

Tunneling–Rotation Spectrum of the Hydrogen Fluoride Dimer

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The tunneling–rotation spectrum of the ground state of the hydrogen fluoride dimer, $\text{HF} \cdots \text{HF}$, has been extended to the submillimeter wavelength region with the RAD-3 submillimeter spectrometer at Gorky in the frequency range 180–380 GHz at 210 K and pressures from 0.5 to 1.5 Torr. The spectrum has been reinvestigated at lower frequencies with a conventional Stark spectrometer at pressures between 0.1 to 0.2 Torr at the National Institute of Standards and Technology. Lines of the a -type $K = 3$ subband have been observed for the first time. The tunneling frequency for the $K = 3$ state is 114 306.35(53) MHz. The rotational constants of this subband are somewhat anomalous as compared with those for the lower K sublevels. For example, the B rotational constant for the B_u state is larger than that for the A_g state, while for all the lower K sublevels the opposite is true. Higher- J R - and P -branch lines of the $K = 0$ through $K = 2$ subbands have been identified and improved rotational constants for these states have been obtained. An atlas of all a - and b -type far infrared and microwave ground state tunneling–rotation transitions for K up to 3 giving frequency, uncertainty, and relative intensity has been prepared. © 1990 Academic Press, Inc.

INTRODUCTION

The microwave spectrum of the hydrogen fluoride dimer was first reported by Dyke, Howard, and Klemperer (1) in 1972. In this remarkable study, it was established that this loosely bound hydrogen-bonded molecule tunnels from a planar bent (C_s) conformation to a symmetrically equivalent form by passing through a symmetric (C_{2h}) conformation. Since that time, the results of several additional microwave studies have been published in which higher frequency as well as higher quantum number a -type transitions have been reported for the ground state tunneling–rotation spectrum of this molecule (2, 3). Recently, while the work reported here was in process, von Puttkamer, Quack, and Suhm (4) reported a study of the far infrared spectrum of $(\text{HF})_2$ in the region 20 to 170 cm^{-1} at medium resolution and observed the b -type tunneling–rotation transitions from $K''_a = 0$ through $K''_a = 3$, although only one symmetry component was measured for the latter subband. Additional, very precise, albeit indirect, ground state data of $(\text{HF})_2$ are available from the near infrared studies of Pine and his coworkers (5, 6) on the ν_1 band for the $K = 0$ through the $K = 2$ states

with somewhat limited data on one of the symmetry components of the $K = 3$ states. A group-theoretic treatment of the large amplitude internal rotation problem in the HF dimer has been made by Hougen and Ohashi (7) as well as by Mills (8).

Using microwave data as well as a variety of additional data, Barton and Howard (9) have derived a potential function for this molecule and have derived a barrier of about 300 cm^{-1} for the very large amplitude tunneling motion. Very recently, Bunker, Gomez, Marshall, Kofranek, Lischka, and Karpfen (10) have derived rotation-tunneling spectra of (HF)₂ and (DF)₂ using an *ab initio* derived potential energy surface (11, 12).

The hydrogen fluoride dimer spectrum, structure, force field, and dynamics have proven to be of wide-ranging interest, both theoretically and experimentally, since it is one of the simplest hydrogen-bonded molecules. In order to assist the theoretical studies on (HF)₂, we have extended the measurement range to much higher frequency than previously recorded. In this paper, we report additional measurements of the ground state submillimeter-wave and microwave tunneling-rotation *a*-type transitions of this molecule. In addition to extending the line assignment to higher-*J* transitions in the $K = 0, 1$, and 2 subbands, we have also been able, with the help of a Padé approximate model, to assign a number of *P*-, *Q*-, and *R*-branch lines in the $K = 3$ subband and, therefore, derive a precise value of the tunneling splitting for the $K = 3$ substate.

Many complexes containing HF as a parent species have been studied in the radio-frequency, microwave, and infrared regions since this molecule forms strong hydrogen bonds and has no quadrupolar nuclei. Since (HF)₂ is always present in the spectra of these complexes, a means of readily identifying lines of the dimer would be most useful. Using the spectroscopic constants obtained in this work, an atlas of both the *a*-type transitions which fall in the microwave and submillimeter-wave regions and the *b*-type far infrared transitions has been prepared. It is hoped that this atlas will expedite future work on the spectrum of (HF)₂ as well as on other HF-containing species.

EXPERIMENTAL DETAILS

This work was initiated by Gorky where the spectrum of (HF)₂ was investigated with the RAD-3 spectrometer (13) using an opto-acoustical detector covering the frequency range 180–380 GHz. The spectra were calibrated using the spectrum of SO₂ whose line frequencies are well known. The calibration spectra were run simultaneously with the dimer spectrum. In a sample in thermodynamic equilibrium, formation of the hydrogen fluoride dimer is favored at lower temperatures and higher pressures. Pressures of HF ranging from 0.5 to 1.5 Torr and temperatures in the vicinity of 210 K were found necessary to produce sufficient (HF)₂ so that the transitions could be measured with a reasonable signal-to-noise level. Unfortunately, at these pressures, the lines are significantly pressure-broadened, and at the higher pressures the linewidths were on the order of 30 MHz. As a result, the frequency measurement precision was degraded, and some of the weaker lines could be measured only to within ± 4 MHz. Figure 1 shows a small portion of the submillimeter spectrum in the frequency range 314–317 GHz run at a pressure of 0.7 Torr. All the assigned lines in the region are labeled. A number of strong unassigned lines remain which may be due to transitions originating in excited states or possibly to impurities.

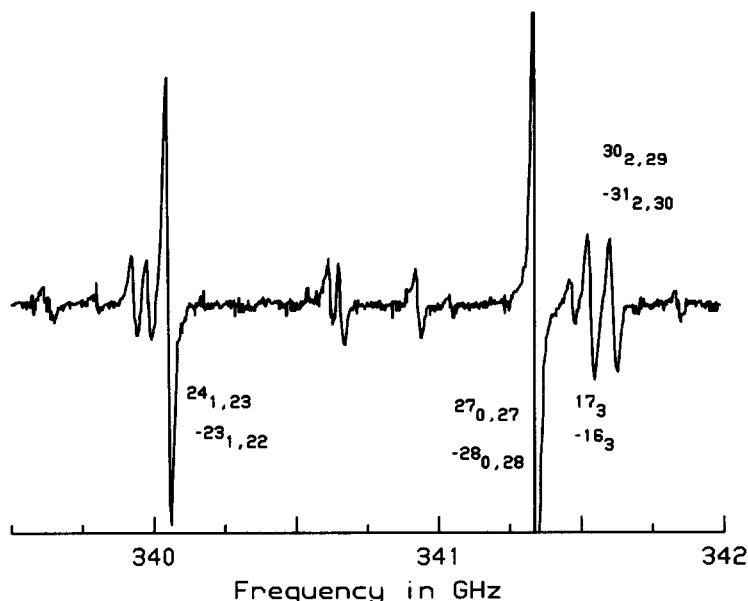


FIG. 1. A portion of the submillimeter spectrum of $(\text{HF})_2$ in the 340 GHz region taken at a total pressure of 0.7 Torr at a temperature at about 210 K. The unassigned lines may be transitions originating in excited vibrational states.

In order to verify the assignment of the $K = 3$ *R*-branch series observed in the submillimeter-wavelength region, it was necessary to make additional measurements at lower frequencies. These measurements were made with a conventional Stark spectrometer (14) in the 60–125 GHz frequency range. Lower frequency transitions were too weak to observe. The 1-m cell was cooled to 195 K, and pressures of HF gas of 0.1 to 0.2 Torr were necessary to produce lines of the dimer. At these conditions, the $(\text{HF})_2$ lines were rather weak, but since reasonably accurate estimates of the line positions could be made using the $K = 3$ submillimeter data as well as a few IR combination differences, they were readily located. These low frequency lines were also pressure-broadened, but, since lower pressures were used, the full width of the lines was only about 4 MHz, and, as a result, they could be measured with a precision of slightly better than 1 MHz. The Stark effect in HF dimer arises from interactions between levels in the two tunneling components. For the $K = 3$ energy levels, the energy difference is quite large, the Stark shifts are second-order and slow, and it is necessary to use electric fields near 2000 V/cm to fully modulate the lines. Figure 2 shows a scan over the first (and strongest) line of the *a*-type $K = 3$ *Q*-branch series taken with a total pressure of 0.15 Torr and path length of 1 m at 190 K. Although the electric field is rather high, the Stark shift is slow and unresolved.

ASSIGNMENTS AND ANALYSIS

The group theory for the tunneling–rotation spectrum of $(\text{HF})_2$ has been developed by Dyke, Howard, and Klemperer (1), Mills (8), and Hougen and Ohashi (7), whose system we follow in this work. The application of the theory has been discussed pre-

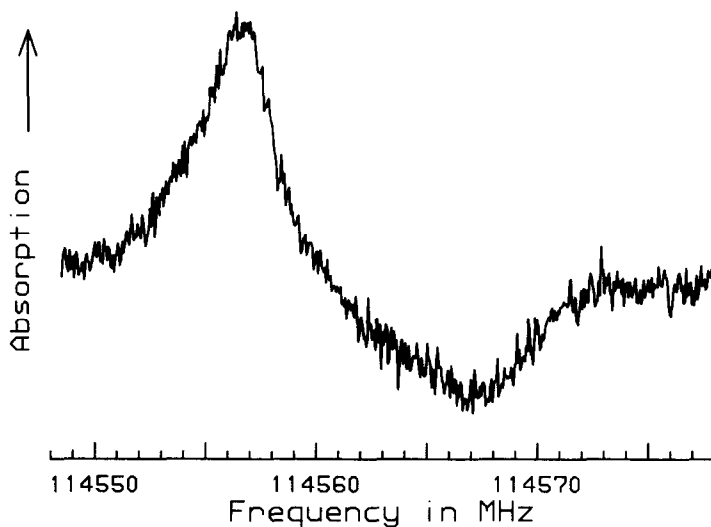


FIG. 2. A scan over the unresolved $3_{3,1}$ - $3_{3,0}$, $3_{3,0}$ - $3_{3,1}$ Q-branch transitions of (HF)₂ taken at a total pressure of 0.15 Torr with a path length of 1 m in a Stark field of 2000 V/cm. The Stark shift is very slow and unresolved.

viously by Lafferty *et al.* (3), and we give here only brief details. The intermediate state (the conformation at the barrier maximum) in (HF)₂ has C_{2h} symmetry, and the symmetry labels of this group can be used to designate the (HF)₂ energy levels. The tunneling splits the ground state into two set of levels; the upper levels have B_u symmetry, and the lower, totally symmetric levels have A_g symmetry. For the ground state tunneling-rotation transitions, the selection rules

$$A_g \leftrightarrow B_u, \quad \Delta K = 0, \pm 1, \quad \Delta J = 0, \pm 1$$

apply, except in the case of the subband with $K = 0$ and $\Delta K = 0$, where there are no $\Delta J = 0$ Q-branch transitions. The A rotational constant of the molecule is quite large, and, while the a -type tunneling-rotation transitions with $\Delta K = 0$ fall in the microwave or submillimeter-wavelength region, the $\Delta K = 1$ transitions fall in the far IR region.

As indicated in Ref. (3), it is necessary to resort to a very empirical, somewhat intuitive treatment in order to account for the observed transitions. While expansions in $J(J+1)$ are well behaved, expansions in K^2 are not convergent; Pine *et al.* (6) have discussed this behavior. Therefore, in fitting the data, we have used a separate expression for each set of K sublevels using expansions in $J(J+1)$, and, with the aid of Polo's (15) expressions, converted the empirical constants obtained to approximate asymmetric rotor constants.

The following expressions were used in the fittings:

$$\begin{aligned} K = 0 \quad E_0^v &= \Delta_0 \delta_{v,1} + B_0^v J(J+1) - D_{J,0}^v J^2(J+1)^2 + H_{J,0}^v J^3(J+1)^3, \\ K = 1 \quad E_1^v &= \Delta_1 \delta_{v,1} + F(1) + B_1^v J(J+1) \pm \frac{1}{4}(B-C)^v J(J+1) \\ &\quad - D_{J,1}^v J^2(J+1)^2 \mp \frac{1}{2} d_1^v J^2(J+1)^2 + H_{J,1}^v J^3(J+1)^3, \\ K = 2 \quad E_2^v &= \Delta_2 \delta_{v,1} + F(2) + B_2^v J(J+1) - (D_{J,2}^v + d_2^v) J^2(J+1)^2 \\ &\quad + (H_{J,2}^v \pm h_2^v) J^3(J+1)^3 \pm l_2^v J^4(J+1)^4, \end{aligned}$$

and

$$K = 3 \quad E_3^v = \Delta_3 \delta_{v,1} + F(3) + B_3^v J(J+1) - D_{J,3}^v J^2(J+1)^2 + H_{J,3}^v J^3(J+1)^3.$$

Here the tunneling splitting for each K is designated Δ_K ; the symbol v is either 0 or 1 and designates the lower A_g tunneling component or the upper B_u component; and the Kronecker delta, $\delta_{v,1}$, indicates that the tunneling splitting applies only to the upper state. The terms which depend on K^2 alone are lumped into the $F(K)$ term. In a well behaved asymmetric rotor, $F(K) = (A - B)K^2 - D_K K^4 + H_K K^6 + \dots$, but, in the case of $(\text{HF})_2$, this series is very nonconvergent; $F(K)$ therefore is the energy of a hypothetical $J = 0$ level of the A_g component of a given K state relative to the $K = 0$ A_g state. The use of Padé (18, 19) and Borel approximants can result in significantly better, but not perfect, accuracy in calculating the observed energy levels and in extrapolating to higher- K states.

The rotational constants B_K^v , $D_{J,K}^v$, and $H_{J,K}^v$ have their usual meaning; these constants differ slightly between the two symmetry components and do not vary smoothly with K^2 , and, therefore, it is necessary to determine them separately for each K sublevel and symmetry state. The constants designated by lower case letters, d_K^v , h_K^v , and l_K^v , are splitting constants. The assignment of the $K = 2$ P - and R -branch series has been considerably expanded in this study and, in order to fit the data to within experimental error, it was necessary to add an additional, previously not required, splitting term proportional to $J^4(J+1)^4$ in order to adequately account for these lines. No asymmetry splitting was observed in the newly assigned $K = 3$ transitions. We have been unable to locate the high- J P -branch transitions which fall in the submillimeter-wavelength region. It is possible that our difficulty may be caused by the fact that the lines are split in these very high- J transitions and, as a result, are weaker and difficult to find by extrapolation from the lower frequency transitions.

Previously (3), only the a -type microwave transitions, together with $\Delta K = 0$ infrared combination differences, were fit subband by subband to obtain the spectroscopic constants. In this work, we have included all the high precision infrared ground state combination differences with $\Delta K = 0, 1$, and 2 taken from the data of Pine *et al.* (5,6). These data include only a handful of $\Delta K = 0$ combination differences for the A_g $K = 3$ states; therefore, we have also included in the fit the somewhat less accurate, but invaluable $K = 3-2$ b -type transitions reported by von Puttkamer *et al.* (4). All the data were fit simultaneously with each datum being assigned an estimated experimental uncertainty and given a weight equal to the square of the reciprocal of this uncertainty.

The data set includes 177 microwave or higher-frequency transitions and 565 infrared combination difference or far infrared tunneling-rotation transitions. The molecular constants obtained are found in Table I, where the uncertainties cited are one standard deviation. Since the $(\text{HF})_2$ molecule is one of the simplest loosely bound hydrogen-bonded species, and since no model exists to satisfactorily account for the observed data, we include here all data used in the fitting as an aid to future efforts. The microwave data are found in Table II and the IR combination differences are given in Table III. The far infrared b -type $K = 3-2$ transitions from Ref. (4) used in the fitting are found in Table IV.

There remain many unassigned lines in both the microwave and the far infrared spectra of $(\text{HF})_2$. In order to assist in extending the line assignment, we have calculated

TABLE I
Rotational Constants for the Ground State Levels of (HF)₂

	A _g	B _u
K=0		
B ₀ (MHz)	6496.8971(54) ^a	6492.7678(67)
D _{J,0} (kHz)	61.765(13)	61.218(16)
H _{J,0} /10 ⁻⁶ (MHz)	-1.3332(72)	-1.3709(97)
Δ ₀ (MHz)	19 747.032(24)	
K=1		
B ₁ (MHz)	6531.2838(16)	6526.7580(15)
(B-C) (MHz)	95.21190(84)	91.18281(98)
D _{J,1} (kHz)	59.602(21)	59.052(22)
d ₁ (kHz)	2.5514(34)	2.2110(35)
H _{J,1} /10 ⁻⁶ (MHz)	-1.180(19)	-1.230(22)
Δ ₁ (MHz)	31 911.041(10)	
F(1) (cm ⁻¹)	35.425080(91)	
K=2		
B ₂ (MHz)	6553.7149(29)	6551.1313(31)
D _{J,2} (kHz)	58.824(88)	58.646(96)
d ₂ (kHz)	-1.007(27)	-0.582(34)
H _{J,2} /10 ⁻⁶ (MHz)	-2.316(82)	-1.957(96)
h ₂ /10 ⁻⁷ (MHz)	-7.67(64)	-8.27(75)
ℓ ₂ /10 ⁻¹⁰ (MHz)	-1.17(46)	0.51(51)
Δ ₂ (MHz)	60 073.48(21)	
F(2) (cm ⁻¹)	116.13300(14)	
K=3		
B ₃ (MHz)	6538.170(72)	6558.936(72)
D _{J,3} (kHz)	52.910(25)	56.119(29)
H _{J,3} /10 ⁻⁶ (MHz)	-2.30(28)	-1.67(42)
Δ ₃ (MHz)	114 306.35(53)	
F(3) (cm ⁻¹)	232.6321(12)	

^a Uncertainties cited are one σ.

a listing of predicted line frequencies of transitions which fall in both of these regions. These listings are included here to facilitate studies in other laboratories. The empirical spectroscopic constants obtained, together with the variance-covariance matrix from the fitting, have also been used to produce an atlas of calculated *a*-type ground state transitions for *K* = 0 through *K* = 3 in the region up to 400 GHz. The atlas, given in Table V, includes the predicted frequency, the estimated uncertainty in the predictions (1σ), which was calculated using the method outlined by Kirchhoff (16), and a crude estimate of the relative intensity of the transition. The intensity estimates were calculated using the symmetric top intensity expressions given by Herzberg (17). The intensities given in the table have been normalized with the strongest line having a relative intensity of 1000; calculated transitions with a relative intensity of less than 1 have not been included in the table. In addition, calculated transitions with an uncertainty greater than 100 MHz have been omitted. A listing of calculated far infrared *b*-type transitions is found in Table VI. Since the near infrared combination differences used in the fitting to determine the *K* intervals are quite precise, these predicted wavenumbers are considerably more accurate than those measured directly. In this line atlas, lines whose calculated wavenumber has an uncertainty greater than 0.01 cm⁻¹

