.45020	(10)	-50	rQ(14, 9)	1572.02126	(30)	-3
rQ(18, 4)	1522.07836	(10)	-14	rQ(27, 6)	1545.86696	(20)	-47	rQ(15, 9)	1572.23208	(60)	12
rQ(19, 4)	1522.47046	(20)	-16	rQ(28, 6)	1546.29354	(20)	-46	rQ(16, 9)	1572.45556	(20)	15
rQ(20, 4)	1522.87846	(20)	-20	rQ(29, 6)	1546.72955	(20)	-17	rQ(17, 9)	1572.69163	(10)	19
rQ(21, 4)	1523.30163	(30)	-18	rQ(30, 6)	1547.17381	(20)	-1	rQ(18, 9)	1572.94000	(20)	21
rQ(22, 4)	1523.73894	(10)	-23	rQ(31, 6)	1547.62567	(40)	20	rQ(19, 9)	1573.20039	(20)	19
rQ(23, 4)	1524.18946	(10)	-26	rQ(32, 6)	1548.08412	(50)	44	rQ(20, 9)	1573.47259	(20)	17
rQ(24, 4)	1524.65199	(20)	-23	rQ(33, 6)	1548.54839	(70)	101	rQ(21, 9)	1573.75640	(20)	25
rQ(25, 4)	1525.12501	(20)	-17	rQ(34, 6)	(1549.01524)			rQ(22, 9)	1574.05114	(20)	3
rQ(26, 4)	1525.60644	(20)	-19	rQ(35, 6)	1549.48673 *		98	rQ(23, 9)	1574.35724	(20)	24
rQ(27, 4)	1526.09392	(30)	-4	rQ(8, 7)	1550.58260	(40)	50	rQ(24, 9)	1574.67365	(20)	15
rQ(28, 4)	1526.58357	(30)	14	rQ(9, 7)	1550.72966	(10)	25	rQ(25, 9)	1575.00052	(20)	22
rQ(29, 4)	1527.06990	(20)	48	rQ(10, 7)	1550.89278	(10)	31	rQ(26, 9)	1575.33726	(20)	21
rQ(30, 4)	1527.54395	(20)	89	rQ(11, 7)	1551.07141	(10)	31	rQ(27, 9)	1575.68348	(50)	7
rQ(31, 4)	1527.99138	(70)	156	rQ(12, 7)	1551.26484	(200)	-21	rQ(28, 9)	1576.03913	(30)	10
rQ(32, 4)	1528.38828	(70)	266	rQ(13, 7)	1551.47440	(20)	26	rQ(29, 9)	1576.40379	(30)	25
rQ(6, 5)	1529.42635	(10)	7	rQ(14, 7)	1551.69826	(10)	15	rQ(30, 9)	1576.77725	(30)	69
rQ(7, 5)	1529.56542	(20)	3	rQ(15, 7)	1551.93675	(10)	7	rQ(31, 9)	1577.15797	(70)	28
rQ(8, 5)	1529.72467	(80)	88	rQ(16, 7)	1552.18960	(10)	1	rQ(11,10)	(1581.51095)		
rQ(9, 5)	1529.90134	(10)	10	rQ(17, 7)	1552.45658	(10)	2	rQ(12,10)	1581.67288	(100)	-130
rQ(10, 5)	1530.09758	(10)	8	rQ(18, 7)	1552.73716	(20)	-10	rQ(13,10)	1581.84899	(100)	-124
rQ(11, 5)	1530.31233	(10)	5	rQ(19, 7)	1553.03127	(20)	-13	rQ(14,10)	1582.03802	(60)	-92
rQ(12, 5)	1530.54531	(10)	3	rQ(20, 7)	1553.33837	(10)	-25	rQ(15,10)	1582.23938	(60)	-73
rQ(13, 5)	1530.79618	(20)	2	rQ(21, 7)	1553.65823	(10)	-36	rQ(16,10)	1582.45317	(20)	-36
rQ(14, 5)	1531.06457	(10)	0	rQ(22, 7)	1553.99053	(10)	-39	rQ(17,10)	1582.67871	(20)	-28
rQ(15, 5)	1531.35010	(10)	-3	rQ(23, 7)	1554.33488	(40)	-36	rQ(18,10)	1582.91630	(20)	3
rQ(16, 5)	1531.65234	(20)	-11	rQ(24, 7)	1554.69057	(20)	-60	rQ(19,10)	1583.16562	(20)	51

Table II. The results of the fit do not of course depend on the choice of labels that we attach to individual spectral lines.

