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FOURIER-TRANSFORM ABSORPTION SPECTRUM OF THE $H_2{}^{17}O$ MOLECULE IN THE 9711–11 335 cm^{-1} SPECTRAL REGION: THE FIRST DECADE OF RESONATING STATES

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Abstract—Fourier transform spectra of ^{18}O-enriched, ^{17}O-enriched, and natural water vapor recorded between 9600 and 11 400 cm^{-1} have been analyzed to assign the $H_2{}^{17}O$ spectral lines. More than 1000 transitions were finally assigned to the $H_2{}^{17}O$ isotopic species leading to 420 precise experimental energy levels of the (0 0 3), (2 0 1), (1 2 1), (1 0 2), (3 0 0), (2 2 0) vibrational states. Rotational, centrifugal distortion, and resonance coupling parameters have been derived from the fit of the experimental energy levels to an effective Hamiltonian based on Padé–Borel approximants well suited to describe the large centrifugal distortion in H_2O. The resulting rms deviation is 0.013 cm^{-1} with 97 varied parameters. © 1999 Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

Water vapor plays an important role in atmospheric absorption and precise information on line positions and line strengths of the water molecule and its main isotopic species is needed for proper modelling of atmospheric spectra.

This paper is a continuation of the experimental and theoretical analyses of the $H_2{}^{16}O$, $H_2{}^{17}O$ and $H_2{}^{18}O$ spectra in the near IR region. The second decades of interacting vibrational states of $H_2{}^{18}O$ and $H_2{}^{16}O$ have been considered in Refs. 1 and 2, respectively, and the corresponding spectral region (11 500–12 840 cm^{-1}) has been analyzed, leading to the determination of an extensive set of precise rotational energy levels for the (2 1 1), (1 3 1), (0 1 3), (1 1 2), (3 1 0), (0 3 2), (2 3 0) vibrational states of both species. In Ref. 3 the transition moment parameters for the second decade of $H_2{}^{16}O$ have been determined from the fit of experimental intensities. Both energy levels and line intensities were accurately modeled in Ref. 4 for the first decade of interacting states of $H_2{}^{18}O$. The present work extends the analysis to the first decade 3ν of interacting vibrational states of $H_2{}^{17}O$ in the 9711–11 335 cm^{-1} region.

The $H_2{}^{17}O$ isotopomer has been recently investigated in the 6.2 μm region[5] where (0 0 0) and (0 1 0) rotational energy levels have been reported. The first hexad of the interacting vibrational states in the 6600–7640 cm^{-1} region has been considered in Ref. 6. The present work deals with the highest vibrational states of $H_2{}^{17}O$ so far analyzed.

2. SPECTRUM ASSIGNMENT AND RESULTS

The ^{18}O-enriched, ^{17}O-enriched, and natural water vapor spectra were recorded using the Fourier transform interferometer built by J.W. Brault at the National Solar Observatory (Kitt Peak, AZ). The experimental procedure and data reduction have been already outlined in Refs. 7 and 8.

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Theoretical analyses of the first decades of $H_2{}^{18}O$ and $H_2{}^{16}O$[4,9] were used for the analysis of the $H_2{}^{17}O$ spectrum and for the determination of spectroscopic parameters. Averages of the corresponding $H_2{}^{18}O$ and $H_2{}^{16}O$ band centers and rotational parameters were taken as an initial approximation for the $H_2{}^{17}O$ spectroscopic parameters. Higher order centrifugal distortion constants and resonance coupling parameters were fixed (in a first step) to the corresponding $H_2{}^{18}O$ values.

For identification purposes, experimental intensities were determined for all spectral lines from peak absorption values (using the method proposed in Ref. 10) with uncertainties varying from 5 to 25% according to the line. The mean value of the water vapor self broadening coefficient was taken as 0.45 cm^{-1} atm^{-1}.

The process of spectral line identification was performed simultaneously with the refinement of spectroscopic parameters from the fit of the observed energy levels. In this way reasonably precise predictions for extending the analysis to higher J values are made. Line assignments were additionally checked using observed and calculated intensities, assuming transition moment parameters for $H_2{}^{17}O$ equal to those of $H_2{}^{18}O$.[4] Finally this procedure yielded 420 precise experimental energy levels values for eight vibrational states of the decade with maximum values of the rotational quantum numbers $J = 14$ and $K_a = 7$. These levels are presented in Table 1 along with the observed − calculated deviations, the number of lines used in the energy level determination and the root-mean square experimental uncertainties when there was more one line reaching the same upper level. Ground state experimental rotational energy levels from Ref. 5 were used in the calculation of the upper states energies. The statistical uncertainty δ on the observed energy levels appearing in Table 1 does not include any absolute wavenumber calibration error (estimated to be less than 0.005 cm^{-1}).

More than 1000 lines were assigned as $H_2{}^{17}O$ transitions in the 9711–11 335 cm^{-1} region. This line list is presented in Table 2. It contains the experimental wavenumbers and calculated intensities followed by the vibro-rotational assignments.

Rotational, centrifugal distortion and resonance coupling parameters obtained from the fit of the energy levels are given in Table 3 along with 65% confidence intervals. Some parameters (without error intervals) were fixed to the corresponding $H_2{}^{18}O$ values.[4] The quality of the fit is characterized by a rms deviation of 0.013 cm^{-1} for 97 varied parameters.

3. THEORETICAL MODEL USED AND FITTING DETAILS

The vibration–rotation Hamiltonian is written as

$$H = \sum_{vv' \in \Gamma} |v\rangle H_{vv'} \langle v'|, \tag{1}$$

where $\Gamma = \{(0\,0\,3), (1\,0\,2), (2\,0\,1), (3\,0\,0), (0\,2\,2), (1\,2\,1), (2\,2\,0), (0\,4\,1), (1\,4\,0), (0\,7\,0)\}$. The vibrational statue (0 7 0) is formally belonging to the second decade of resonating states but should also be included in the calculation because it is close energy to the highest states of the first decade. The (0 6 0) state which should formally appear as a member of the polyad Γ is not included here since its vibrational energy is rather far from the next lowest vibrational state of the decade i.e. (1 4 0). In this condition, the (0 6 0) rotational levels (at least for the set of J or K_a values covered in room temperature spectra) are not perturbing the levels of the other states of the first $3v$ decade (see text below). In fact the (0 6 0) levels[9,11] have to be considered as perturbing the levels of the second hexad $2v + \delta$, as (0 7 0), formally a member of the $3v + \delta$ decade, is perturbing the levels of the first decade.

Because the polyad considered here is involving the highly excited bending states (0 7 0), (1 4 0) and (0 4 1), strong centrifugal distortion effects are to be taken into account. This is done by using the Padé–Borel approximation method[12] where the matrix elements of the H_{vv} operator in the $|jk\rangle$ basis are given by

$$\langle jk|H_{vv}|jk\rangle = E_v + \int_0^\infty \frac{c_0c_1 + (c_1^2 - c_0c_2)t}{c_1 - c_2t}\, e^{-t}\, dt,$$

$$\langle jk|H_{vv}|jk \pm 2\rangle = \langle jk|J_{xy}^2|jk \pm 2\rangle \int_0^\infty \frac{b_0b_1 + (b_1^2 - b_0b_2)t}{b_1 - b_2t}\, e^{-t}\, dt, \tag{2}$$

Table 1. The experimental energy levels of the first decade of $H_2{}^{17}O$ molecule

	(003)				(201)				(121)			
J K_aK_c	E_{obs} (cm^{-1})	o.-c. ($10^{-3}cm^{-1}$)	δ	N	E_{obs} (cm^{-1})	o.-c. ($10^{-3}cm^{-1}$)	δ	N	E_{obs} (cm^{-1})	o.-c. ($10^{-3}cm^{-1}$)	δ	N
0 0 0	11011.8829	0		1	10598.4756	0		1	10311.2025	0		1
1 0 1	11034.9238	-2	0.1	2	10621.7415	5	0.1	2	10334.4383	-5	0.1	2
1 1 1	11045.0893	-1	0.6	2	10632.3436	-2	0.2	2	10351.9456	-4	0.1	2
1 1 0	11050.4414	-1	0.7	2	10637.5525	-2	0.1	2	10357.8378	-7		1
2 0 2	11079.3560	-3	0.4	3	10665.5965	3	0.2	4	10379.5982	-8	0.1	2
2 1 2	11085.8357	-3	0.2	3	10672.5120	-2	0.5	3	10392.4181	1	0.4	2
2 1 1	11101.8683	0	0.1	3	10688.0408	0	2.0	2	10409.9614	-6	0.1	2
2 2 1	11132.1602	2	0.3	2	10721.4280	-3	0.8	2	10461.8918	-14	0.2	3
2 2 0	11133.7817	2	0.1	3	10722.8714	-4	0.1	2	10463.1415	-15	0.1	2
3 0 3	11142.7216	-4	0.6	3	10728.5122	2	0.2	2	10444.4733	-7	0.2	2
3 1 3	11146.0112	-5	0.1	3	10732.0450	0	0.1	2	10452.4414	9	0.1	4
3 1 2	11177.6626	0	0.3	3	10762.5195	-7	0.2	4	10486.6962	-6	0.1	2
3 2 2	11201.3581	0	0.1	3	10789.4088	-5	0.1	3	10531.4682	-7	0.3	4
3 2 1	11208.6193	2	0.3	4	10795.9713	-5	0.1	2	10537.3294	-11	0.6	2
3 3 1	11265.3150	7	2.4	2	10858.0828	-2	0.2	3	10630.5440	-8	0.2	2
3 3 0	11265.6404	5	0.1	2	10858.3468	-2	0.1	3	10630.7417	-2	0.1	2
4 0 4	11223.5374	-7	0.7	4	10808.8131	2	0.3	5	10527.0444	-1	0.1	2
4 1 4	11224.8935	-4	2.4	2	10810.2965	2	0.1	2	10531.3519	13	0.1	3
4 1 3	11275.8502	0	0.5	4	10859.0496	-12	0.3	5	10589.8600	2	1.3	3
4 2 3	11292.1684	-3	0.3	2	10878.8474	-3	0.7	4	10623.1355	-1	1.6	2
4 2 2	11310.4630	3	0.1	4	10895.6442	-6	0.4	4	10638.8174	-10	0.1	3
4 3 2	11360.2609	2	0.7	3	10950.9989	-2	0.5	5	10725.5907	14	0.9	2
4 3 1	11362.3689	1	0.7	3	10952.7315	-2	0.1	3	10726.6622	0	0.6	3
4 4 1	11444.7916	7	0.4	2	11042.6718	2		1	10856.4605	2	0.1	2
4 4 0	11444.8471	7	0.2	2	11042.7094	0		1	10856.4821	3		1
5 0 5	11319.8992	15	0.1	2	10906.1345	1	0.5	3	10626.4277	4	0.2	3
5 1 5	11321.9606	-7	0.2	2	10906.6845	3	0.3	3	10628.5354	10	0.1	3
5 1 4	11393.6912	1	0.4	4	10980.7003	-5	0.4	4	10712.0501	-5	0.1	2
5 2 4	11403.5358	-7	0.5	4	10988.9116	2	0.2	4	10736.0598	-1	0.7	3
5 2 3	11438.0476	1	1.2	2	11020.9390	-5	0.3	3	10767.3280	-16	0.6	2
5 3 3	11478.4790	-2	1.1	2	11066.8924	-1	0.4	4	10844.0809	26	0.7	2
5 3 2	11485.7820	1	0.5	3	11073.0562	-2	0.1	2	10848.2871	9	0.2	2
5 4 2	11564.5787	1	0.1	2	11159.2589	0	0.1	3	10975.4502	-6	0.5	4
5 4 1	11565.0280	0	0.4	2	11159.5776	0	0.4	3	10975.6494	0		1
5 5 1	11669.6535	5	2.9	2	11274.5411	-2		1	11135.9726	-8	1.7	2
5 5 0									11135.9673	-5		1
6 0 6	11436.1969	-1		1	11020.6197	0	1.8	2	10742.5726	3	0.3	2
6 1 6	11437.3564	-15	0.2	2	11020.8270	4	0.3	2	10743.5513	-24	0.4	2
6 1 5	11528.9168	2	0.1	2	11114.0367	-4	0.1	2	10853.8819	-13	0.3	4
6 2 5	11534.4597	-9		1	11116.9197	-13		1	10869.3905	19		1
6 2 4	11589.1268	3	0.1	2	11169.8412	19	0.3	4	10921.2160	-7	0.7	3
6 3 4	11619.0968	-8	1.0	3	11205.0610	5	1.9	3	10985.5829	40	0.5	4
6 3 3	11636.7276	-6	0.5	4	11220.4210	-1	0.1	5	10996.8113	-8	0.1	3
6 4 3	11708.2473	-3	0.8	2	11299.4173	0		1	11120.2083	9	0.7	4
6 4 2	11710.2264	-4	0.9	2	11300.9933	1	0.2	3	11119.2464	-8		1
6 5 2	11816.8039	-11	1.5	2	11414.5649	0	0.1	2				
6 5 1	11816.8697	-7	1.2	2	11414.6493	4	2.6	2	11278.6902	39	1.0	2
6 6 1	11938.4100	-2		1	11553.7754	-2	1.7	2	11468.2561	4	3.8	2
6 6 0	11938.4095	-4		1	11553.7776	0	1.0	2	11468.2583	-2	1.0	2
7 0 7	11568.8342	15		1	11152.4210	0	5.8	2	10875.6794	0	0.7	3
7 1 7	11568.8206	3	0.3	2	11152.9557	-1	0.4	2	10876.0402	-2	0.1	3
7 1 6	11680.7942	1		1	11265.2143	-1	0.5	4	11012.9932	-17	0.7	2
7 2 6	11684.3009	-15	0.1	2	11266.7686	10	0.1	2	11022.1027	-3	0.1	2