TABLE II
Measured a -Type Transitions of $(\text{HF})_2$ in MHz

Transition	Frequency ^a	Dev.	Transition ^a	Frequency	Dev.	Transition	Frequency ^a	Dev.
5(0, 5)-4(0, 4)	84561.67(30) ^c	-0.04	26(1,25)-25(1,24)	364866.7(20) ^d	1.6	20(2,19)-19(2,18)	319239.5(40) ^d	-1.0
6(0, 6)-5(0, 5)	97484.02(30) ^c	0.12	26(1,26)-25(1,25)	363815.3(20) ^d	-0.2	21(2,19)-20(2,18)	332008.4(40) ^d	0.4
7(0, 7)-6(0, 6)	110389.13(30) ^c	-0.05	27(1,26)-26(1,25)	377198.3(20) ^d	-0.1	21(2,20)-20(2,19)	331941.9(40) ^d	3.2
8(0, 8)-7(0, 7)	123276.13(30) ^c	-0.01	27(1,27)-26(1,26)	376155.5(20) ^d	-1.5	22(2,20)-21(2,19)	344684.0(40) ^d	-3.7
13(0,13)-12(0,12)	187388.6(20) ^d	1.7				22(2,21)-21(2,20)	344601.0(40) ^d	-0.5
14(0,14)-13(0,13)	200132.1(20) ^d	-2.4	1(1, 0)-1(1, 1)	31995.190(15) ^b	0.010	23(2,21)-22(2,20)	357329.3(40) ^d	-4.3
15(0,15)-14(0,14)	212851.6(20) ^d	-2.4	1(1, 1)-1(1, 0)	31808.784(15) ^b	-0.020	23(2,22)-22(2,21)	357228.4(40) ^d	1.1
16(0,16)-15(0,15)	225545.0(20) ^d	1.1	3(1, 2)-3(1, 1)	32415.676(30) ^b	0.023	24(2,23)-23(2,22)	369814.5(40) ^d	-0.1
17(0,17)-16(0,16)	238203.9(20) ^d	1.0	3(1, 3)-3(1, 2)	31297.976(30) ^b	0.006	25(2,24)-24(2,23)	382362.7(40) ^d	0.8
20(0,20)-19(0,19)	275976.2(20) ^d	-4.0	4(1, 3)-4(1, 4)	32751.784(20) ^b	0.017			
21(0,21)-20(0,20)	288499.3(20) ^d	-2.0	4(1, 4)-4(1, 5)	30889.733(20) ^b	0.008	2(2, 1)-2(2, 0)	60058.88(96) ^c	0.84
22(0,22)-21(0,21)	300980.8(20) ^d	-3.5	5(1, 4)-5(1, 5)	31171.594(15) ^b	0.014	3(2, 1)-3(2, 2)	60042.78(89) ^c	0.51
23(0,23)-22(0,22)	313428.5(20) ^d	0.8	5(1, 5)-5(1, 4)	30379.961(25) ^b	0.015			
24(0,24)-23(0,23)	325829.7(20) ^d	-0.4	6(1, 5)-6(1, 6)	33674.866(15) ^b	-0.005	3(2, 1)-4(2, 2)	7628.186(20) ^b	0.004
25(0,25)-24(0,24)	338190.9(20) ^d	0.8	6(1, 6)-6(1, 5)	29768.985(25) ^b	0.002	3(2, 2)-4(2, 3)	7627.505(50) ^b	-0.030
26(0,26)-25(0,25)	350509.8(20) ^d	3.9	7(1, 6)-7(1, 7)	34261.371(10) ^b	-0.004	4(2, 2)-5(2, 3)	-5484.82(30) ^b	0.30
27(0,27)-26(0,26)	362781.0(20) ^d	4.7	7(1, 7)-7(1, 6)	29057.251(20) ^b	-0.007	4(2, 3)-5(2, 4)	-5486.20(30) ^b	0.30
28(0,28)-27(0,27)	375001.7(20) ^d	2.2				10(2, 8)-11(2, 9)	-84063.50(40) ^c	-0.32
			1(1, 0)-2(1, 1)	5681.585(20) ^b	0.005	10(2, 9)-11(2, 10)	-84086.50(38) ^c	-0.90
0(0, 0)-1(0, 1)	6753.518(20) ^b	0.033	1(1, 1)-2(1, 2)	5875.943(20) ^b	-0.006	11(2, 9)-12(2, 10)	-97127.35(43) ^c	-0.08
1(0, 1)-2(0, 2)	-6246.835(10) ^b	0.001	2(1, 1)-3(1, 2)	-7446.077(7) ^b	-0.002	11(2, 10)-12(2, 11)	-97158.44(35) ^c	-0.26
2(0, 2)-3(0, 3)	-19252.443(10) ^b	-0.009	2(1, 2)-3(1, 3)	-7148.637(7) ^b	0.003	12(2, 10)-13(2, 11)	-110177.24(27) ^c	0.27
3(0, 3)-4(0, 4)	-32261.797(25) ^b	-0.001	3(1, 2)-4(1, 3)	-20580.365(7) ^b	-0.012	12(2, 11)-13(2, 12)	-110219.19(30) ^c	-0.02
4(0, 4)-5(0, 5)	-71297.33(20) ^b	-0.21	3(1, 3)-4(1, 4)	-20176.030(10) ^b	0.003	13(2, 11)-14(2, 12)	-123211.70(43) ^c	0.33
7(0, 7)-8(0, 8)	-84306.41(20) ^c	-0.31	4(1, 3)-5(1, 4)	-33719.682(30) ^b	0.055	13(2, 12)-14(2, 13)	-123266.50(50) ^c	0.58
8(0, 8)-9(0, 9)	-97310.85(30) ^c	0.18	4(1, 4)-5(1, 5)	-33204.760(30) ^b	0.039	22(2,21)-23(2,22)	-239852.4(40) ^d	1.8
9(0, 9)-10(0,10)	-110709.85(30) ^c	0.44	5(1, 8)-10(1, 9)	-99438.76(36) ^c	-0.12	23(2,22)-24(2,23)	-252684.1(40) ^d	0.5
10(0,10)-11(0,11)	-123301.49(40) ^c	0.75	9(1, 9)-10(1,10)	-98318.44(32) ^c	-0.26	25(2,24)-26(2,25)	-278250.2(40) ^d	0.4
15(0,15)-16(0,16)	-188091.6(20) ^d	1.8	11(1,10)-12(1,11)	-125705.82(23) ^c	0.58	26(2,24)-27(2,25)	-290216.6(40) ^d	-3.0
17(0,17)-18(0,18)	-213896.1(20) ^d	2.6	11(1,11)-12(1,12)	-124321.71(30) ^c	-0.20	26(2,25)-27(2,26)	-290979.8(40) ^d	2.9
18(0,18)-19(0,19)	-226768.9(20) ^d	1.5	16(1,15)-17(1,16)	-191207.9(20) ^d	0.2	27(2,25)-28(2,26)	-302773.6(40) ^d	0.9
22(0,22)-23(0,23)	-278003.1(20) ^d	4.0	16(1,16)-17(1,17)	-189115.2(20) ^d	1.7	27(2,26)-28(2,27)	-303682.8(40) ^d	-4.2
23(0,23)-24(0,24)	-290739.1(20) ^d	5.0	19(1,19)-20(1,20)	-227778.2(20) ^d	5.7	28(2,27)-29(2,28)	-316338.2(40) ^d	-1.7
24(0,24)-25(0,25)	-303452.1(20) ^d	-3.9	23(1,22)-24(1,23)	-282150.2(20) ^d	3.3	29(2,27)-30(2,28)	-327713.2(40) ^d	2.8
25(0,25)-26(0,26)	-316116.8(20) ^d	0.8	23(1,23)-24(1,24)	-279002.1(20) ^d	-0.9	29(2,28)-30(2,29)	-328956.8(40) ^d	-2.0
26(0,26)-27(0,27)	-328748.7(20) ^d	1.4	24(1,23)-25(1,24)	-295035.8(20) ^d	4.7	30(2,29)-31(2,30)	-341538.1(40) ^d	-6.2
27(0,27)-28(0,28)	-341345.1(20) ^d	-1.5	24(1,24)-25(1,25)	-291734.6(20) ^d	1.2	31(2,30)-32(2,31)	-354069.2(40) ^d	-3.1
28(0,28)-29(0,29)	-353897.0(20) ^d	-1.0	25(1,24)-26(1,25)	-307891.3(20) ^d	3.8	32(2,31)-33(2,32)	-366559.3(40) ^d	-3.2
29(0,29)-30(0,30)	-366409.5(20) ^d	-4.3	25(1,25)-26(1,26)	-304438.3(20) ^d	-5.0	33(2,32)-34(2,33)	-378993.6(40) ^d	7.0
30(0,30)-31(0,31)	-378712.1(20) ^d	-3.1	26(1,25)-27(1,26)	-320717.2(20) ^d	-1.9			
			27(1,26)-28(1,27)	-333498.0(20) ^d	1.1	12(3, 9)-11(3, 8)	274016.8(40) ^d	-0.3
5(1, 4)-4(1, 3)	97265.81(30) ^c	-0.29	27(1,27)-28(1,28)	-329728.1(20) ^d	0.6	13(3, 11)-12(3, 10)	287503.8(40) ^d	-1.8
6(1, 5)-5(1, 4)	110288.10(27) ^c	-0.21	28(1,27)-29(1,28)	-346243.0(20) ^d	1.2	14(3, 11)-13(3, 10)	301012.0(40) ^d	-0.2
6(1, 6)-5(1, 5)	109803.05(29) ^c	-0.20	28(1,27)-29(1,28)	-346243.0(20) ^d	1.2	15(3, 13)-14(3, 12)	314530.2(40) ^d	-4.3
7(1, 6)-6(1, 5)	123291.05(26) ^c	0.04	28(1,28)-29(1,29)	-342320.2(20) ^d	0.4	16(3, 13)-15(3, 12)	328070.2(40) ^d	0.1
7(1, 7)-6(1, 6)	122739.59(26) ^c	-0.19	29(1,28)-30(1,29)	-358950.0(20) ^d	-1.5	17(3, 15)-16(3, 14)	341618.0(40) ^d	1.2
13(1,13)-12(1,12)	199960.2(20) ^d	-2.1	29(1,29)-30(1,30)	-354868.7(20) ^d	4.0	18(3, 15)-17(3, 14)	355175.3(40) ^d	3.2
14(1,13)-13(1,12)	213650.6(20) ^d	-0.2	30(1,29)-31(1,30)	-371613.5(20) ^d	-3.7	19(3, 17)-18(3, 16)	368732.4(40) ^d	-1.0
14(1,14)-13(1,13)	212751.6(20) ^d	-2.3	30(1,30)-31(1,31)	-367381.5(20) ^d	1.7	20(3, 17)-19(3, 16)	382304.2(40) ^d	5.8
15(1,14)-14(1,13)	226444.7(20) ^d	-4.6	31(1,30)-32(1,31)	-384227.3(20) ^d	-1.3			
15(1,15)-14(1,14)	225515.8(20) ^d	-3.7				3(3, 1)-3(3, 0)	114556.71(50) ^d	1.63
16(1,16)-15(1,15)	238256.0(20) ^d	-1.5	3(2, 1)-2(2, 0)	99358.48(64) ^c	0.09	4(3, 1)-4(3, 2)	114719.91(50) ^d	-0.48
19(1,18)-18(1,17)	277312.7(20) ^d	-2.6	4(2, 3)-3(2, 2)	112435.82(76) ^c	-0.80	5(3, 3)-5(3, 2)	114926.15(50) ^d	-0.32
19(1,19)-18(1,18)	276286.6(20) ^d	-6.1	5(2, 3)-4(2, 2)	125503.33(86) ^c	-0.37	6(3, 3)-6(3, 4)	115177.76(50) ^d	-0.16
21(0,20)-20(1,19)	302531.7(20) ^d	-1.5	10(2, 9)-9(2, 8)	190624.4(80) ^d	-4.5	7(3, 5)-7(3, 4)	115459.41(50) ^d	0.10
21(1,21)-20(1,20)	301482.6(20) ^d	-3.8	12(2,11)-11(2,10)	216556.1(80) ^d	2.9	8(3, 5)-8(3, 6)	115784.93(50) ^d	-0.19
22(1,21)-21(1,20)	315085.5(20) ^d	1.2	14(2,13)-13(2,12)	242389.0(80) ^d	0.9			
22(1,22)-21(1,21)	314028.7(20) ^d	-1.3	16(2,15)-15(2,14)	268127.3(80) ^d	5.2	3(3, 1)-4(3, 2)	62262.47(50) ^d	-0.81
23(1,22)-22(1,21)	327591.8(20) ^d	-1.8	18(2,16)-17(2,15)	293774.6(40) ^d	-2.5	13(3,11)-14(3,12)	-64496.66(50) ^d	0.58
23(1,23)-22(1,22)	326535.0(20) ^d	-1.2	18(2,17)-17(2,16)	293749.6(40) ^d	6.2	15(3,13)-16(3,14)	-89226.00(50) ^d	-0.10
24(1,23)-23(1,22)	340062.4(20) ^d	1.1	19(2,17)-18(2,16)	306549.1(40) ^d	-2.5	17(3,15)-18(3,16)	-113735.54(50) ^d	-0.28
24(1,24)-23(1,23)	339003.2(20) ^d	-0.3	20(2,18)-19(2,17)	306513.7(40) ^d	5.5			
25(1,24)-24(1,23)	352488.3(20) ^d	2.7	20(2,18)-19(2,17)	319293.4(40) ^d	-2.3			

^a Numbers in parenthesis are estimated experimental uncertainties.

^b Howard et al. (Refs. 1,2).

^c Lafferty et al. (Ref. 3).

^d This work.

or whose relative intensity is less than 0.01 of the strongest transition have not been included.

DISCUSSION

In this work, the microwave spectrum of the a -type $K = 3$ inversion-rotation spectrum is reported for the first time; however, the constants of both the symmetry states of the $K = 3$ levels were recently determined in the far infrared study of von Puttkamer, Quack, and Suhm (4) from the $K = 3-2$ b -type subbands. The B rotational constants determined by these workers agree to within 2 MHz of the more precise values de-

TABLE III

Ground State Combination Differences of (HF)₂^a in cm⁻¹

Quantum Numbers	Com. Diff.	O-C ^b	Sy. ^c	Quantum Numbers	Com. Diff.	O-C	Sy.	Quantum Numbers	Com. Diff.	O-C	Sy.
4(0, 4)-2(0, 2)	3.0342(12) ^d	10 +		14(1, 13)-15(0, 15)	29.3604(16)	-3 +		21(2, 20)-22(0, 22)	107.5898(16)	-1 +	
5(0, 5)-3(0, 3)	3.8997(12)	4 +		15(1, 14)-16(0, 16)	28.9919(16)	0 +		22(2, 21)-23(0, 23)	107.2583(16)	1 +	
6(0, 6)-4(0, 4)	4.7666(12)	-3 +		17(1, 16)-18(0, 18)	28.2688(16)	0 +		24(2, 23)-25(0, 25)	106.6123(16)	1 +	
8(0, 8)-6(0, 6)	6.4946(12)	3 +		21(1, 20)-22(0, 22)	26.8831(16)	7 +		26(2, 25)-27(0, 27)	105.9900(16)	-3 +	
9(0, 9)-7(0, 7)	7.3577(12)	-3 +		22(1, 21)-23(0, 23)	26.5486(16)	0 +		27(2, 26)-28(0, 28)	105.6877(16)	-10 +	
9(0, 9)-7(0, 7)	7.3579(12)	-1 +		31(1, 30)-32(0, 32)	23.7947(16)	7 +		28(2, 27)-29(0, 29)	105.3933(16)	-4 +	
10(0, 10)-8(0, 8)	8.2207(12)	-1 +		33(1, 32)-34(0, 34)	23.2466(16)	-3 +		32(2, 31)-33(0, 33)	104.2805(16)	-6 +	
10(0, 10)-8(0, 8)	8.2209(12)	1 +									
11(0, 11)-9(0, 9)	9.0833(12)	6 +		10(1, 10)-10(0, 10)	35.4651(16)	-2 +		6(2, 4)-6(0, 6)	116.2129(16)	2 +	
11(0, 11)-9(0, 9)	9.0828(12)	1 +		11(1, 11)-11(0, 11)	35.4731(16)	-6 +		6(2, 4)-6(0, 6)	116.2122(16)	-5 +	
12(0, 12)-10(0, 10)	9.9451(12)	16 +		12(1, 12)-12(0, 12)	35.4822(16)	-8 +		8(2, 6)-8(0, 8)	116.2693(16)	-5 +	
12(0, 12)-10(0, 10)	9.9436(12)	1 +		12(1, 12)-12(0, 12)	35.4822(16)	-8 +		8(2, 6)-8(0, 8)	116.2700(16)	2 +	
13(0, 13)-11(0, 11)	10.8030(12)	-1 +		13(1, 13)-13(0, 13)	35.4927(16)	-5 +		9(2, 7)-9(0, 9)	116.3052(16)	12 +	
14(0, 14)-12(0, 12)	11.6614(12)	-1 +		14(1, 14)-14(0, 14)	35.5044(16)	1 +		12(2, 10)-12(0, 12)	116.4297(16)	-3 +	
15(0, 15)-13(0, 13)	12.5193(12)	7 +		14(1, 14)-14(0, 14)	35.5044(16)	1 +		12(2, 10)-12(0, 12)	116.4297(16)	-3 +	
15(0, 15)-13(0, 13)	12.5183(12)	-3 +		15(1, 15)-15(0, 15)	35.5164(16)	-1 +		13(2, 11)-13(0, 13)	116.4802(16)	5 +	
16(0, 16)-14(0, 14)	13.3735(12)	-7 +		16(1, 16)-16(0, 16)	35.5300(16)	3 +		14(2, 12)-14(0, 14)	116.5337(16)	4 +	
17(0, 17)-15(0, 15)	14.2280(12)	-2 +		16(1, 16)-16(0, 16)	35.5303(16)	6 +		15(2, 13)-15(0, 15)	116.5903(16)	-5 +	
17(0, 17)-15(0, 15)	14.2285(12)	3 +		17(1, 17)-17(0, 17)	35.5444(16)	4 +		17(2, 15)-17(0, 17)	116.7175(16)	2 +	
18(0, 18)-16(0, 16)	15.0806(12)	1 +		19(1, 19)-19(0, 19)	35.5764(16)	3 +		17(2, 15)-17(0, 17)	116.7168(16)	-5 +	
18(0, 18)-16(0, 16)	15.0820(12)	15 +		20(1, 20)-20(0, 20)	35.5940(16)	0 +		18(2, 16)-18(0, 18)	116.7859(16)	-4 +	
19(0, 19)-17(0, 17)	15.9307(12)	-3 +		22(1, 22)-22(0, 22)	35.6331(16)	-6 +		18(2, 16)-18(0, 18)	116.7861(16)	-2 +	
20(0, 20)-18(0, 18)	16.7798(12)	1 +		23(1, 23)-23(0, 23)	35.6565(16)	7 +		19(2, 17)-19(0, 19)	116.8596(16)	4 +	
21(0, 21)-19(0, 19)	17.6265(12)	2 +		24(1, 24)-24(0, 24)	35.6792(16)	-1 +		21(2, 19)-21(0, 21)	117.0161(16)	-3 +	
22(0, 22)-20(0, 20)	18.4707(12)	-1 +		26(1, 26)-26(0, 26)	35.7319(16)	7 +		22(2, 20)-22(0, 22)	117.1008(16)	1 +	
23(0, 23)-21(0, 21)	19.3130(12)	-1 +		27(1, 27)-27(0, 27)	35.7603(16)	6 +		23(2, 21)-23(0, 23)	117.1892(16)	6 +	
24(0, 24)-22(0, 22)	20.1545(12)	15 +		28(1, 28)-28(0, 28)	35.7905(16)	4 +		23(2, 21)-23(0, 23)	117.1880(16)	-6 +	
25(0, 25)-23(0, 23)	20.9905(12)	0 +		29(1, 29)-29(0, 29)	35.8235(16)	10 +		24(2, 22)-24(0, 24)	117.2798(16)	-5 +	
25(0, 25)-23(0, 23)	20.9897(12)	-8 +		30(1, 30)-30(0, 30)	35.8572(16)	5 +		25(2, 23)-25(0, 25)	117.3760(16)	6 +	
26(0, 26)-24(0, 24)	21.8252(12)	-2 +		31(1, 31)-31(0, 31)	35.8928(16)	-4 +					
27(0, 27)-25(0, 25)	22.6575(12)	0 +						9(2, 8)-8(0, 8)	120.2000(16)	6 +	
28(0, 28)-26(0, 26)	23.4868(12)	-1 +		9(1, 8)-8(0, 8)	39.4941(16)	-7 +		9(2, 8)-8(0, 8)	120.1992(16)	-2 +	
29(0, 29)-27(0, 27)	24.3127(12)	-6 +		11(1, 10)-10(0, 10)	40.4387(16)	2 +		12(2, 11)-11(0, 11)	121.6187(16)	1 +	
30(0, 30)-28(0, 28)	25.1367(12)	0 +		12(1, 11)-11(0, 11)	40.9153(16)	-1 +		13(2, 12)-12(0, 12)	122.0986(16)	0 +	
31(0, 31)-29(0, 29)	25.9702(12)	1 +		13(1, 12)-12(0, 12)	41.3950(16)	-7 +		14(2, 13)-13(0, 13)	122.5823(16)	3 +	
32(0, 32)-30(0, 30)	26.7739(12)	2 +		14(1, 13)-13(0, 13)	41.8789(16)	-4 +		16(2, 15)-15(0, 15)	123.5593(16)	4 +	
32(0, 32)-30(0, 30)	26.7744(12)	7 +		15(1, 14)-14(0, 14)	42.3665(16)	4 +		16(2, 15)-15(0, 15)	123.5588(16)	-1 +	
33(0, 33)-31(0, 31)	27.5874(12)	3 +		16(1, 15)-15(0, 15)	42.8560(16)	-1 +		17(2, 16)-16(0, 16)	124.0527(16)	2 +	
34(0, 34)-32(0, 32)	28.3984(12)	15 +		17(1, 16)-16(0, 16)	43.3496(16)	3 +		17(2, 16)-16(0, 16)	124.0530(16)	5 +	
35(0, 35)-33(0, 33)	29.2036(12)	6 +		18(1, 17)-17(0, 17)	43.8452(16)	-5 +		18(2, 17)-17(0, 17)	124.5493(16)	-1 +	
35(0, 35)-33(0, 33)	29.2014(12)	-16 +		20(1, 19)-19(0, 19)	44.8472(16)	-4 +		19(2, 18)-18(0, 18)	125.0498(16)	0 +	
36(0, 36)-34(0, 34)	30.0059(12)	6 +		21(1, 20)-20(0, 20)	45.3530(16)	-2 +		19(2, 18)-18(0, 18)	125.0488(16)	-10 +	
37(0, 37)-35(0, 35)	30.8047(12)	10 +		22(1, 21)-21(0, 21)	45.8618(16)	1 +		20(2, 19)-19(0, 19)	125.5535(16)	-1 +	
38(0, 38)-36(0, 36)	31.5974(12)	-3 +		23(1, 22)-22(0, 22)	46.3726(16)	-6 +		20(2, 19)-19(0, 19)	125.5525(16)	-10 +	
39(0, 39)-37(0, 37)	32.3865(12)	-10 +		24(1, 23)-23(0, 23)	46.8877(16)	1 +		21(2, 20)-20(0, 20)	126.0605(16)	-2 +	
39(0, 39)-37(0, 37)	32.3884(12)	8 +		25(1, 24)-24(0, 24)	47.4048(16)	-1 +		22(2, 21)-21(0, 21)	126.5713(16)	0 +	
40(0, 40)-38(0, 38)	33.1731(12)	1 +		27(1, 26)-26(0, 26)	48.4482(16)	1 +		23(2, 22)-22(0, 22)	127.0845(16)	-8 +	
41(0, 41)-39(0, 39)	33.9539(12)	0 +		28(1, 27)-27(0, 27)	48.9741(16)	2 +		24(2, 23)-23(0, 23)	127.6028(16)	1 +	
42(0, 42)-40(0, 40)	34.7295(12)	-5 +		29(1, 28)-28(0, 28)	49.5032(16)	8 +		26(2, 25)-25(0, 25)	128.6482(16)	3 +	
43(0, 43)-41(0, 41)	35.5010(12)	-3 +		30(1, 29)-29(0, 29)	50.0352(16)	15 +		26(2, 25)-25(0, 25)	128.6475(16)	-4 +	
44(0, 44)-42(0, 42)	36.2656(12)	-20 +		31(1, 30)-30(0, 30)	50.5688(16)	10 +		27(2, 26)-26(0, 26)	129.1760(16)	3 +	
								27(2, 26)-26(0, 26)	129.1746(16)	-10 +	
10(1, 10)-12(0, 12)	25.5215(16)	-3 +		12(1, 12)-10(0, 10)	45.4258(16)	-7 +		28(2, 27)-27(0, 27)	129.7080(16)	10 +	
11(1, 11)-13(0, 13)	24.6704(16)	-1 +		14(1, 14)-12(0, 12)	47.1653(16)	-6 +		28(2, 27)-27(0, 27)	129.7065(16)	-5 +	
12(1, 12)-14(0, 14)	23.8213(16)	-1 +		16(1, 16)-14(0, 14)	48.9048(16)	9 +		32(2, 31)-31(0, 31)	131.8679(16)	-3 +	
13(1, 13)-15(0, 15)	22.9741(16)	-5 +		17(1, 17)-15(0, 15)	49.7727(16)	5 +					
14(1, 14)-16(0, 16)	22.1299(16)	-3 +		19(1, 19)-17(0, 17)	51.5068(16)	-3 +					
16(1, 16)-18(0, 18)	20.4492(16)	0 +						8(2, 6)-6(0, 6)	122.7639(16)	-2 +	
20(1, 20)-22(0, 22)	17.1240(16)	8 +						12(2, 10)-10(0, 10)	126.3730(16)	-5 +	
30(1, 30)-32(0, 32)	9.0830(16)	0 +						14(2, 12)-12(0, 12)	128.1951(16)	3 +	
32(1, 32)-34(0, 34)	7.5337(16)	-12 +						15(2, 13)-13(0, 13)	129.1086(16)	-7 +	
								17(2, 15)-15(0, 15)	130.9456(16)	2 +	
9(1, 8)-10(0, 10)	31.2737(16)	-3 +						18(2, 16)-16(0, 16)	131.8665(16)	-3 +	
11(1, 10)-12(0, 12)	30.4951(16)	1 +						19(2, 17)-17(0, 17)	132.7905(16)	3 +	
12(1, 11)-13(0, 13)	30.1125(16)	2 +						21(2, 19)-19(0, 19)	134.6426(16)	-1 +	
13(1, 12)-14(0, 14)	29.7341(16)	0 +						23(2, 21)-21(0, 21)	136.5022(16)	5 +	

^a From Pine *et al.* (Refs. 5,6).^b (Observed - Calculated) × 10⁴ cm⁻¹.^c The symbol + indicates A_g symmetry; - indicates B_u symmetry.^d Numbers in parenthesis are estimated experimental uncertainties.

terminated in this work, attesting to their skill in locating these weak transitions in the maze of as yet unassigned lines falling in the far infrared region. Aside from a refinement of all previously determined spectroscopic constants, the main contribution of the effort reported here is an accurate determination of the tunneling splitting for the K