Using a nonlinear least-squares procedure to minimize the sum of the weighted squares of the differences between the experimental and calculated transition wavenumbers, we obtained the values of 7 parameters of the ν_2 band and of 21 parameters

TABLE III—*Continued*

Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc		Transition	Wavenumber	Obs-Calc	
rQ(20,10)	1583.42604	(20)	77	rR(1, 1)	1489.30166	(20)	24	rR(27, 2)	1556.13890	(10)	-2
rQ(21,10)	1583.69721	(30)	73	rR(2, 1)	1491.14016	(100)	-4	rR(28, 2)	1558.54419	(40)	-52
rQ(22,10)	1583.97927	(30)	79	rR(3, 1)	1493.02378	(10)	0	rR(29, 2)	1560.96339	(20)	15
rQ(23,10)	1584.27177	(30)	77	rR(4, 1)	1494.95249	(60)	67	rR(30, 2)	1563.39337	(30)	26
rQ(24,10)	1584.57549	(30)	175	rR(5, 1)	1496.92414	(100)	20	rR(31, 2)	1565.83362	(30)	40
rQ(25,10)	1584.88755	(30)	116	rR(6, 1)	1498.93953	(10)	4	rR(32, 2)	1568.28319	(30)	60
rQ(26,10)	(1585.20864)			rR(7, 1)	1500.99770	(10)	8	rR(33, 2)	1570.74103	(30)	69
rQ(27,10)	1585.54157	(30)	137	rR(8, 1)	1503.09728	(10)	9	rR(34, 2)	1573.20662	(50)	95
rQ(28,10)	(1585.88070)			rR(9, 1)	1505.23681	(10)	12	rR(35, 2)	1575.68348	(300)	361
rQ(29,10)	(1586.22983)			rR(10, 1)	1507.41415	(10)	12	rR(3, 3)	1514.67131	(40)	-12
rQ(30,10)	(1586.58722)			rR(11, 1)	1509.62617	(200)	7	rR(4, 3)	1516.50761	(10)	-3
rQ(12,11)	(1591.59977)			rR(12, 1)	1511.86692	(20)	13	rR(5, 3)	1518.36959	(10)	-10
rQ(13,11)	(1591.76947)			rR(13, 1)	1514.11586	(10)	12	rR(6, 3)	1520.25710	(30)	-10
rQ(14,11)	1591.94798	(60)	-339	rR(14, 1)	1516.21259	(20)	11	rR(7, 3)	1522.16978	(10)	0
rQ(15,11)	1592.14277	(30)	-253	rR(15, 1)	1518.96580	(20)	5	rR(8, 3)	1524.10690	(10)	-3
rQ(16,11)	1592.34912	(20)	-193	rR(16, 1)	1521.30290	(100)	53	rR(9, 3)	1526.06814	(50)	-1
rQ(17,11)	1592.56711	(30)	-132	rR(17, 1)	1523.69148	(10)	7	rR(10, 3)	1528.05285	(10)	-2
rQ(18,11)	1592.79663	(20)	-58	rR(18, 1)	1526.11137	(20)	2	rR(11, 3)	1530.06050	(10)	1
rQ(19,11)	1593.03680	(20)	-37	rR(19, 1)	1528.55577	(50)	6	rR(12, 3)	1532.09031	(10)	-2
rQ(20,11)	1593.28888	(20)	80	rR(20, 1)	1531.02104	(10)	1	rR(13, 3)	1534.14174	(20)	5
rQ(21,11)	1593.55086	(40)	120	rR(21, 1)	1533.50474	(10)	-4	rR(14, 3)	1536.21379	(20)	1
rQ(22,11)	(1593.82168)			rR(22, 1)	1536.00475	(10)	-18	rR(15, 3)	1538.30575	(30)	-1
rQ(23,11)	(1594.10387)			rR(23, 1)	1538.51967	(10)	0	rR(16, 3)	1540.41663	(20)	-6
rQ(24,11)	(1594.39594)			rR(24, 1)	1541.04739	(10)	-2	rR(17, 3)	1542.54541	(800)	-9
rR(0, 0)	1476.53655	(100)	6	rR(25, 1)	1543.58665	(20)	-4	rR(18, 3)	1544.69094	(10)	-2
rR(1, 0)	1478.51983	(10)	9	rR(26, 1)	1546.13620	(10)	-1	rR(19, 3)	1546.85149	(10)	-6
rR(2, 0)	1480.62532	(10)	4	rR(27, 1)	1548.69478	(10)	3	rR(20, 3)	1549.02518	(100)	-11
rR(3, 0)	1482.83649	(10)	7	rR(28, 1)	1551.26484	(400)	360	rR(21, 3)	1551.20938	(10)	-6
