

**THE PURE ROTATIONAL SPECTRUM OF WATER
VAPOR—A MILLIMETER, SUBMILLIMETER,
AND FAR INFRARED ANALYSIS¹**

J. K. Messer and Frank C. De Lucia

*Department of Physics, Duke University
Durham, North Carolina 27706*

and

Paul Helminger

*Department of Physics, University of South Alabama
Mobile, Alabama 36688*

Received April 11, 1983

Line positions, strengths, and absolute energies are calculated for the pure rotational spectrum of water in the region between 0 cm^{-1} and 877 cm^{-1} . These calculations are done in the context of a reduced centrifugal distortion Hamiltonian, and are based on microwave measurements of this spectrum to 1 THz, and Far Infrared measurements between 32 cm^{-1} and 715 cm^{-1} .

Key words: Rotational spectrum of water, submillimeter spectroscopy.

Introduction

Water is perhaps the most important molecular species, and certainly one of the most pervasive. Because of its strong interaction with radiation, it plays an important role in a wide variety of processes, from propagation through the Earth's atmosphere to energy transfer in cool stars. Water is also one of the most interesting spectroscopic species. It is the prototype bent, tri-atomic X-Y-X or X-Y-Z molecule, whose geometric simplicity conceals great spectroscopic complexity.

¹This work supported by the U.S. Army Research Office.

In this paper we report a detailed, combined analysis of the pure rotational spectrum measured by high resolution microwave techniques to 1 THz (33 cm^{-1}) [1,2], and by Fourier Transform techniques between 32 cm^{-1} and 715 cm^{-1} [3]. This data set, containing 305 transitions, is a representative selection of the pure rotational transitions that absorb significant electromagnetic energy at $T \sim 300\text{ K}$. The analysis then provides a complete map of the pure rotational transitions of water that absorb significant amounts of electromagnetic energy at $\sim 300\text{ K}$.

One of the most important applications of these results is in the calculation of the atmospheric propagation of electromagnetic radiation. Mizushima [4] has addressed this issue recently, using the results of our earlier analysis [2] that included the microwave and infrared data available in 1971. In his paper, Mizushima sets forth useful, straight-forward techniques that lead to a model for atmospheric transmission, which includes the well-known and troublesome far-wing regions.

Experimental

We have previously discussed the spectroscopic techniques that we have developed for high resolution spectroscopy in the shorter millimeter and submillimeter spectral region [1,5]. A block diagram of this system is shown in Figure 1. Briefly, a reflex klystron in the 55 GHz region is phase locked to a signal referenced to a microprocessor controlled frequency synthesizer, which is in turn referenced to WWVB. The output of this klystron is matched into a crystal harmonic generator which produces harmonics over a wide region of the millimeter and submillimeter spectrum. This power is then focused via quasi-optical techniques through the sample cell and detected by a 1.5 K InSb detector. This system has been recently used to measure transitions at frequencies above 1 THz, and to measure 5 new microwave lines of water [1] that were not included in our original study. The complete microwave data set is shown in Table I. Historical references on each of the 15 previously measured lines may be found in reference 2.

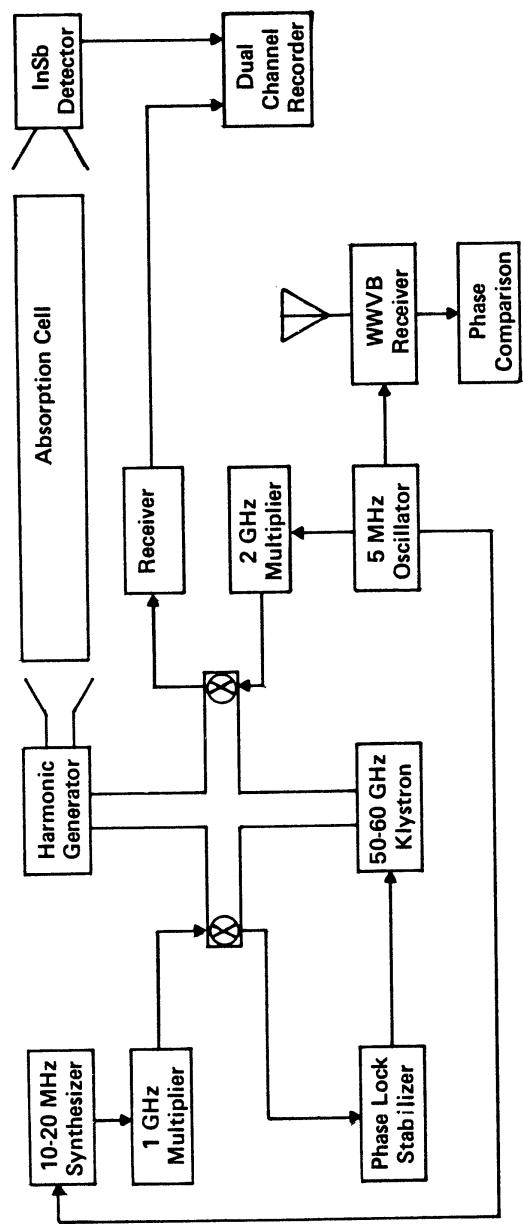


Figure 1. Block diagram of millimeter and submillimeter spectrometer.

TABLE I. Microwave Lines (MHz)

Transition	Measured	Predicted	wt.	Δ
1(1, 0)- 1(0,1)	556936.002	556936.335	10 ⁵	+0.33
2(1, 1)- 2(0,2)	752033.227	752032.636	10 ⁵	-0.59
2(0, 2)- 1(1,1)	987926.764	987929.689	10 ⁵	+2.93
3(1, 3)- 2(2,0)	183310.117	183309.015	10 ⁵	-1.10
4(1, 4)- 3(2,1)	380197.372	380197.637	10 ⁴	+0.27
4(2, 3)- 3(3,0)	448001.075	448001.997	10 ⁴	+0.92
4(2, 2)- 3(3,1)	916171.582	916169.950	10 ⁴	-1.63
5(1, 5)- 4(2,2)	325152.919	325152.867	10 ⁴	-0.05
5(3, 3)- 4(4,0)	474689.127	474690.072	10 ³	+0.95
5(3, 2)- 4(4,1)	620700.807	620702.711	10 ³	+1.90
5(2, 4)- 4(3,1)	970315.022	970316.242	10 ⁴	+1.22
6(1, 6)- 5(2,3)	22235.080	22234.638	10 ⁴	-0.44
6(4, 3)- 5(5,0)	439150.812	439142.394	10 ²	-8.42
6(4, 2)- 5(5,1)	470888.947	470881.284	10 ²	-7.65
7(1, 7)- 6(2,4)	-488491.133	-488490.050	10 ⁴	+1.08
7(5, 3)- 6(6,0)	437346.667	437386.472	5	+39.8
7(5, 2)- 6(6,1)	443018.295	443058.314	5	+40.0
8(6, 2)- 7(7,1)	504482.692	504416.841	1	-65.9
8(6, 3)- 7(7,0)	503568.532	503502.773	1	-65.8
11(2,10)-10(3,7)	-390134.508	-390162.715	10 ²	-28.2

Theory

The problems associated with the analysis of the spectrum of a light asymmetric rotor are substantial. The general theory was described by Wilson and Howard [6] many years ago, but, until the work of Watson [7], a fitting indeterminacy precluded its use for the analysis of most experimental spectra. Watson's reduced Hamiltonian, through 6th order, can be written as

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_r + \mathcal{H}_d^{(4)} + \mathcal{H}_d^{(6)} \\ \mathcal{H}_r &= \frac{1}{2}(B+C)P^2 + [A-\frac{1}{2}(B+C)](P_z^2 - b_p P_-^2) \\ \mathcal{H}_d^{(4)} &= -\Delta_J P^4 - \Delta_{JK} P^2 P_z^2 - \Delta_K P_z^4 - 2\delta_J P^2 P_-^2 \\ &\quad - \delta_K (P_z^2 P_-^2 + P_-^2 P_z^2) \\ \mathcal{H}_d^{(6)} &= H_J P^6 + H_{JK} P^4 P_z^2 + H_{KJ} P^2 P_z^4 + H_K P_z^6 + 2h_J P^4 P_-^2 \\ &\quad + h_{JK} P^2 (P_z^2 P_-^2 + P_-^2 P_z^2) + h_K (P_z^4 P_-^2 + P_-^2 P_z^4)\end{aligned}$$

where $b_p = (C-B)/(2A-B-C)$

and $P_-^2 = P_x^2 - P_y^2$

Its extension to higher order is straightforward [8]. Although each of the spectroscopic quantities in the Hamiltonian above can be related to molecular parameters (e.g. bond lengths or force constants) [9,10], for many applications they can best be viewed as spectral fitting parameters (albeit theoretically well founded parameters). This is especially true for the higher order parameters. In our earlier work, we have discussed extensively the application of these techniques to a number of light asymmetric species (HDS[11], HDO [8], D₂S [12]). Other similar implementations of this theory have also been developed [13,14]. These differ primarily in notation, or in some cases different linear combinations of the parameters have been used. An interesting alternative has been put forth by Kneizys, Freedman, and Clough [15].

There are special problems associated with the analysis of very light, bent triatomic species such as H₂O. Figure 2 shows the geometry of H₂O. Because of the small mass of the hydrogen nuclei, the amplitude of the bending motion is large, and the singularity in the moment of inertia about the a-axis, I_a, at $\theta=180^\circ$ is approached. Thus, the power series in the coefficients of $\langle P_z^{2n} \rangle$ converges very slowly.

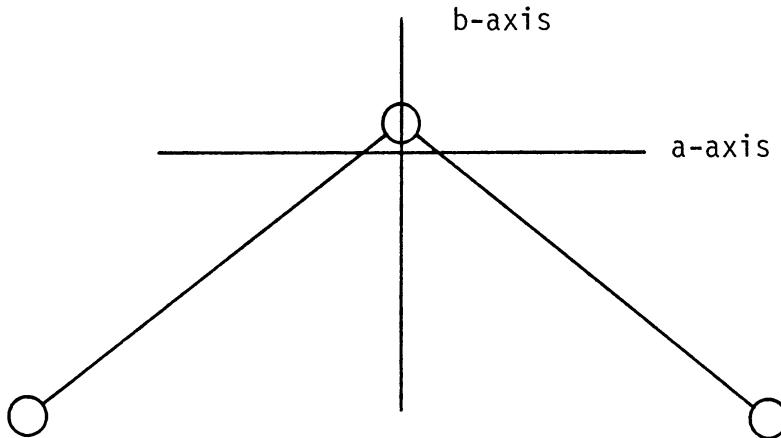


Figure 2. Geometry of the water molecule showing the principal axes of the moments of inertia.