TABLE III—Continued

Quantum Numbers	Com. Diff.	O-C	Sy.	Quantum Numbers	Com. Diff.	O-C	Sy.	Quantum Numbers	Com. Diff.	O-C	Sy.
8(1, 7)-7(1, 7)	3.5825(18)	-5	+	32(1,32)-30(1,30)	26.8479(18)	-9	+	24(0,24)-22(0,22)	20.1426(12)	8	-
8(1, 8)-7(1, 6)	3.3811(18)	7	+	33(1,32)-31(1,30)	27.8496(18)	-2	+	25(0,25)-23(0,23)	20.9792(12)	2	-
11(1,10)-10(1,10)	4.9736(18)	4	+	33(1,33)-31(1,31)	27.6665(18)	-3	+	26(0,26)-24(0,24)	21.8132(12)	-4	-
12(1,11)-11(1,11)	5.4421(18)	4	+	34(1,34)-32(1,32)	28.4814(18)	0	+	27(0,27)-25(0,25)	22.6455(12)	0	-
12(1,12)-11(1,10)	4.9871(18)	-9	+					28(0,28)-26(0,26)	23.4749(12)	3	-
13(1,12)-12(1,12)	5.9128(18)	1	+	9(2, 8)-8(2, 6)	3.9292(16)	-5	+	29(0,29)-27(0,27)	24.3008(12)	1	-
14(1,13)-13(1,13)	6.3862(18)	1	+	10(2, 8)-9(2, 8)	4.3643(16)	8	+	31(0,31)-29(0,29)	25.9441(12)	3	-
14(1,14)-13(1,12)	5.7703(18)	1	+	11(2,10)-10(2, 8)	4.7998(16)	-1	+	32(0,32)-30(0,30)	26.7607(12)	2	-
15(1,14)-14(1,14)	6.8621(18)	3	+	11(2,10)-10(2, 8)	4.7993(16)	-6	+	33(0,33)-31(0,31)	27.5740(12)	3	-
16(1,15)-15(1,15)	7.3396(18)	0	+	12(2,10)-11(2,10)	5.2329(16)	15	+	34(0,34)-32(0,32)	28.3833(12)	0	-
16(1,16)-15(1,14)	6.5383(18)	5	+	13(2,12)-12(2,10)	5.6677(16)	-9	+	36(0,36)-34(0,34)	29.9915(12)	1	-
17(1,16)-16(1,16)	7.8196(18)	0	+	14(2,13)-13(2,11)	6.0964(16)	1	+	37(0,37)-35(0,35)	30.7898(12)	2	-
17(1,17)-16(1,15)	6.9167(18)	6	+	14(2,13)-13(2,11)	6.1021(16)	-1	+	38(0,38)-36(0,36)	31.5842(12)	6	-
18(1,17)-17(1,17)	8.3008(18)	-9	+	15(2,14)-14(2,12)	6.5264(16)	-10	+	39(0,39)-37(0,37)	32.3733(12)	-1	-
19(1,19)-18(1,17)	7.6616(18)	-2	+	15(2,14)-14(2,12)	6.5352(16)	-2	+	41(0,41)-39(0,39)	33.9399(12)	3	-
20(1,19)-19(1,19)	9.2708(18)	-8	+	16(2,14)-15(2,14)	6.9573(16)	-2	+				
20(1,20)-19(1,18)	8.0298(18)	13	+	17(2,15)-16(2,15)	7.3862(16)	-3	+	12(1,12)-10(0,10)	24.2368(16)	-5	-
21(1,20)-20(1,20)	9.7590(18)	-2	+	18(2,16)-17(2,16)	7.8135(16)	-8	+	13(1,13)-15(0,15)	23.3921(16)	7	-
23(1,22)-22(1,22)	10.7395(18)	0	+	18(2,16)-17(2,16)	7.8147(16)	4	+	17(1,17)-19(0,19)	20.0337(16)	0	-
24(1,23)-23(1,23)	11.2312(18)	-7	+	18(2,17)-17(2,15)	7.8325(16)	3	+				
24(1,23)-23(1,23)	11.2307(18)	-12	+	19(2,18)-18(2,16)	8.2629(16)	-6	+	8(1, 7)-9(0, 9)	32.0745(16)	-5	-
24(1,24)-23(1,22)	9.4580(18)	-10	+	19(2,18)-18(2,16)	8.2649(16)	14	+	9(1, 8)-10(0,10)	31.6785(16)	2	-
25(1,24)-24(1,24)	11.7256(18)	0	+	20(2,19)-19(2,18)	8.6670(16)	12	+	13(1,12)-14(0,14)	30.1355(16)	3	-
25(1,25)-24(1,23)	9.8079(18)	6	+	20(2,19)-19(2,17)	8.6953(16)	10	+	16(1,15)-17(0,17)	29.0251(16)	-6	-
26(1,25)-25(1,25)	12.2212(18)	5	+	21(2,19)-20(2,18)	9.1060(16)	10	+	17(1,16)-18(0,18)	28.6653(16)	0	-
26(1,26)-25(1,24)	10.1519(18)	3	+	21(2,19)-20(2,19)	9.0891(16)	-1	+	18(1,17)-19(0,19)	28.3098(16)	0	-
27(1,26)-26(1,26)	12.7166(18)	-3	+	23(2,21)-22(2,21)	9.9309(16)	5	+	12(1,12)-12(0,12)	35.8901(16)	-17	-
27(1,26)-26(1,26)	12.7163(18)	-6	+	23(2,22)-22(2,20)	9.9836(16)	-10	+	13(1,13)-13(0,13)	35.9023(16)	-1	-
27(1,26)-26(1,26)	12.7168(18)	-1	+	25(2,24)-24(2,22)	10.8430(16)	-3	+	13(1,13)-13(0,13)	35.9019(16)	-5	-
27(1,27)-26(1,25)	10.4927(18)	5	+	26(2,25)-25(2,23)	11.2722(16)	-2	+	14(1,14)-14(0,14)	35.9143(16)	2	-
27(1,27)-26(1,25)	10.4939(18)	17	+					17(1,17)-17(0,17)	35.9556(16)	2	-
28(1,27)-27(1,27)	13.2139(18)	-2	+	5(3, 2)-4(3, 2)	2.1789(16)	-10	+	19(1,19)-19(0,19)	35.9888(16)	1	-
28(1,27)-27(1,27)	13.2129(18)	-12	+	7(3, 4)-6(3, 4)	3.0514(16)	6	+	21(1,21)-21(0,21)	36.0273(16)	2	-
28(1,27)-27(1,27)	13.2144(18)	3	+	8(3, 6)-7(3, 4)	3.4860(16)	2	+	23(1,23)-23(0,23)	36.0710(16)	0	-
28(1,28)-27(1,26)	10.8291(18)	2	+	9(3, 6)-8(3, 6)	3.9200(16)	-4	+	25(1,25)-25(0,25)	36.1218(16)	9	-
29(1,28)-28(1,28)	13.7126(18)	3	+	10(3, 8)-9(3, 6)	4.3547(16)	0	+	26(1,26)-26(0,26)	36.1482(16)	-2	-
29(1,28)-28(1,28)	13.7112(18)	-10	+	11(3, 8)-10(3, 8)	4.7883(16)	-2	+	27(1,27)-27(0,27)	36.1777(16)	2	-
29(1,28)-28(1,28)	13.7124(18)	1	+	12(3,10)-11(3, 8)	5.2213(16)	-5	+	31(1,31)-31(0,31)	36.3130(16)	-2	-
29(1,29)-28(1,27)	11.1638(18)	19	+	13(3,10)-12(3,10)	5.6545(16)	-2	+				
30(1,29)-29(1,29)	14.2117(18)	4	+	15(3,12)-14(3,12)	6.5182(16)	-3	+	8(1, 7)-7(0, 7)	39.4285(16)	1	-
31(1,30)-30(1,30)	14.7112(18)	2	+					10(1, 9)-9(0, 9)	40.3630(16)	1	-
31(1,30)-30(1,30)	14.7117(18)	7	+	5(0, 5)-3(0, 3)	3.8967(12)	-1	-	13(1,12)-12(0,12)	41.7888(16)	-9	-
31(1,31)-30(1,29)	11.8167(18)	4	+	6(0, 6)-4(0, 4)	4.7607(12)	-12	-	16(1,15)-15(0,15)	43.2454(16)	0	-
32(1,31)-31(1,31)	15.2114(18)	1	+	7(0, 7)-5(0, 5)	5.6262(12)	-2	-	17(1,16)-16(0,16)	43.7368(16)	-1	-
32(1,32)-31(1,30)	12.1367(18)	-10	+	9(0, 9)-7(0, 7)	7.3540(12)	6	-	18(1,17)-17(0,17)	44.2317(16)	2	-
32(1,32)-31(1,30)	12.1382(18)	4	+	9(0, 9)-7(0, 7)	7.3535(12)	1	-	19(1,18)-18(0,18)	44.7290(16)	-1	-
33(1,32)-32(1,32)	15.7126(18)	6	+	10(0,10)-8(0, 8)	8.2153(12)	4	-	20(1,19)-19(0,19)	45.2305(16)	7	-
33(1,32)-32(1,32)	15.7114(18)	-6	+	11(0,11)-9(0, 9)	9.0771(12)	0	-	22(1,21)-21(0,21)	46.2042(16)	3	-
33(1,32)-32(1,32)	15.7129(18)	9	+	12(0,12)-10(0,10)	9.9382(12)	8	-	23(1,22)-22(0,22)	46.7480(16)	-13	-
33(1,33)-32(1,31)	12.4551(18)	-4	+	13(0,13)-11(0,11)	10.7937(12)	-28	-	24(1,23)-23(0,23)	47.2615(16)	-1	-
33(1,33)-32(1,31)	12.4558(18)	3	+	13(0,13)-11(0,11)	10.7964(12)	-1	-	26(1,25)-25(0,25)	48.2964(16)	17	-
34(1,34)-33(1,32)	12.7693(18)	0	+	14(0,14)-12(0,12)	11.6548(12)	3	-	27(1,26)-26(0,26)	48.8154(16)	0	-
34(1,34)-33(1,32)	12.7688(18)	-5	+	14(0,14)-12(0,12)	11.6533(12)	-12	-	28(1,27)-27(0,27)	49.3396(16)	7	-
35(1,34)-34(1,34)	16.7144(18)	1	+	15(0,15)-13(0,13)	12.5107(12)	-3	-	32(1,31)-31(0,31)	51.4597(16)	-4	-
36(1,36)-35(1,34)	13.3843(18)	-14	+	15(0,15)-13(0,13)	12.5103(12)	-7	-	33(1,32)-32(0,32)	51.9963(16)	-7	-
12(1,12)-10(1,10)	9.9607(18)	-4	+	16(0,16)-14(0,14)	13.3660(12)	-2	-	13(1,13)-11(0,11)	46.6982(16)	-8	-
14(1,14)-12(1,12)	11.6831(18)	2	+	17(0,17)-15(0,15)	14.2200(12)	3	-	20(1,20)-18(0,18)	52.7771(16)	-1	-
16(1,16)-14(1,14)	13.4004(18)	9	+	17(0,17)-15(0,15)	14.2195(12)	-2	-	21(1,21)-19(0,19)	53.6440(16)	7	-
17(1,17)-15(1,15)	14.2563(18)	6	+	18(0,18)-16(0,16)	15.0715(12)	-1	-				
19(1,19)-17(1,17)	15.9624(18)	-7	+	18(0,18)-16(0,16)	15.0715(12)	-1	-	6(2, 5)-7(0, 7)	114.5300(16)	-8	-
25(1,25)-23(1,23)	21.0386(18)	-5	+	19(0,19)-17(0,17)	15.9219(12)	2	-	8(2, 7)-9(0, 9)	113.7268(16)	3	-
27(1,26)-25(1,24)	22.8687(18)	2	+	19(0,19)-17(0,17)	15.9219(12)	2	-	10(2, 9)-11(0,11)	112.9397(16)	-1	-
28(1,27)-26(1,25)	23.7068(18)	5	+	20(0,20)-18(0,18)	16.7698(12)	-2	-	12(2,11)-13(0,13)	112.1711(16)	-4	-
28(1,28)-26(1,26)	23.5457(18)	-1	+	21(0,21)-19(0,19)	17.6162(12)	0	-	14(2,13)-15(0,15)	111.4211(16)	-10	-
31(1,31)-29(1,29)	26.0273(18)	-3	+	22(0,22)-20(0,20)	18.4600(12)	-3	-	15(2,14)-16(0,16)	111.0552(16)	3	-
				23(0,23)-21(0,21)	19.3020(12)	-3	-	16(2,15)-17(0,17)	110.6926(16)	0	-

= 3 levels. This splitting, Δ_3 , was determined to be 114 306.35 (53) MHz. The value for this splitting given by von Puttkamer *et al.* is 114 750 (124) MHz. The estimate of Pine *et al.*, $\Delta_3 = 112\,420\,(200)$, obtained by extrapolating high- J P - and R -branch transitions of the perturbed v_1 $K = 2-1$ and $K = 2-3$ subbands to determine the subband origins, is clearly obsolete.

Some interesting trends in the rotational constants in the ground state of (HF) $_2$ have been noted by von Puttkamer *et al.* (4). Figure 3 gives a plot of the observed B

TABLE III—Continued

Quantum Numbers	Com. Diff.	O-C	Sy.	Quantum Numbers	Com. Diff.	O-C	Sy.	Quantum Numbers	Com. Diff.	O-C	Sy.
17(2,16)-18(0,18)	110.3354(16)	0	-	14(2,13)-13(0,13)	123.9326(16)	-6	-	27(1,27)-26(1,25)	10.5286(18)	3	-
18(2,17)-19(0,19)	109.9836(16)	2	-	15(2,14)-14(0,14)	124.4214(16)	4	-	27(1,27)-26(1,25)	10.5286(18)	3	-
19(2,18)-20(0,20)	109.6370(16)	3	-	16(2,15)-15(0,15)	124.9119(16)	-4	-	28(1,27)-27(1,27)	13.1614(18)	0	-
20(2,19)-21(0,21)	109.2957(16)	2	-	16(2,15)-15(0,15)	124.9124(16)	1	-	28(1,28)-27(1,26)	10.8682(18)	6	-
21(2,20)-22(0,22)	108.9597(16)	-1	-	17(2,16)-16(0,16)	125.4070(16)	0	-	28(1,28)-27(1,26)	10.8657(18)	-19	-
22(2,21)-23(0,23)	108.6301(16)	3	-	18(2,17)-17(0,17)	125.9055(16)	4	-	29(1,28)-28(1,28)	13.6558(18)	-9	-
23(2,22)-24(0,24)	107.9868(16)	-3	-	20(2,19)-19(0,19)	126.9119(16)	2	-	29(1,29)-28(1,27)	11.2036(18)	4	-
25(2,24)-26(0,26)	107.6750(16)	2	-	20(2,19)-19(0,19)	126.9119(16)	2	-	30(1,30)-29(1,28)	11.5361(18)	10	-
26(2,25)-27(0,27)	107.3687(16)	1	-	21(2,20)-20(0,20)	127.4199(16)	-2	-	31(1,30)-30(1,30)	14.6489(18)	-6	-
28(2,27)-29(0,29)	106.7751(16)	-2	-	22(2,21)-21(0,21)	127.9321(16)	1	-	32(1,31)-31(1,31)	15.1465(18)	-3	-
29(2,28)-30(0,30)	106.4875(16)	-10	-	25(2,24)-24(0,24)	129.4880(16)	-4	-	19(1,19)-17(1,17)	15.9543(18)	-7	-
30(2,29)-31(0,31)	106.2083(16)	-1	-	26(2,25)-25(0,25)	130.0142(16)	1	-	20(1,20)-18(1,18)	16.8062(18)	5	-
31(2,30)-32(0,32)	105.9355(16)	4	-	28(2,27)-27(0,27)	131.0759(16)	-2	-	21(1,20)-19(1,18)	17.7759(18)	17	-
34(2,33)-35(0,35)	105.1575(16)	-8	-	30(2,29)-29(0,29)	132.1523(16)	1	-	21(1,21)-19(1,19)	17.6531(18)	-15	-
36(2,35)-37(0,37)	104.6775(16)	-3	-	31(2,30)-30(0,30)	132.6963(16)	7	-	22(1,21)-20(1,19)	18.6262(18)	-1	-
37(2,36)-38(0,38)	104.4497(16)	5	-	33(2,32)-32(0,32)	133.7939(16)	7	-	22(1,22)-20(1,20)	18.5012(18)	-2	-
38(2,37)-39(0,39)	104.2283(16)	-4	-	36(2,35)-35(0,35)	135.4673(16)	0	-	23(1,22)-21(1,20)	19.4744(18)	-19	-
				37(2,36)-36(0,36)	136.0339(16)	10	-	23(1,23)-21(1,21)	19.3469(18)	8	-
5(2, 3)-5(0, 5)	117.5376(16)	10	-	38(2,37)-37(0,37)	136.6016(16)	-5	-	24(1,23)-22(1,21)	20.3270(18)	-10	-
6(2, 4)-6(0, 6)	117.5601(16)	1	-					24(1,24)-22(1,22)	20.1880(18)	-7	-
7(2, 5)-7(0, 7)	117.5876(16)	2	-	10(2, 8)-8(0, 8)	125.9089(16)	2	-	25(1,24)-23(1,22)	21.1689(18)	-4	-
8(2, 6)-8(0, 8)	117.6187(16)	1	-	11(2, 9)-9(0, 9)	126.8135(16)	3	-	25(1,25)-23(1,23)	21.0286(18)	-3	-
9(2, 7)-9(0, 9)	117.6536(16)	-3	-	12(2,10)-10(0,10)	127.7217(16)	10	-	26(1,25)-24(1,23)	22.0120(18)	-1	-
10(2, 8)-10(0,10)	117.6936(16)	6	-	14(2,12)-12(0,12)	129.5432(16)	-7	-	27(1,27)-25(1,25)	22.7019(18)	-1	-
11(2, 9)-11(0,11)	117.7363(16)	1	-	15(2,13)-13(0,13)	130.4592(16)	-4	-	28(1,27)-26(1,25)	23.6899(18)	2	-
12(2,10)-12(0,12)	117.7834(16)	1	-	19(2,17)-17(0,17)	134.1470(16)	3	-	28(1,28)-26(1,26)	23.5339(18)	-8	-
13(2,11)-13(0,13)	117.8347(16)	3	-	21(2,19)-19(0,19)	136.0039(16)	5	-				
14(2,12)-14(0,14)	117.8884(16)	-10	-	22(2,20)-20(0,20)	136.9355(16)	9	-	10(2, 9)-9(2, 7)	4.3630(16)	0	-
15(2,13)-15(0,15)	117.9485(16)	-1	-					11(2, 9)-10(2, 8)	4.7966(16)	3	-
15(2,13)-15(0,15)	117.9487(16)	1	-	13(1,12)-12(1,12)	5.8987(18)	8	-	11(2,10)-10(2, 8)	4.7976(16)	-1	-
16(2,14)-16(0,16)	118.0115(16)	-1	-	20(1,19)-19(1,19)	9.2395(18)	-15	-	12(2,11)-11(2, 9)	5.2344(16)	3	-
18(2,16)-18(0,18)	118.1499(16)	0	-	20(1,20)-19(1,18)	8.0503(18)	21	-	13(2,12)-12(2,10)	5.6650(16)	-6	-
19(2,17)-19(0,19)	118.2251(16)	1	-	21(1,20)-20(1,20)	9.7234(18)	-26	-	14(2,13)-13(2,11)	6.0979(16)	-10	-
19(2,17)-19(0,19)	118.2249(16)	-1	-	21(1,20)-20(1,20)	9.7256(18)	-5	-	15(2,13)-14(2,13)	6.5273(16)	9	-
20(2,18)-20(0,20)	118.3035(16)	-6	-	21(1,21)-20(1,19)	8.4136(18)	1	-	16(2,15)-15(2,13)	6.9631(16)	-6	-
20(2,18)-20(0,20)	118.3044(16)	3	-	21(1,21)-20(1,19)	8.4136(18)	1	-	19(2,17)-18(2,17)	8.2415(16)	-1	-
21(2,19)-21(0,21)	118.3872(16)	0	-	22(1,21)-21(1,21)	10.2126(18)	-2	-	20(2,18)-19(2,18)	8.6665(16)	-8	-
21(2,19)-21(0,21)	118.3877(16)	5	-	22(1,22)-21(1,20)	8.7778(18)	25	-	20(2,19)-19(2,17)	8.8070(16)	3	-
22(2,20)-22(0,22)	118.4753(16)	10	-	23(1,23)-22(1,21)	9.1335(18)	1	-	21(2,19)-20(2,19)	9.0920(16)	3	-
22(2,20)-22(0,22)	118.4746(16)	4	-	24(1,23)-23(1,23)	11.1895(18)	-10	-	22(2,20)-21(2,20)	9.5156(16)	12	-
24(2,22)-24(0,24)	118.6602(16)	0	-	24(1,24)-23(1,22)	9.4866(18)	-10	-	23(2,21)-22(2,21)	9.9360(16)	5	-
25(2,23)-25(0,25)	118.7588(16)	-2	-	25(1,24)-24(1,24)	11.6821(18)	5	-	23(2,22)-22(2,20)	9.9746(16)	15	-
26(2,24)-26(0,26)	118.8628(16)	12	-	25(1,24)-24(1,24)	11.6824(18)	8	-	24(2,23)-23(2,21)	10.4014(16)	5	-
				25(1,25)-24(1,23)	9.8376(18)	-7	-	25(2,24)-24(2,22)	10.9746(16)	14	-
6(2, 5)-5(0, 5)	120.1562(16)	-10	-	26(1,25)-25(1,25)	12.1733(18)	-5	-	26(2,25)-25(2,23)	11.2568(16)	17	-
10(2, 9)-9(0, 9)	122.0168(16)	-1	-	26(1,25)-25(1,25)	12.1743(18)	5	-				
10(2, 9)-9(0, 9)	122.0166(16)	-3	-	26(1,26)-25(1,24)	10.1853(18)	1	-	6(2, 5)-4(2, 3)	4.8052(16)	4	-
14(2,13)-13(0,13)	123.9319(16)	-13	-	27(1,26)-26(1,26)	12.6682(18)	10	-	7(2, 5)-5(2, 3)	5.6770(16)	4	-

TABLE IV

Ground State $K = 3-2$ Transitions of (HF)₂^a in cm⁻¹

Transition	Wavenumber ^b	O-C ^c	Transition	Wavenumber	O-C
12(3, 9) (Bu) - 13(2,12) (Ag)	114.678(6)	4	27(3,25) (Bu) - 26(2,24) (Ag)	132.174(6)	0
13(3,11) (Bu) - 14(2,12) (Ag)	114.259(6)	9			
15(3,13) (Bu) - 16(2,14) (Ag)	113.400(6)	0	5(3, 2) (Ag) - 6(2, 5) (Bu)	111.862(6)	0
16(3,13) (Bu) - 17(2,16) (Ag)	112.977(6)	8	6(3, 4) (Ag) - 7(2, 5) (Bu)	111.426(6)	5
17(3,14) (Bu) - 18(2,17) (Ag)	112.545(6)	-1	7(3, 4) (Ag) - 8(2, 7) (Bu)	110.976(6)	-3
17(3,15) (Bu) - 18(2,16) (Ag)	112.557(6)	0	10(3, 8) (Ag) - 11(2, 9) (Bu)	109.660(6)	6
18(3,15) (Bu) - 19(2,18) (Ag)	112.119(6)	-5	11(3, 8) (Ag) - 12(2,11) (Bu)	109.212(6)	2
18(3,16) (Bu) - 19(2,17) (Ag)	112.138(6)	0	16(3,14) (Ag) - 17(2,15) (Bu)	107.007(6)	3
19(3,16) (Bu) - 20(2,19) (Ag)	111.690(6)	-8	4(3, 2) (Ag) - 3(2, 1) (Bu)	116.233(6)	-1
19(3,17) (Bu) - 20(2,18) (Ag)	111.715(6)	-5	5(3, 2) (Ag) - 4(2, 3) (Bu)	116.667(6)	0
23(3,21) (Bu) - 24(2,22) (Ag)	110.078(6)	1	6(3, 4) (Ag) - 5(2, 3) (Bu)	117.106(6)	8
24(3,21) (Bu) - 25(2,24) (Ag)	109.630(6)	1	7(3, 4) (Ag) - 6(2, 5) (Bu)	117.530(6)	1
25(3,23) (Bu) - 26(2,24) (Ag)	109.272(6)	0	8(3, 6) (Ag) - 7(2, 5) (Bu)	117.953(6)	-4
26(3,23) (Bu) - 27(2,26) (Ag)	108.805(6)	-5	9(3, 6) (Ag) - 8(2, 7) (Bu)	118.386(6)	0
14(3,11) (Bu) - 13(2,12) (Ag)	126.451(6)	0	10(3, 8) (Ag) - 9(2, 7) (Bu)	118.814(6)	1
16(3,13) (Bu) - 15(2,14) (Ag)	127.332(6)	5	11(3, 8) (Ag) - 10(2, 9) (Bu)	119.240(6)	1
17(3,15) (Bu) - 16(2,14) (Ag)	127.769(6)	-1	28(3,25) (Ag) - 27(2,26) (Bu)	126.298(6)	-2
18(3,15) (Bu) - 17(2,16) (Ag)	128.208(6)	5	28(3,26) (Ag) - 27(2,25) (Bu)	126.344(6)	-1
19(3,17) (Bu) - 18(2,16) (Ag)	128.646(6)	-3	29(3,25) (Ag) - 28(2,26) (Bu)	126.753(6)	-5
21(3,19) (Bu) - 20(2,18) (Ag)	129.522(6)	-6	29(3,26) (Ag) - 28(2,27) (Bu)	126.703(6)	-2
22(3,19) (Bu) - 21(2,20) (Ag)	129.949(6)	0	30(3,27) (Ag) - 29(2,28) (Bu)	127.109(6)	0
23(3,21) (Bu) - 22(2,20) (Ag)	130.408(6)	0	30(3,28) (Ag) - 29(2,27) (Bu)	127.168(6)	-3
24(3,21) (Bu) - 23(2,22) (Ag)	130.822(6)	2	31(3,28) (Ag) - 30(2,29) (Bu)	127.511(6)	1
25(3,23) (Bu) - 24(2,22) (Ag)	131.287(6)	-3	31(3,29) (Ag) - 30(2,28) (Bu)	127.582(6)	-3
26(3,23) (Bu) - 25(2,24) (Ag)	131.684(6)	-4			

^a From Puttkamer, Quack & Suhm (Ref. 4).^b Numbers in parenthesis are estimated experimental uncertainties.^c (Observed - Calculated) × 10³ cm⁻¹.

