

# $2\nu_2 - \nu_2$ and $2\nu_2$ bands of $\text{H}_2^{16}\text{O}$ , $\text{H}_2^{17}\text{O}$ , and $\text{H}_2^{18}\text{O}$ : line positions and strengths

Robert A. Toth

*Jet Propulsion Laboratory, California Institute of Technology, Pasadena, California 91109*

Received February 8, 1993; revised manuscript received April 19, 1993

High-resolution spectra of  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{17}\text{O}$ , and  $\text{H}_2^{18}\text{O}$  were recorded with a Fourier-transform spectrometer, covering transitions in the (020)–(010) and (020)–(000) bands. The measured line frequencies were used to determine high-accuracy values of rotational energy levels in the (020) vibrational states for the three isotopic species. Measurements of the line strengths were fitted to a model in which 19 transition moment parameters were determined for each band and molecule. The fitting technique did not consider interactions between the (020), (100), and (001) vibrational states. The experimental results provide a more accurate representation of the line positions and strengths than those currently available for these bands.

## INTRODUCTION

This study involves high-resolution measurements of line positions and absolute line strengths in the (020)–(010) and (020)–(000) bands of  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{17}\text{O}$ , and  $\text{H}_2^{18}\text{O}$ . This task complements my recent studies<sup>1,2</sup> of the (010)–(000) bands of  $\text{H}_2^{16}\text{O}^1$ ,  $\text{H}_2^{17}\text{O}$ , and  $\text{H}_2^{18}\text{O}^2$ . Although the (020) vibrational state is located a few hundred inverse centimeters below the (100) and (001) states for each isotopic species, several rotational levels in the (020) state are strongly perturbed by resonance interactions with levels in the (100) and (001) states. This study does not include perturbation calculations but rather includes computed line-strength values for the unperturbed results derived from a one-band least-squares fit of the experimental line strengths. Similar studies of the (100) and (001) vibrational states (and bands connecting the ground and  $\nu_2$  states) are under way.

Several reports<sup>3–20</sup> have included measurements and calculations of line positions and strengths for the (020)–(010) and (020)–(000) bands of  $\text{H}_2\text{O}$ . High-accuracy measurements of a few rotational transitions in excited vibrational states were obtained by Pearson *et al.*,<sup>20</sup> using millimeter and submillimeter laboratory techniques. They observed transition frequencies in the (000)–(000), (010)–(010), (020)–(020), (100)–(100), and (001)–(001) bands of  $\text{H}_2^{16}\text{O}$ , and here their results are compared with values derived from my recent work<sup>1</sup> on the (000) and (010) states and the results obtained in the present study for the (020) state.

As noted above, several rotational levels in the (020) state are perturbed owing to resonance interactions. Included in the scheme are distant interactions (Fermi type) between like rotational levels in the (020) and (100) states. The latter type interactions result in the borrowing of vibrational strength from one band to another [from the (100)–(000) band to the (020)–(000) band, for example]. The experimental line strengths for each band of each isotopic species were analyzed by the method that I used in my recent reports.<sup>1,2</sup> Briefly, the method is based on the theory developed by Flaud and Camy-Peyret<sup>14</sup> in which the original 8 elements of the dipole moment expansion

are used along with 11 additional terms in a least-squares analysis of the measured line strengths. Transitions that were obviously perturbed by resonance effects were not included in the fits; however, the distant Fermi-type interactions described above did not adversely affect the results.

## EXPERIMENTAL DETAILS

The spectra were obtained with a Fourier-transform spectrometer (FTS) located at the McMath solar telescope facility at the Kitt Peak National Observatory. The experimental conditions and extent of the measurements are given in Table 1. The table lists the unapodized spectral resolution, absorption path lengths, total sample pressures, and percent abundance of each isotopic species for each run. The first 15 runs listed were of samples of normal  $\text{H}_2\text{O}$ , whereas the samples of the final 15 runs listed in the table contained enriched  $^{17}\text{O}$  and  $^{18}\text{O}$ . The  $\text{H}_2^{17}\text{O}$  and  $\text{H}_2^{18}\text{O}$  samples were purchased from Merck and Company, Inc.; the stated isotopic purities were 98.1%  $\text{H}_2^{18}\text{O}$  for one sample and 60.4%  $\text{H}_2^{17}\text{O}$  for the other. Because of slight contamination from various  $\text{H}_2\text{O}$  samples used before a given run of O-enriched  $\text{H}_2\text{O}$ , the values of the isotopic abundances were not always the same as the stated values, as is shown in the latter entries in the table. The method used to determine the correct relative amounts in the samples is described in my earlier report.<sup>2</sup> Briefly, the method is based on the knowledge of the manufacturer's stated isotopic purities and the  $\text{H}_2^{17}\text{O}$  and  $\text{H}_2^{18}\text{O}$  spectral absorptions observed in the  $\text{H}_2^{16}\text{O}$  spectra (initial runs listed in Table 1). The  $\text{H}_2^{17}\text{O}$  and  $\text{H}_2^{18}\text{O}$  liquid samples obtained from the distributor were contained in sealed and evacuated glass tubes. The apparatus and method used to transfer the evaporated gas from the glass containers to the absorption cell are described in Ref. 2.