rR(4, 0)	1485.13598	(10)	8	rR(29, 1)	1553.83482	(30)	16	rR(22, 3)	1553.39965	(50)	-11
rR(5, 0)	1487.50746	(50)	44	rR(30, 1)	1556.41449	(20)	38	rR(23, 3)	1555.58891	(10)	-15
rR(6, 0)	1489.92757	(10)	7	rR(31, 1)	1558.99899	(50)	27	rR(24, 3)	1557.76366	(10)	-4
rR(7, 0)	1492.44281	(50)	13	rR(32, 1)	1561.58842	(20)	66	rR(25, 3)	1559.89533	(10)	7
rR(8, 0)	1494.95249	(60)	-25	rR(33, 1)	1564.18129	(50)	78	rR(26, 3)	1561.92432	(20)	34
rR(9, 0)	1497.50230	(10)	17	rR(34, 1)	1566.77734	(30)	104	rR(27, 3)	1565.90489	(30)	27
rR(10, 0)	1500.07914	(150)	75	rR(35, 1)	1569.37594	(300)	-40	rR(28, 3)	1567.87733	(10)	13
rR(11, 0)	1502.67610	(10)	11	rR(2, 2)	1502.03548	(10)	-5	rR(29, 3)	1570.01411	(30)	21
rR(12, 0)	1505.29105	(20)	13	rR(3, 2)	1503.87113	(10)	-6	rR(30, 3)	1572.24076	(30)	30
rR(13, 0)	1507.92014	(50)	11	rR(4, 2)	1505.73912	(10)	-9	rR(31, 3)	1574.51735	(20)	52
rR(14, 0)	1510.56091	(20)	12	rR(5, 2)	1507.63912	(10)	-1	rR(32, 3)	1576.82477	(20)	70
rR(15, 0)	1513.21121	(20)	6	rR(6, 2)	1509.57043	(10)	-1	rR(33, 3)	1579.15385	(20)	117
rR(16, 0)	1515.86942	(20)	3	rR(7, 2)	1511.53257	(10)	2	rR(34, 3)	1581.49878	(20)	135
rR(17, 0)	1518.53413	(500)	2	rR(8, 2)	1513.52478	(10)	1	rR(35, 3)	1583.85688	(30)	-37
rR(18, 0)	1521.20419	(20)	6	rR(9, 2)	1515.54637	(10)	5	rR(4, 4)	1527.20755	(10)	1
rR(19, 0)	1523.87839	(20)	-4	rR(10, 2)	1517.59639	(10)	2	rR(5, 4)	1529.04570	(10)	-3
rR(20, 0)	1526.55616	(20)	0	rR(11, 2)	1519.67407	(10)	14	rR(6, 4)	1530.90569	(20)	-1
rR(21, 0)	1529.23645	(20)	-12	rR(12, 2)	1521.77800	(20)	8	rR(7, 4)	1532.78715	(10)	2
rR(22, 0)	1531.91889	(10)	-12	rR(13, 2)	1523.90719	(20)	10	rR(8, 4)	1534.68962	(10)	-1
rR(23, 0)	1534.60278	(20)	-12	rR(14, 2)	1526.06019	(50)	27	rR(9, 4)	1536.61289	(10)	2
rR(24, 0)	1537.28756	(10)	-16	rR(15, 2)	1528.23452	(30)	8	rR(10, 4)	1538.55641	(10)	1
rR(25, 0)	1539.97281	(30)	-19	rR(16, 2)	1530.42783	(10)	2	rR(11, 4)	1540.51981	(10)	2
rR(26, 0)	1542.65810	(10)	-21	rR(17, 2)	1532.63532	(30)	8	rR(12, 4)	1542.50250	(10)	-4
rR(27, 0)	1545.34298	(10)	-23	rR(18, 2)	1534.84669	(20)	-2	rR(13, 4)	1544.50417	(10)	0
rR(28, 0)	1548.02703	(30)	-28	rR(19, 2)	1537.03519	(20)	1	rR(14, 4)	1546.52405	(20)	-5
rR(29, 0)	1550.70972	(20)	-42	rR(20, 2)	1539.10883	(10)	-15	rR(15, 4)	1548.56176	(20)	-1
rR(30, 0)	1553.39055	(30)	-62	rR(21, 2)	1542.28236	(10)	-21	rR(16, 4)	1550.61640	(10)	-16
rR(31, 0)	1556.06883	(20)	-83	rR(22, 2)	1544.42637	(50)	-17	rR(17, 4)	1552.68772	(10)	-9
rR(32, 0)	1558.74292	(20)	-146	rR(23, 2)	1546.69697	(10)	-19	rR(18, 4)	1554.77469	(10)	-12
rR(33, 0)	1561.41026	(30)	-243	rR(24, 2)	1549.02518	(1000)	490	rR(19, 4)	1556.87663	(500)	-18
rR(34, 0)	1564.06160	(40)	-503	rR(25, 2)	1551.37320	(10)	-11	rR(20, 4)	1558.99279	(60)	-15
rR(35, 0)	(1566.66953)			rR(26, 2)	1553.74753	(10)	-8	rR(21, 4)	1561.12206	(20)	-21