TABLE V

Calculated B_u-A_g α -Type Transitions in the Ground State Tunneling-Rotation Spectrum of (HF)₂ in MHz

Transition	Freq.	Unc. ^a	Int. ^b	Transition	Freq.	Unc.	Int.	Transition	Freq.	Unc.	Int.
4(2, 2)–5(2, 3)	5485.12	0.05	1	13(2, 11)–13(2, 12)	59603.26	0.91	3	6(3, 3)–6(3, 4)	115172.92	0.26	20
4(2, 3)–5(2, 4)	5486.50	0.05	2	14(2, 13)–14(2, 12)	59627.03	1.55	3	7(3, 5)–7(3, 4)	115459.31	0.31	17
1(1, 1)–2(1, 2)	5875.95	0.01	1	12(2, 10)–12(2, 11)	59670.44	0.79	2	7(3, 4)–7(3, 5)	115459.31	0.31	10
1(0, 1)–2(0, 2)	6246.84	0.01	2	13(2, 12)–13(2, 11)	59673.62	1.27	2	8(3, 6)–8(3, 5)	115785.12	0.38	9
2(1, 2)–3(1, 3)	7148.64	0.01	1	12(2, 11)–12(2, 10)	59720.88	1.02	3	8(3, 5)–8(3, 6)	115785.12	0.38	15
2(1, 1)–3(1, 2)	7446.07	0.01	3	11(2, 9)–11(2, 10)	59732.44	0.68	4	9(3, 7)–9(3, 6)	116149.78	0.43	13
3(2, 2)–4(2, 3)	7627.53	0.03	1	11(2, 10)–11(2, 9)	59767.74	0.81	2	9(3, 6)–9(3, 7)	116149.78	0.43	8
3(2, 1)–4(2, 2)	7628.18	0.02	2	10(2, 8)–10(2, 9)	59789.28	0.57	2	10(3, 8)–10(3, 7)	116552.65	0.49	7
7(3, 5)–8(3, 6)	10957.41	0.79	4	10(2, 9)–10(2, 8)	59813.27	0.63	4	10(3, 7)–10(3, 8)	116552.65	0.49	12
7(3, 4)–8(3, 5)	10957.41	0.79	2	26(2, 25)–26(2, 24)	59821.81	7.50	1	11(3, 9)–11(3, 8)	116993.04	0.56	10
9(3, 7)–10(3, 8)	14400.58	0.81	7	9(2, 7)–9(2, 8)	59840.96	0.48	5	11(3, 8)–11(3, 9)	116993.04	0.56	6
9(3, 6)–10(3, 7)	14400.58	0.81	4	9(2, 8)–9(2, 7)	59856.69	0.49	3	12(3, 10)–12(3, 9)	117470.20	0.66	5
5(2, 3)–6(2, 4)	18596.22	0.09	11	8(2, 6)–8(2, 7)	59887.46	0.41	3	12(3, 9)–12(3, 10)	117470.20	0.66	9
5(2, 4)–6(2, 5)	18598.79	0.08	6	8(2, 7)–8(2, 6)	59897.35	0.39	6	13(3, 11)–13(3, 10)	117983.33	0.79	8
2(0, 2)–3(0, 3)	19252.43	0.01	7	7(2, 5)–7(2, 6)	59928.80	0.34	7	13(3, 10)–13(3, 11)	117983.33	0.79	5
3(1, 3)–4(1, 4)	20176.03	0.01	13	7(2, 6)–7(2, 5)	59934.68	0.32	4	14(3, 12)–14(3, 11)	118531.61	0.94	4
3(1, 2)–4(1, 3)	20580.35	0.01	7	6(2, 4)–6(2, 5)	59964.97	0.29	5	14(3, 11)–14(3, 12)	118531.61	0.94	8
2(2, 1)–3(2, 2)	20741.93	0.05	4	6(2, 5)–6(2, 4)	59968.23	0.27	8	15(3, 13)–15(3, 12)	119114.16	1.05	7
2(2, 0)–3(2, 1)	20742.18	0.05	2	5(2, 3)–5(2, 4)	59995.97	0.25	10	15(3, 12)–15(3, 13)	119114.16	1.05	4
6(3, 4)–7(3, 5)	23711.37	0.73	5	5(2, 4)–5(2, 3)	59997.62	0.24	6	16(3, 14)–16(3, 13)	119730.09	1.10	4
6(3, 3)–7(3, 4)	23711.37	0.73	8	6(1, 5)–7(1, 6)	60007.65	0.03	67	16(3, 13)–16(3, 14)	119730.09	1.10	6
10(3, 8)–11(3, 9)	27003.15	0.77	9	4(2, 2)–4(2, 3)	60021.81	0.23	7	17(3, 15)–17(3, 14)	120378.46	1.07	6
10(3, 7)–11(3, 8)	27003.15	0.77	16	4(2, 3)–4(2, 2)	60022.53	0.22	12	17(3, 14)–17(3, 15)	120378.46	1.07	3
7(1, 7)–7(1, 6)	30957.26	0.02	1	3(2, 1)–3(2, 2)	60042.48	0.22	16	18(3, 16)–18(3, 15)	121058.36	1.13	5
5(1, 5)–5(1, 4)	30379.95	0.01	1	3(2, 2)–3(2, 1)	60042.74	0.21	9	18(3, 15)–18(3, 16)	121058.36	1.13	5
4(1, 4)–4(1, 3)	30889.72	0.01	1	2(2, 0)–2(2, 1)	60057.98	0.21	14	19(3, 17)–19(3, 16)	121768.82	1.76	5
3(1, 3)–3(1, 2)	31297.97	0.01	3	2(2, 1)–2(2, 0)	60058.04	0.21	23	19(3, 16)–19(3, 17)	121768.82	1.76	3
2(1, 2)–2(1, 1)	31604.40	0.01	2	3(3, 1)–4(3, 2)	62263.28	0.53	7	20(3, 18)–20(3, 17)	122508.91	3.24	2
6(2, 4)–7(2, 5)	31703.55	0.12	13	3(3, 0)–4(3, 1)	62263.28	0.53	4	20(3, 17)–20(3, 18)	122508.91	3.24	4
6(2, 5)–7(2, 6)	31707.96	0.11	22	13(3, 11)–14(3, 12)	64497.24	0.48	46	7(1, 7)–6(1, 6)	122739.78	0.03	141
1(1, 1)–1(1, 0)	31808.80	0.01	8	13(3, 10)–14(3, 11)	64497.24	0.48	28	13(2, 12)–14(2, 13)	123267.08	0.28	96
1(1, 0)–1(1, 1)	31995.18	0.01	5	3(1, 3)–2(1, 2)	70907.46	0.01	32	13(2, 11)–14(2, 12)	123267.08	0.28	96
2(1, 1)–2(1, 2)	32163.41	0.01	4	9(2, 7)–10(2, 8)	70987.04	0.19	72	8(0, 8)–7(0, 7)	123276.14	0.18	115
3(0, 3)–4(0, 4)	32261.80	0.02	26	9(2, 8)–10(2, 9)	71002.85	0.16	43	21(3, 19)–21(3, 18)	123277.70	5.68	4
3(1, 2)–3(1, 3)	32415.65	0.01	1	3(1, 2)–2(1, 1)	71168.69	0.02	19	21(3, 18)–21(3, 19)	123277.70	5.68	2
1(0, 1)–1(0, 0)	32732.32	0.04	6	6(0, 6)–7(0, 7)	71297.12	0.06	58	7(1, 6)–6(1, 5)	123291.01	0.03	84
4(1, 3)–4(1, 4)	32751.77	0.01	2	4(0, 4)–3(0, 3)	71624.02	0.09	35	10(0, 10)–11(0, 11)	123302.24	0.14	146
5(1, 4)–5(1, 5)	33171.58	0.01	1	7(1, 7)–8(1, 8)	72284.82	0.04	92	22(3, 20)–22(3, 19)	124074.27	9.27	2
4(1, 4)–5(1, 5)	33204.80	0.01	16	7(1, 6)–8(1, 7)	73153.03	0.04	56	22(3, 19)–22(3, 20)	124074.27	9.27	3
6(1, 5)–6(1, 6)	33674.87	0.01	1	14(3, 12)–15(3, 13)	76888.70	0.43	35	11(1, 11)–12(1, 12)	124321.51	0.12	219
4(1, 3)–5(1, 4)	33719.74	0.01	27	14(3, 11)–15(3, 12)	76888.70	0.43	58	23(3, 21)–23(3, 20)	124897.73	14.27	3
8(1, 7)–8(1, 8)	34930.78	0.02	1	4(1, 4)–3(1, 3)	83885.73	0.02	32	23(3, 20)–23(3, 21)	124897.73	14.27	2
5(3, 3)–6(3, 4)	36514.25	0.65	10	10(2, 8)–11(2, 9)	84063.18	0.20	55	5(2, 3)–4(2, 2)	125503.70	0.49	61
5(3, 2)–6(3, 3)	36514.25	0.65	6	10(2, 9)–11(2, 10)	84085.60	0.18	92	5(2, 4)–4(2, 3)	125503.70	0.49	36
10(1, 9)–10(1, 10)	36516.85	0.04	1	4(1, 3)–3(1, 2)	84225.77	0.02	54	11(1, 10)–12(1, 11)	125706.40	0.11	134
11(3, 9)–12(3, 10)	39553.87	0.69	25	7(0, 7)–8(0, 8)	84306.10	0.08	129	24(3, 22)–24(3, 21)	125747.23	21.03	2
11(3, 8)–12(3, 9)	39553.87	0.69	15	5(0, 5)–4(0, 4)	84561.71	0.11	85	24(3, 21)–24(3, 22)	125747.23	21.03	3
7(2, 5)–8(2, 6)	44805.55	0.15	37	8(1, 8)–9(1, 9)	85304.49	0.05	72	18(3, 16)–19(3, 17)	125906.25	1.07	63
7(2, 6)–8(2, 7)	44812.63	0.13	22	8(1, 7)–9(1, 8)	86297.24	0.05	122	18(3, 15)–19(3, 16)	125906.25	1.07	105
4(0, 4)–5(0, 5)	45273.40	0.03	27	15(3, 13)–16(3, 14)	89225.90	0.41	70	25(3, 23)–25(3, 22)	126621.98	29.94	3
2(0, 2)–1(0, 1)	45707.89	0.05	1	15(3, 12)–16(3, 13)	89225.90	0.41	42	25(3, 22)–25(3, 23)	126621.98	29.94	1
5(1, 5)–6(1, 6)	46233.49	0.02	45	5(1, 5)–4(1, 4)	96851.45	0.02	79	26(3, 24)–26(3, 23)	127521.22	41.46	1
5(1, 4)–6(1, 5)	46862.69	0.02	27	11(2, 9)–12(2, 10)	97127.27	0.20	114	26(3, 23)–26(3, 24)	127521.22	41.46	2
4(3, 2)–5(3, 3)	49365.20	0.58	6	11(2, 10)–12(2, 11)	97158.18	0.20	68	27(3, 25)–27(3, 24)	128444.29	56.10	2
4(3, 1)–5(3, 2)	49365.20	0.58	10	5(1, 4)–4(1, 3)	97266.10	0.02	48	27(3, 24)–27(3, 25)	128444.29	56.10	1
12(3, 10)–13(3, 11)	52052.10	0.58	21	8(0, 8)–9(0, 9)	97311.03	0.09	99	28(3, 26)–28(3, 25)	129390.60	74.46	1
12(3, 9)–13(3, 10)	52052.10	0.58	35	6(0, 6)–5(0, 5)	97483.90	0.13	70	28(3, 25)–28(3, 26)	129390.60	74.46	2
8(2, 6)–9(2, 7)	57900.60	0.17	32	9(1, 9)–10(1, 10)	98318.18	0.07	151	29(3, 27)–29(3, 26)	130359.65	97.20	2
8(2, 7)–9(2, 8)	57911.39	0.15	53	3(2, 1)–2(2, 0)	99358.39	0.38	19	29(3, 26)–29(3, 27)	130359.65	97.20	1
2(1, 2)–1(1, 1)	57918.00	0.01	9	3(2, 2)–2(2, 1)	99358.49	0.38	11	8(1, 8)–7(1, 7)	136559.67	0.04	105
2(1, 1)–1(1, 0)	58096.27	0.01	15	9(1, 8)–10(1, 9)	99438.64	0.07	92	9(0, 9)–8(0, 8)	136143.36	0.21	236
5(0, 5)–6(0, 6)	58285.69	0.04	69	16(3, 14)–17(3, 15)	101508.28	0.43	49	14(2, 12)–15(2, 13)	136228.90	0.37	111
25(2, 23)–25(2, 24)	58394.13	3.17	1	16(3, 13)–17(3, 14)	101508.28	0.43	82	8(1, 7)–7(1, 6)	136272.86	0.04	177
23(2, 21)–23(2, 22)	58647.33	2.70	1	6(1, 6)–5(1, 5)	109803.25	0.02	65	11(0, 11)–12(0, 12)	136285.21	0.17	287
3(0, 3)–2(0, 2)	58672.27	0.07	36	12(2, 10)–13(2, 11)	110177.51	0.23	82	14(2, 13)–15(2, 14)	136300.42	0.35	185
21(2, 19)–21(2, 20)	58879.85	2.26	1	12(2, 11)–13(2, 12)	110219.17	0.23	136	12(1, 12)–13(1, 13)	137308.07	0.14	153
20(2, 18)–20(2, 19)	58988.36	2.06	1	6(1, 5)–5(1, 4)	110288.31	0.02	108	19(3, 17)–20(3, 18)	138020.65	2.11	118
19(2, 17)–19(2, 18)	59091.71	1.86	1	9(0, 9)–10(0, 10)	110310.29	0.12	203	19(3, 16)–20(3, 17)	138020.65	2.11	70
18(2, 16)–18(2, 17)	59189.89	1.68	1	7(0, 7)–6(0, 6)	110389.18	0.16	152	6(2, 4)–5(2, 3)	138558.12	0.55	50
6(1, 6)–7(1, 7)	59260.65	0.03	40	10(1, 10)–11(1, 11)	111324.36	0.09	111	6(2, 5)–5(2, 4)	138559.12	0.54	85
17(2, 15)–17(2, 16)	59282.90	1.50	2	4(2, 2)–3(2, 1)	112436.44	0.44	23	12(1, 11)–13(1, 12)	138829.39	0.14	259
16(2, 14)–16(2, 15)	59370.74	1.34	1	4(2, 3)–3(2, 2)	112436.44	0.44	39	9(1, 9)–8(1, 8)	148561.58	0.06	214
20(2, 19)–20(2, 18)	59446.67	3.22	1	10(1, 9)–11(1, 10)	112575.59	0.09	187	10(0, 10)–9(0, 9)	148989.45	0.23	168
15(2, 13)–15(2, 14)	59653.41	1.19	2	17(3, 15)–18(3, 16)	113735.26	0.56	94	15(2, 13)–16(2, 14)	149226.11	0.51	209
19(2, 18)–19(2, 17)	59655.29	3.01	1	17(3, 14)–18(3, 15)	113735.26	0.56	56	9(1, 8)–8(1, 7)	149232.49	0.06	128
18(2, 17)–18(2, 16)	59675.50	2.76	2	3(3, 1)–3(3, 0)	114555.08	0.37	40	12(0, 12)–13(0, 13)	149257.54	0.19	200
22(2, 21)–22(2, 20)	59675.50	2.76	3	3(3, 0)–3(3, 1)	114555.08	0.37	24	15(2, 14)–16(2, 15)	149271.66	0.44	126
17(2, 16)–17(2, 15)	59504.82	2.47	1	4(3, 2)–4(3, 1)	114720.39	0.29	18	20(3, 18)–21(3,			

TABLE V—Continued

Transition	Freq.	Unc.	Int.	Transition	Freq.	Unc.	Int.	Transition	Freq.	Unc.	Int.
13(1,12)–14(1,13)	151942.82	0.17	178	13(2,11)–12(2,10)	229489.08	0.84	293	22(1,22)–21(1,21)	314029.99	0.59	446
10(1,10)–9(1,9)	161444.14	0.08	152	19(1,18)–20(1,19)	230322.90	0.46	310	15(3,13)–14(3,12)	314534.47	1.88	246
11(0,11)–10(0,10)	161813.01	0.26	328	27(3,25)–28(3,26)	232809.73	57.35	187	15(3,12)–14(3,11)	314534.47	1.88	148
21(3,19)–22(3,20)	162077.05	6.40	140	27(3,24)–28(3,25)	232809.73	57.35	112	22(1,21)–21(1,20)	315083.77	0.59	745
21(3,18)–22(3,19)	162077.05	6.40	83	9(3,7)–8(3,6)	233681.73	0.98	118	28(2,26)–29(2,27)	315276.82	3.00	259
10(1,9)–9(1,8)	162168.58	0.08	256	9(3,6)–8(3,5)	233681.73	0.98	70	25(0,25)–26(0,26)	316117.59	0.69	820
16(2,14)–17(2,15)	162201.56	0.69	140	17(0,17)–16(0,16)	238202.91	0.40	638	28(2,27)–29(2,28)	316336.55	1.75	635
13(0,13)–14(0,14)	162217.50	0.22	379	16(1,16)–15(1,15)	238257.48	0.31	310	26(1,26)–27(1,27)	317099.04	0.75	407
16(2,15)–17(2,16)	162317.27	0.53	233	16(1,15)–15(1,14)	239216.29	0.32	518	20(2,19)–19(2,18)	319240.49	1.02	503
14(1,14)–15(1,15)	163243.17	0.22	199	22(2,20)–23(2,21)	239466.46	2.20	217	20(2,18)–19(2,17)	319295.66	1.35	301
8(2,6)–7(2,5)	164627.00	0.64	82	19(0,19)–20(0,20)	239619.01	0.48	642	26(1,25)–27(1,26)	320715.34	0.68	685
8(2,7)–7(2,6)	164627.06	0.62	137	22(2,21)–23(2,22)	239854.17	1.18	363	24(0,24)–23(0,23)	325830.14	0.68	547
14(1,13)–15(1,14)	165044.95	0.21	335	20(1,20)–21(1,21)	240627.97	0.51	326	23(1,23)–22(1,22)	326536.20	0.63	772
4(3,2)–3(3,1)	167012.19	0.69	11	14(2,13)–13(2,12)	242388.09	0.75	326	23(1,22)–22(1,21)	327593.59	0.62	465
4(3,1)–3(3,0)	167012.19	0.69	19	14(2,12)–13(2,11)	242397.86	0.89	195	29(2,27)–30(2,28)	327715.99	4.26	637
22(3,20)–23(3,21)	174017.64	10.09	89	20(1,19)–21(1,20)	243318.97	0.52	550	16(3,14)–15(3,13)	328070.15	2.01	159
22(3,19)–23(3,20)	174017.64	10.09	150	28(3,26)–29(3,27)	244378.44	75.80	115	16(3,13)–15(3,12)	328070.15	2.01	266
11(1,11)–10(1,10)	174306.02	0.11	296	28(3,25)–29(3,26)	244378.44	75.80	190	26(0,26)–27(0,27)	328750.05	0.71	503
12(0,12)–11(0,11)	174612.64	0.28	226	10(3,8)–9(3,7)	247103.02	1.05	83	29(2,28)–30(2,29)	328954.84	1.78	263
11(1,10)–10(1,9)	175057.78	0.11	149	10(3,7)–9(3,6)	247103.02	1.05	159	17(1,17)–16(1,16)	329773.61	0.80	689
17(2,15)–18(2,16)	175153.06	0.90	25	18(0,18)–19(0,19)	250829.57	0.43	409	21(2,20)–20(2,19)	331938.74	0.88	116
14(0,14)–15(0,15)	175163.36	0.26	254	17(1,17)–16(1,16)	250966.61	0.36	560	21(2,19)–20(2,18)	332008.04	1.52	527
17(2,16)–18(2,17)	175297.66	0.64	155	17(1,16)–16(1,15)	251950.50	0.37	337	27(1,26)–28(1,27)	332499.08	0.69	418
15(1,15)–16(1,16)	176188.52	0.26	370	23(2,21)–24(2,22)	252221.36	2.40	379	25(0,25)–24(0,24)	338190.05	0.71	939
9(2,8)–8(2,7)	177636.98	0.65	100	20(0,20)–21(0,21)	252442.58	0.53	407	24(1,24)–23(1,23)	339003.52	0.67	477
9(2,7)–8(2,6)	177637.37	0.68	166	23(2,22)–24(2,23)	252684.57	1.28	228	24(1,23)–23(1,22)	340067.34	0.65	800
15(1,14)–16(1,15)	178133.99	0.26	224	21(1,21)–22(1,22)	253446.68	0.56	573	30(2,28)–31(2,29)	340081.00	6.35	263
5(3,3)–4(3,2)	180281.66	0.75	38	15(2,14)–14(2,13)	255268.43	0.78	215	27(0,27)–28(0,28)	341343.55	0.75	851
5(3,2)–4(3,1)	180281.66	0.75	23	15(2,13)–14(2,12)	255282.34	0.95	358	30(2,29)–31(2,30)	341531.88	1.80	441
23(3,21)–24(3,22)	185898.76	15.19	158	29(3,27)–30(3,28)	255880.84	98.63	194	17(3,15)–16(3,14)	341616.83	2.04	287
23(3,20)–24(3,21)	185898.76	15.19	95	29(3,26)–30(3,27)	255880.84	98.63	116	17(3,14)–16(3,13)	341616.83	2.04	172
12(1,12)–11(1,11)	187145.84	0.14	203	21(1,20)–22(1,21)	256290.73	0.56	347	28(1,28)–29(1,29)	342320.57	0.91	418
13(0,13)–12(0,12)	187386.94	0.30	430	11(3,9)–10(3,8)	260548.85	1.16	159	22(2,21)–21(2,20)	344601.52	1.14	548
12(1,11)–11(1,10)	187964.77	0.14	340	11(3,8)–10(3,7)	260548.85	1.16	96	21(2,20)–20(2,19)	344687.69	1.83	330
18(2,16)–19(2,17)	188078.31	1.14	168	19(0,19)–18(0,18)	263422.47	0.47	726	28(1,27)–29(1,28)	346244.18	0.74	705
15(0,15)–16(0,16)	188093.38	0.29	469	18(1,18)–17(1,17)	263645.48	0.41	361	26(0,26)–25(0,25)	350505.94	0.76	575
18(2,17)–19(2,18)	188257.23	0.75	282	18(1,17)–17(1,16)	264650.61	0.42	602	25(1,25)–24(1,24)	351430.44	0.74	819
16(1,16)–17(1,17)	189116.91	0.31	244	24(2,22)–25(2,23)	264933.21	2.52	237	31(2,29)–32(2,30)	352384.42	0.91	439
10(2,9)–9(2,8)	190628.93	0.68	197	21(0,21)–22(0,22)	265239.25	0.57	714	25(1,24)–24(1,23)	352485.64	0.70	493
10(2,8)–9(2,7)	190630.11	0.71	119	24(2,23)–25(2,24)	265483.96	1.39	395	28(0,28)–29(0,29)	353895.97	0.86	515
16(1,15)–17(1,16)	191208.15	0.31	411	21(2,22)–22(2,23)	266238.33	0.61	360	31(2,30)–32(2,31)	354066.12	1.95	264
6(3,4)–5(3,3)	193585.13	0.81	34	16(2,15)–15(2,14)	268122.07	0.81	389	29(1,29)–30(1,30)	354872.68	1.10	703
6(3,3)–5(3,2)	193585.13	0.81	57	16(2,14)–15(2,13)	268141.22	1.02	233	18(3,16)–17(3,15)	355172.08	2.03	182
24(3,22)–25(3,23)	197719.55	22.03	100	12(1,12)–11(1,11)	269236.24	0.61	606	18(3,15)–17(3,14)	355172.08	2.03	305
24(3,21)–25(3,22)	197719.55	22.03	166	12(3,10)–11(3,9)	274817.11	1.30	108	23(2,22)–22(2,21)	357227.31	1.23	340
13(1,13)–12(1,12)	199062.27	0.17	384	12(3,9)–11(3,8)	274817.11	1.30	181	23(2,21)–22(2,20)	357333.63	2.36	569
14(0,14)–13(0,13)	200134.52	0.32	289	18(0,18)–19(0,19)	275980.18	0.51	462	29(1,28)–30(1,29)	358948.49	0.86	426
31(1,31)–32(1,32)	200822.18	1.28	231	19(1,19)–18(1,18)	276292.67	0.47	639	27(0,27)–26(0,26)	362776.26	0.83	977
19(2,17)–20(2,18)	200974.90	1.41	303	19(1,18)–18(1,17)	277315.32	0.47	386	26(1,26)–25(1,25)	363815.45	0.85	501
16(0,16)–17(0,17)	201005.77	0.34	308	25(2,23)–26(2,24)	277598.53	2.55	407	32(2,30)–33(2,31)	364602.39	14.57	263
19(2,18)–20(2,19)	201194.34	0.86	182	27(0,27)–28(0,28)	278007.06	0.61	448	26(1,25)–25(1,24)	364845.13	0.78	838
17(1,17)–18(1,18)	202026.72	0.35	442	25(2,24)–26(2,25)	278250.60	1.49	245	29(0,29)–30(0,30)	366405.17	1.06	865
11(2,10)–10(2,9)	203601.48	0.69	136	31(1,31)–32(1,32)	279001.17	0.65	624	32(2,31)–33(2,32)	366556.13	2.48	439
11(2,9)–10(2,8)	203603.87	0.75	229	17(2,16)–16(2,15)	280947.56	0.86	252	30(1,30)–31(1,31)	367383.17	1.38	423
17(1,16)–18(1,17)	204265.59	0.36	268	17(2,15)–16(2,14)	280973.22	1.09	419	19(3,17)–18(3,16)	368733.43	2.31	324
7(3,5)–6(3,4)	206920.86	0.87	76	23(1,22)–24(1,23)	282153.48	0.64	379	19(3,16)–18(3,15)	368733.43	2.31	194
7(3,4)–6(3,3)	206920.86	0.87	46	13(3,11)–12(3,10)	287505.64	1.49	203	24(2,23)–23(2,22)	369814.63	1.35	586
25(3,23)–26(3,24)	209479.04	31.03	174	13(3,10)–12(3,9)	287505.64	1.49	127	24(2,22)–23(2,21)	369944.93	3.21	351
25(3,22)–26(3,23)	209479.04	31.03	104	21(0,21)–22(0,22)	288501.25	0.55	611	28(0,28)–27(0,27)	374933.46	0.80	595
19(1,14)–18(1,13)	212753.91	0.22	256	20(1,20)–19(1,19)	288906.77	0.51	407	27(1,27)–26(1,26)	376157.00	1.03	851
15(0,15)–14(0,14)	212853.98	0.34	532	20(1,19)–19(1,18)	289943.30	0.52	680	33(2,31)–34(2,32)	376734.56	20.76	433
14(1,13)–13(1,12)	213650.85	0.22	430	26(2,24)–27(2,25)	291213.62	2.52	250	17(1,16)–16(1,15)	377198.40	0.94	512
20(2,18)–21(2,19)	213840.28	1.68	194	23(0,23)–24(0,24)	290744.05	0.65	774	30(0,30)–31(0,31)	378888.99	1.40	519
17(0,17)–18(0,18)	213898.73	0.38	559	26(2,25)–27(2,26)	290982.74	1.60	418	32(2,32)–33(2,33)	379000.59	3.72	261
20(2,19)–21(2,20)	214107.33	0.97	326	14(1,14)–15(1,15)	291733.44	0.68	386	31(1,31)–32(1,32)	379850.13	1.80	703
18(1,18)–19(1,19)	214916.29	0.41	287	18(2,17)–17(2,16)	293743.43	0.91	449	20(3,18)–19(3,17)	382298.39	3.41	203
12(2,11)–11(2,10)	216553.16	0.71	261	18(2,16)–17(2,15)	293777.11	1.16	270	20(3,17)–19(3,16)	382298.39	3.41	340
12(2,10)–11(2,9)	216557.31	0.79	157	24(1,23)–25(1,24)	295040.45	0.67	652	25(2,24)–24(2,23)	382681.93	1.51	360
18(1,17)–19(1,18)	217304.47	0.41	683	22(0,22)–21(0,21)	300984.25	0.59	509	25(2,23)–24(2,22)	382520.80	4.44	601
8(3,6)–7(3,5)	220287.02	0.92	58	14(3,12)–13(3,11)	301012.18	1.70	135	29(0,29)–28(0,28)	387173.97	1.12	1000
8(3,5)–7(3,4)	220287.02	0.92	96	14(3,11)–13(3,10)	301012.18	1.70	224	28(1,28)–27(1,27)	388453.53	1.31	517
26(3,24)–27(3,25)	221176.16	42.63	108	21(1,21)–20(1,20)	301486.36	0.56	712	34(2,32)–35(2,33)	388773.97	28.79	256
26(3,23)–27(3,24)	221176.16	42.63	180	21(1,20)–20(1,19)	302533.23	0.56	428	27(1,27)–26(1,26)	389484.05	1.19	864
15(1,15)–14(1,14)	225519.45	0.26	472	27(2,25)–28(2,26)	302774.48	2.55	426	31(0,31)–32(0,32)	391285.21	1.89	865
16(0,16)–15(0,15)	225543.91	0.37	349	24(0,24)–25(0,25)	303448.24	0.67	479	34(2,33)–35(2,34)	391398.33	5.83	430
15(1,14)–14(1,13)	226449.70	0.27	284	27(2,26)–28(2,27)	303678.62	1.69	256				