continued

Table 1 – *continued*

	(003)				(201)				(121)			
J K_aK_c	E_{obs} (cm^{-1})	o.-c. (10^{-3}cm^{-1})	δ	N	E_{obs} (cm^{-1})	o.-c. (10^{-3}cm^{-1})	δ	N	E_{obs} (cm^{-1})	o.-c. (10^{-3}cm^{-1})	δ	N
7 2 5	11760.8479	0		1	11340.1951	47	0.1	2	11098.2952	-16	1.0	2
7 3 5	11781.0420	-14	2.2	2	11364.5568	11	0.3	5	11148.9292	15	0.4	2
7 3 4	11814.4486	0	0.7	2	11394.5005	-6	0.4	3	11172.8692	81	0.8	2
7 4 4	11875.3165	-13		1	11462.8608	7	0.7	4	11285.8217	-12	0.4	2
7 4 3	11881.7829	-3		1	11467.9150	6	0.1	4	11287.8481	-22	1.3	2
7 5 3	11985.8148	10		1	11578.1539	-3	0.1	2	11445.4949	-20	0.8	2
7 5 2	11986.1364	12		1	11578.5210	1	0.6	2				
7 6 2	12102.1252	9		1	11717.6595	-24	1.2	2				
7 6 1	12102.1202	-9		1								
7 7 1	12249.3733	0		1	11888.7041	-1		1				
7 7 0	12249.3730	0		1	11888.7038	-1		1				
8 0 8	11718.9710	6	0.7	3	11300.2369	26	0.4	3	11026.0247	-1	0.1	2
8 1 8	11718.9712	6	2.1	2	11301.4195	3	0.6	3	11026.0236	-10		1
8 1 7	11849.4464	3	4.0	2	11432.7967	-34	0.7	5	11188.4193	-15	0.3	3
8 2 7	11846.0786	4		1	11433.5057	13	0.7	2	11194.1317	1	0.1	2
8 2 6	11950.4114	5	0.7	2	11528.3784	-31	0.2	2	11303.8558	-4	0.2	3
8 3 6					11544.2582	18	0.3	2	11334.5214	1	1.2	2
8 3 5	12016.7533	1	1.8	2	11593.4786	-9	0.6	2	11374.4687	4	0.8	2
8 4 5					11648.9556	4		1				
8 4 4	12079.9423	13	0.4	2	11661.5390	6	0.1	3	11482.2499	-38	0.2	2
8 5 4					11765.2338	-14	0.5	2				
8 5 3					11766.5613	0	0.5	3	11636.0623	-15	0.9	2
8 6 3					11905.1439	26		1				
8 6 2					11905.1738	21		1				
9 0 9					11467.7765	-3	0.1	2				
9 1 9	11886.4883	9	0.7	2	11467.6639	-17	0.1	2	11194.0552	30	0.4	2
9 1 8	12035.0951	-4		1	11617.0916	-29	0.1	2				
9 2 8	12035.0046	3		1	11617.8220	7	0.2	2				
9 2 7					11741.1059	-14		1				
9 3 7	12165.8153	-4		1	11744.0582	31	0.8	2	11539.8451	-21		1
9 3 6					11814.6917	-4	1.3	2				
9 4 6	12276.5956	5		1	11856.7058	6	2.1	3				
9 4 5					11882.2370	-2	0.7	4				
9 5 5	12392.7490	1		1	11975.5022	-29		1	11850.8752	22		1
9 5 4					11979.4288	-3		1				
10 0 10					11651.4800	-3	1.5	2	11378.0911	-23		1
10 1 9	12237.9039	-3		1	11819.1343	14		1	11588.7538	17		1
10 2 9	12237.8860	0		1	11818.4959	0	1.6	2				
10 2 8	12377.8855	6		1	11961.9582	4	1.7	2				
10 3 7					12055.2047	29		1				
10 4 6					12129.0117	-29	2.9	2	11945.7251	-9		1
10 6 4									11964.1539	2		1
11 0 11					11852.3753	-5		1				
11 1 11	12273.6843	-3		1	11852.3784	-2		1				
11 1 10	12457.7805	-2		1	12038.0984	-3		1				
11 2 10	12457.8369	-1		1	12038.0347	-21		1				
11 3 9	12615.8838	3		1								
12 0 12					12070.4313	7	2.1	2				
12 1 12					12070.4354	11	0.4	2				
12 1 11					12274.0576	-12		1				
13 1 12					12527.0897	9		1				
14 0 14					12557.6862	-1		1				
14 1 14					12557.6876	-1		1				

continued

Table 1 — *continued*

J K_aK_c	(102)				(300)				(220)			
	E_{obs} (cm^{-1})	o.-c. ($10^{-3}cm^{-1}$)	δ	N	E_{obs} (cm^{-1})	o.-c. ($10^{-3}cm^{-1}$)	δ	N	E_{obs} (cm^{-1})	o.-c. ($10^{-3}cm^{-1}$)	δ	N
0 0 0	10853.5053	0		1								
1 0 1	10876.2857	0		1	10608.7619	11		1				
1 1 1	10887.3761	2	0.3	2	10619.5641	0		1				
1 1 0	10892.6031	1	0.2	2	10625.2499	5	0.5	2				
2 0 2	10920.3612	0	0.3	2	10652.7611	9	1.3	3				
2 1 2	10927.7093	1	0.1	2	10659.9563	0	0.5	3				
2 1 1	10943.3647	-2	0.4	2	10675.7823	0	1.0	2				
2 2 1	10976.4181	3	0.4	3	10709.7726	-6	0.2	3	10423.2689	-19	3.1	3
2 2 0	10977.8695	2	0.3	3	10711.0897	-8	0.4	3				
3 0 3	10983.4207	-1	0.2	2	10715.7662	6	0.2	2	10402.3193	2	1.6	3
3 1 3	10987.3580	0	0.8	3	10719.5631	0	0.2	2				
3 1 2	11018.3291	-4	0.4	3	10750.4719	0	0.1	2				
3 2 2	11044.7487	2	1.2	2	10778.1552	-9	0.2	3	10493.2193	7	0.2	2
3 2 1	11051.3498	-2	0.4	4	10784.1681	-12	0.2	3	10497.9990	-2	1.3	3
3 3 1	11112.8840	3		1	10847.2367	4		1				
3 3 0	11113.1560	3	0.1	3	10847.4709	7	0.4	4	10595.3494	11	0.5	2
4 0 4	11063.8470	0	0.3	2	10796.1084	2	0.2	2				
4 1 4	11065.6433	2	0.5	3	10797.7688	-1	0.1	2				
4 1 3	11115.7884	-3	1.7	2	10847.6984	1	0.7	3				
4 2 3	11134.5746	-3	0.1	2	10868.4243	-9	0.1	3	10582.4858	14	0.2	2
4 2 2	11151.5140	-4	0.8	3	10883.7628	-12		1				
4 3 2	11206.1843	-1	0.6	3	10940.4760	0	0.1	2	10689.7925	-2	0.1	2
4 3 1	11207.9967	-3	1.5	2	10942.0005	-1	0.1	2				
4 4 1	11297.0459	4	0.7	2								
4 4 0	11297.0504	7		1								
5 0 5	11161.3000	3	0.5	3	10893.3904	-1		1				
5 1 5	11162.0437	2	1.4	2	10894.0331	-3	2.9	3				
5 1 4	11233.3188	-1	0.4	2	10965.1198	5	0.1	3	10668.5034	0	2.3	2
5 2 4	11244.9398	-5		1	10974.1839	-23	0.2	3	10695.5869	15		1
5 2 3	11277.4037	-3	0.8	3	11009.0807	-6	0.4	3				
5 3 3	11324.2161	-24	0.5	2	11056.7989	0	0.1	2				
5 3 2	11328.9207	-1	0.3	3	11062.2784	-3		1	10811.4675	-12	0.6	2
5 4 2	11414.2848	-7	1.5	2								
5 4 1	11414.3891	-3	0.2	3								
5 5 1	11527.5588	4		1	11265.3002	14		1				
5 5 0	11527.5457	3	0.9	2	11265.3105	12	0.7	2				
6 0 6	11275.7714	0		1	11007.7786	-7		1				
6 1 6	11276.1426	3	0.5	2	11008.0099	-4	0.1	2				
6 1 5	11368.5641	0	3.4	3	11100.3233	2		1				
6 2 5	11374.8645	-6	0.3	2	11105.6238	0	0.4	2	10828.5901	-12		1
6 2 4	11426.5877	9	0.7	3								
6 3 4	11462.0407	0	0.1	3	11195.6018	11	0.3	4				
6 3 3	11476.9811	2	1.7	2								
6 4 3	11555.6730	-7		1								
6 4 2	11556.5902	-4		1	11290.5536	32	0.9	2				
6 5 2	11667.8218	-7		1	11405.6024	-12		1				
6 5 1	11667.7440	-2		1	11405.6995	-14		1				
6 6 1	11800.7656	5		1	11545.1586	-3	5.5	1				
6 6 0	11800.7389	4		1								

continued

Table 1 — *continued*

J K_aK_c	(102) E_{obs} (cm^{-1})	o.-c. (10^{-3}cm^{-1})	δ	N	(300) E_{obs} (cm^{-1})	o.-c. (10^{-3}cm^{-1})	δ	N	(220) E_{obs} (cm^{-1})	o.-c. (10^{-3}cm^{-1})	δ	N
7 0 7	11407.6803	2		1	11139.3231	17		1				
7 1 7	11407.8584	0	1.0	2	11139.5064	-6		1				
7 1 6	11520.3513	-5	1.3	3	11251.9877	1	1.8	3				
7 2 6	11523.5186	-8		1	11255.8246	9		1				
7 2 5	11598.6627	0	1.5	2	11329.1109	16	0.7	3				
7 3 5					11356.1530	27	0.4	2				
7 3 4	11651.6366	18		1	11383.3987	2	0.1	2				
7 4 4					11453.0035	-12	1.2	2				
7 4 3	11724.4868	8	2.0	2	11457.3488	-37	0.5	3				
7 5 2	11832.0884	5		1	11569.7754	-16	3.8	2				
7 6 1	11963.2415	-19		1								
7 7 1	12129.3350	0		1								
7 7 0	12129.3345	1		1								
8 0 8	11557.1154	0		1	11288.3246	14		1				
8 1 8	11557.3099	1		1	11287.4465	-18	0.3	2				
8 2 7	11690.3681	-10	0.1	2	11420.8359	8	1.3	2				
8 2 6					11518.7309	-17		1				
8 3 6	11802.6551	12	1.1	3	11537.7556	31	0.7	3				
8 3 5	11857.5090	-3		1								
8 4 5	11908.9230	21	1.5	2	11639.6455	4	0.6	3				
8 5 4					11756.4170	20		1				
9 1 9					11454.3474	2		1				
9 1 8	11874.0446	6		1	11604.8283	-10		1				
9 3 7					11728.4203	7		1				
9 3 6	12076.5002	0		1								
9 4 5	12138.9565	-19		1								
10 1 10	11906.4088	-2	0.1	2	11637.7873	-11		1				
10 2 9					11806.1400	0		1				
10 3 7									11822.6086	20	3.3	2
10 4 7					12083.3903	-3		1				
11 0 11					11838.4124	7	3.2	2				
11 1 11					11838.4028	0	3.2	2				

J K_aK_c	(041) E_{obs} (cm^{-1})	o.-c. (10^{-3}cm^{-1})	δ	N	(022) E_{obs} (cm^{-1})	o.-c. (10^{-3}cm^{-1})	N
1 1 1	9868.3030	24	0.0	2			
2 0 2	9883.1848	0	1.2	2			
2 2 1	10017.8987	-3		1			
2 2 0	10018.7964	4	2.1	2			
3 1 3	9969.6943	-7	3.0	2			
3 2 2	10088.9633	1	0.3	2			
3 3 1	10242.9486	-6		1			
4 0 4	10036.4199	-19	0.6	2			
4 1 3	10112.8859	13		1			
4 2 2	10194.9242	-15		1			
5 1 5	10148.2301	-7		1			
6 0 6	10260.0130	12		1			
9 3 7					11734.8396	-7	1
9 5 4	11620.5490	14	0.2	2			

δ = statistical observed energy error. N = number of lines used to determine the level.