Consequently, a large number of terms are required to fit data for states with large K_{-1} (i.e. those states with large angular momentum about the a-axis). For example, our earlier analysis of H_2O , which included levels only through $K_{-1}=10$ required 21 parameters.

The line strength of an asymmetric top transition between levels (J, τ) and (J', τ') , due to a dipole moment along the g-axis, is given by Gordy and Cook [9] as

$$g_S(J, \tau; J', \tau') = \sum_{F, M, M'} |\langle J, \tau, M | \Phi_{Fg} | J', \tau', M' \rangle|^2,$$

where Φ_{Fg} is the direction-cosine relating the space-fixed axis F to the molecule-fixed axis g. Explicit expressions for $g_S(J, \tau; J', \tau')$ have been given by Moazzen-Ahmadi [16] in a form well suited for evaluation on the computer. These expressions have been used to compute line strengths for the predicted transitions. The accuracy of the computer program used to calculate $g_S(J, \tau; J', \tau')$ was checked by evaluating the strengths for the rigid rotor for $\kappa=\pm 0.5$ for quantum numbers up to $J=12$, and comparing the results with values given in Townes and Schawlow [17].

Analysis

Our original analysis [2] of the rotational structure of the ground vibrational state of H₂O was based on a weighted data set that consisted of 15 microwave lines and the infrared results that were available in the literature at that time. More recently, extensive new near-infrared spectra, due to vibration-rotation transitions of H₂O have been recorded on a large FT spectrometer at Orsay, and analyzed by the techniques discussed above [18,19]. In addition, an excellent FIR FT spectrum of the pure rotational spectrum of H₂O has been published [3].

Since it is our goal to calculate, as accurately as possible, the pure rotational spectrum of water at temperatures ~300 K, we have chosen to fit only the microwave data and the FIR pure rotational data. This is a selection criterion based not upon the relative accuracies of the FIR and IR data, but rather on a recognition that the inclusion of states that are difficult to fit would only decrease the accuracy of our results. The lines included in the FIR data set are highly correlated with the spectrum we wish to predict, so their inclusion seems appropriate.

In any analysis that mixes infrared and microwave data, careful attention must be paid to the weighting scheme. A fit of the FIR data currently available shows an rms deviation of ~30 MHz. The microwave data is ~300 times more accurate. Standard data analysis theory immediately leads to the conclusion that the microwave data should be weighted ~10⁵ relative to the infrared data. However, if this is done, the quality of the fit seriously deteriorates (the rms deviation goes from ~30 MHz to ~60 MHz). The reason for this is that the weighting of data according to the inverse square of its accuracy is valid only if the theoretical model is also accurate at the high level. Clearly, the accuracy of the model can be improved by simply adding higher power terms to the Hamiltonian, but there are already more terms in the Hamiltonian than microwave lines, and it could be argued that this approach is mostly numerology.

Our strategy for weighting the data is as follows. We weight the microwave lines only as heavily as the accuracy of the theoretical model through P₁₀ will allow. This means that the model will not predict some high J,K microwave lines as accurately as they were measured. However,

since we have directly measured all significant lines below 1 THz, this is of no serious practical consequence.

The weights were determined as follows. Since, at low K , the model should be accurate even to microwave accuracy, we initially weighted the $K_1=0$ microwave transitions 10^5 , and ran an analysis on the FIR and $K_1=0$ microwave data. Since the addition of the microwave data did not significantly increase the variance of the fit, we concluded that the assumption of model accuracy to microwave precision was correct through $K_1=0$, and increased the weighting to 10^5 on the next higher K_1 . This process was repeated until the deviation significantly increased ($J=3$, $K_1=2$), and, for this state, a weighting of 10^4 was selected. This process was continued until all of the microwave data was included in the fit. The weights which result are shown in Table I.

Results

Table I shows the measured microwave frequencies. In order to eliminate possibilities of impurity lines at different harmonics, we have measured each of the millimeter and submillimeter lines from two different harmonics (e.g. 17th and 18th). As a further test, each line has been predicted from an analysis that did not contain the line in question. Table I shows this comparison. It should be noted that although the accuracy of the model decreases at higher K_1 , and approaches the accuracy of the FIR data, the error in the prediction of each component of a K_1 doublet is virtually identical. We therefore conclude that the frequency measurements and assignments of these lines are correct.

The spectral constants that result from this analysis are shown in Table II. Since no clear relationship between the higher order spectral constants and the molecular distortions has been derived, the inclusion of such terms in the power series expansion is largely empirical, but based upon statistical tests of significance. We have discussed these tests in detail previously [2,8,11].

In Table III, we show the calculated microwave and FIR pure rotational spectrum of water. These have been sorted according to increasing frequency. The calculated uncer-

TABLE II. Rotational Constants of $H_2^{16}O$ (MHz).

$A = 835839.876 \pm 0.14$	$h_K = (9.4784 \pm 0.05) \times 10^{-1}$
$B = 435346.811 \pm 0.06$	$L_J = (-9.270 \pm 0.2) \times 10^{-6}$
$C = 278140.481 \pm 0.10$	$L_{JK} = (5.807 \pm 0.5) \times 10^{-5}$
$\Delta_J = (3.758280 \pm 0.0005) \times 10^1$	$L_{JK} = (-2.0367 \pm 0.05) \times 10^{-3}$
$\Delta_{JK} = (-1.73361 \pm 0.0003) \times 10^2$	$L_{KKJ} = (8.5898 \pm 0.1) \times 10^{-3}$
$\Delta_K = (9.742470 \pm 0.0003) \times 10^2$	$L_K = (-2.50931 \pm 0.02) \times 10^{-2}$
$\delta_J = (1.521950 \pm 0.0001) \times 10^1$	$\ell_J = (-4.727 \pm 0.1) \times 10^{-6}$
$\delta_K = (3.96461 \pm 0.005) \times 10^1$	$\ell_{KJ} = (3.850 \pm 0.4) \times 10^{-4}$
$H_J = (1.6284 \pm 0.006) \times 10^{-2}$	$\ell_K = (-1.0791 \pm 0.02) \times 10^{-2}$
$H_{JK} = (-5.2534 \pm 0.08) \times 10^{-2}$	$P_{KJ} = (1.7387 \pm 0.2) \times 10^{-5}$
$H_{KJ} = (-5.42802 \pm 0.04) \times 10^{-1}$	$P_{KKJ} = (-5.9902 \pm 0.4) \times 10^{-5}$
$H_K = (3.84436 \pm 0.004) \times 10^0$	$P_K = (1.2065 \pm 0.03) \times 10^{-4}$
$h_J = (8.1611 \pm 0.02) \times 10^{-3}$	$P_{KKJ} = (-3.319 \pm 0.4) \times 10^{-6}$
$h_{JK} = (-2.5607 \pm 0.05) \times 10^{-2}$	$P_K = (5.5019 \pm 0.3) \times 10^{-5}$

tainties, σ_v , in the line positions were calculated via [11]

$$\sigma_v^2 = \sum_{ij} \sigma_i \sigma_j \rho_{ij} c_i c_j$$

where σ_i is the standard error in the i -th spectral constant, c_i the corresponding coefficient in the frequency expression, and ρ_{ij} the correlation coefficients between the i -th and j -th constants and the sum is over the terms retained in the power series. These statistical uncertainties will only be valid for transitions that do not require additional Hamiltonian terms. However, because of the data sets used, and the restrictions placed on which lines would be calculated, the statistical uncertainties of Table III should be generally realistic.

Also included in Table III is the line strength, g_S , and the absolute energy of the lower level, E . Since g_S and E are tabulated separately, these results can be used for systems in which both the temperature and partial pressure of the system vary.

Because the extrapolation of the results of a power series model of this type to high J and K is poor, the predictions of the model have been limited approximately to the range of the input data set. Basically, the predictions include all transitions of significant transition moment (i.e. those down to and including $\Delta K_1=+5$, $\Delta K_1=-3$) whose absolute

TABLE III. PREDICTED SPECTRUM OF WATER. FREQUENCIES IN MHZ., ENERGIES IN RECIPROCAL CENTIMETERS.

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
6(1, 6)- 5(2, 3)	22234.829	0.214D+00	0.0568	446.510953	1	
3(1, 3)- 2(2, 0)	183310.004	0.976D-01	0.1017	136.163990	2	
10(2, 9)- 9(3, 6)	321226.450	0.270D+01	0.0895	1282.919859	3	
5(1, 5)- 4(2, 2)	325152.889	0.213D+00	0.0907	315.779725	4	
4(1, 4)- 3(2, 1)	380197.571	0.162D+00	0.1231	212.156484	5	
11(2, 10)-10(3, 7)	-390136.744	0.313D+01	0.0651	1525.1336733	6	
7(5, 3)- 6(6, 0)	437377.208	0.703D+01	0.0884	1045.058707	7	
6(4, 3)- 5(5, 0)	439145.003	0.181D+01	0.1014	742.077309	8	
7(5, 2)- 6(6, 1)	443049.014	0.703D+01	0.0884	1045.058315	9	
4(2, 3)- 3(3, 0)	448001.366	0.270D+00	0.1325	285.418777	10	
6(4, 2)- 5(5, 1)	470883.639	0.181D+01	0.1018	742.074041	11	
5(3, 3)- 4(4, 0)	474689.662	0.679D+00	0.1183	488.134641	12	
7(1, 7)- 6(2, 4)	-488490.990	0.304D+00	0.0359	586.479543	13	
8(6, 3)- 7(7, 0)	503532.141	0.218D+02	0.0786	1394.816443	14	
8(6, 2)- 7(7, 1)	504446.255	0.218D+02	0.0786	1394.816396	15	
14(3, 12)-13(4, 9)	530366.094	0.316D+02	0.1208	2533.795213	16	
1(1, 0)- 1(0, 1)	556936.073	0.914D-01	1.5000	23.794361	17	
13(3, 10)-12(6, 7)	-571995.962	0.200D+02	0.0772	2414.723116	18	
5(3, 2)- 4(4, 1)	620701.837	0.698D+00	0.1216	488.108168	19	
9(7, 3)- 8(8, 0)	643328.861	0.182D+03	0.0711	1789.126036	20	
9(7, 2)- 8(8, 1)	643468.287	0.182D+03	0.0711	1789.126030	21	
2(1, 1)- 2(0, 2)	752033.052	0.865D-01	2.0730	70.090825	22	
12(2, 10)-11(5, 7)	-766803.274	0.117D+02	0.0792	1960.208020	23	