of the ν_5 band that are listed in Table I. The parameters of the ground state were constrained in this separate fit to the previous values (*11*) except for A_0 and D_K^0, which were taken from Ref. (*9*).

Simultaneous Fit of the Microwave, Submillimeter-Wave, and Infrared Data

Comparison of the parameters obtained from the separate fit of the pure rotational transition frequencies in the states $v_2 = 1$ and $v_5 = 1$ with those obtained from our

TABLE III—*Continued*

Transition	Wavenumber		Obs-Calc	Transition	Wavenumber		Obs-Calc	Transition	Wavenumber		Obs-Calc
rR(22, 4)	1563.26361	(20)	-12	rR(24, 6)	1587.48183	(20)	-50	rR(15, 9)	1599.64225	(20)	13
rR(23, 4)	1565.41579	(50)	-25	rR(25, 6)	1589.57493	(20)	-53	rR(16, 9)	(1601.57282)		
rR(24, 4)	1567.57749	(20)	-14	rR(26, 6)	1591.67718	(80)	-62	rR(17, 9)	(1603.51502)		
rR(25, 4)	1569.74647	(20)	-5	rR(27, 6)	1593.78834	(20)	-33	rR(18, 9)	(1605.46842)		
rR(26, 4)	1571.92003	(30)	-1	rR(28, 6)	1595.90708	(20)	-27	rR(19, 9)	(1607.43270)		
rR(27, 4)	1574.09459	(30)	20	rR(29, 6)	1598.03302	(30)	1	rR(20, 9)	(1609.40755)		
rR(28, 4)	1576.26440	(30)	50	rR(30, 6)	(1600.16476)			oP(8, 3)	1425.42378	(20)	0
rR(29, 4)	1578.42055	(30)	86	rR(7, 7)	1564.19561	(20)	38	oP(14, 3)	1412.21799	(30)	61
rR(30, 4)	1580.54871	(50)	160	rR(8, 7)	1566.04334	(10)	39	oP(15, 3)	1410.47884	(100)	145
rR(31, 4)	1582.62466	(30)	258	rR(9, 7)	1567.90630	(10)	30	oP(15, 4)	1399.87918	(20)	6
rR(32, 4)	1584.61185	(40)	425	rR(10, 7)	1569.78840	(500)	428	oP(16, 3)	1409.04114	(20)	-65
rR(33, 4)	(1586.45963)			rR(11, 7)	1571.67732	(10)	27	oP(16, 4)	1398.58673	(100)	9
rR(34, 4)	(1588.15230)			rR(12, 7)	1573.58480	(10)	27	oP(17, 4)	1397.95261	(30)	0
rR(35, 4)	(1589.70133)			rR(13, 7)	1575.50646	(20)	21	oP(18, 4)	(1396.90396)		
rR(5, 5)	1539.64179	(10)	10	rR(14, 7)	1577.44203	(20)	11	oP(20, 5)	1377.76788	(20)	-22
rR(6, 5)	1541.48271	(10)	8	rR(15, 7)	1579.39127	(10)	7	oP(21, 5)	1376.58166	(20)	-13
rR(7, 5)	1543.34264	(10)	11	rR(16, 7)	1581.35374	(20)	-2	oP(22, 5)	1375.28326	(10)	-17
rR(8, 5)	1545.22117	(10)	7	rR(17, 7)	1583.32658	(300)	-267	oP(23, 5)	1375.08642	(300)	-112
rR(9, 5)	1547.11813	(10)	9	rR(18, 7)	1585.31711	(10)	-18	oP(24, 5)	(1373.86480)		
rR(10, 5)	1549.03300	(500)	-1	rR(19, 7)	1587.31729	(10)	-23	oP(25, 5)	(1372.77159)		
rR(11, 5)	1550.96574	(10)	6	rR(20, 7)	1589.32919	(30)	-33	oP(26, 5)	(1371.73384)		
rR(12, 5)	1552.91567	(10)	2	rR(21, 7)	1591.35250	(30)	-37	oP(26, 6)	1354.60711	(20)	-27
rR(13, 5)	1554.88257	(10)	4	rR(22, 7)	1593.38656	(40)	-60	oP(27, 6)	1353.38592	(20)	-20
rR(14, 5)	1556.86585	(500)	-3	rR(23, 7)	1595.43003	(200)	-190	oP(28, 6)	1352.06541	(20)	4
rR(15, 5)	1558.86521	(10)	-5	rR(24, 7)	1597.48615	(30)	-57	oP(29, 6)	1352.69989	(20)	-6
rR(16, 5)	1560.88005	(10)	-16	rR(25, 7)	1599.55039	(20)	-65	oQ(7, 3)	1439.04645	(50)	17