Table 2. $H_2{}^{17}O$ absorption spectrum in the 9711–11 335 cm^{-1} region

Position (cm^{-1})	Intensity (cm^{-2}/atm)	v'	J upper	K_a upper	K_c upper	J lower	K_a lower	K_c lower	Position (cm^{-1})	Intensity (cm^{-2}/atm)	v'	J upper	K_a upper	K_c upper	J lower	K_a lower	K_c lower
9711.7596	.15E-04	041	4	0	4	5	0	5	10182.2907	.63E-03	121	5	1	5	6	1	6
9745.3932	.21E-04	041	3	1	3	4	1	4	10183.6067	.49E-04	220	4	2	3	5	1	4
9746.6459	.17E-04	041	2	0	2	3	0	3	10184.4510	.37E-03	121	5	2	4	6	2	5
9789.0756	.14E-04	041	1	1	1	2	1	2	10184.6383	.12E-04	121	8	1	7	8	3	6
9807.3628	.15E-04	041	2	2	0	3	2	1	10188.3001	.73E-04	121	5	3	2	6	3	3
9826.1161	.17E-04	041	1	1	1	1	1	0	10190.9812	.68E-03	121	4	1	3	5	1	4
9859.4125	.24E-04	041	2	0	2	1	0	1	10193.0241	.52E-03	121	4	2	2	5	2	3
9877.5279	.15E-04	041	3	2	2	3	2	1	10194.9954	.28E-04	121	7	5	3	8	5	4
9882.4675	.12E-04	041	2	2	1	2	2	0	10195.5658	.28E-04	121	6	4	3	7	4	4
9884.6490	.28E-04	041	2	2	0	2	2	1	10197.0095	.22E-03	121	5	3	3	6	3	4
9890.4639	.24E-04	041	3	1	3	2	1	2	10201.5541	.17E-04	121	6	1	6	6	1	5
9899.8816	.24E-04	041	4	0	4	3	0	3	10202.3834	.92E-03	121	4	0	4	5	0	5
9923.9259	.19E-04	041	5	1	5	4	1	4	10205.4716	.30E-03	121	4	1	4	5	1	5
9935.3520	.17E-04	041	6	0	6	5	0	5	10206.8099	.21E-04	121	6	1	5	6	3	4
9939.7758	.15E-04	041	4	1	3	3	1	2	10206.8500	.15E-04	300	7	4	3	8	5	4
9954.8177	.12E-04	041	3	2	2	2	2	1	10208.0059	.19E-03	121	4	2	3	5	2	4
9959.1809	.33E-04	041	3	3	1	3	3	0	10209.0513	.12E-04	121	4	1	3	4	3	2
9983.4884	.17E-04	041	4	2	2	3	2	1	10211.2998	.21E-04	121	5	0	5	5	2	4
9992.9147	.10E-04	121	6	2	4	7	4	3	10211.5657	.26E-03	121	3	1	2	4	1	3
10013.0153	.12E-04	121	6	1	5	7	3	4	10215.1045	.14E-04	201	4	3	1	5	5	0
10052.0638	.10E-04	121	5	1	4	6	3	3	10218.0885	.68E-04	220	3	2	2	4	1	3
10053.9783	.23E-04	121	10	0	10	11	0	11	10219.4882	.32E-03	121	4	3	1	5	3	2
10071.6356	.14E-04	121	3	1	3	4	3	2	10220.8376	.39E-04	121	5	4	1	6	4	2
10075.3092	.23E-04	220	4	2	3	5	3	2	10221.7460	.11E-03	121	5	4	2	6	4	3
10081.2559	.23E-04	121	4	0	4	5	2	3	10222.2516	.23E-03	121	3	2	1	4	2	2
10082.0136	.48E-04	121	9	1	9	10	1	10	10222.8523	.42E-03	121	3	0	3	4	0	4
10082.3906	.10E-04	220	4	3	2	5	4	1	10223.4178	.18E-03	121	4	3	2	5	3	3
10082.6838	.15E-04	121	4	1	3	5	3	2	10226.5444	.40E-04	300	5	5	1	6	6	0
10093.2012	.19E-04	121	8	3	5	9	3	6	10226.5444	.40E-04	300	5	5	0	6	6	1
10096.8162	.12E-04	121	9	3	7	10	3	8	10226.6398	.15E-04	300	6	1	6	7	2	5
10103.8928	.26E-04	121	8	2	6	9	2	7	10228.1370	.11E-02	121	3	1	3	4	1	4
10107.9226	.10E-03	121	8	0	8	9	0	9	10229.2114	.23E-04	220	3	0	3	3	1	2
10110.1409	.12E-04	220	3	3	0	4	4	1	10229.6560	.80E-04	121	5	1	5	5	1	4
10111.6184	.55E-04	121	8	1	7	9	1	8	10232.0294	.74E-03	121	3	2	2	4	2	3
10116.1113	.26E-04	121	8	2	7	9	2	8	10232.5470	.19E-04	201	10	4	6	11	4	7
10116.7982	.17E-04	121	7	2	5	8	2	6	10235.2079	.42E-04	201	5	2	4	6	4	3
10116.8917	.14E-04	220	5	1	4	6	2	5	10235.4985	.10E-04	300	6	4	2	7	5	3
10117.1945	.17E-04	220	3	2	1	4	3	2	10236.8513	.11E-02	121	2	1	1	3	1	2
10120.9579	.14E-04	121	8	3	6	9	3	7	10238.9874	.26E-04	121	3	0	3	3	2	2
10124.2178	.21E-04	121	7	3	4	8	3	5	10243.0604	.13E-02	121	2	0	2	3	0	3
10124.6914	.14E-04	121	8	4	4	9	4	5	10243.9989	.15E-04	220	4	3	2	5	2	3
10126.1913	.12E-04	121	2	1	1	3	3	0	10244.5431	.14E-04	201	10	3	7	11	3	8
10129.3924	.19E-04	121	3	0	3	4	2	2	10248.5656	.10E-03	121	3	3	0	4	3	1
10131.8935	.40E-04	121	7	1	6	8	1	7	10249.0847	.12E-03	121	4	4	0	5	4	1
10133.2817	.73E-04	121	7	0	7	8	0	8	10249.3012	.48E-04	121	4	4	1	5	4	2
10133.5492	.23E-03	121	7	1	7	8	1	8	10249.7384	.32E-03	121	3	3	1	4	3	2
10138.4507	.11E-03	121	7	2	6	8	2	7	10250.1621	.40E-04	220	2	2	1	3	1	2
10139.4969	.17E-04	220	2	2	1	3	3	0	10250.5153	.45E-03	121	2	1	2	3	1	3
10139.8388	.15E-03	121	6	2	4	7	2	5	10251.7056	.61E-03	121	2	2	0	3	2	1
10145.1499	.68E-04	121	7	3	5	8	3	6	10251.8965	.49E-04	121	5	5	1	6	5	2
10149.1749	.26E-04	121	4	1	4	4	3	1	10256.2215	.49E-04	121	4	1	4	4	1	3
10149.1749	.26E-04	201	7	1	7	8	3	6	10256.2215	.49E-04	121	7	7	1	8	7	2
10150.9962	.23E-03	121	6	1	5	7	1	6	10256.4099	.21E-03	121	2	2	1	3	2	2
10155.9464	.11E-03	121	6	3	3	7	3	4	10258.4388	.19E-04	121	6	6	1	7	6	2
10157.6321	.40E-03	121	6	0	6	7	0	7	10258.4388	.19E-04	121	6	6	0	7	6	1
10158.3898	.15E-03	121	6	1	6	7	1	7	10259.6125	.24E-04	201	5	1	5	6	3	4
10158.9086	.21E-04	121	7	4	3	8	4	4	10259.8575	.12E-04	220	5	3	2	6	2	5
10164.6235	.10E-04	300	7	5	2	8	6	3	10261.6460	.15E-04	201	9	5	5	10	5	6
10165.1654	.15E-04	201	6	3	3	7	5	2	10262.8673	.31E-03	121	1	1	0	2	1	1
10165.3678	.11E-03	121	5	2	3	6	2	4	10263.9108	.46E-04	300	7	3	4	8	4	5
10166.3332	.40E-04	121	7	4	4	8	4	5	10264.4338	.43E-03	121	1	0	1	2	0	2
10167.6621	.14E-04	121	7	0	7	7	2	6	10264.7594	.66E-04	300	6	2	5	7	3	4
10170.0534	.14E-03	121	5	1	4	6	1	5	10266.1204	.30E-04	201	5	2	3	6	4	2
10170.9728	.44E-04	121	6	3	4	7	3	5	10267.3053	.58E-04	300	6	3	4	7	4	3
10173.1543	.24E-04	121	7	1	7	7	1	6	10267.8349	.39E-04	201	12	0	12	13	0	13
10178.0133	.35E-04	220	3	0	3	4	1	4	10267.8349	.39E-04	201	12	1	12	13	1	13
10180.7087	.22E-03	121	5	0	5	6	0	6	10268.3372	.12E-04	201	9	4	5	10	4	6

continued

Table 2 — *continued*

Position (cm^{-1})	Intensity (cm^{-2}/atm)	v'	J (upper)	K_a (upper)	K_c (upper)	J (lower)	K_a (lower)	K_c (lower)
10271.6897	.21E-04	201	4	2	3	5	4	2
10272.7181	.92E-03	121	1	1	1	2	1	2
10273.6930	.12E-04	220	3	2	1	4	1	4
10274.5770	.26E-04	201	10	2	8	11	2	9
10278.5337	.15E-04	201	9	3	6	10	3	7
10279.0165	.28E-04	201	9	4	6	10	4	7
10279.3314	.25E-03	121	3	1	3	3	1	2
10284.0714	.30E-04	300	11	0	11	12	1	12
10284.0714	.30E-04	300	11	1	11	12	0	12
10287.4290	.80E-03	121	0	0	0	1	0	1
10288.2462	.57E-04	201	4	2	2	5	4	1
10293.8771	.40E-04	201	8	5	3	9	5	4
10293.9270	.23E-04	300	4	0	4	5	3	3
10293.9270	.23E-04	121	6	3	3	7	1	6
10296.7153	.19E-04	201	10	2	9	11	2	10
10297.4480	.16E-03	121	2	1	2	2	1	1
10298.0407	.88E-04	201	11	0	11	12	0	12
10298.0407	.88E-04	201	11	1	11	12	1	12
10300.8230	.14E-04	220	10	3	7	11	2	10
10301.0163	.97E-04	201	9	3	7	10	3	8
10301.9873	.37E-04	300	5	3	3	6	4	2
10303.9833	.88E-04	201	8	4	4	9	4	5
10305.7386	.31E-04	201	9	2	7	10	2	8
10308.0587	.17E-03	121	4	2	3	4	2	2
10308.0587	.17E-03	121	7	3	5	7	3	4
10308.1086	.21E-04	201	4	1	4	5	3	3
10308.5737	.12E-03	300	5	3	2	6	4	3
10309.3013	.14E-04	201	7	3	5	7	5	2
10309.7588	.11E-02	121	1	1	1	1	1	0
10311.4661	.31E-04	201	8	4	5	9	4	6
10312.5102	.26E-04	201	7	6	2	8	6	3
10313.6657	.19E-04	300	10	1	10	11	0	11
10314.1968	.64E-04	300	5	2	4	6	3	3
10320.0327	.75E-03	121	3	2	2	3	2	1
10323.0917	.12E-04	220	3	0	3	2	1	2
10324.8893	.40E-04	220	3	2	1	3	1	2
10325.3287	.82E-04	300	7	2	5	8	3	6
10325.5958	.40E-04	121	6	3	4	6	3	3
10326.4605	.54E-03	121	2	2	1	2	2	0
10326.8635	.49E-04	201	9	1	8	10	1	9
10327.0232	.18E-03	201	9	2	8	10	2	9
10327.2339	.58E-04	201	7	5	2	8	5	3
10327.6551	.88E-04	201	7	5	3	8	5	4
10327.7861	.14E-04	121	4	3	1	5	1	4
10328.4152	.82E-04	201	8	2	6	9	2	7
10328.9963	.16E-02	121	2	2	0	2	2	1
10329.2645	.24E-04	201	5	3	3	5	5	0
10330.3211	.24E-04	041	9	5	4	10	1	9
10330.7328	.61E-03	121	2	1	1	2	1	2
10331.8469	.27E-03	121	3	2	1	3	2	2
10333.0785	.18E-03	300	4	3	2	5	4	1
10334.4382	.28E-03	121	1	0	1	0	0	0
10334.8412	.66E-04	300	4	3	1	5	4	2
10334.9645	.12E-04	300	3	0	3	4	3	2
10336.3406	.17E-04	201	6	3	3	6	5	2
10336.9058	.31E-03	121	5	3	3	5	3	2
10338.9767	.12E-03	201	7	4	3	8	4	4
10339.3783	.34E-03	121	4	2	2	4	2	3
10342.3224	.15E-04	300	9	1	9	10	0	10
10343.3733	.21E-03	201	7	4	4	8	4	5
10343.4137	.23E-03	121	4	3	2	4	3	1
10343.8448	.12E-04	220	5	1	4	5	0	5
10343.9602	.49E-04	201	6	6	1	7	6	2
10343.9602	.49E-04	201	6	6	0	7	6	1
10344.0426	.79E-04	220	2	2	1	2	1	2
10344.0426	.79E-04	300	8	2	7	9	1	8
10345.8553	.77E-03	121	4	3	1	4	3	2
10345.8553	.77E-03	201	7	3	4	8	3	5
10346.1077	.10E-03	121	5	3	2	5	3	3
10346.7760	.14E-02	121	3	3	1	3	3	0
10347.1802	.48E-03	121	3	3	0	3	3	1
10349.7393	.12E-03	121	6	3	3	6	3	4
10351.2392	.80E-04	201	3	1	3	4	3	2
10351.3172	.35E-04	220	3	2	2	3	1	3
10351.8782	.27E-03	201	4	1	3	5	3	2
10355.4862	.50E-03	121	2	1	2	1	1	1
10355.4862	.50E-03	201	8	2	7	9	2	8
10355.6229	.42E-03	201	9	1	9	10	1	10
10355.7516	.16E-03	201	9	0	9	10	0	10
10355.8249	.15E-02	121	2	0	2	1	0	1
10355.9954	.45E-03	201	8	1	7	9	1	8
10358.2593	.17E-04	121	7	3	4	7	3	5
10358.3767	.26E-04	300	8	4	5	9	3	6
10358.6990	.12E-03	201	7	2	5	8	2	6
10359.3914	.16E-03	201	6	5	1	7	5	2
10359.5107	.57E-04	201	6	5	2	7	5	3
10360.6830	.17E-04	201	10	0	10	10	2	9
10360.7751	.41E-03	201	7	3	5	8	3	6
10362.0083	.29E-03	300	3	3	1	4	4	0
10362.0083	.29E-03	300	5	2	3	6	3	4
10362.1047	.68E-04	201	6	2	5	6	4	2
10362.2620	.24E-03	300	3	3	0	4	4	1
10362.7617	.23E-04	121	8	4	4	8	4	5
10363.0191	.66E-04	201	4	0	4	5	2	3
10365.5470	.29E-03	121	4	1	3	4	1	4
10365.5470	.29E-03	121	6	4	2	6	4	3
10365.6747	.26E-04	220	5	3	2	5	2	3
10367.7744	.10E-02	121	2	1	1	1	1	0
10368.0525	.41E-03	121	5	4	2	5	4	1
10368.3356	.10E-03	300	7	1	6	8	2	7
10369.3448	.57E-04	300	8	1	8	9	0	9
10369.6076	.66E-04	121	6	2	4	6	2	5
10370.1841	.35E-04	300	8	0	8	9	1	9
10371.2236	.32E-03	121	4	4	1	4	4	0
10372.6976	.43E-03	201	6	4	2	7	4	3
10373.2140	.16E-02	121	3	1	3	2	1	2
10374.4689	.69E-03	121	3	0	3	2	0	2
10374.6620	.13E-03	300	7	3	5	8	2	6
10379.5562	.86E-03	201	6	3	3	7	3	4
10380.3439	.75E-04	201	3	1	2	4	3	1
10381.5169	.42E-04	201	5	2	4	5	4	1
10382.1346	.65E-03	201	8	0	8	9	0	9
10382.3549	.19E-04	220	6	2	5	6	1	6
10383.1166	.89E-03	201	7	2	6	8	2	7
10383.2789	.34E-03	201	8	1	8	9	1	9
10383.9131	.33E-04	220	3	3	0	3	2	1
10384.1147	.34E-03	201	7	1	6	8	1	7
10385.5627	.33E-04	121	8	5	3	8	5	4
10385.7541	.31E-03	121	8	2	6	9	0	9
10388.9523	.37E-04	201	2	1	2	3	3	1
10389.4494	.56E-03	121	4	1	4	3	1	3
10389.7515	.19E-04	201	9	0	9	9	2	8
10390.2405	.88E-04	121	7	5	3	7	5	2
10390.3538	.57E-04	220	4	3	2	4	2	3
10390.4538	.52E-03	201	5	5	1	6	5	2
10390.4538	.52E-03	201	6	3	4	7	3	5
10390.5069	.17E-02	121	4	0	4	3	0	3
10391.7256	.45E-03	121	3	1	2	2	1	1
10391.8875	.21E-04	121	2	2	1	2	0	2
10392.3070	.91E-04	300	6	1	5	7	2	6
10394.6114	.24E-03	121	6	5	1	6	5	2
10394.9301	.75E-04	121	3	2	2	3	0	3
10395.9789	.88E-04	300	3	2	2	4	3	1
10396.8323	.12E-03	300	7	0	7	8	1	8
10397.3232	.83E-03	121	3	2	2	2	2	1
10398.3467	.67E-03	121	5	5	1	5	5	0
10398.3467	.67E-03	121	5	5	0	5	5	1
10398.8704	.23E-04	300	8	5	4	9	4	5