TABLE VI

Calculated *b*-Type Transitions in the Ground State Tunneling-Rotation Spectrum of (HF)₂ in cm⁻¹

Transition	Wavenumber	Int	Transition	Wavenumber	Int	Transition	Wavenumber	Int	
52(1,52)Ag - 53(0,53)Bu	15.3589(91) ^a	2 ^b	13(1,13)Bu - 14(0,14)Ag	30.4914	1	34(1,33)Ag - 34(0,34)Bu	37.2669	2	24
51(1,51)Ag - 52(0,52)Bu	15.5942(79)	1	8(1, 8)Ag - 9(0, 9)Bu	30.9098	1	21(1,20)Bu - 21(0,21)Ag	37.3128	1	32
50(1,50)Ag - 51(0,51)Bu	15.8383(68)	2	12(1,12)Bu - 13(0,13)Ag	30.9131	1	9(2, 2)Bu - 10(1,1)Ag	37.3577	1	3
49(1,49)Ag - 50(0,50)Bu	16.0908(59)	1	7(1, 7)Ag - 8(0, 8)Bu	31.3332	1	6(1, 6)Ag - 5(0, 5)Bu	37.3843	1	13
48(1,48)Ag - 49(0,49)Bu	16.3513(51)	3	11(1,11)Bu - 12(0,12)Ag	31.3360	1	22(1,21)Bu - 22(0,22)Ag	37.3925	1	53
47(1,47)Ag - 48(0,48)Bu	16.6197(43)	2	6(1, 6)Ag - 7(0, 7)Bu	31.7579	1	35(1,34)Ag - 35(0,35)Bu	37.4164	3	38
46(1,46)Ag - 47(0,47)Bu	16.8956(37)	4	10(1,10)Bu - 11(0,11)Ag	31.7603	1	23(1,22)Bu - 23(0,23)Ag	37.4760	1	32
45(1,45)Ag - 46(0,46)Bu	17.1788(31)	2	5(1, 5)Ag - 6(0, 6)Bu	32.1841	1	24(1,23)Bu - 24(0,24)Ag	37.5634	1	53
44(1,44)Ag - 45(0,50)Ag	17.3245(68)	3	9(1, 9)Bu - 10(0,10)Ag	32.1858	1	36(1,35)Ag - 36(0,36)Bu	37.5705	4	22
43(1,44)Ag - 45(0,45)Bu	17.4689(26)	4	4(1, 4)Ag - 5(0, 5)Bu	32.6115	1	25(1,24)Bu - 25(0,25)Ag	37.6548	1	31
42(1,48)Ag - 49(0,49)Bu	17.6004(58)	2	8(1, 8)Bu - 9(0, 9)Ag	32.6123	1	37(1,36)Ag - 37(0,37)Bu	37.7293	6	35
41(1,43)Ag - 44(0,44)Bu	17.7658(22)	3	7(1, 7)Bu - 8(0, 8)Ag	33.0399	1	26(1,25)Bu - 26(0,26)Ag	37.7502	1	52
40(1,47)Ag - 48(0,48)Bu	17.8841(50)	3	3(1, 3)Ag - 4(0, 4)Bu	33.0402	1	31(1, 3)Bu - 32(0, 2)Ag	37.7924	1	8
39(1,42)Ag - 43(0,43)Bu	18.0692(18)	5	6(1, 6)Bu - 7(0, 7)Ag	33.4685	1	6(1, 6)Bu - 6(0, 6)Bu	37.8234	1	9
38(1,38)Ag - 39(0,39)Bu	18.1751(43)	2	2(1, 2)Ag - 3(0, 3)Bu	33.4701	1	3(21,26)Bu - 27(0,27)Ag	37.8495	1	30
37(1,41)Ag - 42(0,42)Bu	18.3788(15)	3	5(1, 5)Bu - 6(0, 6)Ag	33.8979	1	38(1,37)Ag - 38(0,38)Bu	37.8928	7	20
36(1,44)Ag - 40(0,40)Bu	18.4733(36)	4	1(1, 1)Ag - 2(0, 2)Bu	33.9011	1	28(1,27)Bu - 28(0,28)Ag	37.9530	1	50
40(1,40)Ag - 41(0,41)Bu	18.6944(12)	6	4(1, 4)Bu - 5(0, 5)Ag	34.3282	1	29(1,28)Bu - 29(0,29)Ag	38.0605	1	29
44(1,44)Bu - 45(0,45)Ag	18.7784(31)	3	3(1, 3)Bu - 4(0, 4)Ag	34.7592	1	39(1,38)Ag - 39(0,39)Bu	38.0611	9	32
39(1,39)Ag - 40(0,40)Bu	19.0158(10)	4	1(1, 0)Ag - 1(0, 1)Bu	34.7705	1	30(1,29)Bu - 30(0,30)Ag	38.1722	1	47
43(1,43)Ag - 44(0,44)Bu	19.0900(26)	5	2(1, 1)Ag - 2(0, 2)Bu	34.7789	1	5(41, 4)Ag - 3(0, 3)Ag	38.2275	1	6
38(1,38)Ag - 39(0,39)Bu	19.3427(8)	7	3(1, 2)Ag - 3(0, 3)Bu	34.7913	1	40(1,39)Ag - 40(0,40)Bu	38.2342	1	18
42(1,42)Ag - 43(0,43)Ag	19.4081(21)	3	4(1, 3)Ag - 4(0, 4)Bu	34.8080	1	8(1, 8)Ag - 7(0, 7)Bu	38.2632	1	17
37(1,37)Ag - 38(0,38)Bu	19.6501(6)	5	5(1, 4)Ag - 5(0, 5)Bu	34.8288	1	31(1,30)Bu - 31(0,31)Ag	38.2880	1	27
41(1,41)Ag - 42(0,42)Ag	19.7322(17)	6	6(1, 5)Ag - 6(0, 6)Bu	34.8537	1	32(1,31)Bu - 32(0,32)Ag	38.4082	1	44
36(1,36)Ag - 37(0,37)Bu	20.0125(5)	9	7(1, 6)Ag - 7(0, 7)Bu	34.8808	1	41(1,40)Ag - 41(0,41)Bu	38.4132	1	28
35(1,35)Ag - 36(0,36)Bu	20.0623(14)	4	8(1, 7)Ag - 8(0, 8)Bu	34.9161	1	33(1,32)Bu - 33(0,33)Ag	38.5326	2	26
35(1,35)Ag - 36(0,36)Bu	20.3549(4)	5	9(1, 8)Ag - 9(0, 9)Bu	34.9536	1	32(41,41)Ag - 42(0,42)Bu	38.5952	1	17
39(1,39)Bu - 40(0,40)Ag	20.3980(12)	7	10(1, 9)Ag - 10(0,10)Bu	34.9952	1	34(1,33)Bu - 34(0,34)Ag	38.6614	3	41
34(1,34)Ag - 35(0,35)Bu	20.7021(3)	10	11(1,10)Ag - 11(0,11)Bu	35.0410	1	5(1, 5)Bu - 4(0, 4)Ag	38.6628	1	12
38(1,38)Bu - 39(0,39)Ag	20.7931(9)	5	12(1,11)Ag - 12(0,12)Bu	35.0910	1	24(91, 9)Ag - 8(0, 8)Bu	38.7037	1	11
33(1,33)Ag - 34(0,34)Bu	21.0538(2)	6	13(1,12)Ag - 13(0,13)Bu	35.1451	1	43(1,42)Ag - 43(0,43)Bu	38.7832	2	25
37(1,37)Bu - 38(0,38)Ag	21.0854(7)	9	2(1, 2)Bu - 3(0, 3)Ag	35.1909	1	35(1,34)Ag - 35(0,35)Ag	38.7947	4	24
32(1,32)Ag - 33(0,33)Bu	21.4100(2)	11	1(1, 1)Ag - 0(0, 0)Bu	35.2005	1	36(1,35)Bu - 36(0,36)Ag	38.9324	5	38
36(1,36)Bu - 37(0,37)Ag	21.4368(6)	5	14(1,13)Ag - 14(0,14)Bu	35.2035	1	44(1,43)Ag - 44(0,44)Bu	38.9763	2	14
31(1,31)Ag - 32(0,32)Bu	21.7704(1)	7	15(1,14)Ag - 15(0,15)Bu	35.2660	1	37(1,36)Bu - 37(0,37)Ag	39.0747	7	22
35(1,35)Bu - 36(0,36)Ag	21.7929(4)	10	16(1,15)Ag - 16(0,16)Bu	35.3328	1	6(1, 6)Bu - 5(0, 5)Ag	39.0984	1	8
30(1,30)Ag - 31(0,31)Bu	22.1349(1)	12	17(1,16)Ag - 17(0,17)Bu	35.4037	1	10(1,10)Ag - 9(0, 9)Bu	39.1449	1	21
35(1,35)Bu - 36(0,36)Ag	22.1536(3)	6	18(1,17)Ag - 18(0,18)Bu	35.4789	1	45(1,44)Ag - 45(0,45)Bu	39.1746	1	24
29(1,29)Ag - 30(0,30)Bu	22.5033(1)	8	19(1,18)Ag - 19(0,19)Bu	35.5583	1	38(1,37)Bu - 38(0,38)Ag	39.2216	1	31
33(1,33)Bu - 34(0,34)Ag	22.5187(1)	11	1(1, 1)Bu - 2(0, 2)Ag	35.6232	1	39(1,38)Bu - 39(0,39)Ag	39.3732	1	19
28(1,28)Ag - 29(0,29)Bu	22.8754(1)	14	2(1, 2)Ag - 1(0, 1)Bu	35.6356	1	46(1,45)Ag - 46(0,46)Bu	39.3781	1	36
32(1,32)Bu - 33(0,33)Ag	22.8880(2)	7	20(1,19)Ag - 20(0,20)Bu	35.6419	1	40(1,39)Bu - 40(0,40)Ag	39.5295	1	31
27(1,27)Ag - 28(0,28)Bu	23.2511(1)	8	21(1,20)Ag - 21(0,21)Bu	35.7298	1	7(1, 7)Bu - 6(0, 6)Ag	39.5343	1	16
31(1,31)Bu - 32(0,32)Ag	23.2614(1)	12	22(1,21)Ag - 22(0,22)Bu	35.8220	1	30(11,11)Ag - 10(0,10)Bu	39.5866	1	13
26(1,26)Ag - 27(0,27)Bu	23.6303(1)	15	23(1,22)Ag - 23(0,23)Bu	35.9184	1	47(1,46)Ag - 47(0,47)Bu	39.5870	2	19
30(1,30)Bu - 31(0,31)Ag	23.6386(1)	8	24(1,23)Ag - 24(0,24)Bu	36.0191	1	41(1,40)Bu - 41(0,41)Ag	39.6908	1	17
25(1,25)Ag - 26(0,26)Bu	24.0128(1)	9	3(1, 3)Ag - 2(0, 2)Bu	36.0715	1	48(1,47)Ag - 48(0,48)Bu	39.8013	1	49
29(1,29)Bu - 30(0,30)Ag	24.0194(1)	14	25(1,24)Ag - 25(0,25)Bu	36.1241	1	42(1,41)Bu - 42(0,42)Ag	39.8569	2	27
24(1,24)Ag - 25(0,25)Bu	24.3985(1)	16	26(1,25)Ag - 26(0,26)Bu	36.2335	1	8(1, 8)Bu - 7(0, 7)Ag	39.9703	1	11
28(1,28)Bu - 29(0,29)Ag	24.4038(1)	8	27(1,26)Ag - 27(0,27)Bu	36.3472	1	49(1,48)Ag - 49(0,49)Bu	40.0212	1	57
23(1,23)Ag - 24(0,24)Bu	24.7872(1)	9	28(1,27)Ag - 28(0,28)Bu	36.4652	1	43(1,42)Bu - 43(0,43)Ag	40.0281	2	15
27(1,27)Bu - 28(0,28)Ag	24.7915(1)	15	1(1, 0)Bu - 2(0, 1)Ag	36.4930	1	12(1,12)Ag - 11(0,11)Bu	40.0290	1	24
22(1,22)Ag - 23(0,23)Bu	25.1789(1)	6	2(1, 1)Bu - 2(0, 2)Ag	36.5001	1	44(1,43)Ag - 44(0,44)Ag	40.2643	1	24
26(1,26)Bu - 27(0,27)Ag	25.1825(1)	9	4(1, 4)Ag - 3(0, 3)Bu	36.5083	1	50(1,49)Ag - 50(0,50)Bu	40.2667	1	66
21(1,21)Ag - 22(0,22)Bu	25.5734(1)	10	3(1, 2)Bu - 3(0, 3)Ag	36.5106	1	45(1,44)Bu - 45(0,45)Ag	40.3858	1	36
25(1,25)Bu - 26(0,26)Ag	25.5764(1)	16	4(1, 3)Bu - 4(0, 4)Ag	36.5247	1	9(1, 9)Bu - 8(0, 8)Ag	40.4066	1	20
20(1,20)Ag - 21(0,21)Bu	25.9706(1)	17	5(1, 4)Bu - 5(0, 5)Ag	36.5423	1	13(1,13)Ag - 12(0,12)Bu	40.4719	1	15
24(1,24)Bu - 25(0,25)Ag	25.9732(1)	10	6(1, 5)Bu - 6(0, 6)Ag	36.5634	1	51(1,50)Ag - 51(0,51)Bu	40.4780	1	77
19(1,19)Ag - 20(0,20)Bu	26.3704(1)	17	29(1,28)Ag - 29(0,29)Bu	36.5877	1	46(1,45)Bu - 46(0,46)Ag	40.5725	2	21
23(1,23)Bu - 24(0,24)Ag	26.3728(1)	17	7(1, 6)Bu - 7(0, 7)Ag	36.5880	1	52(1,51)Ag - 52(0,52)Bu	40.7151	1	88
18(1,18)Ag - 19(0,19)Bu	26.7726(1)	17	8(1, 7)Bu - 8(0, 8)Ag	36.6163	1	47(1,46)Bu - 47(0,47)Ag	40.7646	1	49
22(1,22)Bu - 23(0,23)Ag	26.7750(1)	10	9(1, 8)Bu - 9(0, 9)Ag	36.6480	1	10(1,10)Bu - 9(0, 9)Ag	40.8430	1	13
17(1,17)Ag - 18(0, 8)Bu	27.1772(1)	10	10(1, 9)Bu - 10(0,10)Ag	36.6834	1	14(1,14)Ag - 13(0,13)Bu	40.9153	1	27
21(1,21)Ag - 22(0,22)Ag	27.1797(1)	18	30(1,29)Ag - 30(0,30)Bu	36.7146	1	48(1,47)Bu - 48(0,48)Ag	40.9623	1	58
16(1,16)Ag - 17(0,17)Bu	27.5841(1)	17	11(1,10)Bu - 11(0,11)Ag	36.7223	1	49(1,48)Bu - 49(0,49)Ag	41.1555	1	70
20(1,20)Bu - 21(0,21)Ag	27.5867(1)	11	12(1,11)Bu - 12(0,12)Ag	36.7648	1	11(1,11)Bu - 10(0,10)Ag	41.2795	1	23
15(1,15)Ag - 16(0,16)Bu	27.9932(1)	10	13(1,12)Bu - 13(0,13)Ag	36.8110	1	15(1,15)Ag - 14(0,14)Bu	41.3593	1	17
19(1,19)Bu - 20(0,20)Ag	27.9959(1)	18	31(1,30)Ag - 31(0,31)Bu	36.8459	1	50(1,49)Bu - 50(0,50)Ag	41.3744	1	77
14(1,14)Ag - 15(0,15)Bu	28.4043(1)	16	14(1,13)Bu - 14(0,14)Ag	36.8608	1	51(1,50)Bu - 51(0,51)Ag	41.5892	1	89
18(1,18)Bu - 19(0,19)Ag	28.4072(1)	11	15(1,14)Bu - 15(0,15)Ag	36.9142	1	12(1,12)Bu - 11(0,11)Ag	41.7162	1	15
13(1,13)Ag - 14(0,14)Bu	28.8174(1)	9	1(1, 1)Bu - 0(0, 0)Ag	36.9234	1	16(1,16)Ag - 15(0,15)Bu	41.8038	1	29
17(1,17)Bu - 18(0,18)Ag	28.8206(1)	18	5(1, 5)Ag - 4(0, 4)Bu	36.9459	1	13(1,13)Bu - 12(0,12)Ag	42.1530	1	27
12(1,12)Ag - 13(0,13)Bu	29.2324(1)	15	16(1,15)Bu - 16(0,16)Ag	36.9713	1	17(1,17)Ag - 16(0,16)Bu	42.2488	1	18
16(1,16)Ag - 17(0,17)Bu	29.2357(1)	17	32(1,31)Ag - 32(0,32)Bu	36.9817	1	14(1,14)Bu - 13(0,13)Ag	42.5899	1	17
11(1,11)Ag - 12(0,12)Bu	29.6492(1)	9	17(1,16)Bu - 17(0,17)Ag	37.0321	1	18(1,18)Ag - 17(0,17)Bu	42.6943	1	31
15(1,15)Bu - 16(0,16)Ag	29.6527(1)	18	18(1,17)Bu - 18(0,18)Ag	37.0966	1	15(1,15)Bu - 14(0,14)Ag	43.0268	1	29
10(1,10)Ag - 11(0,11)Bu	30.0678(1)	14	33(1,32)Ag - 33(0,33)Bu	37.1220	1	19(1,19)Ag - 18(0,18)Bu	43.1403	1	19
14(1,14)Bu - 15(0,15)Ag	30.0713(1)	10	19(1,18)Bu - 19(0,19)Ag	37.1649	1	16(1,16)Bu - 15(0,15)Ag	43.4639	1	18
9(1, 9)Ag - 10(0,10)Bu	30.4880(1)	7	20(1,19)Bu - 20(0,20)Ag	37.2369	1	20(1,20)Ag - 19(0,19)Bu	43.5868	1	33

^a Numbers in parenthesis are one standard deviation.^b Relative intensity. Intensity normalized to strongest line = 100.