TABLE III. CONTINUED (2)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
11(2, 9)-10(5, 6)	-841073.593	0.9690+01	0.0673	1690.664992	24	
10(8, 3)- 9(9, 0)	846047.928	0.9240+03	0.0653	2226.129627	25	
10(8, 2)- 9(9, 1)	846068.633	0.9240+03	0.0653	2226.129626	26	
13(2,11)-12(5, 8)	-854053.383	0.1660+02	0.0835	2246.885715	27	
9(2, 8)- 8(3, 5)	906205.524	0.2640+01	0.1317	1050.158405	28	
4(2, 2)- 3(3, 1)	916171.415	0.3090+00	0.1632	285.219540	29	
5(2, 4)- 4(3, 1)	970315.178	0.3040+00	0.2639	383.842826	30	
2(0, 2)- 1(1, 1)	987926.855	0.1010+00	0.7562	37.137136	31	
14(2,12)-13(5, 9)	-1068691.028	0.2870+02	0.0824	2550.884458	32	
3(1, 2)- 3(0, 3)	1097364.636	0.2120+00	2.1838	136.761699	33	
12(3, 9)-11(6, 6)	-1101190.771	0.1560+02	0.0486	2105.868396	34	
10(2, 8)- 9(5, 5)	-1109631.008	0.8200+01	0.0482	1437.969201	35	
1(1, 1)- 0(0, 0)	1113343.499	0.1900+00	1.0000	0.000000	36	
8(1, 8)- 7(2, 5)	-1146620.402	0.9460+00	0.0247	744.163105	37	
3(1, 2)- 2(2, 1)	1153125.565	0.2820+00	0.3016	134.901715	38	
12(2,11)-11(3, 8)	-1153377.509	0.5780+01	0.0513	1774.751712	39	
6(3, 4)- 5(4, 1)	1158326.188	0.1750+01	0.2825	610.341762	40	
3(2, 1)- 3(1, 2)	1162914.460	0.6310+00	2.5384	173.365838	41	
8(5, 4)- 7(6, 1)	1168402.308	0.8600+01	0.2311	1216.194757	42	
7(4, 4)- 6(5, 1)	1172525.455	0.4040+01	0.2578	888.633693	43	
8(5, 3)- 7(6, 2)	1190873.049	0.8560+01	0.2316	1216.190015	44	
4(2, 2)- 4(1, 3)	1207642.613	0.8910+00	3.6416	275.497109	45	
9(6, 4)- 8(7, 1)	1215828.159	0.1670+02	0.2093	1590.691804	46	
9(6, 3)- 8(7, 2)	1219970.393	0.1670+02	0.2093	1590.691159	47	

TABLE III. CONTINUED (3)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
2(2, 0)- 2(1, 1)	1228790.890	0.4080+00	1.2603	95.175944	48
13(3, 11)-12(4, 8)	1271461.249	0.1540+02	0.1598	2205.654682	49
7(4, 3)- 6(5, 2)	1278266.767	0.4070+01	0.2612	888.599790	50
8(2, 7)- 7(3, 4)	1296408.169	0.2160+01	0.1977	842.357333	51
9(1, 8)- 8(4, 5)	-1307977.999	0.5050+01	0.0438	1079.080152	52
6(2, 5)- 5(3, 2)	1322062.974	0.6600+00	0.3157	508.812550	53
10(7, 4)- 9(8, 1)	1333152.289	0.1420+03	0.1918	2009.879176	54
10(7, 3)- 9(8, 2)	1333857.167	0.1420+03	0.1918	2009.879089	55
6(1, 7)- 7(4, 4)	-1344693.419	0.3590+01	0.0355	882.890789	56
5(2, 3)- 5(1, 4)	1410622.868	0.1220+01	4.2184	399.457645	57
10(1, 9)- 9(4, 6)	-1435015.419	0.6540+01	0.0466	1293.018771	58
7(2, 6)- 6(3, 3)	1440778.190	0.1360+01	0.2756	661.549569	59
11(8, 4)-10(9, 1)	1512504.262	0.7550+03	0.1778	2471.868118	60
11(8, 3)-10(9, 2)	1512618.931	0.7550+03	0.1778	2471.868106	61
6(3, 3)- 5(4, 2)	1541969.404	0.2070+01	0.3093	610.115013	62
7(1, 6)- 6(4, 3)	-1574247.221	0.2690+01	0.0223	704.214380	63
9(2, 7)- 8(5, 4)	-1596287.106	0.6840+01	0.0270	1201.922059	64
4(1, 3)- 4(0, 4)	1602218.809	0.4730+00	2.0483	222.052850	65
2(2, 1)- 2(1, 2)	1661009.213	0.3220+00	0.8333	79.496419	66
2(1, 2)- 1(0, 1)	1669905.942	0.2740+00	1.5000	23.794361	67
11(1, 10)-10(4, 7)	-1693467.099	0.7820+01	0.0455	1524.848504	68
5(0, 5)- 4(3, 2)	-1713887.642	0.1450+01	0.0108	325.348067	69
3(0, 3)- 2(1, 2)	1716770.141	0.2340+00	1.7428	79.496419	70
6(0, 6)- 5(3, 3)	-1716963.988	0.1670+01	0.0157	446.696836	71

TABLE III. CONTINUED (4)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
6(3, 3)- 6(2, 4)	1762052.092	0.180D+01	4.8036	602.773846	72	
7(3, 5)- 6(4, 2)	1766197.466	0.257D+01	0.4389	757.781026	73	
6(2, 4)- 6(1, 5)	1794793.558	0.156D+01	4.2430	542.905986	74	
7(3, 4)- 7(2, 5)	1797168.920	0.241D+01	5.9079	782.410239	75	
11(3, 8)-10(6, 5)	-1851256.822	0.134D+02	0.0247	1813.224239	76	
5(3, 2)- 5(2, 3)	1867755.157	0.152D+01	3.4279	446.510953	77	
9(1, 9)- 8(2, 6)	-1879749.120	0.256D+01	0.0187	920.210515	78	
7(0, 7)- 6(3, 4)	-1880762.350	0.205D+01	0.0175	586.243889	79	
8(4, 5)- 7(5, 2)	1884878.147	0.571D+01	0.4390	1059.836837	80	
4(0, 4)- 3(3, 1)	-1893690.006	0.119D+01	0.0041	222.052850	81	
9(5, 5)- 8(6, 2)	1898873.488	0.111D+02	0.4072	1411.642910	82	
13(2, 12)-12(3, 9)	-1903502.302	0.134D+02	0.0430	2042.374403	83	
12(3, 10)-11(4, 7)	1903633.381	0.975D+01	0.2236	1899.099568	84	
5(2, 3)- 4(3, 2)	1918484.803	0.866D+00	0.4392	382.517197	85	
3(2, 2)- 3(1, 3)	1919361.367	0.612D+00	1.2963	142.278553	86	
10(6, 5)- 9(7, 2)	1930234.770	0.170D+02	0.3750	1810.589819	87	
10(6, 4)- 9(7, 3)	1945026.666	0.169D+02	0.3755	1810.585174	88	
9(5, 4)- 8(6, 3)	1969236.353	0.111D+02	0.4100	1411.612465	89	
6(1, 5)- 5(4, 2)	-2014876.246	0.240D+01	0.0092	542.905986	90	
8(3, 5)- 8(2, 6)	2015991.170	0.309D+01	6.4062	982.912187	91	
11(7, 5)-10(8, 2)	2022549.995	0.142D+03	0.3477	2254.351434	92	
11(7, 4)-10(8, 3)	2025345.630	0.142D+03	0.3478	2254.350744	93	
4(3, 1)- 4(2, 2)	2040480.726	0.133D+01	2.1654	315.79725	94	
12(1, 11)-11(4, 8)	-2050971.346	0.955D+01	0.0425	1774.616748	95	

TABLE III. CONTINUED (5)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
4(1, 3)-3(2, 2)	2074431.032	0.634D+00	0.8358	206.301547	96
6(4, 4)-7(5, 3)	2162363.362	0.595D+01	0.4575	1059.648039	97
3(1, 3)-2(0, 2)	2164133.946	0.476D+00	2.1575	70.090825	98
8(0, 8)-7(3, 5)	-2177420.806	0.297D+01	0.0171	744.064094	99
3(3, 0)-3(2, 1)	2196348.598	0.101D+01	1.0948	212.156484	100
5(1, 4)-5(0, 5)	2221749.577	0.920D+00	1.9181	325.348067	101
8(3, 6)-7(4, 3)	2244804.544	0.329D+01	0.5329	931.238174	102
4(2, 3)-4(1, 4)	2264152.393	0.971D+00	1.5658	224.838508	103
8(2, 6)-7(5, 3)	-2300483.271	0.586D+01	0.0109	982.912187	104
9(4, 5)-9(3, 6)	2317891.766	0.453D+01	7.0643	1282.919859	105
7(2, 5)-7(1, 6)	2344253.212	0.176D+01	4.0126	704.214380	106
10(4, 6)-10(3, 7)	2347489.784	0.581D+01	8.1599	1538.150293	107
11(3, 9)-10(4, 6)	2356830.466	0.806D+01	0.3191	1616.454112	108
3(3, 1)-3(2, 2)	2365902.229	0.991D+00	1.0370	206.301547	109
13(4, 9)-12(7, 6)	-2368558.584	0.289D+02	0.0193	2533.795213	110
4(0, 4)-3(1, 3)	2391573.591	0.554D+00	2.8321	142.278553	111
9(3, 6)-9(2, 7)	2428253.291	0.358D+01	6.3358	1201.922059	112
8(4, 4)-8(3, 5)	2446855.464	0.351D+01	5.6165	1050.158405	113
4(3, 2)-4(2, 3)	2462936.444	0.126D+01	1.8465	300.362492	114
13(1, 12)-12(4, 9)	-2477504.722	0.142D+02	0.0391	2042.310749	115
9(3, 7)-8(4, 4)	2531909.135	0.475D+01	0.5268	1131.776706	116
9(4, 6)-8(5, 3)	2547410.854	0.596D+01	0.6154	1255.913258	117
7(3, 4)-6(4, 3)	2567174.911	0.317D+01	0.5584	756.725607	118
11(4, 7)-11(3, 8)	2571779.833	0.733D+01	8.6099	1813.224239	119