continued

Table 2 — *continued*

Position	Intensity	v'	J	K_a	K_c	J	K_a	K_c
(cm^{-1})	(cm^{-2}/atm)		upper			lower		
10399.5096	.44E-04	201	5	1	5	5	3	2
10401.5207	.31E-04	121	4	2	3	4	0	4
10403.3620	.37E-03	300	3	2	1	4	3	2
10403.5257	.19E-04	201	9	1	8	9	3	7
10403.7869	.19E-04	300	8	1	8	8	2	7
10404.2310	.15E-02	121	5	1	5	4	1	4
10404.3451	.23E-04	300	7	4	4	8	3	5
10404.4848	.82E-04	300	3	1	3	4	2	2
10404.7692	.26E-03	201	5	4	1	6	4	2
10404.8065	.50E-03	121	5	0	5	4	0	4
10405.5540	.69E-03	201	5	4	2	6	4	3
10406.4389	.32E-03	121	7	3	5	8	1	8
10407.6363	.44E-04	121	6	1	5	6	1	6
10409.3755	.28E-03	220	4	2	3	3	1	2
10410.4644	.16E-02	201	7	1	7	8	1	8
10411.1508	.20E-02	201	6	1	5	7	1	6
10411.3994	.60E-04	121	5	2	4	5	0	5
10412.1922	.26E-03	121	6	4	3	7	2	6
10413.0664	.62E-03	201	5	3	2	6	3	3
10413.5105	.38E-03	300	5	1	4	6	2	5
10414.2247	.29E-03	300	6	3	4	7	2	5
10416.1363	.57E-04	201	6	2	4	6	4	3
10416.5847	.97E-04	201	8	0	8	8	2	7
10416.7512	.10E-02	121	4	1	3	3	1	2
10417.0559	.14E-04	300	8	2	7	8	3	6
10417.9113	.10E-02	121	6	0	6	5	0	5
10418.2595	.15E-04	300	8	3	6	8	4	5
10418.9786	.95E-03	201	5	2	3	6	2	4
10419.8235	.23E-02	201	5	3	3	6	3	4
10420.3198	.39E-04	201	8	1	8	8	1	7
10420.4564	.24E-04	220	5	2	4	4	1	3
10423.0691	.22E-03	300	6	1	6	7	0	7
10423.6688	.30E-04	121	6	2	5	6	0	6
10423.8441	.33E-04	121	5	4	2	6	2	5
10426.0045	.39E-03	300	2	2	1	3	3	0
10427.3818	.98E-03	121	4	2	2	3	2	1
10427.5275	.20E-03	300	2	2	0	3	3	1
10429.0167	.86E-04	201	8	1	7	8	3	6
10429.4940	.20E-03	121	6	6	1	6	6	0
10429.4940	.20E-03	121	6	6	0	6	6	1
10429.7107	.19E-04	220	6	2	5	5	1	4
10429.7953	.71E-03	121	7	1	7	6	1	6
10429.9604	.24E-03	121	7	0	7	6	0	6
10431.4809	.40E-04	300	7	1	7	7	2	6
10432.1874	.24E-03	300	5	2	4	6	1	5
10432.5694	.21E-03	300	4	1	3	5	2	4
10435.5125	.31E-03	201	4	4	1	5	4	2
10436.6198	.10E-02	121	5	2	4	4	2	3
10436.9194	.37E-03	121	5	1	4	4	1	3
10437.1661	.33E-04	121	7	2	6	7	0	7
10437.3020	.28E-02	201	5	2	4	6	2	5
10438.7039	.10E-02	201	5	1	4	6	1	5
10439.3702	.24E-04	121	2	2	0	1	0	1
10440.8617	.14E-03	121	8	1	8	7	1	7
10441.0840	.41E-03	121	8	0	8	7	0	7
10442.0300	.15E-03	121	4	3	2	3	3	1
10442.8950	.44E-03	121	4	3	1	3	3	0
10443.5865	.15E-04	121	6	3	4	6	1	5
10444.3988	.88E-04	201	7	0	7	7	2	6
10445.2047	.39E-04	121	5	3	3	5	1	4
10445.5571	.23E-02	201	4	3	1	5	3	2
10445.9255	.17E-04	121	8	1	7	8	1	8
10447.1454	.42E-03	300	5	0	5	6	1	6
10448.3098	.18E-03	300	5	1	5	6	0	6
10448.5210	.43E-03	300	2	1	2	3	2	1
10448.8187	.77E-03	201	4	3	2	5	3	3
10449.8507	.42E-02	201	4	2	2	5	2	3
10450.5028	.16E-03	121	9	0	9	8	0	8
10450.6043	.49E-04	201	7	1	6	7	3	5
10451.0331	.60E-03	300	3	1	2	4	2	3
10451.5648	.23E-03	121	9	1	9	8	1	8
10451.9961	.11E-03	121	7	7	1	7	7	0
10451.9961	.11E-03	201	8	2	7	8	2	6
10452.2489	.28E-03	121	5	2	3	4	2	2
10453.5681	.35E-04	300	7	4	3	8	3	6
10454.1610	.17E-03	201	2	0	2	3	2	1
10454.2625	.23E-03	121	6	2	5	5	2	4
10454.8380	.11E-03	300	5	3	3	6	2	4
10455.0027	.76E-03	121	6	1	5	5	1	4
10456.4004	.69E-04	300	6	1	6	6	2	5
10457.4306	.10E-04	121	3	3	1	3	1	2
10458.5512	.10E-03	300	6	2	5	6	3	4
10459.9891	.13E-03	121	10	0	10	9	0	9
10460.1698	.41E-02	201	4	1	3	5	1	4
10462.7906	.28E-04	201	9	3	7	9	3	6
10463.7206	.15E-02	201	4	2	3	5	2	4
10465.7818	.24E-04	300	6	0	6	6	1	5
10466.1083	.35E-03	121	5	3	2	4	3	1
10466.9644	.16E-03	201	6	1	5	6	3	4
10469.0122	.31E-03	201	6	0	6	6	2	5
10469.5449	.27E-02	300	4	2	3	5	1	4
10470.2280	.21E-03	300	4	0	4	5	1	5
10470.3015	.18E-03	300	2	1	1	3	2	2
10470.4935	.41E-03	121	7	2	6	6	2	5
10470.6128	.44E-04	300	7	1	6	7	2	5
10470.9971	.17E-03	121	7	1	6	6	1	5
10472.0015	.10E-03	300	5	2	4	5	3	3
10473.1077	.30E-03	300	4	1	4	5	0	5
10475.4216	.55E-03	121	6	2	4	5	2	3
10475.9438	.26E-04	300	6	4	2	7	3	5
10476.1710	.78E-03	201	3	3	0	4	3	1
10477.2768	.23E-02	201	3	3	1	4	3	2
10478.2443	.34E-03	201	4	1	3	4	3	2
10478.5203	.44E-04	201	5	1	4	5	3	3
10478.8305	.10E-03	201	6	1	6	6	1	5
10478.9077	.42E-04	300	5	1	5	5	2	4
10478.9577	.42E-04	201	3	1	2	3	3	1
10480.8968	.29E-02	201	3	2	1	4	2	2
10483.4026	.15E-03	121	6	3	4	5	3	3
10484.1524	.96E-02	201	4	0	4	5	0	5
10484.4162	.27E-02	201	4	1	4	5	1	5
10485.3914	.18E-03	201	7	2	6	7	2	5
10485.5328	.25E-03	121	8	1	7	7	1	6
10486.1155	.15E-03	121	8	2	7	7	2	6
10486.8057	.15E-04	220	5	3	2	5	0	5
10486.8057	.15E-04	201	8	1	8	7	3	5
10487.3889	.25E-02	201	3	1	2	4	1	3
10488.2470	.26E-04	300	7	2	5	7	3	4
10488.7813	.15E-04	102	5	5	1	6	6	0
10488.7813	.15E-04	102	5	5	0	6	6	1
10489.6368	.37E-03	121	6	3	3	5	3	2
10489.9699	.59E-02	201	3	2	2	4	2	3
10490.2411	.21E-03	121	5	4	2	4	4	1
10491.0057	.22E-03	201	5	0	5	5	2	4
10491.1041	.47E-03	300	1	1	0	2	2	1
10491.4622	.88E-03	300	3	0	3	4	1	4
10496.3354	.91E-04	121	7	2	5	6	2	4
10497.9445	.66E-04	300	3	1	3	4	0	4
10499.7401	.24E-04	300	7	3	4	8	2	7
10499.9630	.23E-04	201	8	6	3	8	6	2
10500.0257	.62E-04	201	8	6	2	8	6	3
10500.4076	.33E-04	300	3	2	1	3	3	0
10500.4076	.33E-04	003	6	4	2	7	6	1
10500.4076	.33E-04	102	6	4	3	7	5	2
10501.5888	.39E-04	300	4	2	2	4	3	1
10502.2851	.48E-04	121	4	2	2	3	0	3
10502.2851	.48E-04	201	7	7	1	7	7	0
10502.2851	.48E-04	201	7	7	0	7	7	1