rR(17, 5)	1562.91003	(20)	-18	rR(26, 7)	(1601.62441)			oQ(13, 3)	1436.04259	(20)	69
rR(18, 5)	1564.95449	(10)	-26	rR(27, 7)	(1603.70627)			oQ(14, 3)	1436.00165	(100)	149
rR(19, 5)	1567.01300	(10)	-26	rR(28, 7)	(1605.79609)			oQ(15, 3)	1436.25596	(500)	-613
rR(20, 5)	1569.08481	(20)	-36	rR(29, 7)	(1607.89328)			oQ(14, 4)	1425.39888	(20)	6
rR(21, 5)	1571.16943	(20)	-44	rR(30, 7)	(1609.99722)			oQ(15, 4)	1425.80374	(10)	7
rR(22, 5)	1573.26616	(30)	-51	rR(8, 8)	1576.31058	(10)	25	oQ(16, 4)	1426.86621	(30)	2
rR(23, 5)	1575.37413	(20)	-75	rR(9, 8)	1578.16219	(10)	20	oQ(17, 4)	(1427.51328)		
rR(24, 5)	1577.49233	(20)	-137	rR(10, 8)	1580.02797	(10)	25	oQ(19, 5)	1411.76139	(30)	40
rR(25, 5)	1579.61403	*	-824	rR(11, 8)	1581.90761	(10)	33	oQ(20, 5)	1412.26739	(20)	-1
rR(26, 5)	1581.76291	(30)	326	rR(12, 8)	1583.80072	(10)	27	oQ(21, 5)	1412.66067	(10)	-10
rR(27, 5)	1583.90691	(30)	223	rR(13, 8)	1585.70721	(20)	28	oQ(22, 5)	1414.15520	(20)	-31
rR(28, 5)	1586.05831	(20)	226	rR(14, 8)	1587.62666	(10)	19	oQ(23, 5)	(1414.62232)		
rR(29, 5)	1588.21512	(30)	296	rR(15, 8)	1589.55898	(10)	20	oQ(24, 5)	(1415.21750)		
rR(30, 5)	1590.37449	(40)	343	rR(16, 8)	1591.50359	(10)	5	oQ(25, 5)	(1415.86692)		
rR(31, 5)	1592.53479	(30)	461	rR(17, 8)	1593.46054	(10)	9	oQ(25, 6)	1398.73191	(20)	-23
rR(32, 5)	1594.69250	*	633	rR(18, 8)	1595.43003	(50)	86	oQ(26, 6)	1399.20447	(1000)	797
rR(6, 6)	1551.97188	(10)	23	rR(19, 8)	1597.40923	(10)	-11	oQ(27, 6)	1399.56012	(10)	7
rR(7, 6)	1553.81607	(20)	26	rR(20, 8)	1599.40056	(30)	-8	oQ(28, 6)	1401.87755	(20)	-3
rR(8, 6)	1555.67704	(10)	19	rR(21, 8)	(1601.40269)			oQ(29, 6)	1402.18904	(30)	-17
rR(9, 6)	1557.55474	(10)	21	rR(22, 8)	(1603.41510)			oQ(30, 6)	(1402.66713)		
rR(10, 6)	1559.44877	(10)	20	rR(23, 8)	(1605.43747)			oR(6, 3)	(1450.96680)		
rR(11, 6)	1561.35888	(10)	21	rR(24, 8)	(1607.46941)			oR(12, 3)	(1458.16747)		
rR(12, 6)	1563.28469	(20)	16	rR(25, 8)	(1609.51048)			oR(13, 3)	1459.82623	(100)	156
rR(13, 6)	1565.22585	(10)	5	rR(26, 8)	(1611.56027)			oR(14, 3)	(1461.78486)		
rR(14, 6)	1567.18220	(20)	8	rR(27, 8)	(1613.61831)			oR(13, 4)	(1449.22046)		
rR(15, 6)	1569.15304	(10)	-8	rR(28, 8)	(1615.68414)			oR(14, 4)	1451.32347	(10)	11
rR(16, 6)	1571.13833	(10)	-9	rR(29, 8)	(1617.75728)			oR(15, 4)	(1454.08321)		
rR(17, 6)	1573.13742	(20)	-20	rR(30, 8)	(1619.83722)			oR(16, 4)	(1456.42686)		
rR(18, 6)	1575.15006	(20)	-21	rR(9, 9)	1588.31471	(10)	-32	oR(18, 5)	(1444.06018)		
rR(19, 6)	1577.17561	(20)	-33	rR(10, 9)	1590.17071	(10)	-29	oR(19, 5)	(1446.26029)		
rR(20, 6)	1579.21380	(20)	-35	rR(11, 9)	1592.03989	(10)	-14	oR(20, 5)	1448.34617	(30)	-21
rR(21, 6)	1581.26393	(20)	-49	rR(12, 9)	1593.92187	(10)	-4	oR(21, 5)	1451.53194	(100)	-89
rR(22, 6)	1583.32658	(80)	34	rR(13, 9)	1595.81636	(20)	-4	oR(22, 5)	(1453.69030)		
rR(23, 6)	1585.39858	(10)	-48	rR(14, 9)	1597.72335	(20)	12	oR(23, 5)	(1455.97502)		