TABLE III. CONTINUED (6)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
10(3, 8)-9(4, 5)	2574997.916	0.659D+01	0.4357	1360.236395	120	
9(0, 9)-8(3, 6)	-2576654.653	0.460D+01	0.0157	920.168847	121	
14(2, 13)-13(3, 10)	-2602479.486	0.293D+02	0.0375	2327.913757	122	
10(5, 6)-9(6, 3)	2618243.714	0.113D+02	0.5999	1631.384986	123	
10(1, 10)-9(2, 7)	-2619334.447	0.518D+01	0.0153	1114.550479	124	
5(3, 3)-5(2, 4)	2630964.885	0.145D+01	2.4848	416.209052	125	
4(1, 4)-3(0, 3)	2640476.668	0.788D+00	3.0063	136.761699	126	
11(6, 6)-10(7, 3)	2645021.037	0.141D+02	0.5637	2054.371769	127	
5(1, 4)-4(4, 1)	-2657676.189	0.233D+01	0.0019	399.457645	128	
7(4, 3)-7(3, 4)	2664580.940	0.280D+01	4.2232	842.357333	129	
5(2, 4)-5(1, 5)	2685643.015	0.131D+01	1.7129	326.625656	130	
11(6, 5)-10(7, 4)	2689143.763	0.142D+02	0.5658	2054.348343	131	
12(7, 6)-11(8, 3)	2712467.886	0.150D+03	0.5286	2522.323635	132	
12(7, 5)-11(8, 4)	2721710.438	0.149D+03	0.5290	2522.319822	133	
2(2, 1)-1(1, 0)	2773979.082	0.514D+00	1.5000	42.371746	134	
10(3, 7)-9(6, 4)	-2790983.252	0.119D+02	0.0101	1538.150293	135	
10(5, 5)-9(6, 4)	2801841.611	0.119D+02	0.6120	1631.247460	136	
12(5, 7)-12(4, 8)	2848980.938	0.117D+02	9.2686	2205.654682	137	
6(3, 4)-6(2, 5)	2880032.839	0.167D+01	2.9535	552.911818	138	
6(1, 5)-6(0, 6)	2884278.158	0.146D+01	1.8642	446.696836	139	
6(4, 2)-6(3, 3)	2884946.907	0.244D+01	3.0649	661.549569	140	
14(1, 13)-13(4, 10)	-2947362.414	0.267D+02	0.0357	2327.883373	141	
6(2, 4)-5(3, 3)	2962107.729	0.156D+01	0.8640	503.968582	142	
2(2, 0)-1(1, 1)	2968750.797	0.458D+00	1.2438	37.137136	143	

TABLE III. CONTINUED (7)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
5(1, 4)- 4(2, 3)	2970798.379	0.123D+01	1.6348	300.362492	144
12(4, 8)-12(3, 9)	2991518.018	0.952D+01	8.4862	2105.868396	145
11(5, 6)-11(4, 7)	2997532.402	0.839D+01	7.7731	1899.009568	146
8(2, 6)- 8(1, 7)	2998566.515	0.199D+01	3.8126	882.890789	147
10(3, 7)-10(2, 8)	3003353.982	0.393D+01	6.0255	1437.969201	148
5(0, 5)- 4(1, 4)	3013201.195	0.976D+00	3.9098	224.838508	149
5(4, 1)- 5(3, 2)	3043769.625	0.199D+01	2.0686	508.812550	150
10(0, 10)- 9(3, 7)	-3048868.987	0.691D+01	0.0142	1114.532784	151
10(4, 7)- 9(5, 4)	3118962.256	0.716D+01	0.7495	1477.299110	152
4(4, 0)- 4(3, 1)	3126590.401	0.151D+01	1.0924	383.842826	153
5(1, 5)- 4(0, 4)	3135014.311	0.115D+01	3.9731	222.052850	154
9(4, 5)- 8(5, 4)	3149857.950	0.689D+01	0.6882	1255.168458	155
4(4, 1)- 4(3, 2)	3165538.123	0.153D+01	1.0866	382.517197	156
6(2, 5)- 6(1, 6)	3167583.302	0.158D+01	1.7895	447.252627	157
5(4, 2)- 5(3, 3)	3182190.417	0.195D+01	2.0240	503.968582	158
7(2, 5)- 6(5, 2)	-3183483.093	0.480D+01	0.0030	782.410239	159
7(3, 5)- 7(2, 6)	3210366.183	0.218D+01	3.2671	709.608750	160
6(4, 3)- 6(3, 4)	3230151.715	0.228D+01	2.8683	648.979359	161
10(5, 5)-10(4, 6)	3245335.079	0.640D+01	6.2884	1616.454112	162
11(5, 7)-10(6, 4)	3307357.337	0.123D+02	0.7912	1875.464271	163
11(1, 11)-10(2, 8)	-3323230.592	0.852D+01	0.0132	1327.118176	164
7(4, 4)- 7(3, 5)	3329192.801	0.251D+01	3.6131	816.695024	165
3(2, 2)- 2(1, 1)	3331462.260	0.981D+00	1.6667	95.175944	166
12(6, 7)-11(7, 4)	3354493.768	0.182D+02	0.7649	2321.908993	167

TABLE III. CONTINUED (8)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
12(6, 6)-11(7, 5)	3468213.774	0.182D+02	0.7729	2321.816431	168	
12(4, 8)-11(7, 5)	-3482442.093	0.192D+02	0.0083	2205.654682	169	
8(4, 5)- 8(3, 6)	3495365.089	0.303D+01	4.2307	1006.116783	170	
9(5, 4)- 9(4, 5)	3509452.406	0.524D+01	5.0330	1360.236395	171	
7(1, 6)- 7(0, 7)	3536666.843	0.195D+01	1.8571	586.243889	172	
11(4, 8)-10(5, 5)	3547233.475	0.105D+02	0.8005	1724.706823	173	
11(0, 11)-10(3, 8)	-3568085.802	0.983D+01	0.0127	1327.110553	174	
13(4, 9)-13(3, 10)	3569692.165	0.176D+02	8.1190	2414.723116	175	
6(0, 6)- 5(1, 5)	3599643.912	0.142D+01	4.9535	326.625656	176	
8(3, 6)- 8(2, 7)	3612977.315	0.295D+01	3.4606	885.600849	177	
6(1, 6)- 5(0, 5)	3654607.273	0.152D+01	4.9762	325.348067	178	
8(3, 5)- 7(4, 4)	3669864.266	0.427D+01	0.9026	927.744927	179	
11(3, 8)-11(2, 9)	3674234.312	0.477D+01	5.7637	1690.664992	180	
9(2, 7)- 9(1, 8)	3682708.233	0.275D+01	3.7234	1079.080152	181	
7(2, 6)- 7(1, 7)	3691321.272	0.183D+01	1.8307	586.479543	182	
11(5, 6)-10(6, 5)	3718055.413	0.131D+02	0.8341	1874.975511	183	
8(5, 3)- 8(4, 4)	3721520.728	0.460D+01	3.9855	1131.776706	184	
9(4, 6)- 9(3, 7)	3737022.447	0.360D+01	4.7027	1216.232093	185	
13(4, 10)-12(5, 7)	3762705.944	0.168D+02	0.6153	2300.686444	186	
12(4, 9)-11(5, 6)	3776034.237	0.139D+02	0.7471	1998.996473	187	
6(1, 5)- 5(2, 4)	3798279.055	0.187D+01	2.6597	416.209052	188	
4(2, 3)- 3(1, 2)	3807264.424	0.155D+01	1.9718	173.365838	189	
7(5, 2)- 7(4, 3)	3855291.485	0.414D+01	3.0348	931.238174	190	
9(3, 6)- 8(6, 3)	-3858107.819	0.112D+02	0.0033	1282.919859	191	

TABLE III. CONTINUED (9)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
6(5, 1)- 6(4, 2)	3922864.812	0.300D+01	2.0955	757.781026	192
12(5, 8)-11(6, 5)	3937035.604	0.153D+02	0.9568	2144.048511	193
5(5, 0)- 5(4, 1)	3949332.900	0.233D+01	1.1081	610.341762	194
6(5, 2)- 6(4, 3)	3953489.084	0.301D+01	2.0897	756.725607	195
7(5, 3)- 7(4, 4)	3954356.367	0.404D+01	3.0052	927.744927	196
5(5, 1)- 5(4, 2)	3956032.672	0.234D+01	1.1074	610.115013	197
8(5, 4)- 8(4, 5)	3971017.340	0.420D+01	3.8722	1122.709596	198
3(2, 1)- 2(1, 2)	3977049.238	0.874D+00	0.9239	779.496419	199
12(1,12)-11(2, 9)	-3981743.685	0.125D+02	0.0117	1557.848338	200
7(2, 5)- 6(3, 4)	4000157.706	0.251D+01	1.5000	648.979359	201
9(5, 5)- 9(4, 6)	4020120.778	0.454D+01	4.6812	1340.885726	202
10(4, 7)-10(3, 8)	4053416.746	0.387D+01	5.0346	1446.129068	203
9(3, 7)- 9(2, 8)	4072559.074	0.383D+01	3.5753	1080.386163	204
12(6, 6)-12(5, 7)	4101674.929	0.117D+02	6.9894	2300.686444	205
12(0,12)-11(3, 9)	-4113887.918	0.134D+02	0.0115	1557.844992	206
10(5, 6)-10(4, 7)	4118660.448	0.569D+01	5.4049	1581.336478	207
8(1, 7)- 8(0, 8)	4161920.188	0.260D+01	1.8660	744.064094	208
7(0, 7)- 6(1, 6)	4166853.792	0.184D+01	5.9751	447.252627	209
6(2, 4)- 5(5, 1)	-4176115.360	0.359D+01	0.0005	602.773846	210
7(1, 7)- 6(0, 6)	4190580.727	0.187D+01	5.9836	446.696836	211
5(2, 4)- 4(1, 3)	4218438.517	0.206D+01	2.4459	275.497109	212
8(2, 7)- 8(1, 8)	4240197.491	0.241D+01	1.8561	744.163105	213
10(4, 6)- 9(5, 5)	4241212.758	0.859D+01	0.9746	1474.982502	214
11(5, 7)-11(4, 8)	4279719.073	0.719D+01	6.0135	1843.029779	215