continued

Table 2 — *continued*

Position (cm^{-1})	Intensity (cm^{-2}/atm)	v'	J (upper)	K_a (upper)	K_c (upper)	J (lower)	K_a (lower)	K_c (lower)
10503.0248	.36E-03	300	3	2	2	4	1	3
10506.8911	.38E-02	201	3	0	3	4	0	4
10507.7369	.12E-01	201	3	1	3	4	1	4
10507.8054	.72E-03	201	5	1	5	5	1	4
10509.3740	.74E-03	201	4	0	4	4	2	3
10509.7604	.51E-04	201	6	2	5	5	4	2
10510.6690	.11E-03	300	5	3	2	6	2	5
10510.8598	.31E-03	300	2	0	2	3	1	3
10511.4357	.52E-02	201	2	2	0	3	2	1
10511.8490	.21E-03	121	6	4	2	5	4	1
10511.9528	.53E-04	121	10	1	9	9	1	8
10512.8816	.75E-04	121	7	3	4	6	3	3
10513.0558	.39E-04	121	6	4	3	5	4	2
10513.0558	.39E-04	201	7	2	6	6	4	3
10513.9432	.40E-04	201	8	5	4	8	5	3
10514.9286	.96E-02	201	2	1	1	3	1	2
10515.0112	.78E-03	201	6	6	1	6	6	0
10515.0112	.78E-03	201	6	6	0	6	6	1
10515.9471	.19E-02	201	2	2	1	3	2	2
10518.2509	.75E-04	121	6	4	3	6	2	4
10519.3262	.16E-03	300	5	1	4	5	2	3
10519.9119	.62E-04	121	8	3	6	7	3	5
10520.9781	.86E-04	300	4	0	4	4	1	3
10522.8987	.35E-03	201	7	5	3	7	5	2
10523.4675	.12E-03	201	7	5	2	7	5	3
10523.6926	.32E-03	201	7	3	5	7	3	4
10525.8102	.21E-03	300	2	1	2	2	2	1
10529.0586	.12E-01	201	2	0	2	3	0	3
10529.5346	.84E-03	300	1	0	1	2	1	2
10530.1731	.51E-04	102	5	4	2	6	5	1
10530.3113	.40E-04	102	5	4	1	6	5	2
10530.4512	.32E-03	201	6	5	2	6	5	1
10530.5626	.24E-02	201	6	5	1	6	5	2
10530.6088	.38E-02	201	2	1	2	3	1	3
10531.4514	.33E-03	201	2	0	2	2	2	1
10532.1170	.14E-03	121	7	4	4	6	4	3
10532.1582	.60E-04	300	3	3	1	4	2	2
10532.1582	.60E-04	102	7	3	4	8	4	5
10532.6200	.73E-04	300	4	1	3	4	2	2
10533.0377	.53E-04	121	7	4	3	6	4	2
10533.6030	.10E-03	121	8	3	5	7	3	4
10533.7491	.17E-04	102	6	3	4	7	4	3
10534.0031	.12E-04	102	6	2	5	7	3	4
10534.5641	.35E-03	201	7	4	4	7	4	3
10536.0638	.66E-04	121	9	3	7	8	3	6
10536.6627	.42E-03	300	2	2	1	3	1	2
10536.9170	.23E-02	201	5	5	1	5	5	0
10539.0345	.25E-03	300	3	1	2	3	2	1
10540.3501	.71E-04	300	2	1	1	2	2	0
10541.0671	.90E-04	121	6	5	1	5	5	0
10541.5252	.23E-04	022	8	2	7	7	3	4
10542.0508	.11E-03	201	8	4	4	8	4	5
10542.5820	.27E-02	201	1	1	0	2	1	1
10542.6559	.38E-03	300	3	0	3	3	1	2
10543.1181	.11E-02	201	5	2	4	5	2	3
10543.2737	.14E-03	201	7	4	3	7	4	4
10544.6055	.41E-03	201	6	4	3	6	4	2
10544.7478	.24E-04	201	9	4	5	9	4	6
10547.2884	.99E-03	201	6	4	2	6	4	3
10548.0320	.13E-03	300	3	3	0	4	2	3
10549.5594	.42E-03	300	1	1	1	2	0	2
10551.7367	.38E-02	201	1	0	1	2	0	2
10551.8613	.26E-02	201	5	4	2	5	4	1
10552.4181	.83E-03	201	5	4	1	5	4	2
10553.1160	.89E-02	201	1	1	1	2	1	2
10553.9543	.82E-04	121	8	4	4	7	4	3
10554.8859	.10E-04	102	5	1	5	5	4	2
10557.5004	.64E-02	201	4	4	0	4	4	1
10557.7914	.17E-03	300	2	0	2	2	1	1
10559.4298	.64E-04	102	4	4	1	5	5	0
10559.4298	.64E-04	102	4	4	0	5	5	1
10559.7181	.21E-02	201	5	3	3	5	3	2
10559.8638	.15E-03	300	3	2	1	4	1	4
10562.8353	.33E-04	300	5	2	3	6	1	6
10563.7686	.93E-03	201	4	2	3	4	2	2
10568.8223	.17E-02	201	4	3	2	4	3	1
10569.1856	.58E-04	300	2	2	0	3	1	3
10570.8765	.66E-03	201	5	3	2	5	3	3
10571.9256	.50E-02	201	4	3	1	4	3	2
10573.3489	.69E-03	201	6	3	3	6	3	4
10574.3153	.12E-01	201	3	3	1	3	3	0
10574.7021	.80E-02	201	0	0	0	1	0	1
10574.7849	.38E-02	201	3	3	0	3	3	1
10575.2161	.40E-04	102	5	3	2	6	4	3
10575.2822	.42E-04	201	4	1	3	3	3	0
10577.5420	.15E-02	201	2	1	2	2	1	1
10577.9732	.64E-02	201	3	2	2	3	2	1
10579.8895	.79E-04	201	7	3	4	7	3	5
10580.8080	.51E-04	121	8	5	3	7	5	2
10582.2874	.12E-04	102	10	1	10	11	0	11
10584.6572	.19E-04	300	4	2	3	3	3	0
10584.9645	.17E-04	102	5	2	4	6	3	3
10585.9960	.48E-02	201	2	2	1	2	2	0
10586.3381	.46E-04	201	2	2	0	3	0	3
10588.1594	.21E-04	121	10	4	6	9	4	5
10588.2010	.30E-04	300	6	3	4	5	4	1
10588.7260	.12E-01	201	2	2	0	2	2	1
10590.1569	.10E-01	201	1	1	1	1	1	0
10590.4893	.20E-02	201	3	2	1	3	2	2
10591.0566	.39E-04	201	5	0	5	4	2	2
10591.9319	.26E-04	201	8	1	7	7	3	4
10596.2055	.25E-02	201	4	2	2	4	2	3
10597.3777	.18E-03	201	4	0	4	3	2	1
10598.7861	.51E-04	102	4	3	2	5	4	1
10600.3765	.31E-04	121	9	5	5	8	5	4
10600.6214	.34E-02	201	1	1	0	1	1	1
10601.3416	.30E-04	300	7	3	5	6	4	2
10601.4769	.64E-03	300	1	1	0	1	0	1
10602.0213	.11E-03	300	7	3	4	7	2	5
10605.8062	.36E-03	201	5	2	3	5	2	4
10606.6037	.10E-04	121	10	6	4	9	4	5
10606.8652	.12E-03	201	6	1	5	5	3	2
10608.6323	.21E-03	300	4	2	2	4	1	3
10608.8040	.49E-02	201	2	1	1	2	1	2
10609.4589	.28E-04	300	8	3	6	7	4	3
10610.2020	.42E-03	300	5	2	3	5	1	4
10611.0583	.73E-03	300	3	2	1	3	1	2
10613.5673	.23E-04	102	8	2	7	9	1	8
10613.9342	.59E-03	300	3	1	2	3	0	3
10615.8282	.69E-04	300	2	0	2	1	1	1
10615.8282	.69E-04	300	4	3	2	5	0	5
10616.1197	.19E-03	300	2	2	0	2	1	1
10618.2315	.31E-03	201	6	2	4	6	2	5
10620.3244	.26E-04	121	8	6	3	7	6	2
10620.6172	.61E-03	201	3	1	2	3	1	3
10621.7417	.16E-02	201	1	0	1	0	0	0
10626.0785	.13E-03	300	4	1	3	4	0	4
10626.2250	.11E-03	300	7	2	5	7	1	6
10626.9221	.16E-03	300	4	3	1	4	2	2
10627.9468	.86E-04	102	3	3	0	4	4	1
10629.6982	.15E-04	300	7	3	4	6	4	3
10630.5453	.59E-03	300	2	2	1	2	1	2
10632.1823	.33E-04	201	7	2	5	7	2	6
10634.7453	.64E-03	201	4	1	3	4	1	4
10635.5812	.34E-02	201	2	1	2	1	1	1
10635.8637	.57E-04	300	8	4	5	8	3	6
10636.0356	.45E-03	300	3	3	0	3	2	1
10636.1831	.23E-02	300	2	1	2	1	0	1

continued

Table 2 – *continued*

Position	Intensity	v'	J	K_a	K_c	J	K_a	K_c
(cm^{-1})	(cm^{-2}/atm)		upper			lower		
10636.2530	.28E-03	300	3	2	2	3	1	3
10636.6975	.51E-04	102	7	1	6	8	2	7
10636.9290	.42E-04	300	8	5	4	8	4	5
10637.6319	.23E-04	300	8	2	6	8	1	7
10638.3940	.31E-04	300	7	4	4	7	3	5
10638.9749	.28E-04	102	8	0	8	9	1	9
10640.4589	.23E-03	300	5	1	4	5	0	5
10641.0373	.53E-03	300	4	3	2	4	2	3
10641.4834	.71E-04	300	7	5	2	7	4	3
10641.8229	.12E-01	201	2	0	2	1	0	1
10642.4174	.75E-04	102	7	2	6	8	1	7
10643.9926	.29E-03	300	6	3	4	6	2	5
10644.1200	.85E-03	300	4	2	3	4	1	4
10645.8559	.12E-01	201	2	1	1	1	1	0
10648.1362	.64E-04	300	7	3	5	7	2	6
10648.3062	.48E-04	300	5	2	4	5	1	5
10649.0438	.82E-04	022	4	4	1	4	3	2
10649.3337	.42E-04	102	4	2	2	5	3	3
10649.5582	.53E-03	300	3	1	3	2	0	2
10650.8877	.64E-04	300	6	5	1	6	4	2
10651.4205	.10E-03	201	2	2	1	2	0	2
10651.8973	.11E-03	300	6	5	2	6	4	3
10652.8176	.12E-01	201	3	1	3	2	1	2
10654.1036	.11E-03	300	8	3	6	8	2	7
10654.8205	.28E-03	201	5	1	4	5	1	5
10655.2634	.73E-02	201	3	2	2	2	2	1
10657.2264	.22E-03	201	4	2	3	4	0	4
10658.1409	.64E-04	300	5	5	1	5	4	2
10658.5078	.55E-02	201	3	0	3	2	0	2
10659.3830	.24E-04	300	6	2	5	6	1	6
10660.5403	.24E-02	201	3	2	1	2	2	0
10661.0808	.55E-04	300	6	6	1	6	5	2
10661.2313	.11E-02	300	4	1	4	3	0	3
10661.6680	.99E-04	201	7	3	5	7	1	6
10662.5739	.51E-04	102	3	2	2	4	3	1
10663.0666	.42E-04	201	6	3	4	6	1	5
10663.1595	.17E-04	201	8	3	6	8	1	7
10664.2505	.46E-03	201	5	2	4	5	0	5
10665.1895	.11E-03	102	7	0	7	8	1	8
10665.4609	.39E-04	102	7	1	7	8	0	8
10667.0448	.66E-04	300	7	1	6	7	0	7
10667.4372	.13E-02	201	4	3	2	3	3	1
10668.0124	.22E-03	201	5	3	3	5	1	4
10668.3942	.52E-02	201	4	1	4	3	1	3
10668.9637	.38E-02	201	4	3	1	3	3	0
10670.5438	.11E-03	102	3	2	1	4	3	2
10671.5882	.14E-04	121	8	3	5	7	1	6
10671.9789	.71E-04	102	6	2	5	7	1	6
10672.2754	.12E-01	201	4	0	4	3	0	3
10672.4137	.30E-03	300	5	1	5	4	0	4
10673.3649	.31E-02	201	4	2	3	3	2	2
10674.0498	.14E-02	201	5	4	2	4	4	1
10674.1585	.53E-04	300	2	2	0	1	1	1
10674.3403	.46E-03	201	5	4	1	4	4	0
10674.4902	.48E-04	121	6	4	3	6	0	6
10675.8692	.40E-04	201	4	3	2	4	1	3
10676.0106	.42E-04	121	5	4	2	4	2	3
10678.8954	.11E-03	201	7	6	2	6	6	1
10678.8954	.11E-03	003	9	5	5	10	5	6
10680.0519	.75E-04	201	7	1	6	7	1	7
10681.7067	.12E-03	102	5	1	4	6	2	5
10683.1935	.71E-04	300	3	2	2	2	1	1
10684.2091	.89E-02	201	4	2	2	3	2	1
10684.5138	.43E-02	201	5	0	5	4	0	4
10684.9712	.40E-04	201	3	3	1	3	1	2
10685.9392	.12E-01	201	4	1	3	3	1	2
10686.0865	.42E-02	201	5	3	3	4	3	2
10686.7324	.35E-04	300	9	1	8	9	0	9
10689.4731	.80E-02	201	5	2	4	4	2	3
10690.3050	.10E-03	201	8	1	7	8	1	8
10690.8803	.13E-02	201	5	3	2	4	3	1
10691.1004	.37E-04	201	8	2	7	8	0	8
10691.2012	.18E-03	102	6	1	6	7	0	7
10692.6500	.16E-03	102	2	2	1	3	3	0
10693.5956	.14E-02	201	6	4	2	5	4	1
10693.7872	.10E-03	300	7	1	7	6	0	6
10694.3074	.55E-04	102	2	2	0	3	3	1
10694.4065	.12E-03	201	7	5	2	6	5	1
10694.9464	.33E-02	201	6	1	6	5	1	5
10695.3142	.10E-02	300	4	2	3	3	1	2
10695.9568	.12E-01	201	6	0	6	5	0	5
10699.0535	.19E-02	300	5	2	4	4	1	3
10702.5053	.15E-03	300	8	1	8	7	0	7
10702.6838	.70E-03	121	7	3	5	6	1	6
10702.8789	.11E-02	201	6	3	4	5	3	3
10704.7857	.24E-04	102	7	0	7	7	1	6
10704.9401	.33E-04	300	3	2	1	2	1	2
10705.0801	.97E-03	121	6	4	3	5	2	4
10705.5693	.16E-02	201	5	1	4	4	1	3
10705.8600	.24E-02	201	5	2	3	4	2	2
10706.7077	.80E-02	201	7	0	7	6	0	6
10706.7077	.80E-02	201	7	1	7	6	1	6
10709.1552	.96E-03	201	7	4	4	6	4	3
10710.1792	.12E-03	201	8	5	4	7	5	3
10711.3054	.28E-03	201	8	5	3	7	5	2
10711.8111	.77E-04	300	3	3	1	2	2	0
10713.1032	.31E-03	201	7	4	3	6	4	2
10713.2467	.30E-02	201	6	3	3	5	3	2
10713.3250	.17E-03	300	3	3	0	2	2	1
10713.8278	.80E-04	300	7	2	6	6	1	5
10715.0551	.28E-03	102	5	0	5	6	1	6
10715.1576	.89E-02	201	6	1	5	5	1	4
10715.1576	.89E-02	201	7	2	6	6	2	5
10715.2966	.27E-02	201	8	0	8	7	0	7
10717.4846	.19E-02	201	7	3	5	6	3	4
10717.9486	.15E-03	300	8	2	7	7	1	6
10718.9146	.13E-02	121	8	2	6	7	0	7
10719.6942	.49E-04	300	10	1	10	9	0	9
10721.1764	.69E-04	300	9	1	8	8	2	7
10721.5201	.24E-04	102	5	3	2	5	4	1
10722.3936	.15E-04	003	8	4	4	9	4	5
10722.7689	.19E-04	102	4	3	1	4	4	0
10722.7689	.19E-04	003	9	3	7	10	3	8
10723.2176	.11E-02	201	7	1	6	6	1	5
10724.0475	.45E-02	201	6	2	4	5	2	3
10725.0035	.12E-03	201	9	5	5	8	5	4
10725.1730	.20E-02	201	9	1	9	8	1	8
10725.3778	.71E-03	201	9	0	9	8	0	8
10725.4886	.64E-03	201	8	2	7	7	2	6
10726.3745	.42E-04	300	11	0	11	10	1	10
10726.3745	.42E-04	300	11	1	11	10	0	10
10728.1377	.48E-04	201	9	5	4	8	5	3
10729.3390	.26E-04	300	10	2	9	9	1	8
10729.6471	.34E-03	201	8	3	6	7	3	5
10729.9106	.19E-02	201	8	1	7	7	1	6
10733.2432	.51E-03	201	8	4	4	7	4	3
10733.3765	.10E-02	201	10	0	10	9	0	9
10733.7841	.49E-04	102	6	0	6	6	1	5
10734.1704	.95E-03	201	9	2	8	8	2	7
10734.5144	.57E-03	201	7	3	4	6	3	3
10735.4831	.24E-04	003	8	3	5	9	3	6
10735.6952	.99E-04	102	4	2	3	5	1	4
10735.9926	.24E-03	201	9	1	8	8	1	7
10737.2157	.26E-03	201	9	4	6	8	4	5
10737.8825	.68E-04	102	2	1	1	3	2	2
10737.9599	.13E-03	102	4	0	4	5	1	5
10738.2345	.67E-03	201	7	2	5	6	2	4
10739.4497	.90E-04	041	9	5	4	8	1	7