TABLE VI—Continued

Transition	Wavenumber	Int	Transition	Wavenumber	Int	Transition	Wavenumber	Int
17(1,17)Bu - 16(0,16)Ag	43.9010(1)	32	44(2,43)Bu - 45(1,44)Ag	63.9102(52)	14	15(2,14)Ag - 16(1,15)Bu	72.7233(1)	32
21(1,21)Ag - 20(0,20)Bu	44.0537(1)	20	36(2,35)Ag - 37(1,36)Bu	64.2109(8)	13	16(2,14)Ag - 17(1,17)Bu	72.7510(1)	34
18(1,18)Bu - 17(0,17)Ag	44.3383(1)	19	44(2,42)Bu - 44(1,43)Ag	64.2769(40)	9	24(2,22)Bu - 25(1,25)Ag	72.8338(1)	22
22(1,22)Ag - 21(0,21)Bu	44.4812(1)	34	32(2,34)Ag - 33(1,35)Bu	64.5904(6)	24	15(2,13)Ag - 16(1,16)Bu	73.1269(1)	19
19(1,19)Bu - 18(0,18)Ag	44.7556(1)	33	42(2,41)Bu - 43(1,42)Ag	64.6676(30)	16	21(2,20)Bu - 22(1,21)Ag	73.1378(1)	22
23(1,23)Ag - 22(0,22)Bu	44.9291(1)	20	34(2,33)Ag - 35(1,34)Bu	64.9733(5)	15	14(2,13)Ag - 15(1,14)Bu	73.1492(1)	18
20(1,20)Bu - 19(0,19)Ag	45.2130(1)	20	39(2,37)Ag - 40(1,40)Bu	64.9857(98)	11	23(2,21)Bu - 24(1,24)Ag	73.1878(1)	37
26(1,24)Ag - 23(0,23)Bu	45.3775(1)	34	41(2,40)Bu - 42(1,41)Ag	65.0221(23)	10	14(2,12)Ag - 15(1,15)Bu	73.5065(1)	31
21(1,21)Bu - 20(0,20)Ag	45.6505(1)	35	38(2,36)Ag - 39(1,39)Bu	65.3037(79)	20	22(2,20)Bu - 23(1,23)Ag	73.5451(1)	22
25(1,25)Ag - 24(0,24)Bu	45.8264(1)	20	33(2,32)Ag - 34(1,33)Bu	65.3593(4)	26	20(2,19)Bu - 21(1,20)Ag	73.5657(1)	37
22(1,22)Bu - 21(0,21)Ag	46.0881(1)	21	40(2,39)Bu - 41(1,40)Ag	65.4004(17)	18	13(2,12)Ag - 14(1,13)Bu	73.5763(1)	30
26(1,26)Ag - 25(0,25)Bu	46.2758(1)	34	37(2,35)Ag - 38(1,38)Bu	65.6211(63)	13	13(2,11)Ag - 14(1,14)Bu	73.8898(1)	18
23(1,23)Bu - 22(0,22)Ag	46.5258(1)	35	32(2,31)Ag - 33(1,32)Bu	65.7485(3)	16	21(2,19)Bu - 22(1,22)Ag	73.9060(1)	37
27(1,27)Ag - 26(0,26)Bu	46.7257(1)	20	39(2,38)Bu - 40(1,39)Ag	65.7823(13)	11	19(2,18)Bu - 20(1,19)Ag	73.9948(1)	22
24(1,24)Bu - 23(0,23)Ag	46.9637(1)	21	36(2,34)Ag - 37(1,37)Bu	65.9386(50)	23	12(2,11)Ag - 13(1,12)Bu	74.0045(1)	17
28(1,28)Ag - 27(0,27)Bu	47.1761(1)	32	32(2,30)Ag - 33(1,31)Bu	66.1406(1)	29	20(2,18)Bu - 21(1,21)Ag	74.2703(1)	22
25(1,25)Bu - 24(0,24)Ag	47.4031(1)	35	38(2,37)Bu - 39(1,38)Ag	66.1677(40)	21	12(2,10)Ag - 13(1,13)Bu	74.2770(1)	28
29(1,29)Ag - 28(0,28)Bu	47.6271(1)	19	35(2,33)Ag - 36(1,36)Bu	66.2565(39)	14	18(2,17)Bu - 19(1,18)Ag	74.4251(1)	36
26(1,26)Bu - 25(0,25)Ag	47.8400(1)	21	30(2,29)Ag - 31(1,30)Bu	66.3555(2)	18	11(2,10)Ag - 12(1,11)Bu	74.4338(1)	26
30(1,30)Ag - 29(0,29)Bu	48.0787(1)	32	37(2,36)Bu - 38(1,37)Ag	66.5565(7)	13	19(2,17)Bu - 20(1,20)Ag	74.6382(1)	37
27(1,27)Bu - 26(0,26)Ag	48.2844(1)	35	34(2,32)Ag - 35(1,35)Bu	66.5754(30)	26	11(2,9)Ag - 12(1,12)Bu	74.6680(1)	15
31(1,31)Ag - 30(0,30)Bu	48.5309(1)	19	33(2,31)Ag - 34(1,34)Bu	66.8954(23)	16	17(2,16)Bu - 18(1,17)Ag	74.8565(1)	21
28(1,28)Bu - 27(0,27)Ag	48.7172(1)	20	30(2,28)Ag - 31(1,29)Bu	66.9331(1)	31	10(2,9)Ag - 11(1,10)Bu	74.8641(1)	14
32(1,32)Ag - 31(0,31)Bu	48.9837(1)	31	36(2,35)Bu - 37(1,36)Ag	66.9485(6)	23	18(2,16)Bu - 19(1,19)Ag	75.0095(1)	22
29(1,29)Bu - 28(0,28)Ag	49.1561(1)	34	32(2,30)Ag - 33(1,33)Bu	67.2171(17)	28	10(2,8)Ag - 11(1,11)Bu	75.0626(1)	14
33(1,33)Ag - 32(0,32)Bu	49.4372(1)	18	28(2,27)Ag - 29(1,28)Bu	67.3332(1)	19	16(2,15)Bu - 17(1,16)Ag	75.2888(1)	35
30(1,30)Bu - 29(0,29)Ag	49.5954(1)	20	35(2,34)Bu - 36(1,35)Ag	67.3437(5)	15	9(2,8)Ag - 10(1,9)Bu	75.2953(1)	22
34(1,34)Ag - 33(0,33)Bu	49.8914(2)	29	31(2,29)Ag - 32(1,32)Bu	67.5407(13)	17	17(2,15)Bu - 18(1,18)Ag	75.3844(1)	36
31(1,31)Bu - 30(0,30)Ag	50.0331(1)	32	27(2,26)Ag - 28(1,27)Bu	67.7358(1)	33	9(2,7)Ag - 10(1,10)Bu	75.4611(1)	13
35(1,35)Ag - 34(0,34)Bu	50.3463(3)	17	34(2,33)Bu - 35(1,34)Ag	67.7419(4)	25	15(2,14)Bu - 16(1,17)Ag	75.7221(1)	20
32(1,32)Bu - 31(0,31)Ag	50.5475(1)	29	30(2,28)Ag - 31(1,31)Bu	67.8664(9)	30	8(2,7)Ag - 9(1,8)Bu	75.7228(1)	11
36(1,36)Ag - 35(0,35)Bu	50.8021(4)	27	26(2,25)Ag - 27(1,26)Bu	68.1408(1)	20	16(2,14)Bu - 17(1,17)Ag	75.7628(1)	21
33(1,33)Bu - 32(0,32)Ag	50.9156(2)	31	33(2,32)Bu - 34(1,33)Ag	68.1430(3)	16	8(2,6)Ag - 9(1,9)Bu	75.8632(1)	19
37(1,37)Ag - 36(0,36)Bu	51.2586(6)	15	29(2,27)Ag - 30(1,30)Bu	68.1946(7)	19	15(2,13)Bu - 16(1,16)Ag	76.1447(1)	34
34(1,34)Ag - 33(0,33)Bu	51.3566(3)	18	37(2,35)Bu - 38(1,38)Ag	68.5061(81)	23	14(2,12)Ag - 15(1,14)Bu	76.1562(1)	32
38(1,38)Ag - 37(0,37)Bu	51.7161(7)	25	28(2,26)Ag - 29(1,29)Bu	68.5254(5)	32	7(2,6)Ag - 8(1,7)Bu	76.1601(1)	16
35(1,35)Bu - 34(0,34)Ag	51.7982(4)	29	32(2,31)Bu - 33(1,32)Ag	68.5469(2)	29	7(2,5)Ag - 8(1,8)Bu	76.2690(1)	10
39(1,39)Ag - 38(0,38)Bu	52.1745(9)	14	25(2,24)Ag - 26(1,25)Bu	68.5480(1)	34	14(2,12)Ag - 15(1,15)Bu	76.5302(1)	19
36(1,36)Bu - 35(0,35)Ag	52.2403(6)	16	36(2,34)Bu - 37(1,37)Ag	68.8244(65)	14	13(2,12)Bu - 14(1,13)Ag	76.5910(1)	18
40(1,40)Ag - 39(0,39)Bu	52.6404(11)	23	27(2,25)Ag - 28(1,28)Bu	68.8590(9)	20	6(2,5)Ag - 7(1,6)Bu	76.5936(1)	8
37(1,37)Bu - 36(0,36)Ag	52.6831(7)	27	31(2,30)Bu - 32(1,31)Ag	68.9534(2)	18	6(2,4)Ag - 7(1,7)Bu	76.6784(1)	14
41(1,41)Ag - 40(0,40)Bu	53.0945(14)	13	24(2,23)Ag - 25(1,24)Bu	68.9574(1)	21	13(2,11)Bu - 14(1,14)Ag	76.9191(1)	31
38(1,38)Bu - 37(0,37)Ag	53.1286(9)	15	31(2,33)Bu - 32(1,36)Ag	69.1444(51)	25	12(2,11)Bu - 13(1,12)Ag	77.0264(1)	29
42(1,42)Ag - 41(0,41)Bu	53.5562(17)	20	26(2,24)Ag - 27(1,27)Bu	69.1957(2)	34	5(2,4)Ag - 6(1,5)Bu	77.0278(1)	11
39(1,39)Bu - 38(0,38)Ag	53.5710(11)	24	30(2,29)Bu - 31(1,30)Ag	69.2625(2)	31	5(2,3)Ag - 6(1,6)Bu	77.0915(1)	6
40(1,40)Bu - 39(0,39)Ag	54.0162(14)	14	23(2,22)Ag - 24(1,23)Bu	69.3688(1)	35	12(2,10)Bu - 13(1,13)Ag	77.3114(1)	17
43(1,43)Ag - 42(0,42)Bu	54.0191(21)	11	34(2,32)Bu - 35(1,35)Ag	69.4665(40)	16	11(2,10)Bu - 12(1,11)Ag	77.4624(1)	16
41(1,41)Ag - 40(0,40)Ag	54.4623(17)	22	25(2,23)Ag - 26(1,26)Bu	69.5354(2)	21	4(2,3)Ag - 5(1,4)Bu	77.4626(1)	4
44(1,44)Ag - 43(0,43)Bu	54.4834(25)	18	29(2,28)Bu - 30(1,29)Ag	69.7739(1)	19	4(2,2)Ag - 5(1,5)Bu	77.5081(1)	8
42(1,42)Bu - 41(0,41)Ag	54.9094(21)	12	22(2,21)Ag - 23(1,22)Bu	69.7822(1)	21	11(2,9)Bu - 12(1,12)Ag	77.7072(1)	27
45(1,45)Ag - 44(0,44)Bu	54.9490(30)	10	33(2,31)Bu - 34(1,34)Ag	69.7908(31)	28	3(2,2)Ag - 4(1,3)Bu	77.8979(1)	5
43(1,43)Bu - 42(0,42)Ag	55.3577(25)	20	24(2,22)Ag - 25(1,25)Bu	69.8785(1)	35	10(2,9)Bu - 11(1,10)Ag	77.8988(1)	25
46(1,46)Ag - 45(0,45)Bu	55.4161(35)	16	32(2,30)Bu - 33(1,33)Ag	70.1174(23)	17	3(2,1)Ag - 4(1,4)Bu	77.9283(1)	3
44(1,44)Bu - 43(0,43)Ag	55.8071(30)	11	28(2,27)Bu - 29(1,28)Ag	70.1877(1)	33	10(2,8)Bu - 11(1,11)Ag	78.1064(1)	15
47(1,47)Ag - 46(0,46)Bu	55.8848(41)	9	21(2,20)Ag - 22(1,21)Bu	70.1975(1)	36	2(2,1)Ag - 3(1,2)Bu	78.3337(1)	1
45(1,45)Bu - 44(0,44)Ag	56.2578(36)	17	23(2,21)Ag - 24(1,24)Bu	70.2249(1)	21	9(2,8)Bu - 10(1,9)Ag	78.3357(1)	13
48(1,48)Ag - 47(0,47)Bu	56.3533(48)	15	30(2,32)Bu - 31(1,32)Ag	70.3303(18)	30	9(2,7)Ag - 10(1,10)Bu	78.3526(1)	2
46(1,46)Bu - 45(0,45)Ag	56.7098(42)	10	22(2,20)Ag - 23(1,23)Bu	70.5795(1)	36	9(2,6)Ag - 10(1,10)Ag	78.5000(1)	23
49(1,49)Ag - 48(0,48)Bu	56.8275(56)	7	27(2,26)Bu - 28(1,27)Ag	70.6035(1)	20	8(2,7)Bu - 9(1,8)Ag	78.7729(1)	20
47(1,47)Bu - 46(0,46)Ag	57.1634(49)	15	20(2,19)Ag - 21(1,20)Bu	70.6145(1)	21	8(2,6)Ag - 9(1,9)Bu	78.9149(1)	12
50(1,50)Ag - 49(0,49)Bu	57.3016(65)	12	30(2,28)Bu - 31(1,31)Ag	70.7786(13)	19	7(2,6)Bu - 8(1,7)Ag	79.2104(1)	10
48(1,48)Bu - 47(0,47)Ag	57.6185(58)	8	21(2,19)Ag - 22(1,22)Bu	70.9284(1)	21	7(2,5)Bu - 8(1,8)Ag	79.3241(1)	17
51(1,51)Ag - 50(0,50)Bu	57.7778(75)	6	26(2,25)Bu - 27(1,26)Ag	71.0215(1)	35	39(2,37)Ag - 39(1,38)Bu	79.6287(98)	33
49(1,49)Bu - 48(0,48)Ag	58.0753(67)	13	19(2,18)Ag - 20(1,19)Bu	71.0332(1)	35	2(2,0)Ag - 3(1,1)Bu	79.6443(1)	12
52(1,52)Ag - 51(0,51)Bu	58.2561(87)	10	29(2,27)Bu - 30(1,30)Ag	71.1134(9)	33	3(2,1)Ag - 3(1,2)Bu	79.6451(1)	12
50(1,50)Bu - 49(0,49)Ag	58.5338(77)	7	20(2,18)Ag - 21(1,21)Bu	71.2855(1)	36	4(2,2)Ag - 4(1,3)Bu	79.6463(1)	28
53(1,53)Ag - 52(0,52)Bu	58.7368(99)	5	25(2,24)Bu - 26(1,25)Ag	71.4413(1)	21	5(2,3)Ag - 5(1,4)Bu	79.6477(1)	21
51(1,51)Bu - 50(0,50)Ag	58.9943(89)	11	28(2,26)Bu - 29(1,29)Ag	71.4511(6)	20	6(2,5)Bu - 7(1,6)Ag	79.6480(1)	14
46(2,45)Ag - 47(1,46)Bu	60.6399(92)	6	18(2,17)Ag - 19(1,18)Bu	71.4535(1)	21	6(2,4)Ag - 6(1,5)Bu	79.6493(1)	43
44(2,46)Ag - 45(1,45)Bu	60.9754(73)	12	19(2,17)Ag - 20(1,20)Bu	71.6663(3)	21	7(2,5)Ag - 7(1,6)Bu	79.6513(1)	29
44(2,43)Ag - 45(1,44)Bu	61.3163(58)	8	27(2,25)Bu - 28(1,28)Ag	71.7920(4)	35	38(2,36)Ag - 38(1,37)Bu	79.6531(79)	59
47(2,42)Ag - 44(1,43)Bu	61.6625(46)	14	24(2,23)Bu - 25(1,24)Ag	71.8610(1)	36	2(2,1)Ag - 2(1,2)Bu	79.6534(1)	7
42(2,41)Ag - 43(1,42)Bu	62.0136(36)	9	17(2,16)Ag - 18(1,17)Bu	71.8754(1)	34	8(2,6)Ag - 8(1,7)Bu	79.6535(1)	55
41(2,40)Ag - 42(1,41)Bu	62.3693(28)	16	18(2,16)Ag - 19(1,19)Bu	72.0108(1)	35	9(2,7)Ag - 9(1,8)Bu	79.6560(1)	36
40(2,39)Ag - 41(1,40)Bu	62.7296(22)	10	26(2,24)Bu - 27(1,27)Ag	72.1360(3)	21	10(2,8)Ag - 10(1,9)Bu	79.6588(1)	66
39(2,38)Ag - 40(1,39)Bu	63.0940(17)	19	23(2,22)Bu - 24(1,23)Ag	72.2864(1)	22	11(2,9)Ag - 11(1,10)Bu	79.6618(1)	43
46(2,45)Bu - 47(1,46)Ag	63.1889(87)	11	16(2,15)Ag - 17(1,16)Bu	72.2986(1)	20	3(2,2)Ag - 3(1,3)Bu	79.6634(1)	20
38(2,37)Ag - 39(1,38)Bu	63.4625(13)	12	17(2,15)Ag - 18(1,18)Bu	72.3790(1)	20	12(2,10)Ag - 12(1,11)Bu	79.6652(1)	76
45(2,44)Bu - 46(1,45)Ag	63.5475(68)	7	25(2,23)Bu - 26(1,26)Ag	72.4832(1)	26	13(2,11)Ag - 13(1,12)Bu	79.6687(1)	48
37(2,36)Ag - 38(1,37)Bu	63.8348(10)	21	22(2,21)Bu - 23(1,22)Ag	72.7114(1)	37	14(2,12)Ag - 14(1,13)Bu	79.6725(1)	83

while the difference between the B constants of the A_g and B_u states through the $K = 2$ states is small, with the A_g constant being slightly larger than that of the B_u state, for the $K = 3$ states this difference is quite large and the A_g state B constant is smaller than that of the B_u state. In fact, when the high- J R -branch transitions of the $K = 3$

TABLE VI—Continued

Transition	Wavenumber	Int	Transition	Wavenumber	Int	Transition	Wavenumber	Int
37(2,35)Ag - 37(1,36)Bu	79.6731(63)	37	41(2,40)Ag - 41(1,41)Bu	82.4940(25)	51	30(2,29)Bu - 30(1,30)Ag	84.0735(2)	88
15(2,13)Ag - 15(1,14)Bu	79.6766(1)	52	36(2,34)Bu - 36(1,35)Ag	82.5125(65)	40	10(2, 8)Ag - 9(1, 9)Bu	84.1564(1)	41
4(2, 3)Ag - 4(1, 4)Bu	79.6767(1)	17	35(2,33)Bu - 35(1,34)Ag	82.5301(51)	71	31(2,30)Bu - 31(1,31)Ag	84.1647(2)	51
16(2,14)Ag - 16(1,15)Bu	79.6808(1)	89	34(2,32)Bu - 34(1,33)Ag	82.5499(40)	44	32(2,31)Bu - 32(1,32)Ag	84.2589(2)	82
17(2,15)Ag - 17(1,16)Bu	79.6852(1)	55	33(2,31)Bu - 33(1,32)Ag	82.5601(31)	77	33(2,32)Bu - 33(1,33)Ag	84.3561(3)	47
36(2,34)Ag - 36(1,35)Bu	79.6893(50)	65	32(2,30)Bu - 32(1,31)Ag	82.5729(23)	48	34(2,33)Bu - 34(1,34)Ag	84.4562(3)	76
18(2,16)Ag - 18(1,17)Bu	79.6897(1)	93	31(2,29)Bu - 31(1,30)Ag	82.5844(18)	83	4(2, 3)Bu - 3(1, 2)Ag	84.4579(1)	22
5(2, 4)Ag - 5(1, 5)Bu	79.6933(1)	36	30(2,28)Bu - 30(1,29)Ag	82.5949(13)	52	11(2,10)Ag - 10(1, 9)Bu	84.4587(1)	44
19(2,17)Ag - 19(1,18)Bu	79.6943(1)	56	29(2,27)Bu - 29(1,28)Ag	82.6044(9)	89	4(2, 2)Bu - 3(1, 3)Ag	84.4769(1)	13
20(2,18)Ag - 20(1,19)Bu	79.6990(1)	95	28(2,26)Bu - 28(1,27)Ag	82.6130(6)	54	35(2,34)Bu - 35(1,35)Ag	84.5593(4)	43
35(2,33)Ag - 35(1,34)Bu	79.7022(39)	41	27(2,25)Bu - 27(1,26)Ag	82.6209(4)	91	11(2, 9)Ag - 10(1,10)Bu	84.6238(1)	26
21(2,19)Ag - 21(1,20)Bu	79.7037(1)	57	26(2,24)Bu - 26(1,25)Ag	82.6282(3)	57	36(2,35)Bu - 36(1,36)Ag	84.6563(5)	69
22(2,20)Ag - 22(1,21)Bu	79.7082(1)	96	42(2,41)Ag - 42(1,42)Bu	82.6336(33)	29	37(2,36)Bu - 37(1,37)Ag	84.7742(6)	39
34(2,32)Ag - 34(1,33)Bu	79.7121(30)	72	25(2,23)Bu - 25(1,24)Ag	82.6595(2)	97	38(2,37)Bu - 38(1,38)Ag	84.8660(8)	63
23(2,21)Ag - 23(1,22)Bu	79.7127(1)	57	24(2,22)Bu - 24(1,23)Ag	82.6411(1)	58	5(2, 4)Bu - 4(1, 3)Ag	84.8934(1)	15
6(2, 5)Ag - 6(1, 6)Bu	79.7132(1)	25	23(2,21)Bu - 23(1,22)Ag	82.6469(1)	99	12(2,11)Ag - 11(1,10)Bu	84.8963(1)	28
24(2,22)Ag - 24(1,23)Bu	79.7168(1)	94	22(2,20)Bu - 22(1,21)Ag	82.6523(1)	59	5(2, 3)Bu - 4(1, 4)Ag	84.9251(1)	26
33(2,31)Ag - 33(1,32)Bu	79.7194(23)	45	21(2,19)Bu - 21(1,20)Ag	82.6573(1)	99	39(2,38)Bu - 39(1,39)Ag	85.0007(11)	35
25(2,23)Ag - 25(1,24)Bu	79.7206(2)	56	20(2,18)Bu - 20(1,19)Ag	82.6621(1)	59	12(2,10)Ag - 11(1,11)Bu	85.0940(1)	47
26(2,24)Ag - 26(1,25)Bu	79.7240(2)	92	19(2,17)Bu - 19(1,18)Ag	82.6667(1)	98	40(2,39)Bu - 40(1,40)Ag	85.1182(15)	56
32(2,30)Ag - 32(1,31)Bu	79.7246(17)	78	18(2,16)Bu - 18(1,17)Ag	82.6710(1)	58	41(2,40)Bu - 41(1,41)Ag	85.2385(21)	31
27(2,25)Ag - 27(1,26)Bu	79.7267(3)	54	17(2,15)Bu - 17(1,16)Ag	82.6750(1)	95	6(2, 5)Bu - 5(1, 4)Ag	85.3285(1)	30
31(2,29)Ag - 31(1,30)Bu	79.7278(13)	48	16(2,14)Bu - 16(1,15)Ag	82.6789(1)	55	13(2,12)Ag - 12(1,11)Bu	85.3337(1)	49
28(2,26)Ag - 28(1,27)Bu	79.7286(5)	88	15(2,13)Bu - 15(1,14)Ag	82.6825(1)	90	42(2,41)Bu - 42(1,42)Ag	85.3616(28)	49
30(2,28)Ag - 30(1,29)Bu	79.7293(9)	83	14(2,12)Bu - 14(1,13)Ag	82.6860(1)	52	6(2, 4)Bu - 5(1, 5)Ag	85.3760(1)	18
29(2,27)Ag - 29(1,28)Bu	79.7295(6)	51	13(2,11)Bu - 13(1,12)Ag	82.6892(1)	83	43(2,42)Bu - 43(1,43)Ag	85.4874(38)	28
7(2, 6)Ag - 7(1, 7)Bu	79.7364(1)	49	12(2,10)Bu - 12(1,11)Ag	82.6923(1)	47	13(2,11)Ag - 12(1,12)Bu	85.5667(1)	29
8(2, 7)Ag - 8(1, 8)Bu	79.7366(1)	8	11(2, 9)Bu - 11(1,10)Ag	82.6952(1)	74	44(2,43)Bu - 44(1,44)Ag	85.6158(50)	43
9(2, 8)Ag - 9(1, 9)Bu	79.7392(1)	33	10(2, 8)Bu - 10(1, 9)Ag	82.6978(1)	41	45(2,44)Bu - 45(1,45)Ag	85.7468(66)	24
10(2, 9)Ag - 10(1,10)Bu	79.8261(1)	40	9(2, 7)Bu - 9(1, 8)Ag	82.7003(1)	63	7(2, 6)Bu - 6(1, 5)Ag	85.7630(1)	20
11(2,10)Ag - 11(1,11)Bu	79.8626(1)	71	8(2, 6)Bu - 8(1, 7)Ag	82.7025(1)	134	14(2,13)Ag - 13(1,12)Bu	85.7710(1)	31
12(2,11)Ag - 12(1,12)Bu	79.9024(1)	45	7(2, 5)Bu - 7(1, 6)Ag	82.7045(1)	51	7(2, 5)Bu - 6(1, 6)Ag	85.8294(1)	33
13(2,12)Ag - 13(1,13)Bu	79.9456(1)	80	6(2, 4)Bu - 6(1, 5)Ag	82.7063(1)	26	46(2,45)Bu - 46(1,46)Ag	85.8803(85)	37
14(2,13)Ag - 14(1,14)Bu	79.9921(1)	50	5(2, 3)Bu - 5(1, 4)Ag	82.7073(1)	12	14(2,12)Ag - 13(1,13)Bu	86.0419(1)	51
15(2,14)Ag - 15(1,15)Bu	80.0491(1)	87	4(2, 2)Bu - 4(1, 3)Ag	82.7078(1)	37	8(2, 7)Bu - 7(1, 6)Ag	86.1970(1)	37
5(2, 4)Bu - 6(1, 5)Ag	80.0858(1)	7	3(2, 1)Bu - 3(1, 2)Ag	82.7102(1)	21	15(2,14)Ag - 14(1,13)Bu	86.2080(1)	53
16(2,15)Ag - 16(1,16)Bu	80.0950(1)	54	2(2, 0)Bu - 2(1, 1)Ag	82.7110(1)	7	8(2, 6)Bu - 7(1, 7)Ag	86.2855(1)	22
17(2,16)Ag - 17(1,17)Bu	80.1534(1)	92	2(2, 1)Bu - 2(1, 2)Ag	82.7205(1)	12	15(2,13)Ag - 14(1,14)Bu	86.5195(1)	32
5(2, 3)Bu - 6(1, 4)Ag	80.1523(1)	11	3(2, 2)Bu - 3(1, 3)Ag	82.7292(1)	13	9(2, 8)Bu - 8(1, 7)Ag	86.6305(1)	24
18(2,17)Ag - 18(1,18)Bu	80.2112(1)	56	4(2, 3)Bu - 4(1, 4)Ag	82.7409(1)	29	9(2, 7)Bu - 8(1, 8)Ag	86.6447(1)	33
19(2,18)Ag - 19(1,19)Bu	80.2742(1)	95	5(2, 4)Bu - 5(1, 5)Ag	82.7554(1)	22	16(2,14)Ag - 15(1,13)Bu	86.9994(1)	55
20(2,19)Ag - 20(1,20)Bu	80.3406(1)	57	7(2, 5)Ag - 6(1, 6)Bu	82.7708(1)	19	10(2, 9)Bu - 9(1, 8)Ag	87.0633(1)	13
21(2,20)Ag - 21(1,21)Bu	80.4102(1)	96	6(2, 5)Bu - 6(1, 6)Ag	82.7729(1)	44	17(2,16)Ag - 16(1,15)Bu	87.0812(1)	56
22(2,21)Ag - 22(1,22)Bu	80.4832(1)	58	43(2,42)Ag - 43(1,43)Bu	82.7768(43)	45	10(2, 8)Bu - 9(1, 9)Ag	87.2050(1)	26
2(2, 1)Ag - 1(1, 0)Bu	80.5181(1)	8	7(2, 6)Bu - 7(1, 7)Ag	82.7933(1)	30	17(2,15)Ag - 16(1,16)Bu	87.4815(1)	34
2(2, 0)Bu - 1(1, 1)Ag	80.5212(1)	14	8(2, 7)Bu - 8(1, 8)Ag	82.8166(1)	57	11(2,10)Bu - 10(1, 9)Ag	87.4955(1)	27
4(2, 3)Bu - 5(1, 4)Ag	80.5236(1)	8	9(2, 8)Bu - 9(1, 9)Ag	82.8429(1)	38	18(2,17)Ag - 17(1,16)Bu	87.5173(1)	34
23(2,22)Ag - 23(1,23)Bu	80.5594(1)	96	10(2, 9)Bu - 10(1,10)Ag	82.8720(1)	69	11(2, 9)Bu - 10(1,10)Ag	87.6684(1)	46
4(2, 2)Bu - 5(1, 5)Ag	80.5712(1)	5	11(2,10)Bu - 11(1,11)Ag	82.9041(1)	44	12(2,11)Ag - 11(1,10)Ag	87.9271(1)	48
24(2,23)Ag - 24(1,24)Bu	80.6390(1)	57	44(2,43)Ag - 44(1,44)Bu	82.9237(55)	25	19(2,18)Ag - 18(1,17)Bu	87.9332(1)	58
25(2,24)Ag - 25(1,25)Bu	80.7218(1)	94	12(2,11)Bu - 12(1,12)Ag	82.9391(1)	79	18(2,16)Ag - 17(1,17)Bu	87.9658(1)	58
26(2,25)Ag - 26(1,26)Bu	80.8079(1)	56	13(2,12)Bu - 13(1,13)Ag	82.9770(1)	50	12(2,10)Bu - 11(1,11)Ag	88.1340(1)	29
27(2,26)Ag - 27(1,27)Bu	80.8972(1)	91	14(2,13)Bu - 14(1,14)Ag	83.0179(1)	87	13(2,12)Bu - 12(1,13)Ag	88.3579(1)	30
3(2, 2)Ag - 2(1, 1)Bu	80.9558(1)	18	15(2,14)Bu - 15(1,15)Ag	83.0617(1)	93	20(2,19)Ag - 19(1,18)Bu	88.3887(1)	35
3(2, 2)Bu - 4(1, 3)Ag	80.9615(1)	3	45(2,44)Ag - 45(1,45)Bu	83.0746(70)	39	18(1,18)Bu - 18(1,19)Ag	88.4520(1)	58
3(2, 1)Ag - 2(1, 2)Bu	80.9649(1)	11	16(2,15)Bu - 16(1,16)Ag	83.1085(1)	91	13(2,11)Bu - 12(1,12)Ag	88.6026(1)	51
28(2,27)Ag - 28(1,28)Bu	80.9899(1)	53	8(2, 7)Ag - 7(1, 6)Bu	83.1453(1)	21	14(2,13)Bu - 13(1,12)Ag	88.7881(1)	53
3(2, 1)Bu - 4(1, 4)Ag	80.9932(1)	5	17(2,16)Bu - 17(1,17)Ag	83.1581(1)	57	21(2,20)Ag - 20(1,19)Bu	88.8238(1)	60
29(2,28)Ag - 29(1,29)Bu	81.0858(1)	87	18(2,17)Bu - 18(1,18)Ag	83.2108(1)	97	20(2,18)Ag - 19(1,19)Bu	88.9400(1)	60
30(2,29)Ag - 30(1,30)Bu	81.1849(1)	51	46(2,45)Ag - 46(1,46)Bu	83.2294(89)	22	14(2,12)Bu - 13(1,13)Ag	89.0721(1)	32
31(2,30)Ag - 31(1,31)Bu	81.2874(2)	82	8(2, 6)Ag - 7(1, 7)Bu	83.2298(1)	35	15(2,14)Bu - 14(1,13)Ag	89.2175(1)	33
32(2,31)Ag - 32(1,32)Bu	81.3931(2)	47	19(2,18)Bu - 19(1,19)Ag	83.2664(1)	59	22(2,21)Ag - 21(2,20)Bu	89.2585(1)	36
4(2, 3)Ag - 3(1, 2)Bu	81.3935(1)	13	20(2,19)Bu - 20(1,20)Ag	83.3249(1)	100	21(2,19)Ag - 20(1,20)Bu	89.4298(1)	36
2(2, 1)Bu - 3(1, 2)Ag	81.3993(1)	2	21(2,20)Bu - 21(1,21)Ag	83.3864(1)	60	15(2,13)Bu - 14(1,14)Ag	89.5443(1)	55
4(2, 2)Ag - 3(1, 3)Bu	81.4177(1)	22	22(2,21)Bu - 22(1,22)Ag	83.4508(1)	100	16(2,15)Bu - 15(1,14)Ag	89.6462(1)	57
2(2, 0)Bu - 3(1, 3)Ag	81.4189(1)	1	23(2,22)Bu - 23(1,23)Ag	83.5183(1)	60	23(2,22)Ag - 22(1,21)Bu	89.6928(1)	60
33(2,32)Ag - 33(1,33)Bu	81.5021(3)	76	9(2, 8)Ag - 8(1, 7)Bu	83.5832(1)	38	22(2,20)Ag - 21(2,19)Bu	89.9210(1)	60
34(2,33)Ag - 34(1,34)Bu	81.6143(4)	44	2(2, 1)Bu - 1(1, 0)Ag	83.5855(1)	15	16(2,14)Bu - 15(1,13)Ag	90.0185(1)	34
35(2,34)Ag - 35(1,35)Bu	81.7299(5)	70	24(2,23)Bu - 24(1,24)Ag	83.5887(1)	99	17(2,16)Bu - 16(1,15)Ag	90.0742(1)	35
5(2, 4)Ag - 4(1, 3)Bu	81.8314(1)	25	2(2, 0)Bu - 1(1, 1)Ag	83.5887(1)	9	24(2,23)Ag - 23(2,22)Bu	90.1267(1)	36
36(2,35)Ag - 36(1,36)Bu	81.8488(7)	40	25(2,24)Bu - 25(1,25)Ag	83.6620(1)	58	23(2,21)Ag - 22(2,20)Bu	90.4136(1)	36
5(2, 3)Ag - 4(1, 4)Bu	81.8617(1)	15	9(2, 7)Ag - 8(1, 8)Bu	83.6917(1)	23	17(2,15)Bu - 16(1,16)Ag	90.4946(1)	59
37(2,36)Ag - 37(1,37)Bu	81.9710(9)	64	26(2,25)Bu - 26(1,26)Ag	83.7383(1)	96	18(2,17)Ag - 17(1,16)Ag	90.5014(1)	59
38(2,37)Ag - 38(1,38)Bu	82.0966(11)	36	27(2,26)Bu - 27(1,27)Ag	83.8177(1)	57	25(2,24)Ag - 24(2,23)Bu	90.5601(1)	59
39(2,38)Ag - 39(1,39)Bu	82.2256(15)	57	28(2,27)Bu - 28(1,28)Ag	83.9000(1)	93	24(2,22)Ag - 23(2,21)Bu	90.9074(1)	60
6(2, 5)Ag - 5(1, 4)Bu	82.2693(1)	17	29(2,28)Bu - 29(1,29)Ag	83.9852(1)	54	19(2,18)Bu - 18(1,17)Ag	90.9278(1)	36
6(2, 4)Ag - 5(1, 5)Bu	82.3148(1)	29	10(2, 9)Ag - 9(1, 8)Bu	84.0210(1)	25	18(2,16)Bu - 17(1,17)Ag	90.9726(1)	36
40(2,39)Ag - 40(1,40)Bu	82.3580(19)	32	3(2, 2)Bu - 2(1, 1)Ag	84.0219(1)	11	26(2,25)Ag - 25(1,24)Bu	90.9931(1)	35
37(2,35)Bu - 37(1,36)Ag	82.4929(81)	64	3(2, 1)Bu - 2(1, 2)Ag	84.0314(1)	19	20(2,19)Bu - 19(1,18)Ag	91.3534(1)	61