TABLE III. CONTINUED (10)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
10(2, 8)-10(1, 9)	4345505.189	0.372D+01	3.7069	1293.018771	216	
11(6, 5)-11(5, 6)	4348551.333	0.980D+01	5.8904	1998.996473	217	
12(3, 9)-12(2, 10)	4366788.819	0.755D+01	5.6338	1960.208020	218	
11(4, 8)-11(3, 9)	4435738.089	0.442D+01	5.2530	1695.069503	219	
13(5, 9)-12(6, 6)	4467764.902	0.202D+02	1.0642	2437.503573	220	
3(3, 1)-2(2, 0)	4468573.600	0.158D+01	2.3942	136.163990	221	
12(5, 8)-12(4, 9)	4509552.700	0.882D+01	6.4897	2124.951399	222	
3(3, 0)-2(2, 1)	4512388.623	0.157D+01	2.3651	134.901715	223	
10(6, 4)-10(5, 5)	4519595.211	0.929D+01	4.9192	1724.706823	224	
7(1, 6)-6(2, 5)	4535937.333	0.239D+01	3.7787	552.911818	225	
10(3, 8)-10(2, 9)	4571663.232	0.468D+01	3.6453	1293.634818	226	
6(2, 5)-5(1, 4)	4600440.999	0.241D+01	3.1282	399.457645	227	
13(1, 13)-12(2, 10)	-4602885.866	0.184D+02	0.0105	1806.672296	228	
9(6, 3)-9(5, 4)	4619378.989	0.864D+01	3.9967	1477.299110	229	
11(4, 7)-10(7, 4)	-4656939.972	0.164D+02	0.0032	1899.009568	230	
8(6, 2)-8(5, 3)	4668658.144	0.796D+01	3.0777	1255.913258	231	
13(0, 13)-12(3, 10)	-4671880.519	0.189D+02	0.0104	1806.670794	232	
10(6, 5)-10(5, 6)	4684417.541	0.908D+01	4.8534	1718.720183	233	
9(6, 4)-9(5, 5)	4684706.226	0.857D+01	3.9773	1474.982502	234	
7(6, 1)-7(5, 2)	4687493.180	0.632D+01	2.1312	1059.836837	235	
6(6, 0)-6(5, 1)	4689504.614	0.676D+01	1.1227	888.633693	236	
8(6, 3)-8(5, 4)	4690074.003	0.798D+01	3.0730	1255.168458	237	
6(6, 1)-6(5, 2)	4690509.238	0.675D+01	1.1227	888.599790	238	
7(6, 2)-7(5, 3)	4693011.041	0.634D+01	2.1304	1059.648039	239	

TABLE III. CONTINUED (11)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
11(6, 6)-11(5, 7)	4701176.316	0.952D+01	5.6966	1985.785821	240
8(0, 8)- 7(1, 7)	4724266.649	0.228D+01	6.9853	586.479543	241
8(1, 8)- 7(0, 7)	4734299.654	0.226D+01	6.9886	586.243889	242
12(5, 7)-11(6, 6)	4739308.184	0.153D+02	1.0852	2142.600161	243
12(6, 7)-12(5, 8)	4749582.003	0.104D+02	6.4880	2275.373865	244
9(1, 8)- 9(0, 9)	4764041.742	0.383D+01	1.8790	920.168847	245
9(2, 8)- 9(1, 9)	4801945.814	0.370D+01	1.8751	920.210515	246
9(3, 6)- 8(4, 5)	4802983.524	0.608D+01	1.3994	1122.709596	247
13(5, 9)-13(4, 10)	4806733.887	0.124D+02	6.8374	2426.196787	248
12(4, 9)-12(3, 10)	4869933.257	0.644D+01	5.3923	1962.507934	249
11(2, 9)-11(1, 10)	4971053.954	0.486D+01	3.7198	1524.848504	250
8(3, 5)- 7(6, 2)	-4977503.142	0.991D+01	0.0009	1050.158405	251
8(2, 6)- 7(3, 5)	4983065.897	0.377D+01	2.3838	816.695024	252
7(2, 6)- 6(1, 5)	4997623.841	0.263D+01	4.0005	542.905986	253
13(3, 10)-13(2, 11)	5031639.425	0.142D+02	5.5973	2246.885715	254
11(3, 9)-11(2, 10)	5094456.993	0.577D+01	3.6928	1525.136733	255
4(3, 2)- 3(2, 1)	5107286.408	0.222D+01	2.3198	212.156484	256
8(1, 7)- 7(2, 6)	5194865.565	0.278D+01	4.8841	709.608750	257
14(1, 14)-13(2, 11)	-5197469.663	0.302D+02	0.0096	2073.516812	258
4(2, 2)- 3(1, 3)	5201435.012	0.154D+01	0.6107	142.278553	259
14(0, 14)-13(3, 11)	-5232876.142	0.303D+02	0.0095	2073.516123	260
12(7, 5)-12(6, 6)	5264437.967	0.180D+02	5.8524	2437.503573	261
9(0, 9)- 8(1, 8)	5276520.153	0.292D+01	7.9895	744.163105	262
9(1, 9)- 8(0, 8)	5280737.584	0.287D+01	7.9909	744.064094	263

TABLE III. CONTINUED (12)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
4(3, 1)- 3(2, 2)	5322554.370	0.220D+01	2.1642	206.301547	264	
11(7, 4)-11(6, 5)	5332123.839	0.120D+02	4.9505	2144.048511	265	
13(4, 10)-13(3, 11)	5340225.633	0.114D+02	5.4835	2248.066058	266	
10(1, 9)-10(0, 10)	5350876.015	0.573D+01	1.8935	1114.532784	267	
7(7, 0)- 7(6, 1)	5354944.169	0.217D+02	1.1362	1216.194757	268	
7(7, 1)- 7(6, 2)	5355084.939	0.217D+02	1.1362	1216.190015	269	
10(7, 3)-10(6, 4)	5363512.617	0.117D+02	4.0480	1875.464271	270	
12(7, 6)-12(6, 7)	5366254.788	0.183D+02	5.8130	2433.802845	271	
8(7, 1)- 8(6, 2)	5367751.555	0.145D+02	2.1644	1411.642910	272	
8(7, 2)- 8(6, 3)	5368644.949	0.145D+02	2.1643	1411.612465	273	
10(2, 9)-10(1, 10)	5368814.187	0.568D+01	1.8918	1114.550479	274	
9(7, 2)- 9(6, 3)	5372426.485	0.144D+02	3.1260	1631.384986	275	
11(7, 5)-11(6, 6)	5372769.339	0.118D+02	4.9378	2142.600161	276	
9(7, 3)- 9(6, 4)	5376410.157	0.144D+02	3.1252	1631.247460	277	
10(7, 4)-10(6, 5)	5377462.983	0.117D+02	4.0445	1874.975511	278	
11(4, 7)-10(5, 6)	5404940.552	0.109D+02	1.3613	1718.720183	279	
8(2, 7)- 7(1, 6)	5437830.301	0.276D+01	4.9793	1704.214380	280	
12(2, 10)-12(1, 11)	5563887.145	0.799D+01	3.7426	1774.616748	281	
12(3, 10)-12(2, 11)	5628790.724	0.847D+01	3.7301	1774.751712	282	
15(3, 3)- 4(2, 2)	5641760.789	0.272D+01	2.3265	3115.779725	283	
15(1, 15)-14(2, 12)	-5773428.376	0.572D+02	0.0088	2358.303643	284	
15(0, 15)-14(3, 12)	-5791481.488	0.572D+02	0.0088	2358.303318	285	
9(1, 8)- 8(2, 7)	5800364.404	0.320D+01	5.9482	885.600849	286	
10(4, 6)- 9(7, 3)	-5819903.625	0.168D+02	0.0011	1616.454112	287	

TABLE III. CONTINUED (13)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
10(0,10)- 9(1, 9)	5825635.901	0.398D+01	8.9904	920.210515	288
10(1,10)- 9(0, 9)	5827415.529	0.393D+01	8.9910	920.168847	289
9(2, 7)- 8(3, 6)	5870095.322	0.509D+01	3.4659	1.006.116783	290
10(3, 7)- 9(4, 6)	5913843.752	0.813D+01	2.1086	1.340.885726	291
9(2, 8)- 8(1, 7)	5920763.209	0.292D+01	5.9889	882.890789	292
11(1,10)-11(0,11)	5928035.449	0.802D+01	1.9087	1327.110553	293
11(2,10)-11(1,11)	5936447.831	0.803D+01	1.9079	1327.118176	294
8(8, 0)- 8(7, 1)	5948909.454	0.178D+03	1.1490	1590.691804	295
8(8, 1)- 8(7, 2)	5948928.591	0.178D+03	1.1490	1590.691159	296
9(8, 1)- 9(7, 2)	5974545.464	0.140D+03	2.1953	1810.589819	297
9(8, 2)- 9(7, 3)	5974682.116	0.140D+03	2.1952	1810.585174	298
10(8, 2)-10(7, 3)	5995240.381	0.140D+03	3.1728	2054.371769	299
10(8, 3)-10(7, 4)	5995921.972	0.140D+03	3.1727	2054.348343	300
11(8, 3)-11(7, 4)	6008280.670	0.148D+03	4.1045	2321.908993	301
11(8, 4)-11(7, 5)	6010941.304	0.148D+03	4.1038	2321.816431	302
6(3, 4)- 5(2, 3)	6069850.971	0.302D+01	2.4582	446.510953	303
4(4, 1)- 3(3, 0)	6076475.933	0.267D+01	3.3913	285.418777	304
7(3, 4)- 6(6, 1)	-6076823.411	0.821D+01	0.0001	842.357333	305
4(4, 0)- 3(3, 1)	6083242.543	0.267D+01	3.3883	285.219540	306
13(2,11)-13(1,12)	6133004.039	0.147D+02	3.7692	2042.310749	307
13(3,11)-13(2,12)	6166481.568	0.143D+02	3.7631	2042.374403	308
5(3, 2)- 4(2, 3)	6249176.404	0.279D+01	1.8471	300.362492	309
11(0,11)-10(1,10)	6372391.617	0.545D+01	9.9890	1114.550479	310
11(1,11)-10(0,10)	6373150.612	0.541D+01	9.9893	1114.532784	311