continued

Table 2 — *continued*

Position (cm^{-1})	Intensity (cm^{-2}/atm)	v'	J (upper)	K_a (upper)	K_c (upper)	J (lower)	K_a (lower)	K_c (lower)	Position (cm^{-1})	Intensity (cm^{-2}/atm)	v'	J (upper)	K_a (upper)	K_c (upper)	J (lower)	K_a (lower)	K_c (lower)
10740.4740	.20E-03	201	10	2	9	9	2	8	10799.6960	.79E-04	003	7	1	6	8	1	7
10740.9829	.49E-03	102	4	1	4	5	0	5	10800.6491	.99E-04	003	7	2	6	8	2	7
10741.7173	.15E-04	300	5	3	3	4	2	2	10800.7082	.55E-04	102	4	1	3	4	2	2
10741.9696	.19E-04	102	6	4	2	7	3	5	10800.8328	.39E-04	003	8	1	8	9	1	9
10742.3333	.47E-03	201	10	1	9	9	1	8	10800.8681	.11E-03	003	8	0	8	9	0	9
10744.1972	.39E-04	003	9	2	8	10	2	9	10802.1219	.14E-04	300	10	4	7	9	3	6
10744.5916	.35E-04	220	10	3	7	9	2	8	10803.3086	.49E-04	102	2	2	1	3	1	2
10745.7622	.71E-04	121	10	4	6	9	2	7	10803.9407	.14E-04	300	4	3	2	3	0	3
10746.3076	.23E-03	201	12	0	12	11	0	11	10804.4870	.42E-04	003	6	3	4	7	3	5
10746.3076	.23E-03	201	12	1	12	11	1	11	10806.8937	.19E-03	102	3	1	2	3	2	1
10746.9244	.19E-04	102	5	1	5	5	2	4	10807.9364	.77E-04	102	2	1	1	2	2	0
10746.9244	.19E-04	300	9	3	7	8	2	6	10809.0970	.37E-04	201	4	3	2	3	1	3
10747.0014	.77E-03	201	8	2	6	7	2	5	10810.2189	.31E-04	003	5	4	1	6	4	2
10747.2362	.17E-03	201	11	2	10	10	2	9	10810.3108	.18E-03	102	3	0	3	3	1	2
10747.8702	.62E-04	201	11	1	10	10	1	9	10810.8736	.84E-04	003	5	4	2	6	4	3
10749.8087	.16E-03	300	6	3	4	5	2	3	10816.5742	.73E-04	102	0	0	0	1	1	1
10750.4492	.33E-04	003	8	2	6	9	2	7	10817.3718	.58E-04	102	1	1	1	2	0	2
10751.2358	.91E-04	300	4	4	1	3	3	0	10821.5417	.31E-03	201	6	3	3	5	1	4
10752.5401	.13E-03	201	12	1	11	11	1	10	10825.3910	.93E-04	102	2	0	2	2	1	1
10752.6144	.12E-02	201	8	3	5	7	3	4	10825.7946	.69E-04	003	5	3	2	6	3	3
10753.2981	.10E-03	201	9	4	5	8	4	4	10826.0307	.21E-03	003	6	1	5	7	1	6
10753.3437	.51E-04	022	9	3	7	8	2	6	10826.3302	.20E-03	003	7	1	7	8	1	8
10753.7703	.95E-04	102	4	2	3	4	3	2	10826.4385	.12E-03	003	6	2	5	7	2	6
10754.1926	.10E-03	300	7	3	5	6	2	4	10826.4385	.12E-03	003	7	0	7	8	0	8
10754.4622	.14E-04	300	7	4	3	7	1	6	10827.0450	.17E-04	102	3	2	1	4	1	4
10755.0876	.31E-04	201	14	0	14	13	0	13	10828.1163	.23E-04	300	8	5	4	7	4	3
10755.0876	.31E-04	201	14	1	14	13	1	13	10831.4080	.20E-03	003	5	3	3	6	3	4
10755.8285	.42E-04	003	7	4	4	8	4	5	10835.3199	.12E-04	003	8	0	8	8	2	7
10756.3792	.40E-03	300	8	3	6	7	2	5	10836.0880	.10E-03	003	5	2	3	6	2	4
10756.3792	.40E-03	201	13	1	12	12	1	11	10837.4494	.99E-04	003	4	4	0	5	4	1
10757.7962	.28E-04	102	7	2	5	7	3	4	10837.6318	.37E-04	003	4	4	1	5	4	2
10758.4581	.22E-03	102	1	1	0	2	2	1	10841.4267	.15E-04	102	6	2	4	7	1	7
10759.1105	.85E-03	102	3	0	3	4	1	4	10842.5887	.91E-04	201	5	3	3	4	1	4
10759.1105	.85E-03	201	4	2	2	3	0	3	10844.4997	.23E-04	201	5	4	1	4	2	2
10760.3944	.30E-04	102	4	3	2	5	2	3	10845.1807	.13E-03	201	6	2	4	5	0	5
10761.1858	.21E-04	102	3	2	2	3	3	1	10845.6692	.10E-04	003	8	1	7	8	3	6
10761.6183	.17E-04	003	6	5	1	7	5	2	10851.2560	.44E-03	003	6	0	6	7	0	7
10761.9935	.16E-03	201	10	2	8	9	2	7	10851.6946	.13E-03	003	5	1	4	6	1	5
10762.4212	.49E-04	102	5	0	5	5	1	4	10851.9268	.34E-03	003	5	2	4	6	2	5
10763.3762	.39E-04	201	3	3	0	2	1	1	10852.1942	.11E-03	003	6	1	6	7	1	7
10764.1910	.35E-04	121	10	6	4	9	2	7	10852.5034	.55E-04	201	7	3	4	6	1	5
10765.7378	.12E-03	102	3	1	3	4	0	4	10855.1939	.40E-03	003	4	3	1	5	3	2
10765.7824	.21E-04	003	7	3	4	8	3	5	10855.1939	.40E-03	201	6	4	2	5	2	3
10766.0360	.15E-03	201	9	3	6	8	3	5	10857.6881	.14E-04	102	9	4	5	9	3	6
10766.2045	.68E-04	102	4	1	4	4	2	3	10858.0822	.97E-04	003	4	3	2	5	3	3
10766.6000	.26E-04	102	6	1	5	6	2	4	10859.8182	.57E-04	201	5	4	2	4	2	3
10766.6000	.26E-04	102	6	2	4	6	3	3	10862.9543	.21E-04	003	7	7	1	7	7	0
10767.5797	.60E-04	102	3	2	1	3	3	0	10862.9543	.21E-04	003	7	7	0	7	7	1
10769.3330	.24E-04	102	4	2	2	4	3	1	10864.6695	.49E-03	003	4	2	2	5	2	3
10769.6228	.37E-04	102	3	2	2	4	1	3	10865.9542	.82E-04	201	7	4	3	6	2	4
10770.2304	.57E-04	102	5	2	3	5	3	2	10867.9186	.30E-04	003	2	0	2	3	2	1
10771.4530	.88E-04	201	10	4	6	9	4	5	10868.8293	.35E-03	102	1	1	0	1	0	1
10773.9363	.11E-03	201	10	3	7	9	3	6	10870.2593	.57E-04	102	7	3	4	7	2	5
10774.4464	.68E-04	003	9	1	9	10	1	10	10873.3605	.13E-03	102	2	1	1	2	0	2
10778.4585	.12E-03	102	2	0	2	3	1	3	10874.1799	.14E-03	003	5	0	5	6	0	6
10778.8552	.60E-04	201	3	3	1	2	1	2	10875.0221	.44E-04	102	6	3	3	6	2	4
10779.6089	.36E-03	201	4	3	1	3	1	2	10875.7159	.62E-03	003	5	1	5	6	1	6
10780.1023	.26E-04	300	5	5	0	4	4	1	10876.3829	.10E-03	102	4	2	2	4	1	3
10781.8750	.60E-04	102	3	1	3	3	2	2	10876.9712	.63E-03	003	4	1	3	5	1	4
10783.6066	.26E-04	003	6	4	3	7	4	4	10877.0400	.17E-03	003	4	2	3	5	2	4
10785.5729	.39E-04	003	5	5	1	6	5	2	10878.2402	.35E-03	102	3	2	1	3	1	2
10787.5249	.97E-04	102	5	1	4	5	2	3	10878.5244	.21E-03	102	5	2	3	5	1	4
10788.7168	.37E-04	102	4	0	4	4	1	3	10879.1807	.26E-04	201	6	3	4	5	1	5
10791.1717	.30E-03	102	2	1	2	3	0	3	10880.1636	.71E-04	201	8	4	4	7	2	5
10795.8621	.11E-03	003	6	3	3	7	3	4	10881.7908	.32E-03	102	3	1	2	3	0	3
10797.0584	.36E-03	102	1	0	1	2	1	2	10881.8424	.48E-04	003	6	1	5	6	3	4
10797.9275	.12E-03	201	5	3	2	4	1	3	10882.8992	.80E-04	102	2	2	0	2	1	1
10798.7815	.46E-04	300	8	4	5	7	3	4	10883.1268	.15E-03	102	5	3	2	5	2	3
10799.3183	.10E-03	201	5	2	3	4	0	4	10883.4642	.10E-03	003	3	3	0	4	3	1