All the data were obtained with the sample temperatures near or at room temperature (296 K) with sample temperatures inferred from readings of one or more thermistor probes in thermal contact with the absorption cell walls. Total sample pressures were measured with a Baratron gauge. The spectral runs obtained with path lengths

**Table 1. Experimental Conditions of Measurements**

Spectral Range (cm <sup>-1</sup> )	Unapodized Resolution (cm <sup>-1</sup> )	Path Length (m)	Sample Pressure (Torr)	Percent Abundance of Isotopic Species		
				H <sub>2</sub> <sup>16</sup> O <sup>a</sup>	H <sub>2</sub> <sup>17</sup> O	H <sub>2</sub> <sup>18</sup> O
1066–2200	0.0056	2.39	0.37	99.6	0.04	0.2
1066–2250	0.0056	2.39	1.18	99.6	0.04	0.2
1300–2300	0.0052	25	0.92	99.6	0.04	0.2
1300–2300	0.0052	97	0.86	99.6	0.04	0.2
1300–2300	0.0052	193	0.92	99.6	0.04	0.2
1300–2300	0.0052	433	0.87	99.6	0.04	0.2
1900–4506	0.011	433	7.10	99.6	0.04	0.2
1900–4506	0.011	433	13.1	99.6	0.04	0.2
2900–4200	0.011	2.39	0.34	99.6	0.04	0.2
2900–4200	0.011	2.39	2.25	99.6	0.04	0.2
2819–4356	0.011	25	1.18	99.6	0.04	0.2
2732–4364	0.011	25	3.86	99.6	0.04	0.2
2693–4364	0.011	76	3.86	99.6	0.04	0.2
2622–4457	0.011	193	3.98	99.6	0.04	0.2
2622–4506	0.011	433	4.01	99.6	0.04	0.2
1170–2149	0.0056	2.39	0.25	ND	0.62	98.1
1061–2192	0.0056	2.39	0.65	ND	0.62	98.1
1009–2192	0.0056	2.39	1.41	ND	0.62	98.1
1009–2299	0.0056	2.39	4.99	ND	0.62	98.1
1170–2129	0.0056	2.39	0.31	ND	42.9	35.8
1102–2198	0.0056	2.39	1.33	ND	52.1	30.7
1061–2224	0.0056	2.39	5.21	ND	59.9	27.3
2954–4124	0.011	2.39	0.30	25	0.47	73.5
2922–4235	0.011	2.39	1.08	17	0.52	81.3
2890–4254	0.011	2.39	5.30	6	0.58	92.2
2881–4298	0.011	2.39	13.8	4	0.60	94.0
2967–4131	0.011	2.39	0.52	15	52.6	31.7
2948–4196	0.011	2.39	1.07	15	54.1	30.5
2887–4292	0.011	2.39	5.06	14	56.8	28.1
2881–4298	0.011	2.39	13.8	14	57.7	26.6

<sup>a</sup>ND, not determined.

greater than 2.4 m (H<sub>2</sub><sup>16</sup>O samples) were made with the use of a 6-m-base-length multiple transversal cell. Unfortunately, when the 6-m cell was used a small amount of formamine was found to be absorbed onto the cell walls, and this was always present in the recorded spectra. Although the presence was minute, it made certain regions inaccessible for measurements of H<sub>2</sub>O, namely, the 1550–1640- and 1711–1800-cm<sup>-1</sup> regions, several areas between 3500 and 3600 cm<sup>-1</sup>, and the entire region below 1300 cm<sup>-1</sup>. This problem was noted in Ref. 1.

Another hindrance with either the 2.39-m cell or the 6-m-base-length cell was the added contributions from a combination of narrow, low-pressure absorptions as a result of a small amount of water vapor (50–200-μm total pressure) in the vacuum tank that enclosed the FTS and air-broadened H<sub>2</sub><sup>16</sup>O absorptions that were due to the H<sub>2</sub>O content in the open spaces between the infrared source (a Globar) and the vacuum tank.

## SPECTRAL ANALYSIS AND ENERGY LEVELS

The line centers were measured with two computer programs. One, labeled LINEFINDER, determines line-center positions and relative absorption peaks, and the other (NLLS) uses the technique of nonlinear least squares, in which absorption line positions, strengths, linewidths, and continuum parameters are fitted simultaneously in an

interactive mode. The NLLS technique was used to determine experimental values of line strengths and the majority of line-center values. These computer algorithms have been used in several previous studies and recently in the analysis of data of the ν<sub>2</sub> bands of H<sub>2</sub><sup>16</sup>O<sup>1</sup> and H<sub>2</sub><sup>17</sup>O and H<sub>2</sub><sup>18</sup>O<sup>2</sup>. The input to the NLLS program for the stronger H<sub>2</sub><sup>16</sup>O lines in the (020)–(000) band included two line positions: one representing the slightly shifted, pressure-broadened contribution and the other for the desired low-pressure feature.