subband were first observed, the fact that the value of $(B' - B'')$ for this subband was positive led to the suspicion that the series originated in levels other than those of $K = 3$, and it was not until the P - and Q -branch lines of this subband were observed that we considered the line assignment firm. Bunker *et al.* (10) have calculated the

TABLE VI—Continued

Transition	Wavenumber	Int	Transition	Wavenumber	Int	Transition	Wavenumber	Int
25(2,23)Ag - 24(1,24)Bu	91.4022(1)	36	32(3,30)Ag - 33(2,31)Bu	100.1734(48)	26	7(3, 4)Ag - 8(2, 7)Bu	110.9792(11)	11
27(2,26)Ag - 26(1,25)Bu	91.4255(1)	58	37(2,35)Bu - 36(1,36)Ag	100.2097(81)	44	7(3, 5)Ag - 8(2, 6)Bu	110.9794(11)	7
19(2,17)Bu - 18(1,18)Ag	91.4524(1)	61	32(2,31)Bu - 32(2,31)Bu	100.4756(32)	27	20(3,17)Bu - 21(2,18)Ag	111.2858(11)	34
21(2,20)Bu - 20(1,19)Ag	91.7782(1)	37	42(2,41)Bu - 41(1,40)Ag	100.5056(26)	33	20(3,18)Bu - 21(2,19)Ag	111.3055(11)	20
28(2,27)Ag - 27(1,26)Bu	91.8575(1)	34	31(3,29)Ag - 32(2,30)Bu	100.5796(37)	16	6(3, 3)Ag - 7(2, 6)Bu	111.4207(11)	5
26(2,24)Ag - 25(1,25)Bu	91.8977(2)	59	30(3,27)Ag - 31(2,30)Bu	100.9010(25)	17	6(3, 4)Ag - 7(2, 5)Bu	111.4209(11)	9
20(2,18)Bu - 19(1,19)Ag	91.9337(1)	37	43(2,42)Bu - 42(1,41)Ag	100.9113(36)	18	19(3,16)Bu - 20(2,19)Ag	111.7043(11)	20
22(2,21)Bu - 21(1,20)Ag	92.2022(1)	62	30(3,28)Ag - 31(2,29)Bu	100.9898(28)	28	19(3,17)Bu - 20(2,18)Ag	111.7202(11)	34
29(2,28)Ag - 28(1,27)Bu	92.2890(1)	55	44(2,43)Bu - 43(1,42)Ag	101.3160(48)	29	5(3, 2)Ag - 6(2, 5)Bu	111.8618(12)	6
27(2,25)Ag - 26(1,26)Bu	92.3937(3)	35	29(3,26)Ag - 30(2,29)Bu	101.3282(19)	29	5(3, 3)Ag - 6(2, 4)Bu	111.8619(12)	3
23(2,19)Bu - 20(1,20)Ag	92.4166(1)	62	29(3,27)Ag - 30(2,28)Bu	101.4036(21)	17	18(3,15)Bu - 19(2,18)Ag	112.1244(12)	33
23(2,22)Bu - 22(1,21)Ag	92.6254(1)	37	45(2,44)Bu - 44(1,43)Ag	101.7195(64)	16	18(3,16)Bu - 19(2,17)Ag	112.1371(12)	20
30(2,29)Ag - 29(1,28)Bu	92.7199(1)	32	28(3,25)Ag - 29(2,28)Bu	101.7569(15)	18	4(3, 1)Ag - 5(2, 4)Bu	112.3024(12)	2
28(2,26)Ag - 27(1,27)Bu	92.8900(5)	57	28(3,26)Ag - 29(2,27)Bu	101.8207(16)	30	4(3, 2)Ag - 5(2, 3)Bu	112.3025(12)	4
22(2,20)Bu - 21(1,21)Ag	92.9008(1)	37	46(2,45)Bu - 45(1,44)Ag	102.1219(83)	25	17(3,14)Bu - 18(2,17)Ag	112.5460(12)	19
24(2,23)Bu - 23(1,22)Ag	93.0477(1)	61	27(3,24)Ag - 28(2,27)Bu	102.1873(12)	31	17(3,15)Bu - 18(2,16)Ag	112.5561(12)	32
31(2,30)Ag - 30(1,29)Bu	93.1503(2)	53	27(3,25)Ag - 28(2,28)Bu	102.2359(18)	18	3(3, 0)Ag - 4(2, 3)Bu	112.7424(12)	1
29(2,27)Ag - 28(1,28)Bu	93.3862(6)	33	26(3,23)Ag - 27(2,26)Bu	102.6191(11)	19	3(3, 1)Ag - 4(2, 2)Bu	112.7424(12)	1
23(2,21)Bu - 22(1,22)Ag	93.3863(1)	62	26(3,24)Ag - 27(2,25)Bu	102.6640(12)	31	16(3,13)Bu - 17(2,16)Ag	112.9690(12)	31
25(2,24)Bu - 24(1,23)Ag	93.4693(1)	36	25(3,22)Ag - 26(2,25)Bu	103.0523(11)	32	16(3,14)Bu - 17(2,15)Ag	112.9769(12)	18
32(2,31)Ag - 31(1,30)Bu	93.5802(2)	30	25(3,23)Ag - 26(2,24)Bu	103.0896(11)	19	15(3,12)Bu - 16(2,15)Ag	113.3934(11)	18
24(2,22)Bu - 23(1,23)Ag	93.8729(1)	37	24(3,21)Ag - 25(2,24)Bu	103.4868(11)	19	15(3,13)Bu - 16(2,14)Ag	113.3994(11)	30
30(2,28)Ag - 29(1,29)Bu	93.8871(9)	55	25(3,22)Ag - 25(3,22)Ag	103.5177(11)	32	14(3,11)Bu - 15(2,14)Ag	113.8190(11)	28
26(2,25)Bu - 25(1,24)Ag	93.9000(1)	60	23(3,20)Ag - 24(2,23)Bu	103.9225(11)	32	14(3,12)Bu - 15(2,13)Ag	113.8236(11)	17
33(2,32)Ag - 32(1,31)Bu	94.0095(3)	49	23(3,21)Ag - 24(2,22)Bu	103.9479(11)	19	35(3,33)Ag - 35(2,34)Bu	114.1497(87)	39
27(2,26)Bu - 26(1,25)Ag	94.3099(1)	35	22(3,19)Ag - 23(2,22)Bu	104.3593(11)	19	34(3,32)Ag - 34(2,33)Bu	114.1619(69)	69
25(2,23)Bu - 24(1,24)Ag	94.3605(2)	62	23(3,20)Ag - 23(3,20)Ag	104.3801(11)	33	33(3,31)Ag - 33(2,32)Bu	114.1742(54)	43
31(2,29)Ag - 30(1,30)Bu	94.3772(13)	32	21(3,18)Ag - 22(2,21)Bu	104.7972(11)	32	32(3,30)Ag - 32(2,31)Bu	114.1866(42)	75
34(2,33)Ag - 33(1,32)Bu	94.4383(3)	28	21(3,19)Ag - 22(2,20)Bu	104.8140(11)	19	31(3,29)Ag - 31(2,30)Bu	114.1991(32)	46
28(2,27)Bu - 27(1,26)Ag	94.7289(1)	58	20(3,17)Ag - 21(2,20)Bu	105.2359(12)	19	30(3,28)Ag - 30(2,29)Bu	114.2118(25)	80
26(2,24)Bu - 25(1,25)Ag	94.8488(3)	36	20(3,18)Ag - 21(2,19)Bu	105.2495(12)	32	29(3,27)Ag - 29(2,28)Bu	114.2245(19)	49
35(2,34)Ag - 34(1,33)Bu	94.8666(4)	46	19(3,16)Ag - 20(2,19)Bu	105.6755(12)	32	28(3,26)Ag - 28(2,27)Bu	114.2374(15)	85
32(2,30)Ag - 31(1,31)Bu	94.8714(17)	52	19(3,17)Ag - 20(2,18)Bu	105.6863(12)	19	13(3,10)Bu - 14(2,13)Ag	114.2458(11)	16
29(2,28)Ag - 28(1,27)Ag	95.1471(1)	34	34(2,33)Ag - 34(2,33)Ag	106.0171(97)	16	13(3,11)Bu - 14(2,12)Ag	114.2492(11)	26
26(2,25)Ag - 25(1,24)Bu	95.2944(6)	26	18(3,15)Ag - 19(2,18)Bu	106.1158(12)	18	27(3,25)Ag - 27(2,26)Bu	114.2504(12)	52
37(2,35)Bu - 36(1,36)Ag	95.3378(4)	60	18(3,16)Ag - 19(2,17)Bu	106.1244(12)	31	26(3,24)Ag - 26(2,25)Bu	114.2634(11)	88
33(2,31)Ag - 32(1,32)Bu	95.3640(23)	30	32(3,29)Ag - 33(2,32)Ag	106.4093(77)	28	25(3,23)Ag - 25(2,24)Bu	114.2765(11)	54
30(2,29)Bu - 29(1,28)Ag	95.5645(1)	56	17(3,14)Ag - 18(2,17)Bu	106.5568(12)	30	30(3,27)Ag - 30(2,28)Bu	114.2872(26)	48
37(2,36)Ag - 36(1,35)Bu	95.7217(7)	42	17(3,15)Ag - 18(2,16)Bu	106.5635(12)	18	31(3,28)Ag - 31(2,29)Bu	114.2879(34)	78
28(2,26)Bu - 27(1,27)Ag	95.8271(6)	35	33(3,30)Ag - 33(3,30)Ag	106.5785(78)	17	29(3,26)Ag - 29(2,27)Bu	114.2883(20)	83
34(2,32)Ag - 33(1,33)Bu	95.8548(30)	48	31(3,28)Bu - 32(2,31)Ag	106.8039(59)	17	24(3,22)Ag - 24(2,23)Bu	114.2895(11)	91
31(2,30)Bu - 30(1,29)Ag	95.9810(2)	32	31(3,29)Bu - 32(2,30)Ag	106.9488(61)	29	32(3,29)Ag - 32(2,30)Bu	114.2906(45)	45
38(2,37)Ag - 37(1,36)Bu	96.1486(10)	24	16(3,13)Ag - 17(2,16)Bu	106.9982(11)	17	28(3,25)Ag - 28(2,26)Bu	114.2910(15)	51
29(2,27)Bu - 28(1,28)Ag	96.3167(9)	58	17(3,15)Bu - 17(3,15)Bu	107.0034(12)	29	27(3,24)Ag - 27(2,25)Bu	114.2953(13)	87
35(2,33)Ag - 34(1,34)Bu	96.3432(39)	28	30(3,27)Ag - 31(2,30)Bu	107.2009(46)	30	33(3,31)Ag - 33(2,32)Bu	114.2956(58)	72
32(2,31)Ag - 31(1,30)Ag	96.3967(2)	52	30(3,28)Bu - 31(2,29)Ag	107.3245(46)	18	26(3,23)Ag - 26(2,24)Bu	114.3008(11)	53
39(2,38)Ag - 38(1,37)Bu	96.5750(13)	38	15(3,12)Ag - 16(2,15)Bu	107.4401(11)	28	23(3,21)Ag - 23(2,22)Bu	114.3026(11)	55
30(2,28)Bu - 29(1,29)Ag	96.8062(13)	34	15(3,13)Ag - 16(2,14)Bu	107.4441(11)	17	34(3,31)Ag - 34(2,32)Bu	114.3030(74)	41
33(2,32)Bu - 32(1,31)Ag	96.8115(2)	30	29(3,26)Bu - 30(2,29)Ag	107.6001(34)	18	25(3,22)Ag - 25(2,23)Bu	114.3074(11)	90
36(2,34)Ag - 35(1,35)Bu	96.8288(49)	44	29(3,27)Bu - 30(2,28)Ag	107.7052(35)	31	35(3,32)Ag - 35(2,33)Bu	114.3131(94)	66
40(2,39)Ag - 39(1,38)Bu	97.0010(18)	21	15(2,14)Ag - 15(2,14)Ag	107.8823(11)	16	24(3,21)Ag - 24(2,22)Bu	114.3150(11)	54
34(2,33)Bu - 33(1,32)Ag	97.2255(3)	49	14(3,12)Ag - 15(2,13)Bu	107.8853(11)	27	22(3,20)Ag - 22(2,21)Bu	114.3156(11)	92
31(2,29)Bu - 30(1,30)Ag	97.2955(18)	55	28(3,25)Bu - 29(2,28)Ag	108.0015(26)	32	23(3,20)Ag - 23(2,21)Bu	114.3234(11)	92
37(2,35)Ag - 36(1,36)Bu	97.3110(63)	25	28(3,26)Bu - 29(2,27)Ag	108.0905(26)	19	21(3,19)Ag - 21(2,20)Bu	114.3284(11)	55
41(2,40)Ag - 40(1,39)Bu	97.4267(23)	34	14(3,13)Bu - 14(3,13)Bu	108.3248(11)	25	22(3,19)Ag - 22(2,20)Bu	114.3324(11)	55
35(2,34)Bu - 34(1,33)Ag	97.6387(3)	28	14(3,12)Bu - 14(3,12)Bu	108.3270(11)	15	20(3,18)Ag - 20(2,19)Bu	114.3412(11)	92
32(2,30)Bu - 31(1,31)Ag	97.7842(13)	32	27(3,24)Bu - 28(2,27)Ag	108.4802(19)	27	21(3,18)Ag - 21(2,19)Bu	114.3420(11)	92
37(2,36)Ag - 36(1,37)Bu	97.8877(78)	40	28(3,25)Bu - 29(2,28)Ag	108.4802(19)	32	20(3,17)Ag - 20(2,18)Bu	114.3453(13)	55
42(2,41)Ag - 41(1,40)Bu	97.8522(31)	19	12(3, 9)Ag - 13(2,12)Bu	108.7674(11)	14	19(3,17)Ag - 19(2,18)Bu	114.3537(12)	54
36(2,35)Bu - 35(1,34)Ag	98.0509(4)	45	13(2,11)Bu - 13(2,11)Bu	108.7690(11)	23	19(3,16)Ag - 19(2,17)Bu	114.3622(12)	91
29(3,27)Ag - 38(1,38)Bu	98.2628(97)	23	26(3,23)Bu - 27(2,26)Ag	108.8109(15)	33	18(3,16)Ag - 18(2,17)Bu	114.3660(12)	89
33(2,31)Bu - 32(1,32)Ag	98.2721(31)	51	26(3,24)Bu - 27(2,25)Ag	108.8739(15)	20	18(3,15)Ag - 18(2,16)Bu	114.3727(12)	53
43(2,42)Ag - 42(1,41)Bu	98.2775(40)	30	11(3, 8)Ag - 12(2,11)Bu	109.2100(11)	21	17(3,15)Ag - 17(2,16)Bu	114.3780(12)	52
37(2,36)Bu - 36(1,35)Ag	98.4623(5)	26	11(3, 9)Ag - 12(2,10)Bu	109.2112(11)	12	17(3,14)Ag - 17(2,15)Bu	114.3831(12)	88
44(2,43)Ag - 43(1,42)Bu	98.7028(52)	17	25(3,22)Bu - 26(2,25)Ag	109.2187(12)	20	16(3,14)Ag - 16(2,15)Bu	114.3896(11)	85
34(2,32)Bu - 33(1,33)Ag	98.7590(40)	30	25(3,23)Bu - 26(2,24)Ag	109.2714(12)	34	16(3,13)Ag - 16(2,14)Bu	114.3936(11)	51
35(3,32)Ag - 36(2,35)Bu	98.7923(87)	23	24(3,21)Bu - 25(2,24)Ag	109.6284(11)	34	15(3,13)Ag - 15(2,14)Bu	114.4009(11)	49
38(2,37)Bu - 37(1,36)Ag	98.8729(7)	41	10(3, 7)Ag - 11(2,10)Bu	109.6526(11)	11	15(3,12)Ag - 15(2,13)Bu	114.4038(11)	83
45(2,44)Ag - 44(1,43)Bu	99.1280(67)	26	10(3, 8)Ag - 11(2, 9)Bu	109.6534(11)	19	14(3,12)Ag - 14(2,13)Bu	114.4117(11)	80
34(3,31)Ag - 35(2,34)Bu	99.2102(69)	14	24(3,22)Bu - 25(2,23)Ag	109.6722(11)	20	14(3,11)Ag - 14(2,12)Bu	114.4139(11)	48
35(2,33)Bu - 34(1,34)Ag	99.2444(51)	48	24(3,23)Bu - 25(2,24)Ag	110.0401(11)	20	13(3,11)Ag - 13(2,12)Bu	114.4220(11)	45
39(2,38)Bu - 38(1,37)Ag	99.2825(10)	23	23(3,21)Bu - 24(2,22)Ag	110.0763(11)	34	13(3,10)Ag - 13(2,11)Bu	114.4236(11)	76
34(3,32)Ag - 35(2,35)Bu	99.3737(80)	24	9(3, 6)Ag - 10(2, 9)Bu	110.0950(11)	17	12(3,10)Ag - 12(2,11)Bu	114.4318(11)	72
46(2,45)Ag - 45(1,44)Bu	99.5535(86)	14	9(3, 7)Ag - 10(2, 8)Bu	110.0956(11)	10	12(3, 9)Ag - 12(2,10)Bu	114.4330(11)	43
33(3,31)Bu - 34(2,33)Ag	99.6302(54)	25	23(3,22)Ag - 23(3,22)Ag	110.4536(11)	34	11(3, 9)Ag - 11(2,10)Bu	114.4411(11)	40
40(2,39)Bu - 39(1,38)Ag	99.6911(14)	37	22(3,20)Bu - 23(2,21)Ag	110.4834(11)	20	11(3, 8)Ag - 11(2, 9)Bu	114.4419(11)	67
36(2,34)Bu - 35(1,35)Ag	99.7281(64)	27	8(3, 5)Ag - 9(2, 8)Bu	110.5373(11)	8	10(3, 8)Ag - 10(2, 9)Bu	114.4497(11)	62
33(3,31)Ag - 34(2,32)Bu	99.7713(62)	15	8(3, 6)Ag - 9(2, 7)Bu	110.5376(11)	14	10(3, 7)Ag - 10(2, 8)Bu	114.4503(11)	37
32(3,29)Ag - 33(2,32)Bu	100.0520(42)	16	21(3,18)Bu - 22(2,21)Ag	110.8688(11)	20	9(3, 7)Ag - 9(2, 8)Bu	114.4577(11)	34
41(2,40)Bu - 40(1,39)Ag	100.0989(19)	21	21(3,19)Bu - 22(2,20)Ag	110.8931(11)	34	9(3, 6)Ag - 9(2, 7)Bu	114.4581(11)	57

energy levels and the B rotational constants for several quanta of the trans-bending vibration. In their calculations the B rotational constants for the A_g states are larger than those of the B_u states for $K = 0$ through $K = 4$. Because of this, we are led to suggest that the $K = 3$ A_g states must be perturbed. The A_g and B_u states have energies