TABLE III. CONTINUED (14)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
10(1, 9)-9(2, 8)	6374566.102	0.376D+01	6.9804	1080.386163	312
7(3, 5)-6(2, 4)	6413196.465	0.340D+01	2.7576	602.773846	313
10(2, 9)-9(1, 8)	6432187.973	0.334D+01	6.9984	1079.080152	314
3(3, 1)-2(0, 2)	6449397.542	0.198D+01	0.0133	70.090825	315
9(9, 0)-9(8, 1)	6483026.333	0.880D+03	1.1616	2009.879176	316
9(9, 1)-9(8, 2)	6483028.915	0.880D+03	1.1616	2009.879089	317
12(1,11)-12(0,12)	6498654.661	0.106D+02	1.9246	1557.844992	318
12(2,11)-12(1,12)	6502600.488	0.107D+02	1.9242	1557.848338	319
10(9, 1)-10(8, 2)	6520987.037	0.737D+03	2.2246	2254.351434	320
10(9, 2)-10(8, 3)	6521007.368	0.737D+03	2.2246	2254.350744	321
12(4, 8)-11(5, 7)	6591503.562	0.140D+02	1.9059	1985.785821	322
12(5, 7)-11(8, 4)	-6644402.459	0.148D+03	0.0013	2300.686444	323
5(2, 3)-4(1, 4)	6645573.639	0.239D+01	0.3892	224.838508	324
10(2, 8)-9(3, 7)	6647512.217	0.613D+01	4.6241	1216.232093	325
14(2,12)-14(1,13)	6685405.274	0.252D+02	3.7979	2327.883373	326
14(3,12)-14(2,13)	6702537.745	0.242D+02	3.7948	2327.913757	327
8(3, 6)-7(2, 5)	6706554.404	0.405D+01	3.2617	782.410239	328
5(4, 2)-4(3, 1)	6783470.480	0.314D+01	3.2675	383.842826	329
5(4, 1)-4(3, 2)	6830009.585	0.316D+01	3.2465	382.517197	330
9(4, 5)-8(7, 2)	-6908861.002	0.177D+02	0.0003	1360.236395	331
12(0,12)-11(1,11)	6917016.906	0.718D+01	10.9861	1327.118176	332
12(1,12)-11(0,11)	6917345.718	0.716D+01	10.9862	1327.110553	333
11(1,10)-10(2, 9)	6931612.879	0.451D+01	7.9934	1293.634818	334
11(3, 8)-10(4, 7)	6951821.167	0.957D+01	3.0533	1581.336478	335

TABLE III. CONTINUED (15)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
11(2,10)-10(1, 9)	6958722.428	0.418D+01	8.0016	1293.018771	336
9(3, 7)- 8(2, 6)	6994755.768	0.468D+01	3.9865	982.912187	337
13(1,12)-13(0,13)	7064309.054	0.157D+02	1.9413	1806.670796	338
13(2,12)-13(1,13)	7066172.384	0.158D+02	1.9411	1806.672296	339
10(3, 8)- 9(2, 7)	7321142.972	0.506D+01	4.8916	1201.922059	340
11(2, 9)-10(3, 8)	7331003.601	0.685D+01	5.7622	1446.129068	341
6(3, 3)- 5(2, 4)	7355124.706	0.339D+01	1.4265	416.209052	342
4(3, 2)- 3(0, 3)	7367565.504	0.293D+01	0.0508	136.761699	343
6(4, 3)- 5(3, 2)	7432247.528	0.335D+01	3.1571	508.812550	344
13(0,13)-12(1,12)	7459510.692	0.967D+01	11.9818	1557.848338	345
13(1,13)-12(0,12)	7459655.939	0.967D+01	11.9818	1557.844992	346
12(1,11)-11(2,10)	7479223.736	0.569D+01	8.9952	1525.136733	347
12(2,11)-11(1,10)	7491910.757	0.561D+01	8.9991	1524.848504	348
6(4, 2)- 5(3, 3)	7609106.727	0.339D+01	3.0697	503.968582	349
5(5, 1)- 4(4, 0)	7612912.751	0.349D+01	4.3935	488.134641	350
5(5, 0)- 4(4, 1)	7613804.362	0.349D+01	4.3931	488.108168	351
14(1,13)-14(0,14)	7625739.360	0.295D+02	1.9587	2073.516123	352
14(2,13)-14(1,14)	7626629.602	0.296D+02	1.9586	2073.516812	353
11(5, 6)-10(8, 3)	-7655329.542	0.140D+03	0.0005	1998.996473	354
11(3, 9)-10(2, 8)	7707674.232	0.578D+01	5.8909	1437.969201	355
13(4, 9)-12(5, 8)	7747278.207	0.244D+02	2.6600	2275.373865	356
12(3, 9)-11(4, 8)	7879704.618	0.110D+02	4.1784	1843.029779	357
8(4, 4)- 7(7, 1)	-7885732.617	0.227D+02	0.0001	1131.776706	358
12(2,10)-11(3, 9)	7948653.888	0.781D+01	6.8519	1695.069503	359

TABLE III. CONTINUED (16)

TRANSITION	FREQUENCY	STB.	DEV.	STR.	ENERGY	#
7(4, 4)- 6(3, 3)	7980337.174	0.369D+01	3.0648	661.549569	360	
14(0,14)-13(1,13)	7999777.810	0.158D+02	12.9764	1806.672296	361	
14(1,14)-13(0,13)	7999843.430	0.158D+02	12.9764	1806.670796	362	
13(1,12)-12(2,11)	8021219.258	0.835D+01	9.9900	1774.751712	363	
13(2,12)-12(1,11)	8027173.662	0.851D+01	9.9918	1774.616748	364	
12(3,10)-11(2, 9)	8149647.527	0.737D+01	6.9141	1690.664992	365	
6(2, 4)- 5(1, 5)	8278715.628	0.325D+01	0.2592	326.625656	366	
6(5, 2)- 5(4, 1)	8341966.987	0.382D+01	4.2595	610.341762	367	
6(5, 1)- 5(4, 2)	8349781.123	0.383D+01	4.2567	610.115013	368	
8(4, 5)- 7(3, 4)	8404750.573	0.469D+01	3.0459	842.357333	369	
5(3, 3)- 4(0, 4)	8451622.211	0.376D+01	0.0958	222.052850	370	
7(4, 3)- 6(3, 4)	8461907.566	0.369D+01	2.7911	648.979359	371	
13(2,11)-12(3,10)	8525432.574	0.956D+01	7.9013	1962.507934	372	
15(0,15)-14(1,14)	8537685.860	0.307D+02	13.9701	2073.516812	373	
15(1,15)-14(0,14)	8537716.258	0.307D+02	13.9701	2073.516123	374	
10(5, 5)- 9(8, 2)	-8549250.661	0.142D+03	0.0002	1724.706823	375	
14(1,13)-13(2,12)	8559344.787	0.148D+02	10.9799	2042.374403	376	
14(2,13)-13(1,12)	8562163.978	0.150D+02	10.9808	2042.310749	377	
13(3,11)-12(2,10)	8629768.086	0.948D+01	7.9321	1960.208020	378	
7(3, 4)- 6(2, 5)	8677359.465	0.402D+01	1.0195	552.911818	379	
13(3,10)-12(4, 9)	8687138.742	0.153D+02	5.3718	2124.951399	380	
9(4, 6)- 8(3, 5)	8715787.046	0.586D+01	3.1681	1050.158405	381	
10(4, 7)- 9(3, 6)	8946306.428	0.651D+01	3.4810	1282.919859	382	
7(5, 3)- 6(4, 2)	9049746.635	0.406D+01	4.1411	757.781026	383	

TABLE III. CONTINUED (17)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
14(2,12)-13(3,11)	9078268.492	0.134D+02	8.9237	2248.066058	384
6(6, 1)- 5(5, 0)	9083143.325	0.647D+01	5.3939	742.077309	385
6(6, 0)- 5(5, 1)	9083253.065	0.647D+01	5.3939	742.074041	386
7(5, 2)- 6(4, 3)	9087047.336	0.404D+01	4.1278	756.725607	387
14(3,12)-13(2,11)	9131697.684	0.133D+02	8.9394	2246.885715	388
11(4, 8)-10(3, 7)	9140058.338	0.721D+01	4.0153	1538.150293	389
12(4, 9)-11(3, 8)	9345346.471	0.926D+01	4.7719	1813.224239	390
9(5, 4)- 8(8, 1)	-9348337.187	0.183D+03	0.0000	1477.299110	391
4(4, 1)- 3(1, 2)	9435738.991	0.414D+01	0.0044	173.365838	392
8(4, 4)- 7(3, 5)	9445912.531	0.455D+01	2.3776	816.695024	393
13(4,10)-12(3, 9)	9603204.899	0.119D+02	5.7006	2105.868396	394
6(3, 4)- 5(0, 5)	9702223.415	0.437D+01	0.1241	325.348067	395
8(5, 4)- 7(4, 3)	9711186.973	0.448D+01	4.0158	931.238174	396
7(6, 2)- 6(5, 1)	9819892.863	0.618D+01	5.2518	888.633693	397
7(6, 1)- 6(5, 2)	9821051.432	0.618D+01	5.2514	888.599790	398
11(6, 5)-10(9, 2)	-9827785.578	0.861D+03	0.0001	2144.048511	399
8(5, 3)- 7(4, 4)	9838240.458	0.425D+01	3.9673	927.744927	400
5(4, 2)- 4(1, 3)	10031593.818	0.493D+01	0.0227	275.497109	401
7(2, 5)- 6(1, 6)	10047773.847	0.392D+01	0.1886	447.252627	402
8(3, 5)- 7(2, 6)	10209423.250	0.467D+01	0.7161	709.608750	403
9(5, 5)- 8(4, 4)	10289052.360	0.554D+01	3.8799	1131.776706	404
4(4, 0)- 3(1, 3)	10368506.139	0.417D+01	0.0016	142.278553	405
7(7, 1)- 6(6, 0)	10485473.188	0.209D+02	6.3930	1045.058707	406
7(7, 0)- 6(6, 1)	10485486.363	0.209D+02	6.3930	1045.058315	407