continued

Table 2 — *continued*

Position	Intensity	v'	J	K_a	K_c	J	K_a	K_c	Position	Intensity	v'	J	K_a	K_c	J	K_a	K_c
(cm^{-1})	(cm^{-2}/atm)		upper			lower			(cm^{-1})	(cm^{-2}/atm)		upper			lower		
10883.6199	.40E-04	102	7	4	3	7	3	4	10932.7906	.53E-04	003	6	5	1	6	5	2
10884.1841	.31E-04	102	3	1	2	2	2	1	10933.5835	.12E-04	201	9	3	6	8	1	7
10884.5067	.27E-03	003	3	3	1	4	3	2	10933.8803	.68E-04	102	5	1	4	4	2	3
10884.5910	.10E-03	003	6	0	6	6	2	5	10934.2309	.30E-03	102	2	2	1	1	1	0
10884.5910	.10E-03	102	6	2	4	6	1	5	10935.4112	.42E-04	102	7	1	6	7	0	7
10887.3758	.79E-04	102	1	1	1	0	0	0	10936.9951	.18E-03	102	5	0	5	4	1	4
10890.5920	.11E-03	201	8	3	5	7	1	6	10937.2407	.37E-04	003	3	0	3	3	2	2
10891.5109	.15E-04	003	5	1	4	5	3	3	10938.3567	.17E-04	102	7	2	6	7	1	7
10892.3068	.30E-04	003	7	6	2	7	6	1	10940.1749	.24E-04	003	7	3	5	7	3	4
10892.3068	.30E-04	003	7	6	1	7	6	2	10940.4214	.68E-04	102	5	1	5	4	0	4
10892.9167	.82E-04	102	4	3	1	4	2	2	10940.9386	.93E-04	102	2	2	0	1	1	1
10893.5404	.21E-03	003	3	2	1	4	2	2	10940.9386	.93E-04	201	8	4	5	7	2	6
10893.7391	.39E-04	201	5	5	1	4	3	2	10942.8180	.13E-02	003	2	0	2	3	0	3
10894.1693	.79E-04	102	4	1	3	4	0	4	10943.4394	.17E-04	201	8	2	6	7	0	7
10894.4791	.19E-04	201	7	2	5	6	0	6	10943.9332	.39E-03	003	2	1	2	3	1	3
10895.0434	.33E-04	003	4	1	3	4	3	2	10945.2113	.55E-04	003	2	0	2	2	2	1
10895.7820	.53E-04	102	7	2	5	7	1	6	10949.8912	.48E-04	102	6	0	6	5	1	5
10896.6034	.33E-04	102	5	2	3	4	3	2	10951.4822	.13E-03	102	6	1	6	5	0	5
10896.6034	.33E-04	102	6	4	2	6	3	3	10953.4347	.49E-04	003	6	4	3	6	4	2
10898.8757	.87E-03	003	4	0	4	5	0	5	10953.4347	.49E-04	102	6	1	5	5	2	4
10899.0157	.35E-03	003	4	1	4	5	1	5	10955.4716	.28E-03	003	1	1	0	2	1	1
10899.6441	.99E-04	003	6	6	1	6	6	0	10956.5204	.10E-03	003	6	4	2	6	4	3
10899.6441	.99E-04	003	6	6	0	6	6	1	10957.7425	.11E-03	003	5	2	4	5	2	3
10900.7404	.17E-04	201	9	4	5	8	2	6	10957.8692	.80E-04	003	5	4	1	5	4	2
10901.7202	.15E-03	102	3	3	0	3	2	1	10959.1086	.30E-04	003	6	3	4	6	3	3
10901.9186	.87E-03	003	3	2	2	4	2	3	10959.1086	.30E-04	201	8	3	6	7	1	7
10902.5322	.30E-03	003	3	1	2	4	1	3	10959.5552	.20E-03	003	4	4	1	4	4	0
10903.7925	.21E-04	102	7	5	2	7	4	3	10959.6383	.61E-03	003	4	4	0	4	4	1
10903.9358	.29E-03	102	2	1	2	1	0	1	10961.4614	.18E-03	102	4	2	3	3	1	2
10904.1931	.25E-03	102	3	0	3	2	1	2	10962.1381	.26E-04	102	7	1	7	6	0	6
10905.1402	.15E-04	102	8	4	5	8	3	6	10964.9192	.42E-03	003	1	0	1	2	0	2
10906.7456	.17E-03	102	4	3	2	4	2	3	10965.8626	.10E-02	003	1	1	1	2	1	2
10907.2150	.84E-04	102	5	4	1	5	3	2	10968.7431	.33E-04	102	7	1	6	6	2	5
10907.4022	.49E-04	102	3	3	1	3	2	2	10969.8093	.40E-04	102	5	2	4	4	1	3
10907.4776	.24E-04	201	6	5	1	5	3	2	10971.3036	.20E-03	003	5	3	3	5	3	2
10907.9862	.28E-04	102	7	6	1	7	5	2	10972.1228	.13E-03	102	3	2	1	2	1	2
10908.6008	.48E-04	102	6	4	3	6	3	4	10972.3690	.39E-04	102	8	1	8	7	0	7
10910.2704	.18E-03	102	4	2	3	4	1	4	10972.9012	.23E-03	003	3	1	3	3	1	2
10910.4315	.68E-04	102	6	3	4	6	2	5	10973.0569	.10E-04	201	9	4	6	8	2	7
10910.4315	.68E-04	300	7	3	5	6	0	6	10978.0849	.17E-03	003	4	3	2	4	3	1
10911.2523	.42E-04	201	7	4	4	6	2	5	10979.0110	.31E-03	102	3	3	0	2	2	1
10912.1036	.23E-04	102	5	4	2	5	3	3	10981.5497	.14E-02	003	3	3	1	3	3	0
10912.3894	.12E-04	201	6	5	2	5	3	3	10981.5497	.14E-02	003	4	3	1	4	3	2
10914.1167	.42E-04	102	6	5	2	6	4	3	10982.0789	.38E-03	003	3	3	0	3	3	1
10916.2407	.75E-04	102	4	4	1	4	3	2	10983.6030	.69E-04	003	5	3	2	5	3	3
10916.6250	.17E-04	102	6	6	0	6	5	1	10987.4820	.21E-04	102	8	2	7	7	1	6
10916.6878	.66E-04	102	6	6	1	6	5	2	10988.1094	.96E-03	003	0	0	0	1	0	1
10917.3539	.97E-04	102	3	1	3	2	0	2	10988.3066	.14E-04	102	10	1	10	9	0	9
10918.3116	.37E-04	201	7	3	5	6	1	6	10989.6551	.69E-04	003	6	3	3	6	3	4
10919.0031	.48E-04	102	8	3	6	8	2	7	10989.9224	.67E-03	003	3	2	2	3	2	1
10920.1533	.53E-04	102	5	5	0	5	4	1	10990.3927	.14E-04	003	6	0	6	5	2	3
10920.3996	.23E-04	102	5	5	1	5	4	2	10990.3927	.14E-04	102	9	1	8	8	2	7
10921.1002	.38E-03	003	3	0	3	4	0	4	10990.8655	.15E-03	003	2	1	2	2	1	1
10921.7070	.11E-02	003	3	1	3	4	1	4	10994.7492	.18E-03	102	4	3	2	3	2	1
10921.9443	.86E-04	102	4	0	4	3	1	3	10996.7287	.49E-03	003	2	2	1	2	2	0
10922.3457	.57E-03	003	2	2	0	3	2	1	10998.7030	.14E-04	201	9	2	7	8	0	8
10922.8496	.46E-04	102	6	1	5	6	0	6	10999.6365	.14E-02	003	2	2	0	2	2	1
10923.0810	.68E-04	003	5	1	5	5	1	4	11002.5164	.64E-04	102	4	3	1	3	2	2
10924.0997	.88E-04	003	4	0	4	4	2	3	11002.9017	.10E-02	003	1	1	1	1	1	0
10925.6962	.24E-04	201	8	5	3	7	3	4	11003.1372	.22E-03	003	3	2	1	3	2	2
10926.6788	.20E-03	003	2	2	1	3	2	2	11009.1382	.39E-04	102	5	3	3	4	2	2
10928.6193	.79E-04	102	6	2	5	6	1	6	11009.6129	.23E-04	102	4	2	2	3	1	3
10928.7581	.10E-02	003	2	1	1	3	1	2	11011.0242	.28E-03	003	4	2	2	4	2	3
10929.0517	.17E-04	201	10	4	6	9	2	7	11012.1016	.33E-04	003	4	0	4	3	2	1
10929.1049	.25E-03	102	4	1	4	3	0	3	11013.2774	.22E-03	102	4	4	1	3	3	0
10931.0829	.23E-04	003	7	5	2	7	5	3	11013.5095	.37E-03	003	1	1	0	1	1	1
10931.0829	.23E-04	201	7	5	3	6	3	4	11016.2471	.60E-04	102	6	3	4	5	2	3
10932.0324	.28E-03	003	5	5	1	5	5	0	11021.2764	.19E-04	102	8	3	6	7	2	5
10932.6885	.19E-04	003	6	5	2	6	5	1	11021.7413	.14E-04	003	6	1	5	5	3	2

continued

Table 2 — *continued*

Position	Intensity	v'	J	K_a	K_c	J	K_a	K_c
(cm^{-1})	(cm^{-2}/atm)		upper			lower		
11022.6409	.47E-03	003	2	1	1	2	1	2
11029.4819	.93E-04	102	5	3	2	4	2	3
11032.1103	.44E-04	102	5	4	2	4	3	1
11033.5828	.11E-03	102	5	4	1	4	3	2
11034.9237	.29E-03	003	1	0	1	0	0	0
11035.7606	.82E-04	003	3	1	2	3	1	3
11037.5174	.55E-04	003	6	2	4	6	2	5
11042.3358	.12E-03	102	5	5	0	4	4	1
11048.9045	.37E-03	003	2	1	2	1	1	1
11051.5460	.13E-03	003	4	1	3	4	1	4
11053.0984	.15E-04	102	5	2	3	4	1	4
11055.5824	.15E-02	003	2	0	2	1	0	1
11059.6816	.10E-02	003	2	1	1	1	1	0
11060.5847	.21E-04	102	6	5	1	5	4	2
11061.8514	.15E-04	102	6	3	3	5	2	4
11063.3613	.14E-04	003	7	6	2	6	6	1
11063.3613	.14E-04	003	7	6	1	6	6	0
11064.8204	.75E-04	003	3	2	2	3	0	3
11066.7838	.15E-02	003	3	1	3	2	1	2
11067.2128	.75E-03	003	3	2	2	2	2	1
11067.8108	.23E-04	003	5	1	4	5	1	5
11068.0597	.15E-04	102	8	4	5	7	3	4
11070.5461	.28E-04	003	4	2	3	4	0	4
11072.7167	.57E-03	003	3	0	3	2	0	2
11073.1884	.25E-03	003	3	2	1	2	2	0
11076.6983	.14E-03	003	4	3	2	3	3	1
11077.4167	.21E-04	102	7	4	3	6	3	4
11078.1590	.33E-04	003	7	3	5	7	1	6
11078.6022	.40E-03	003	4	3	1	3	3	0
11078.8739	.58E-04	003	5	2	4	5	0	5
11079.1848	.35E-04	003	6	5	2	5	5	1
11079.2468	.11E-03	003	6	5	1	5	5	0
11079.6077	.28E-04	003	5	3	3	5	1	4
11079.7907	.73E-04	003	5	4	1	4	4	0
11082.6916	.50E-03	003	3	1	2	2	1	1
11082.9886	.55E-03	003	4	1	4	3	1	3
11086.6869	.41E-03	003	4	2	3	3	2	2
11086.9994	.16E-02	003	4	0	4	3	0	3
11090.5691	.30E-04	102	7	7	1	6	6	0
11090.5691	.30E-04	102	7	7	0	6	6	1
11097.6585	.17E-02	003	5	1	5	4	1	4
11097.6585	.17E-02	003	5	3	3	4	3	2
11098.2785	.31E-03	003	5	0	5	4	0	4
11099.0271	.93E-03	003	4	2	2	3	2	1
11101.7370	.62E-04	003	7	5	3	6	5	2
11102.0225	.24E-04	003	7	5	2	6	5	1
11102.5948	.20E-03	102	5	3	3	4	0	4
11102.7404	.13E-02	003	4	1	3	3	1	2
11102.8300	.18E-03	003	6	4	2	5	4	1
11104.0972	.86E-03	003	5	2	4	4	2	3
11110.0084	.42E-04	003	2	2	0	1	0	1
11111.4765	.37E-03	003	6	1	6	5	1	5
11116.9175	.12E-03	003	6	3	4	5	3	3
11118.5613	.33E-03	003	5	1	4	4	1	3
11119.3317	.26E-03	003	6	2	5	5	2	4
11122.5753	.70E-03	003	7	1	7	6	1	6
11122.9679	.32E-03	003	5	2	3	4	2	2
11123.1150	.22E-03	003	7	0	7	6	0	6
11126.9711	.28E-04	003	7	4	3	6	4	2
11129.5538	.32E-03	003	6	3	3	5	3	2
11130.0375	.63E-03	003	6	1	5	5	1	4
11132.6914	.40E-03	003	7	2	6	6	2	5
11133.8071	.14E-03	003	8	1	8	7	1	7
11133.9720	.23E-03	003	7	3	5	6	3	4
11134.0301	.44E-03	003	8	0	8	7	0	7
11137.3796	.46E-04	102	6	3	4	5	0	5
11138.0623	.33E-04	003	4	3	1	4	1	4
11138.0623	.33E-04	003	8	2	7	7	2	6
11138.6149	.35E-04	003	3	2	1	2	0	2
11138.7974	.12E-03	003	7	1	6	6	1	5
11142.2503	.21E-04	003	9	5	5	8	5	4
11143.3334	.53E-03	003	6	2	4	5	2	3
11143.9982	.24E-03	003	9	1	9	8	1	8
11146.5564	.20E-03	003	8	1	7	7	1	6
11149.4927	.51E-04	102	8	3	5	7	2	6
11151.3527	.10E-03	003	9	2	8	8	2	7
11151.6468	.66E-04	003	8	4	4	7	4	3
11152.4193	.33E-04	102	7	2	5	6	1	6
11153.9961	.39E-04	003	9	1	8	8	1	7
11154.4611	.95E-04	003	7	3	4	6	3	3
11157.1076	.35E-04	003	9	4	6	8	4	5
11158.8871	.11E-03	003	7	2	5	6	2	4
11159.8657	.19E-04	003	10	2	9	9	2	8
11161.1029	.51E-04	003	10	1	9	9	1	8
11161.6432	.64E-04	003	11	1	11	10	1	10
11162.0340	.58E-04	003	9	3	7	8	3	6
11167.0384	.23E-04	003	11	2	10	10	2	9
11167.5523	.15E-04	003	11	1	10	10	1	9
11169.0334	.13E-03	003	8	2	6	7	2	5
11172.8427	.14E-04	003	11	3	9	10	3	8
11173.9253	.84E-04	003	4	2	2	3	0	3
11175.8903	.10E-03	003	8	3	5	7	3	4
11177.9226	.28E-04	003	10	2	8	9	2	7
11186.0783	.14E-04	003	3	3	1	2	1	2
11189.2584	.51E-04	003	4	3	1	3	1	2
11192.8483	.14E-04	102	9	3	6	8	2	7
11210.6515	.24E-04	003	5	3	2	4	1	3
11216.4300	.15E-04	003	5	2	3	4	0	4
11217.7157	.12E-04	102	8	3	6	7	0	7
11237.8486	.53E-04	003	6	3	3	5	1	4
11254.1696	.21E-04	003	5	3	3	4	1	4
11264.4607	.31E-04	003	6	2	4	5	0	5
11265.1398	.14E-04	003	5	4	2	4	2	3
11272.4525	.15E-04	003	7	3	4	6	1	5
11293.2242	.14E-04	003	6	3	4	5	1	5
11298.5646	.15E-04	003	8	4	4	7	2	5
11334.8027	.12E-04	003	7	3	5	6	1	6