infrared measurements in Table I demonstrates that both sets of data are compatible. Some parameters obtained from the analysis of the pure rotational transitions in the excited states $v_2 = 1$ and $v_5 = 1$ (for instance A_2, A_5 and $A\zeta_5^z$) have larger dispersions than those obtained from the separate analysis of the infrared data because of the selection rules $\Delta K = 0$ and $\Delta l = 0$ for the pure rotational transitions, but all parameters from the separate fits of the submillimeter and infrared data agree within three error intervals. A remarkable agreement for the parameter E_5 between both sets has been

TABLE III—*Continued*

Transition	Wavenumber		Obs-Calc	Transition	Wavenumber		Obs-Calc	Transition	Wavenumber		Obs-Calc
oR(24, 5)	(1458.31283)			sP(29, 3)	1467.04184	(80)	110	sQ(27, 3)	1518.33153	(20)	28
oR(24, 6)	(1441.17005)			sQ(6, 0)	(1478.87876)			sQ(28, 3)	1516.24171	(20)	57
oR(25, 6)	(1443.32126)			sQ(7, 0)	1478.54710	(400)	405	sQ(29, 3)	1516.15909	(30)	117
oR(26, 6)	1445.37038	(60)	-4	sQ(11, 0)	1476.83077	(10)	24	sR(5, 0)	(1489.10108)		
oR(27, 6)	(1449.37227)			sQ(12, 0)	1476.32586	(20)	7	sR(6, 0)	1490.47978	(50)	19
sP(7, 0)	(1466.95890)			sQ(13, 0)	1475.80437	(10)	-20	sR(7, 0)	1491.77116	(100)	0
sP(8, 0)	1464.93254	(10)	-6	sQ(14, 0)	1475.33394	(100)	23	sR(8, 0)	1493.07428	(600)	544
sP(9, 0)	1462.82076	(500)	66	sQ(15, 0)	1474.53971	(100)	134	sR(9, 0)	(1494.32320)		
sP(10, 0)	1460.70263	(2000)	-1189	sQ(16, 0)	1473.95977	(500)	506	sR(10, 0)	(1495.54308)		
sP(11, 0)	1458.56523	(200)	-131	sQ(17, 0)	(1473.32888)			sR(13, 1)	1515.33922	(10)	0
sP(12, 0)	(1456.38509)			sQ(18, 0)	1472.67297	(500)	-488	sR(14, 1)	1516.85078	(500)	4
sP(15, 1)	1465.98491	(40)	-21	sQ(19, 0)	(1472.00616)			sR(15, 1)	1517.71246	(50)	4
sP(16, 1)	1464.10034	(10)	-5	sQ(14, 1)	1491.51144	(500)	2	sR(16, 1)	1518.99258 *		-337
sP(17, 1)	(1461.56732)			sQ(15, 1)	1491.32450	(10)	5	sR(18, 2)	1537.54782	(20)	-23
sP(18, 1)	(1459.45770)			sQ(16, 1)	(1490.48837)			sR(19, 2)	1538.94094	(10)	-21
sP(20, 2)	(1471.23204)			sQ(17, 1)	(1490.07491)			sR(20, 2)	1540.45018	(20)	-32
sP(21, 2)	1469.23698	(80)	-53	sQ(19, 2)	1505.23681	(100)	-39	sR(21, 2)	1540.86073	(10)	-19
sP(22, 2)	1467.36099	(20)	-20	sQ(20, 2)	1504.93592	(100)	-7	sR(22, 2)	1542.30053	(30)	-55