TABLE III. CONTINUED (18)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
10(6, 4)- 9(9, 1)	-10512684.365	0.100D+04	0.0000	1875.464271	408
8(6, 3)- 7(5, 2)	10545969.490	0.6557D+01	5.1326	1059.836837	409
8(6, 2)- 7(5, 3)	10552542.234	0.6558D+01	5.1305	1059.648039	410
9(4, 5)- 8(3, 6)	10616240.379	0.607D+01	1.8784	1006.116783	411
9(5, 4)- 8(4, 5)	10630327.696	0.519D+01	3.7329	1122.709596	412
6(4, 3)- 5(1, 4)	10710625.553	0.517D+01	0.0690	399.457645	413
10(5, 6)- 9(4, 5)	10747075.109	0.685D+01	3.7627	1360.236395	414
11(5, 7)- 10(4, 6)	11072287.628	0.882D+01	3.7294	1616.454112	415
7(3, 5)- 6(0, 6)	11092268.182	0.481D+01	0.1325	446.696836	416
8(7, 2)- 7(6, 1)	11227121.260	0.141D+02	6.2419	1216.194757	417
8(7, 1)- 7(6, 2)	11227282.748	0.141D+02	6.2419	1216.190015	418
9(6, 4)- 8(5, 3)	11252237.858	0.714D+01	5.0164	1255.913258	419
9(6, 3)- 8(5, 4)	11278689.345	0.713D+01	5.0080	1255.168458	420
12(5, 8)-11(4, 7)	11283119.339	0.122D+02	3.8497	1899.009568	421
13(5, 9)-12(4, 8)	11418420.769	0.168D+02	4.1718	2205.654682	422
10(5, 5)- 9(4, 6)	11506668.615	0.736D+01	3.3816	1340.885726	423
7(4, 4)- 6(1, 5)	11537182.825	0.544D+01	0.1441	542.905986	424
5(4, 1)- 4(1, 4)	11557098.422	0.524D+01	0.0046	224.838508	425
8(8, 1)- 7(7, 0)	11821105.682	0.170D+03	7.3909	1394.816443	426
6(8, 0)- 7(7, 1)	11821107.263	0.170D+03	7.3909	1394.816396	427
8(2, 6)- 7(1, 7)	11884753.352	0.459D+01	0.1508	586.479543	428
9(3, 6)- 8(2, 7)	11911325.928	0.566D+01	0.5230	885.600849	429
10(6, 5)- 9(5, 4)	11922040.244	0.831D+01	4.8898	1477.299110	430
9(7, 3)- 8(6, 2)	11959989.870	0.136D+02	6.1187	1411.642910	431

TABLE III. CONTINUED (19)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
9(7, 2)- 8(6, 3)	11961041.828	0.136D+02	6.1183	1411.612465	432	
10(4, 6)- 9(3, 7)	11998355.983	0.799D+01	1.4082	1216.232093	433	
10(6, 4)- 9(5, 5)	12006143.048	0.830D+01	4.8624	1474.982502	434	
11(5, 6)-10(4, 7)	12521133.402	0.104D+02	2.9009	1581.336478	435	
11(6, 6)-10(5, 5)	12528128.864	0.962D+01	4.7452	1724.706823	436	
8(4, 5)- 7(1, 6)	12546172.705	0.629D+01	0.2211	704.214380	437	
9(8, 2)- 8(7, 1)	12566920.431	0.138D+03	7.2304	1590.691804	438	
9(8, 1)- 8(7, 2)	12566942.343	0.138D+03	7.2304	1590.691159	439	
8(3, 6)- 7(0, 7)	12587474.459	0.526D+01	0.1294	586.243889	440	
10(7, 4)- 9(6, 3)	12680124.239	0.122D+02	6.0070	1631.384986	441	
10(7, 3)- 9(6, 4)	12684949.439	0.123D+02	6.0056	1631.247460	442	
11(6, 5)-10(5, 6)	12751024.287	0.949D+01	4.6668	1718.720183	443	
5(5, 1)- 4(2, 2)	12779983.878	0.588D+01	0.0019	315.779725	444	
6(4, 2)- 5(1, 5)	12925714.627	0.581D+01	0.0072	326.625656	445	
12(6, 7)-11(5, 6)	13035168.940	0.121D+02	4.5888	1998.996473	446	
9(9, 1)- 8(8, 0)	13101039.892	0.825D+03	8.3880	1789.126036	447	
9(9, 0)- 8(8, 1)	13101040.085	0.825D+03	8.3880	1789.126030	448	
5(5, 0)- 4(2, 3)	13242278.930	0.587D+01	0.0015	300.362492	449	
6(5, 2)- 5(2, 3)	13253491.769	0.662D+01	0.0086	446.510953	450	
10(8, 3)- 9(7, 2)	13303619.725	0.139D+03	7.1007	1810.589819	451	
10(8, 2)- 9(7, 3)	13303779.663	0.139D+03	7.1007	1810.585174	452	
11(7, 5)-10(6, 4)	13381302.993	0.116D+02	5.8955	1875.464271	453	
11(7, 4)-10(6, 5)	13398730.585	0.117D+02	5.8903	1874.975511	454	
12(6, 6)-11(5, 7)	13542159.429	0.113D+02	4.3866	1985.785821	455	

TABLE III. CONTINUED (20)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
11(4, 7)-10(3, 8)	13577017.746	0.9360+01	1.0483	1446.129068	456	
7(5, 3)- 6(2, 4)	13696745.634	0.6680+01	0.0268	602.773846	457	
12(5, 7)-11(4, 8)	13720203.574	0.1260+02	2.3478	1843.029779	458	
9(2, 7)- 8(1, 8)	13723270.128	0.5780+01	0.1297	744.163105	459	
10(3, 7)- 9(2, 8)	13723425.273	0.7130+01	0.4095	1080.386163	460	
9(4, 6)- 8(1, 7)	13730344.731	0.7240+01	0.2722	882.890789	461	
10(9, 2)- 9(8, 1)	13850081.629	0.7210+03	8.2175	2009.879176	462	
10(9, 1)- 9(8, 2)	13850084.585	0.7210+03	8.2175	2009.879089	463	
11(8, 4)-10(7, 3)	14028731.680	0.1480+03	6.9886	2054.371769	464	
11(8, 3)-10(7, 4)	14029548.272	0.1480+03	6.9884	2054.348343	465	
12(7, 6)-11(6, 5)	14052872.395	0.1700+02	5.7752	2144.048511	466	
12(7, 5)-11(6, 6)	14105421.080	0.1700+02	5.7593	2142.600161	467	
9(3, 7)- 8(0, 8)	14155242.472	0.6000+01	0.1218	744.064094	468	
6(5, 1)- 5(2, 4)	14162936.425	0.6690+01	0.0053	416.209052	469	
8(5, 4)- 7(2, 5)	14172936.833	0.6950+01	0.0687	782.410239	470	
7(4, 3)- 6(1, 6)	14509523.707	0.6190+01	0.0080	447.252627	471	
9(5, 5)- 8(2, 6)	14751898.993	0.7960+01	0.1463	982.912187	472	
10(4, 7)- 9(1, 8)	15057267.951	0.7820+01	0.2932	1079.080152	473	
7(5, 2)- 6(2, 5)	15197231.890	0.6830+01	0.0110	552.911818	474	
12(4, 8)-11(3, 9)	15306960.724	0.1100+02	0.8078	1695.069503	475	
10(5, 6)- 9(2, 7)	15493220.166	0.8480+01	0.2529	1201.922059	476	
10(2, 8)- 9(1, 9)	15522017.105	0.7280+01	0.1163	920.210515	477	
11(3, 8)-10(2, 9)	15576901.145	0.8450+01	0.3448	1293.634818	478	
5(5, 1)- 4(0, 4)	15589845.299	0.6770+01	0.0000	222.052850	479	

TABLE III. CONTINUED (21)

TRANSITION	FREQUENCY	STD. DEV.	STR.	ENERGY	#
10(3, 8)- 9(0, 9)	15767892.948	0.701D+01	0.1133	920.168847	480
6(6, 1)- 5(3, 2)	16076245.850	0.905D+01	0.0012	508.812550	481
6(6, 0)- 5(3, 3)	16221476.154	0.903D+01	0.0011	503.968582	482
8(4, 4)- 7(1, 7)	16347599.986	0.687D+01	0.0067	586.479543	483
8(5, 3)- 7(2, 6)	16377799.442	0.711D+01	0.0171	709.608750	484
11(5, 7)-10(2, 8)	16423131.394	0.914D+01	0.3573	1437.969201	485
11(4, 8)-10(1, 9)	16488917.510	0.862D+01	0.2941	1293.018771	486
7(6, 2)- 6(3, 3)	16627704.582	0.967D+01	0.0046	661.549569	487
6(5, 2)- 5(0, 5)	16885864.214	0.765D+01	0.0002	325.348067	488
7(6, 1)- 6(3, 4)	17004692.231	0.968D+01	0.0041	648.979359	489
8(6, 3)- 7(3, 4)	17065841.915	0.100D+02	0.0122	842.357333	490
13(4, 9)-12(3, 10)	17126764.164	0.223D+02	0.6592	1962.507934	491
11(2, 9)-10(1, 10)	17271481.020	0.838D+01	0.1066	1114.550479	492
11(3, 9)-10(0, 10)	17404055.436	0.804D+01	0.1054	1114.532784	493
12(3, 9)-11(2, 10)	17409899.700	0.101D+02	0.3068	1525.136733	494
9(6, 4)- 8(3, 5)	17420614.049	0.984D+01	0.0286	1050.158405	495
12(5, 8)-11(2, 9)	17529133.484	0.122D+02	0.4306	1690.664992	496
9(5, 4)- 8(2, 7)	17738670.100	0.844D+01	0.0209	885.600849	497
10(6, 5)- 9(3, 6)	17749384.416	0.105D+02	0.0625	1282.919859	498
8(6, 2)- 7(3, 5)	17836091.403	0.993D+01	0.0095	816.695024	499
12(4, 9)-11(1, 10)	17990634.737	0.105D+02	0.2851	1524.848504	500
11(6, 6)-10(3, 7)	18120953.728	0.116D+02	0.1269	1538.150293	501
7(5, 3)- 6(0, 6)	18375817.350	0.770D+01	0.0004	446.696836	502
9(4, 5)- 8(1, 8)	18469415.184	0.792D+01	0.0044	744.163105	503