with

$$c_0 = \left[A - \frac{B+C}{2}\right]k^2 + \frac{B+C}{2}j(j+1),$$

$$c_1 = -\Delta_k k^4 - \Delta_{jk}k^2 j(j+1) - \Delta_j j^2(j+1)^2,$$

$$2c_2 = H_k k^6 + H_{kj}k^4 j(j+1) + H_{jk}k^2 j^2(j+1)^2 + H_j j^3(j+1)^3 + L_k k^8 + \cdots, \quad (3)$$

$$b_0 = \frac{B-C}{2},$$

$$b_1 = -\delta_k[k^2 + (k \pm 2)^2] - 2\delta_j j(j+1),$$

$$2b_2 = h_k[k^4 + (k \pm 2)^4] + h_{jk}[k^2 + (k \pm 2)^2]j(j+1) + 2h_j j^2(j+1)^2 + \cdots. \quad (4)$$

Table 3. Band origins, rotational, centrifugal distortion and resonance coupling constants for the vibrational states of the first decade of the $H_2{}^{17}O$ molecule (in cm^{-1})

Parameter		(003)	(201)	(102)	(300)
E_v		11011.88290	10598.47560	10853.5053	10586.037250(5100)
A		24.3770854(8000)	25.126631(1300)	25.108285(1300)	25.293061(1200)
B		14.2052102(1200)	13.9759919(2400)	14.0111977(4100)	13.9381690(7200)
C		8.84324475(9900)	8.7577290(2200)	8.7751174(2700)	8.7806736(2800)
Δ_k	10^{-1}	0.2440195(6400)	0.243237(1400)	0.281634(1200)	0.2340654(9700)
Δ_{jk}	10^{-2}	-0.581058(1100)	-0.502553(3700)	-0.539612(360)	-0.547068(6600)
Δ_j	10^{-2}	0.137	0.13110-02	0.12890323(9600)	0.1316828(7000)
δ_k	10^{-2}	0.107357(1000)	0.109150(3100)	0.105218(2000)	0.126913(2900)
δ_j	10^{-3}	0.555	0.505129(1200)	0.523158(1700)	0.535296(3300)
H_k	10^{-4}	0.77407(1300)	1.04808(5000)	0.75950(3200)	0.79
H_{kj}	10^{-4}	-0.19	-0.18195(1800)	-0.12	-0.12
H_{jk}	10^{-5}	-0.20	-0.20	-0.20	-0.20
H_j	10^{-6}	0.79	0.53	0.66	0.66
h_k	10^{-4}	0.24	0.24	0.24	0.24
h_{jk}	10^{-5}	0.00	-0.24246(2400)	0.00	0.00
h_j	10^{-6}	0.33	0.33	0.33	0.33
L_k	10^{-6}	-0.12	-0.12	-0.12	-0.12
L_{kkj}	10^{-6}	0.12	0.12	0.12	0.12
L_{jjk}	10^{-7}	-0.57	-0.57	-0.57	-0.57

Parameter		(121)	(022)	(220)
E_v		10311.2025	10502.5	10269.69027(1700)
A		32.162643(1300)	30.94423(2200)	33.066034(4900)
B		14.5713622(6600)	14.821049(9400)	14.449491(1800)
C		8.643934(4100)	8.574609(2700)	8.608269(1400)
Δ_k	10^{-1}	0.873194(1500)	0.73515(1700)	0.995580(4800)
Δ_{jk}	10^{-2}	-0.990427(6600)	-1.21283(4200)	-0.89121(1500)
Δ_j	10^{-2}	0.158034(1000)	0.192	0.102976(1400)
δ_k	10^{-2}	0.759722(3600)	0.83969(1900)	0.40
δ_j	10^{-3}	0.727495(2900)	0.82	0.74
H_k	10^{-3}	1.062598(8000)	0.77	0.88
H_{kj}	10^{-4}	-0.84513(5400)	-0.50	-0.50
H_{jk}	10^{-4}	0.19752(1300)	0.23	0.23
H_j	10^{-5}	0.080460(4100)	0.12	0.12
h_k	10^{-3}	0.20	0.20	0.20
h_{jk}	10^{-5}	0.85	0.85	0.85
h_j	10^{-6}	0.60	0.60	0.60
L_k	10^{-5}	-0.24	-0.24	-0.24
L_{kkj}	10^{-5}	0.12	0.12	0.12
L_{jjk}	10^{-6}	-0.60	-0.60	-0.60
l_k	10^{-5}	0.60	0.60	0.60
l_{kj}	10^{-6}	-0.40	-0.40	-0.40
P_k	10^{-8}	0.43	0.43	0.43

continued

Table 3 — *continued*

Parameter		(041)	(140)	(070)
E_v		9813.343183(9500)	9710.63	10195.0
A		46.768706(3400)	50.32360(9700)	118.6425(1500)
B		15.115175(1100)	14.99	15.15642(4400)
C		8.4866385(4600)	8.411	7.96564(1200)
Δ_k		0.4675253(5400)	0.564269(3500)	3.5
Δ_{jk}	10^{-1}	-0.209217(1300)	-0.19	-2.4
Δ_j	10^{-2}	0.207	0.19	0.24
δ_k	10^{-1}	0.53	0.60	3.0
δ_j	10^{-3}	0.85	0.93	1.2
H_k	10^{-1}	0.19	0.24	30.0
H_{kj}	10^{-3}	-0.49	-0.45	-9.0
H_{jk}	10^{-3}	0.13	0.13	
H_j	10^{-5}	0.32	0.32	
h_k	10^{-2}	0.66	0.66	6.6
h_j	10^{-5}	0.12	0.12	
L_k	10^{-3}	-0.16	-0.24	-250.0
L_{kkj}	10^{-5}	0.70	0.70	120.0
L_{jjk}	10^{-5}	-0.60	-0.60	
l_k	10^{-3}	0.11	0.11	
l_{kj}	10^{-6}	-0.80	-0.80	
P_k	10^{-5}	0.20	0.20	2500.0
p_k	10^{-5}	0.25	0.25	

Resonance coupling constants

	F_k	$F_j\times10$	$F_{xy}\times10$	$F_{xyk}\times10^3$
201-003	-0.5			
121-201	-0.407087(2400)	-1.05186(1600)	0.320147(4900)	-0.93
041-121	-0.679084(6500)		1.1	
300-102	-0.917591(5500)			
022-102	-0.371202(7400)	-0.72081(4500)		
022-300	-0.101435(1100)	-0.179476(6200)	-0.11	
220-102			0.19887(5200)	
220-300	-0.575349(9500)	-0.49522(7300)		
220-022		1.8	1.14266(4500)	
070-022			-0.95	
070-220	-3.05		-0.14	
140-220	-1.61			

	$C_{xz}\times10$	C_y	$C_{xzj}\times10^3$	$C_{yj}\times10^2$
102-003	-3.487077(1900)			
102-201	-1.77539(1500)			
300-201	-4.60479(1900)	0.473	0.43522(2800)	
300-121	0.57880(1100)			
022-201	-0.28979(2100)	-0.184		
022-121	-1.3	-0.74		
022-041	2.6670(1000)			
220-003	-0.37718(6800)			
220-201	0.26513(1200)			
220-121	-3.87265(1300)	0.34		
220-041	0.61754(5800)			
070-121		-0.300924(5800)		0.21
140-121	2.16745(4300)			
140-041	-1.9			

The integrals in Eqs. (2) can be estimated in the following way:

$$\langle jk|H_{vv}|jk\rangle = E_v + (c_0c_2 - c_1^2)/c_2 + c_1Ei(c_1/c_2)(c_1/c_2)^2\exp(-c_1/c_2), \quad (5)$$

where $Ei(-x) = -\int_x^\infty e^{-t}t^{-1}\,dt$ is the exponential integral.

The same evaluation takes place for the $\langle jk|H_{vv}|jk \pm 2\rangle$ matrix elements replacing c_n by b_n. It should be stressed that the rotational and centrifugal distortion constants in Eqs. (3) and (4) have their usual meaning as accepted in the literature on asymetric rotors in the A-representation.

The resonance couplings were taken into account by appropriate rotation–vibration operators (off-diagonal operators with respect to v) for the Fermi-type, Darling–Dennison-type and other anharmonic-type interactions.

$$F_{vv'} = F_0^{vv'} + F_k^{vv'}J_z^2 + F_j^{vv'}J^2 + F_{xy}^{vv'}J_{xy}^2 + F_{xyk}^{vv'}\{J_{xy}^2, J_z^2\} \quad (6)$$

or for the Coriolis-type interactions:

$$C_{vv'} = C_y^{vv'}iJ_y + C_{xz}^{vv'}\{J_x, J_z\} + C_{yj}^{vv'}iJ_yJ^2 + C_{xzj}^{vv'}J^2\{J_x, J_z\} \quad (7)$$

As for the first decades of $H_2{}^{16}O$ and $H_2{}^{18}O$, a new type of resonance, the so-called HEL-resonance[11] where HEL stands for 'highly excited local', has been taken into account. These resonances are coupling levels of the (2 2 0), (0 0 2), (1 2 1) vibrational states of the first decade with levels of the highly excited bending state (0 7 0) formally belonging to the second decade.

The fitting procedure for the first decade of $H_2{}^{17}O$ states was made much easier by using the results previously obtained from the fit for $H_2{}^{18}O$.[4] Parameters for the (0 4 1), (1 4 0), (0 7 0) and (0 2 2) states, which are dark states in the present analysis, were initially fixed to the $H_2{}^{18}O$ values. This resulted in a more stable and rapid fitting process. It has been found that the resonance scheme for the first decade of $H_2{}^{18}O$ is very similar to what is observed for $H_2{}^{16}O$ and $H_2{}^{18}O$. In particular, starting at $J = 7$, the $K_a = 0$ energy levels of the (1 2 1) vibrational state are perturbed by the $K_a = 1$ energy levels of (0 7 0). The mixing reaches a maximum of 10% for the level [8 0 8] (1 2 1), but is not large enough to cause the weak $7v_2$ band transitions to manifest. The $K_a = 1$ levels of the (2 2 0) state greatly perturbed by (0 7 0) in $H_2{}^{16}O$ and $H_2{}^{18}O$ have not been observed for $H_2{}^{17}O$ due to weakness of the corresponding transitions. Similar to the $H_2{}^{18}O$ case, the (0 6 0) vibrational state does not affect other members of the decade, at least for the observed energy levels, and this explains why this particular state was not considered as a member of the polyad.

As for $H_2{}^{16}O$ and $H_2{}^{18}O$, numerous resonance perturbations with unobserved dark states are complicating the fitting procedure. This explains why the (0 0 3) and (1 0 2) vibrational states which are less perturbed by resonances, show very good observed − calculated values (a few 10^{-3} cm^{-1} as a rule), whereas the residuals for (1 2 1), (3 0 0), (2 0 1) states show clear signs of incomplete modelling of the resonances with the dark states.

Surprising examples of the intensity redistribution due to resonances and giving rise to observable transitions, otherwise too weak to be observed, is provided by the [9 5 4] (0 4 1) and [10 3 7] (2 2 0) energy levels involved in transitions borrowing their intensities from the strong $2v_1 + v_3$ and $v_1 + 2v_2 + v_3$ perturbing partners.

Overall, the fit is rather satisfactory, and, even if the precision of the fit is one order of the magnitude worse than the experimental precision on line positions, one should not try to increase unwisely the number of variable parameters. Our goal was rather to achieve a fit which allows one to get unambiguous assignments of the spectral lines and which provide satisfactory predictions of unobserved lines.

4. CONCLUSIONS

The $H_2{}^{17}O$ high resolution absorption spectrum in the 9711–11 335 cm^{-1} spectral region has been properly analyzed using an improved theoretical model taking into account the influence of dark states. The spectroscopic parameters obtained reproduce the observed 420 energy levels with an average precision of 0.013 cm^{-1}. About 30% of the experimental energy levels are derived from single transitions. These results again demonstrate that, when the combination difference method is inoperative the correct assignment of highly excited vibro-rotational transitions is only possible if an adequate calculation of the line positions and intensities is available.

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Note added in proof

A recent calculation of the rovibrational levels of water has been performed by Partrige et al.[13] Our experimental energy levels for $H_2{}^{17}O$ are in good agreement with these theoretical calculations (within 0.04–0.09 cm^{-1} on the average) for all considered vibrational states.

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