sP(23, 2)	1464.38732	(100)	-72	sQ(21, 2)	1504.75175	(20)	-25	sR(23, 2)	(1543.61396)		
sP(24, 2)	(1462.44679)			sQ(22, 2)	1503.46991	(20)	-21	sR(24, 2)	(1544.87303)		
sP(25, 2)	(1460.38052)			sQ(23, 2)	(1503.21901)			sR(24, 3)	1561.16698	(20)	35
sP(26, 2)	(1458.26282)			sQ(24, 2)	(1502.84173)			sR(25, 3)	1562.61399	(100)	-1
sP(26, 3)	1474.56430	(100)	45	sQ(25, 2)	(1502.41181)			sR(26, 3)	1564.16301	(10)	17
sP(27, 3)	1472.63813	(100)	92	sQ(25, 3)	1518.70936	(10)	29	sR(27, 3)	1563.75839	(10)	58
sP(28, 3)	1470.81489	(30)	31	sQ(26, 3)	1518.46917	(20)	37	sR(28, 3)	1565.35914	(20)	83

obtained, although there is only indirect information involved in the pure rotational transition frequencies on the energy E_5 of that vibrational state. A simultaneous fit of the frequencies of the rotational transitions in the ground state and the vibration–rotational wavenumbers to the states $v_2 = 1$ and $v_5 = 1$ confirmed also the compatibility of these data. The experimental wavenumbers of the vibration–rotational transitions are compared in Table III with the values calculated from the parameters of the simultaneous fit.

Intensity Perturbations

Already noticed by di Lauro and Mills (*1*) in their low-resolution spectra of H_3CF through the band contours, there are strong perturbations of intensity due to the x–y Coriolis interactions in the ν_2 and ν_5 bands of H_3CF. These perturbations are certainly more pronounced in our high-resolution spectra of H_3CF. In an attempt to analyze them, we have extracted the intensity information from the absorbance spectrum of H_3CF. From the intensities of 72 lines of the ν_2 and ν_5 bands, using the fitting program described previously (*13*), we have determined the vibrational transition moments $\langle 0, 0^0 | \mu_x | 0, 1^{\pm 1} \rangle$, $\langle 0, 0^0 | \mu_z | 1, 0^0 \rangle$,

$$\langle 0, 0^0 | \mu_x | 0, 1^{\pm 1} \rangle = 0.0680(6) \times 10^{-30}\ \mathrm{Cm} \tag{7}$$

$$\langle 0, 0^0 | \mu_z | 1, 0^0 \rangle = 0.0549(11) \times 10^{-30}\ \mathrm{Cm}, \tag{8}$$

which gives

$$\partial \mu_x / \partial q_{5a} = 0.1360(12) \times 10^{-30}\ \mathrm{Cm} \tag{9}$$

$$\partial \mu_z / \partial q_2 = 0.0776(15) \times 10^{-30}\ \mathrm{Cm} \tag{10}$$

and

$$(\partial\mu_x/\partial q_{5a})/(\partial\mu_z/\partial q_2) = 1.75(2). \tag{11}$$