TABLE III. CONTINUED (22)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
12(6, 7)-11(3, 8)	18604481.175	0.145D+02	0.2307	1813.224239	504	
9(6, 3)- 8(3, 6)	18745071.774	0.967D+01	0.0173	1006.116783	505	
13(5, 9)-12(2, 10)	18776727.606	0.183D+02	0.4675	1960.208020	506	
12(2, 10)-11(1, 11)	18979558.712	0.976D+01	0.0990	1327.118176	507	
12(3, 10)-11(0, 11)	19048736.929	0.970D+01	0.0985	1327.110553	508	
7(7, 1)- 6(4, 2)	19097842.614	0.222D+02	0.0009	757.781026	509	
7(7, 0)- 6(4, 3)	19129484.685	0.222D+02	0.0009	756.725607	510	
13(3, 10)-12(2, 11)	19185862.722	0.154D+02	0.2820	1774.751712	511	
10(5, 5)- 9(2, 8)	19316250.136	0.100D+02	0.0207	1080.386163	512	
6(6, 1)- 5(1, 4)	19354623.875	0.102D+02	0.0000	399.457645	513	
13(4, 10)-12(1, 11)	19533880.863	0.133D+02	0.2724	1774.616748	514	
10(6, 4)- 9(3, 7)	19763286.273	0.110D+02	0.0263	1216.232093	515	
8(7, 2)- 7(4, 3)	19769905.925	0.166D+02	0.0031	931.238174	516	
8(7, 1)- 7(4, 4)	19874650.156	0.166D+02	0.0030	927.744927	517	
8(5, 4)- 7(0, 7)	20053856.888	0.786D+01	0.0005	586.243889	518	
7(6, 2)- 6(1, 5)	20184550.233	0.104D+02	0.0001	542.905986	519	
9(7, 3)- 8(4, 4)	20350168.742	0.151D+02	0.0075	1131.776706	520	
9(7, 2)- 8(4, 5)	20622133.171	0.153D+02	0.0071	1122.709596	521	
13(2, 11)-12(1, 12)	20656823.786	0.141D+02	0.0928	1557.848338	522	
13(3, 11)-12(0, 12)	20692309.891	0.141D+02	0.0926	1557.844992	523	
10(7, 4)- 9(4, 5)	20808955.634	0.136D+02	0.0155	1360.236395	524	
10(4, 6)- 9(1, 9)	20872860.871	0.934D+01	0.0025	920.210515	525	
11(6, 5)-10(3, 8)	20923101.481	0.133D+02	0.0342	1446.129068	526	
11(5, 6)-10(2, 9)	21146213.380	0.116D+02	0.0168	1293.634818	527	

TABLE III. CONTINUED (23)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
11(7, 5)-10(4, 6)	21146233.283	0.154D+02	0.0299	1616.454112	528	
8(6, 3)- 7(1, 6)	21207264.047	0.105D+02	0.0004	704.214380	529	
10(7, 3)- 9(4, 6)	21389776.442	0.139D+02	0.0136	1340.885726	530	
12(7, 6)-11(4, 7)	21398956.130	0.185D+02	0.0563	1899.009568	531	
8(8, 1)- 7(5, 2)	21863543.031	0.183D+03	0.0007	1059.836837	532	
8(8, 0)- 7(5, 3)	21869203.243	0.183D+03	0.0007	1059.648039	533	
9(5, 5)- 8(0, 8)	21912385.697	0.910D+01	0.0006	744.064094	534	
11(7, 4)-10(4, 7)	22201808.574	0.161D+02	0.0227	1581.336478	535	
12(6, 6)-11(3, 9)	22257616.591	0.158D+02	0.0380	1695.069503	536	
14(2, 12)-13(1, 13)	22310922.444	0.244D+02	0.0877	1806.672296	537	
14(3, 12)-13(0, 13)	22329010.778	0.241D+02	0.0876	1806.670796	538	
9(6, 4)- 8(1, 7)	22435171.734	0.104D+02	0.0008	882.890789	539	
9(8, 2)- 8(5, 3)	22603330.130	0.143D+03	0.0023	1255.913258	540	
9(8, 1)- 8(5, 4)	22625661.295	0.143D+03	0.0023	1255.168458	541	
12(7, 5)-11(4, 8)	23086316.470	0.193D+02	0.0337	1843.029779	542	
12(5, 7)-11(2, 10)	23250398.656	0.138D+02	0.0115	1525.1336733	543	
10(8, 3)- 9(5, 4)	23295425.200	0.141D+03	0.0054	1477.299110	544	
10(8, 2)- 9(5, 5)	23364896.046	0.141D+03	0.0053	1474.982502	545	
11(4, 7)-10(1, 10)	23517495.165	0.108D+02	0.0014	1114.550479	546	
7(7, 1)- 6(2, 4)	23744841.613	0.228D+02	0.0000	602.773846	547	
10(6, 5)- 9(1, 8)	23860345.940	0.111D+02	0.0013	1079.080152	548	
11(8, 4)-10(5, 5)	23911839.507	0.147D+03	0.0104	1724.706823	549	
10(5, 6)- 9(0, 9)	23939970.141	0.103D+02	0.0005	920.168847	550	
11(8, 3)-10(5, 6)	24091428.796	0.147D+03	0.0101	1718.720183	551	

TABLE III, CONTINUED (24)

TRANSITION	FREQUENCY	STD.	DEV.	STR.	ENERGY	#
8(7, 2)- 7(2, 5)	24231655+785	0.170D+02	0.0000	782.410239	552	
9(9, 1)- 8(6, 2)	24417700+901	0.100D+04	0.0005	1411.642910	553	
9(9, 0)- 8(6, 3)	24418613+625	0.100D+04	0.0005	1411.612465	554	
9(7, 3)- 8(2, 6)	24813015+376	0.157D+02	0.0001	982.912187	555	

energy falls below 2625 cm⁻¹. Note that in a few cases the line strength is zero to 4 places. We have decided not to exclude these lines, and point out that, in these cases, $gS < 5 \times 10^{-5}$. Readers in need of parameters for higher energy states are referred to reference 20.

There are two ways that the results of this work can be used. First, the spectral constants of Table II can be used along with the computational techniques that we have described. We offer two cautions about this approach. First, the significant figures published in Table II are absolutely necessary to accurately calculate the spectrum, even though they greatly exceed the statistical uncertainty in the constants. This is because some of these constants are highly correlated. Secondly, all of our calculations and constants are in the context of a basis set which includes centrifugal distortion. Calculations which use operators evaluated in a rigid rotor basis must consider "2nd order corrections". While these are small for most molecules, they can be large in molecules with extreme centrifugal distortion. For a more detailed discussion of this, readers are referred to references 8 and 9.

The other approach is to simply use the results tabulated in Table III. The authors can make this table available to interested readers on magnetic media, preferably DEC RX02 floppy disks. Alternatively, DEC VAX11/780 tape could be produced.

References

1. P. Helminger, J.K. Messer, and F.C. De Lucia, Appl. Phys. Letters 42, 309 (1983).
2. F.C. De Lucia, P. Helminger, R.L. Cook, and W. Gordy, Phys. Rev. A5, 487 (1972).
3. J. Kauppinen, T. Karkkainen, and E. Kyrö, J. Mol. Spectrosc. 71, 15 (1978).
4. Masataka Mizushima, Int. J. of Infrared and Millimeter Waves 3, 379 (1982).
5. P. Helminger, F.C. De Lucia, and W. Gordy, Phys. Rev. Letters 25, 1397 (1970).

6. E.B. Wilson, Jr. and J.B. Howard, *J. Chem. Phys.* 4, 260 (1936).
7. J.K.G. Watson, *J. Chem. Phys.* 46, 1935 (1967).
8. F.C. De Lucia, R.L. Cook, P. Helminger, and W. Gordy, *J. Chem. Phys.* 55, 5334 (1971).
9. W. Gordy and R.L. Cook, Microwave Molecular Spectra, Interscience, New York, 1970.
10. R.L. Cook, F.C. De Lucia, and P. Helminger, *J. Mol. Spectrosc.* 53, 62 (1974).
11. P. Helminger, R.L. Cook, and F.C. De Lucia, *J. Mol. Spectrosc.* 40, 125 (1971).
12. R.L. Cook, F.C. De Lucia, and P. Helminger, *J. Mol. Spectrosc.* 41, 123 (1972).
13. W.H. Kirchhoff, *J. Mol. Spectrosc.* 41, 333 (1972).
14. G. Steenbeckeliers and J. Bellet, *J. Mol. Spectrosc.* 45, 10 (1973).
15. F.X. Kneizys, J.N. Freedman, and S.A. Clough, *J. Chem. Phys.* 44, 2552 (1966).
16. M.N. Moazzen-Ahmadi and J.A. Roberts, *J. Quant. Spec. Rad. Trans.* (1983) to be published.
17. C.H. Townes and A.L. Schawlow, Microwave Spectroscopy, McGraw-Hill, New York, 1955.
18. J.M. Flaud and C. Camy-Peyret, *Mol. Phys.* 26, 811 (1973).
19. C. Camy-Peyret, J.M. Flaud, G. Guelachvili, and C. Amiot, *Mol. Phys.* 26, 825 (1973).
20. J.-M. Flaud, C. Camy-Peyret, and R.A. Toth, Water Vapour Line Parameters From Microwave to Medium Infrared, Pergamon, New York, 1981.