TABLE VI—Continued

Transition	Wavenumber	Int	Transition	Wavenumber	Int	Transition	Wavenumber	Int
8(3, 6)Ag - 8(2, 7)Bu	114.4650(11)	51	13(3, 11)Bu - 13(2, 12)Ag	120.3455(11)	80	23(3, 20)Ag - 22(2, 21)Bu	124.2588(11)	58
8(3, 5)Ag - 8(2, 6)Bu	114.4652(11)	30	13(3, 10)Bu - 13(2, 11)Ag	120.3480(11)	58	23(3, 21)Ag - 22(2, 20)Bu	124.2757(11)	35
7(3, 5)Ag - 7(2, 6)Bu	114.4716(11)	26	14(3, 12)Bu - 14(2, 13)Ag	120.3510(11)	40	24(3, 21)Ag - 23(2, 22)Bu	124.6696(11)	35
7(3, 4)Ag - 7(2, 5)Bu	114.4717(11)	44	14(3, 11)Bu - 14(2, 12)Ag	120.3544(11)	84	24(3, 22)Ag - 23(2, 21)Bu	124.6904(11)	58
6(3, 4)Ag - 6(2, 5)Bu	114.4774(11)	37	15(3, 13)Bu - 15(2, 14)Ag	120.3569(11)	87	10(3, 7)Bu - 9(2, 8)Ag	124.6962(11)	45
6(3, 3)Ag - 6(2, 4)Bu	114.4775(11)	22	15(3, 12)Bu - 15(2, 13)Ag	120.3615(11)	52	10(3, 8)Bu - 9(2, 7)Ag	124.6968(11)	27
5(3, 3)Ag - 5(2, 4)Bu	114.4824(12)	18	16(3, 14)Bu - 16(2, 15)Ag	120.3634(12)	54	25(3, 22)Ag - 24(2, 23)Bu	125.0792(11)	57
5(3, 2)Ag - 5(2, 3)Bu	114.4825(12)	30	16(3, 13)Bu - 16(2, 14)Ag	120.3694(12)	90	25(3, 23)Ag - 24(2, 22)Bu	125.1047(11)	34
4(3, 2)Ag - 4(2, 3)Bu	114.4867(12)	21	17(3, 15)Bu - 17(2, 16)Ag	120.3704(12)	92	11(3, 8)Bu - 10(2, 9)Ag	125.1350(11)	28
4(3, 1)Ag - 4(2, 2)Bu	114.4867(12)	13	18(3, 16)Bu - 18(2, 17)Ag	120.3779(12)	56	11(3, 9)Bu - 10(2, 8)Ag	125.1359(11)	48
3(3, 0)Ag - 3(2, 1)Bu	114.4901(12)	12	17(3, 14)Bu - 17(2, 15)Ag	120.3782(12)	55	26(3, 23)Ag - 25(2, 24)Bu	125.4876(11)	34
3(3, 1)Ag - 3(2, 2)Bu	114.4901(12)	7	19(3, 17)Bu - 19(2, 18)Ag	120.3860(11)	96	26(3, 24)Ag - 25(2, 23)Bu	125.5185(11)	56
12(3, 9)Bu - 13(2, 12)Ag	114.6737(11)	24	18(3, 15)Bu - 18(2, 16)Ag	120.3879(12)	94	12(3, 9)Bu - 11(2, 10)Ag	125.5737(11)	50
12(3, 10)Bu - 13(2, 11)Ag	114.6763(11)	14	20(3, 18)Bu - 20(2, 19)Ag	120.3947(11)	58	12(3, 10)Bu - 11(2, 9)Ag	125.5750(11)	30
11(3, 8)Bu - 12(2, 11)Ag	115.1027(11)	13	19(3, 16)Bu - 19(2, 17)Ag	120.3987(11)	57	27(3, 24)Ag - 26(2, 25)Bu	125.8947(12)	55
11(3, 9)Bu - 12(2, 10)Ag	115.1045(11)	22	21(3, 19)Bu - 21(2, 20)Ag	120.4039(11)	97	27(3, 25)Ag - 26(2, 24)Bu	125.9321(12)	33
10(3, 7)Bu - 11(2, 10)Ag	115.5327(11)	20	20(3, 17)Bu - 20(2, 18)Ag	120.4105(11)	96	13(3, 10)Bu - 12(2, 11)Ag	126.0122(11)	31
10(3, 8)Bu - 11(2, 9)Ag	115.5340(11)	12	22(3, 20)Bu - 22(2, 21)Ag	120.4138(11)	58	13(3, 11)Bu - 12(2, 10)Ag	126.0141(11)	52
3(3, 0)Ag - 2(2, 1)Bu	115.8010(12)	21	21(3, 18)Bu - 21(2, 19)Ag	120.4237(11)	97	28(3, 25)Ag - 27(2, 26)Bu	126.3005(15)	32
3(3, 1)Ag - 2(2, 0)Bu	115.8010(12)	12	23(3, 21)Bu - 23(2, 22)Ag	120.4243(11)	97	27(3, 26)Ag - 26(2, 27)Bu	126.3454(15)	54
9(3, 6)Bu - 10(2, 9)Ag	115.9636(11)	10	24(3, 22)Bu - 24(2, 23)Ag	120.4355(11)	57	14(3, 11)Bu - 13(2, 12)Ag	126.4507(11)	54
9(3, 7)Bu - 10(2, 8)Ag	115.9636(11)	17	23(3, 19)Bu - 23(2, 20)Ag	120.4381(11)	97	14(3, 12)Bu - 13(2, 13)Ag	126.4507(11)	54
4(3, 1)Ag - 3(2, 2)Bu	116.2344(12)	14	25(3, 23)Bu - 25(2, 24)Ag	120.4473(12)	95	29(3, 26)Ag - 28(2, 27)Bu	126.7050(19)	53
4(3, 2)Ag - 3(2, 1)Bu	116.2344(12)	24	23(3, 20)Bu - 23(2, 21)Ag	120.4541(11)	58	29(3, 27)Ag - 28(2, 26)Bu	126.7586(19)	32
8(3, 5)Bu - 9(2, 8)Ag	116.3955(11)	15	26(3, 24)Bu - 26(2, 25)Ag	120.4598(15)	56	15(3, 12)Bu - 14(2, 13)Ag	126.8889(11)	34
8(3, 6)Bu - 9(2, 7)Ag	116.3960(11)	9	24(3, 21)Bu - 24(2, 22)Ag	120.4717(11)	96	15(3, 13)Bu - 14(2, 12)Ag	126.8924(11)	56
5(3, 2)Ag - 4(2, 3)Bu	116.6667(12)	28	27(3, 25)Bu - 27(2, 26)Ag	120.4730(19)	92	30(3, 27)Ag - 29(2, 28)Bu	127.1081(25)	31
3(3, 0)Ag - 4(2, 2)Bu	116.6667(12)	16	28(3, 26)Bu - 28(2, 27)Ag	120.4869(26)	53	30(3, 28)Ag - 29(2, 27)Bu	127.1719(25)	52
7(3, 4)Bu - 8(2, 7)Ag	116.8281(11)	7	25(3, 22)Bu - 25(2, 23)Ag	120.4911(12)	57	16(3, 13)Bu - 15(2, 14)Ag	127.3270(12)	58
7(3, 5)Bu - 8(2, 6)Ag	116.8285(11)	12	29(3, 27)Bu - 29(2, 28)Ag	120.5015(34)	87	16(3, 14)Bu - 15(2, 13)Ag	127.3316(12)	34
6(3, 3)Ag - 5(2, 4)Bu	117.0980(11)	18	14(3, 11)Ag - 13(2, 12)Bu	120.5089(11)	31	31(3, 28)Ag - 30(2, 29)Bu	127.5098(32)	50
6(3, 4)Ag - 5(2, 3)Bu	117.0980(11)	31	14(3, 12)Ag - 13(2, 11)Bu	120.5105(11)	52	31(3, 29)Ag - 30(2, 28)Bu	127.5852(33)	30
6(3, 3)Bu - 7(2, 6)Ag	117.2615(11)	9	26(3, 23)Bu - 26(2, 24)Ag	120.5125(15)	93	17(3, 14)Bu - 16(2, 15)Ag	127.7647(12)	35
6(3, 4)Bu - 7(2, 5)Ag	117.2617(11)	5	30(3, 28)Bu - 30(2, 29)Ag	120.5168(46)	51	17(3, 15)Bu - 16(2, 14)Ag	127.7708(12)	59
7(3, 4)Ag - 6(2, 5)Bu	117.5282(11)	36	31(3, 29)Bu - 31(2, 30)Ag	120.5338(59)	82	32(3, 29)Ag - 31(2, 30)Bu	127.9201(42)	29
7(3, 5)Ag - 6(2, 4)Bu	117.5283(11)	20	27(3, 24)Bu - 27(2, 25)Ag	120.5360(19)	55	32(3, 30)Ag - 31(2, 29)Bu	127.9988(43)	48
5(3, 2)Bu - 6(2, 5)Ag	117.6956(12)	4	32(3, 30)Bu - 32(2, 31)Ag	120.5495(77)	47	18(3, 15)Bu - 17(2, 16)Ag	128.2023(12)	60
5(3, 3)Bu - 6(2, 4)Ag	117.6957(12)	6	28(3, 25)Bu - 28(2, 26)Ag	120.5619(26)	90	18(3, 16)Bu - 17(2, 15)Ag	128.2101(12)	36
8(3, 5)Ag - 7(2, 6)Bu	117.9574(11)	22	33(3, 31)Bu - 33(2, 32)Ag	120.5668(97)	76	33(3, 30)Ag - 32(2, 31)Bu	128.3088(54)	47
8(3, 6)Ag - 7(2, 5)Bu	117.9575(11)	37	29(3, 26)Bu - 29(2, 27)Ag	120.5905(35)	52	33(3, 31)Ag - 32(2, 30)Bu	128.4128(56)	28
4(3, 1)Bu - 5(2, 4)Ag	118.1303(12)	4	30(3, 27)Bu - 30(2, 28)Ag	120.6218(46)	85	19(3, 16)Bu - 18(2, 17)Ag	128.6395(11)	36
4(3, 2)Bu - 5(2, 3)Ag	118.1304(12)	2	31(3, 28)Bu - 31(2, 29)Ag	120.6564(60)	49	19(3, 17)Bu - 18(2, 16)Ag	128.6495(11)	61
9(3, 6)Ag - 8(2, 7)Bu	118.3854(11)	40	32(3, 29)Bu - 32(2, 30)Ag	120.6943(77)	79	34(3, 31)Ag - 33(2, 32)Bu	128.7059(69)	27
9(3, 7)Ag - 8(2, 6)Bu	118.3857(11)	24	33(3, 30)Bu - 33(2, 31)Ag	120.7360(98)	46	34(3, 32)Ag - 33(2, 31)Bu	128.8273(71)	45
3(3, 0)Bu - 4(2, 3)Ag	118.5657(12)	1	15(3, 12)Ag - 14(2, 13)Bu	120.9302(11)	54	20(3, 17)Bu - 19(2, 18)Ag	129.0763(11)	61
3(3, 1)Bu - 4(2, 2)Ag	118.5657(12)	1	15(3, 13)Ag - 14(2, 12)Bu	120.9324(11)	32	20(3, 18)Bu - 19(2, 17)Ag	129.0894(11)	37
10(3, 7)Ag - 9(2, 8)Bu	118.8124(11)	26	16(3, 13)Ag - 15(2, 14)Bu	121.3503(11)	33	35(3, 32)Ag - 34(2, 33)Bu	129.1013(87)	43
10(3, 8)Ag - 9(2, 7)Bu	118.8128(11)	43	16(3, 14)Ag - 15(2, 13)Bu	121.3533(11)	55	35(3, 33)Ag - 34(2, 32)Bu	129.2424(90)	26
11(3, 8)Ag - 10(2, 9)Bu	119.2382(11)	46	31(3, 0)Bu - 2(2, 1)Ag	121.6255(12)	13	21(3, 18)Bu - 20(2, 19)Ag	129.5128(11)	37
11(3, 9)Ag - 10(2, 8)Bu	119.2388(11)	27	3(3, 1)Bu - 2(2, 0)Ag	121.6255(12)	22	21(3, 19)Bu - 20(2, 18)Ag	129.5287(11)	61
12(3, 9)Ag - 11(2, 10)Bu	119.6629(11)	29	17(3, 14)Ag - 16(2, 15)Bu	121.7693(12)	56	32(3, 19)Bu - 31(2, 20)Ag	129.9489(11)	61
12(3, 10)Ag - 11(2, 9)Bu	119.6637(11)	48	17(3, 15)Ag - 16(2, 14)Bu	121.7733(12)	34	22(3, 20)Bu - 21(2, 19)Ag	129.9686(11)	37
13(3, 10)Ag - 12(2, 11)Bu	120.0865(11)	50	4(3, 1)Bu - 3(2, 2)Ag	122.0638(12)	26	23(3, 20)Bu - 22(2, 21)Ag	130.3845(11)	37
13(3, 11)Ag - 12(2, 10)Bu	120.0877(11)	30	4(3, 2)Bu - 3(2, 1)Ag	122.0638(12)	15	23(3, 21)Bu - 22(2, 20)Ag	130.4089(11)	61
3(3, 1)Bu - 3(2, 2)Ag	120.3140(12)	12	18(3, 15)Ag - 17(2, 16)Bu	122.1871(12)	34	24(3, 21)Bu - 23(2, 22)Ag	130.8197(11)	61
3(3, 0)Bu - 3(2, 1)Ag	120.3140(12)	7	18(3, 16)Ag - 17(2, 15)Bu	122.1923(12)	57	24(3, 22)Bu - 23(2, 21)Ag	130.8495(11)	36
4(3, 2)Bu - 4(2, 3)Ag	120.3154(12)	13	5(3, 2)Bu - 4(2, 3)Ag	122.5023(12)	17	25(3, 22)Bu - 24(2, 23)Ag	131.2543(12)	36
4(3, 1)Bu - 4(2, 2)Ag	120.3155(12)	22	5(3, 3)Bu - 4(2, 2)Ag	122.5024(12)	29	25(3, 23)Bu - 24(2, 22)Ag	131.2906(12)	60
5(3, 3)Bu - 5(2, 4)Ag	120.3172(12)	31	19(3, 16)Ag - 18(2, 17)Bu	122.6038(12)	58	26(3, 23)Bu - 25(2, 24)Ag	131.6884(15)	59
5(3, 2)Bu - 5(2, 3)Ag	120.3173(12)	19	19(3, 17)Ag - 18(2, 16)Bu	122.6105(12)	34	26(3, 24)Bu - 25(2, 23)Ag	131.7322(15)	35
6(3, 4)Ag - 6(2, 5)Ag	120.3194(11)	23	6(3, 3)Bu - 5(2, 4)Ag	122.9410(11)	33	27(3, 24)Bu - 26(2, 25)Ag	132.1219(19)	35
6(3, 3)Bu - 6(2, 4)Ag	120.3195(11)	39	6(3, 4)Bu - 5(2, 3)Ag	122.9410(11)	19	27(3, 25)Bu - 26(2, 24)Ag	132.1746(19)	58
7(3, 5)Bu - 7(2, 6)Ag	120.3219(11)	47	20(3, 17)Ag - 19(2, 18)Bu	123.0193(11)	53	28(3, 25)Bu - 27(2, 26)Ag	132.5547(26)	37
7(3, 4)Bu - 7(2, 5)Ag	120.3221(11)	28	19(3, 18)Ag - 19(2, 17)Bu	123.0279(12)	58	28(3, 26)Bu - 27(2, 25)Ag	132.6177(26)	34
8(3, 6)Bu - 8(2, 7)Ag	120.3248(11)	32	7(3, 4)Bu - 6(2, 5)Ag	123.3797(11)	21	29(3, 26)Bu - 28(2, 27)Ag	132.9858(34)	33
8(3, 5)Bu - 8(2, 6)Ag	120.3251(11)	53	7(3, 5)Bu - 6(2, 4)Ag	123.3799(11)	36	29(3, 27)Bu - 28(2, 26)Ag	133.0619(34)	56
9(3, 7)Bu - 9(2, 8)Ag	120.3281(11)	60	21(3, 18)Ag - 20(2, 19)Bu	123.4337(11)	59	30(3, 27)Bu - 29(2, 28)Ag	133.4181(46)	54
9(3, 6)Bu - 9(2, 7)Ag	120.3287(11)	36	21(3, 19)Ag - 20(2, 18)Bu	123.4445(11)	35	30(3, 28)Bu - 29(2, 27)Ag	133.5071(45)	37
10(3, 8)Bu - 10(2, 9)Ag	120.3318(11)	39	8(3, 5)Bu - 7(2, 6)Ag	123.8185(11)	39	31(3, 28)Bu - 30(2, 29)Ag	133.8487(59)	31
10(3, 7)Bu - 10(2, 8)Ag	120.3327(11)	65	8(3, 6)Bu - 7(2, 5)Ag	123.8188(11)	23	31(3, 29)Bu - 30(2, 28)Ag	133.9537(59)	53
11(3, 9)Bu - 11(2, 10)Ag	120.3359(11)	71	22(3, 19)Ag - 21(2, 20)Bu	123.8468(11)	35	32(3, 29)Bu - 31(2, 30)Ag	134.2783(77)	51
11(3, 8)Bu - 11(2, 9)Ag	120.3372(11)	42	22(3, 20)Ag - 21(2, 19)Bu	123.8604(11)	59	32(3, 30)Bu - 31(2, 29)Ag	134.4019(77)	30
12(3, 10)Bu - 12(2, 11)Ag	120.3405(11)	45	9(3, 6)Bu - 8(2, 7)Ag	124.2574(11)	25	33(3, 30)Bu - 32(2, 31)Ag	134.7069(97)	29
12(3, 9)Bu - 12(2, 10)Ag	120.3423(11)	76	9(3, 7)Bu - 8(2, 6)Ag	124.2577(11)	42	33(3, 31)Bu - 32(2, 30)Ag	134.8518(98)	49

of 232.6 and 236.4 cm^{-1} above the $K = 0$, $J = 0$ A_g level. (Bunker *et al.* (10) calculate 227.2 and 231.6 cm^{-1} for the energies of these states.) According to Ref. (10), the $K = 1$ levels of the bending state lie in the vicinity of 215 cm^{-1} with a tunneling splitting of 25 cm^{-1} . A $\Delta K = \pm 2$ Coriolis interaction between these levels is possible. Such an interaction would require the A_g levels of the bending mode to fall close to 233 cm^{-1} .

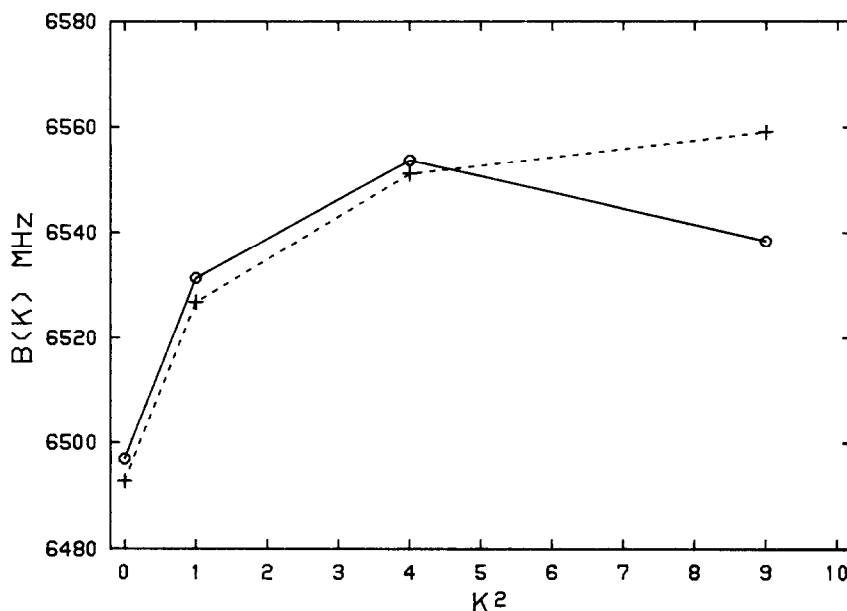


FIG. 3. A plot of the B rotational constant of both the A_g (\circ) and B_u (+) states of (HF)₂ as a function of K^2 . Note the anomalous shift in this constant for the $K = 3$ states suggesting a perturbation of the levels of this state.

Since the splitting in the bending mode is very large, the B_u levels would not be affected by the interaction. An equally valid possibility to account for this resonance is an interaction with a low- K sublevel of the van der Waals stretching vibration. The tunneling splitting in this mode should be close to that of the ground state. A low- K sublevel would have smaller splitting than the $K = 3$ ground state sublevels, and, thus, one of the $K = 3$ ground state levels would be more perturbed than the other.

One advantage of using backward wave oscillators is the ability to scan over large segments of the spectrum. As in every portion of the spectrum of (HF)₂, a large number of unidentified lines remain in the higher frequency spectrum, some of which may arise from impurities, but many of which must originate in excited vibrational states. Now that the ground state transitions have been catalogued, and with the guidance of the calculations of Bunker *et al.*, it is hoped to extend the line assignments to those originating in excited vibrational states.

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REFERENCES

1. T. R. DYKE, B. J. HOWARD, AND W. KLEMPERER, *J. Chem. Phys.* **56**, 2442-2454 (1972).
2. B. J. HOWARD, T. R. DYKE, AND W. KLEMPERER, *J. Chem. Phys.* **81**, 5417-5425 (1984).
3. W. J. LAFFERTY, R. D. SUENRAM, AND F. J. LOVAS, *J. Mol. Spectrosc.* **123**, 434-452 (1987).
4. K. VON PUTTKAMER, M. QUACK, AND M. A. SUHM, *Mol. Phys.* **65**, 1025 (1988).
5. A. S. PINE AND W. J. LAFFERTY, *J. Chem. Phys.* **78**, 2154-2162 (1983).
6. A. S. PINE, W. J. LAFFERTY, AND B. J. HOWARD, *J. Chem. Phys.* **81**, 2939-2950 (1984).
7. J. T. HOUGEN AND N. OHASHI, *J. Mol. Spectrosc.* **109**, 134-165 (1985).
8. I. M. MILLS, *J. Phys. Chem.* **88**, 532-536 (1984).
9. A. E. BARTON AND B. J. HOWARD, *Faraday Discuss. Chem. Soc.* **73**, 45 (1982).
10. P. R. BUNKER, P. C. GOMEZ, M. D. MARSHALL, M. KOFRANEK, H. LISCHKA, AND A. KARPFEN, *J. Chem. Phys.* **91**, 5154-5159 (1989).
11. M. KOFRANEK, H. LISCHKA, AND A. KARPFEN, *Chem. Phys.* **1988**, 137-153.
12. P. R. BUNKER, M. KOFRANEK, H. LISCHKA, AND A. KARPFEN, *J. Chem. Phys.* **89**, 3002-3007 (1988).
13. S. P. BELOV AND M. YU. TRETYAKOV, "IX Int. Conf. on High Res. IR Spectrosc., Prague, 1968," p. 68.
14. R. D. SUENRAM AND F. J. LOVAS, *J. Amer. Chem. Soc.* **102**, 7189-7184 (1980).
15. S. R. POLO, *Canad. J. Phys.* **35**, 880 (1972).
16. W. H. KIRCHHOFF, *J. Mol. Spectrosc.* **41**, 333-380 (1972).
17. G. HERZBERG, "Infrared and Raman Spectra," Van Nostrand, New York, 1945.
18. O. L. POLYANSKY, *J. Mol. Spectrosc.* **112**, 79-87 (1985).
19. O. L. POLYANSKY AND I. N. KOZIN, to be published.