Because $\zeta^y_{2,5a} < 0$ [cf. Ref. (*1*)], we have a negative perturbation of intensity corresponding to a classical model in which the vibrational angular momentum and the dipole moment rotate in the opposite sense in the plane perpendicular to the axis y. This result is in agreement with the conclusion of di Lauro and Mills (*1*) although they reached it by considering perturbations of the band contour. The ratio of the dipole moment derivatives [Eq. (11)] is comparable with the value estimated by di Lauro and Mills (*1*),

$$(\partial\mu_x/\partial q_{5a})/(\partial\mu_z/\partial q_2) = 2.3 \pm 0.6. \tag{12}$$

The results of our intensity analysis should be considered preliminary because the sample temperature was not measured accurately during the measurements and the total pressure might also have increased due to a small leak of air into the sample cell. Both the ratio of the vibrational transition moments and their relative signs are of course determined here much more accurately than their absolute values.

DISCUSSION

Both the standard deviation 8.0×10^{-4} cm^{-1} for the infrared data in the simultaneous fit of the wavenumbers of 2046 vibration–rotational transitions and 0.38 MHz for the frequencies of 202 purely rotational transitions in the $v_2 = 1$ and $v_5 = 1$ states and the relatively small dispersions of parameters indicated in Table I constitute a satisfactory result for experimental data in such a large set pertaining to a system of strongly perturbed vibration–rotational levels. However, on close inspection of the differences between experimental and calculated wavenumbers of vibration–rotational transitions in Table III one sees that for certain values of the rotational quantum number K there are systematic trends in these differences which reach +0.023 cm^{-1} for $J = 30$ in the $^PQ(J, 8)$ lines, −0.020 cm^{-1} for $^PQ(32, 9)$ but only +0.0020 cm^{-1} for the line $^PQ(34, 6)$. These differences, which are evident especially in the ν_5 band, are more pronounced in the $\Delta K = -1$ transitions. Although we endeavored to introduce several other terms of higher order both diagonal and off-diagonal in our model Hamiltonian, we have been unable to eliminate these differences. Their irregular dependence on K indicates that they are probably not caused by interactions within the system of the states $v_2 = 1$ and $v_5 = 1$. Because interactions with other vibrational states have not been taken explicitly into account in our model Hamiltonian, we speculate that for the largest values of J these interactions are already so strong that they cannot be absorbed into the effective values of parameters which in our model Hamiltonian describe the interactions between and within the states $v_2 = 1$ and $v_5 = 1$. The nearby vibrational states have the term values $\nu_3\,(A_1) = 1048.611$ cm^{-1} (*11*), $\nu_6\,(E) = 1182.674$ cm^{-1} (*14*), $\nu_1\,(A_1) = 2916.643$ cm^{-1} and $\nu_4\,(E) = 2998.438$ cm^{-1} (*15*); the state of vibrational term value nearest the states $v_2 = 1$ and $v_5 = 1$ is therefore the state $v_6 = 1$. Although crossings of energy levels and coincidences occur for large values of J between the states $v_6 = 1$ and $v_2 = 1$, $v_5 = 1$ which have the same overall symmetry species, because they occur for $\Delta K > 3$ the effects should be extremely small.

ACKNOWLEDGMENTS

We thank Dr. J. Pola (Prague) and Dr. R. Fajgar (Prague) for preparing the sample of H_3CF and K. Lattner (Giessen) for his expert assistance in recording the infrared spectra. The laboratory work in Giessen was supported in part by the Deutsche Forschungsgemeinschaft and the Fonds der Chemischen Industrie. D.P. thanks the National Science Council of the Republic of China for appointment as Visiting Research Professor at the Academia Sinica Institute of Atomic and Molecular Sciences, and the research of J.F.O. is also supported by the National Science Council of the Republic of China.

RECEIVED: October 16, 1991

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