The measured line positions obtained by both techniques were calibrated and corrected to H<sub>2</sub>O and N<sub>2</sub>O calibration frequencies. The H<sub>2</sub>O frequencies measured in the (020)–(010) bands were calibrated to those of the (010)–(000) bands.<sup>1,2</sup> Several of the well-measured transitions in the (020)–(010) band were then used (after correction) to determine a preliminary set of upper state, (020), rotational levels using the values of the (010) state rotational levels given in Refs. 1 and 2. These preliminary values were then used to compute rotational transitions in the (020)–(000) bands. The N<sub>2</sub>O calibration was derived from my recent work on N<sub>2</sub>O frequencies.<sup>21</sup> The N<sub>2</sub>O spectra obtained in the 2500–4300 cm<sup>-1</sup> region also contained H<sub>2</sub>O features because of a small amount of water vapor in the FTS vacuum tank and air-broadened H<sub>2</sub><sup>16</sup>O absorptions. The H<sub>2</sub>O low-pressure contributions were measured in the N<sub>2</sub>O spectra with the aid of the LINEFINDER program. The computed transitions in the (020)–(000)

band and the measured H<sub>2</sub><sup>16</sup>O frequencies in the (020)–(000) band derived from N<sub>2</sub>O were found to be in excellent agreement, and these H<sub>2</sub>O transitions were used to calibrate the remainder of the H<sub>2</sub>O lines in the 2600–4300-cm<sup>-1</sup> region observed in the H<sub>2</sub>O spectra.

The rotational energy levels in the (020) vibrational

states of the three isotopic species were derived by the addition to each measured transition frequency of the (020)–(010) and (020)–(000) bands, the appropriate lower state level given in Ref. 1 for H<sub>2</sub><sup>16</sup>O and Ref. 2 for H<sub>2</sub><sup>17</sup>O and H<sub>2</sub><sup>18</sup>O. These results were weighted and then averaged for each level. Table 2 lists values of the rotational

Table 2. Rotational Energy Levels (cm<sup>-1</sup>) of the (020) Vibrational States of H<sub>2</sub><sup>16</sup>O, H<sub>2</sub><sup>17</sup>O, and H<sub>2</sub><sup>18</sup>O<sup>a</sup>

J	K <sub>a</sub>	K <sub>c</sub>	H <sub>2</sub> <sup>16</sup> O	H <sub>2</sub> <sup>17</sup> O		H <sub>2</sub> <sup>18</sup> O		J	K <sub>a</sub>	K <sub>c</sub>	H <sub>2</sub> <sup>16</sup> O	H <sub>2</sub> <sup>17</sup> O		H <sub>2</sub> <sup>18</sup> O	
0	0	0	3151.63015	5	3144.98051	12	3139.04970	7	8	4	5	4381.73551	8	4370.97458	165
1	0	1	3175.44134	3	3168.76987	7	3162.82037	3	8	4	4	4386.31325	6	4366.71745	25
1	1	1	3196.09338	3	3189.17376	5	3183.00501	3	8	5	4	4564.03483	10	4551.56987	50
1	1	0	3201.91337	5	3195.01050	18	3188.85719	4	8	5	3	4564.36667	5	4540.37063	40
2	0	2	3221.96118	3	3215.22971	2	3209.22624	5	8	6	3	4774.80498	6	4760.32400	300
2	1	2	3237.91733	4	3230.93737	4	3224.71452	6	8	6	2	4775.08841	8	4759.39835	40
2	1	1	3255.34594	3	3248.41705	10	3242.23924	10	8	7	2	5008.96301	21		
2	2	1	3316.14537	5	3308.49234	8	3301.67406	5	8	7	1	5008.96310	30		
2	2	0	3317.21063	4	3309.57493	8	3302.77181	15	8	8	1	5261.47098	40		
3	0	3	3289.24254	3	3282.38741	4	3276.27338	2	8	8	0	5261.47098	40		
3	1	3	3299.99111	6	3292.91109	3	3286.59870	4	9	0	9	4068.70392	4	4060.04533	25
3	1	2	3334.62656	6	3327.64464	10	3321.41967	3	9	1	9	4068.93111	12	4060.25980	19
3	2	2	3387.68067	6	3379.96116	15	3373.08318	4	9	1	8	4263.15049	6	4254.22548	135
3	2	1	3392.74937	4	3385.10552	8	3378.29607	4	9	2	8	4268.24095	7	4259.07123	50
3	3	1	3500.51111	6	3491.69413	40	3483.84567	8	9	2	7	4399.54219	6	4383.37656	40
3	3	0	3500.63874	2	3491.82603	13	3483.98060	5	9	3	7	4436.94054	10	4418.47205	40
4	0	4	3375.29786	4	3368.24726	15	3361.95836	5	9	3	6	4493.80443	8	4477.17310	50
4	1	4	3381.70430	6	3374.47825	5	3368.03562	4	9	4	6	4600.49746	10		
4	1	3	3438.57499	2	3431.49385	23	3425.17952	12	9	4	5	4611.79486	7	4591.95867	50
4	2	3	3482.06452	3	3474.24200	3	3467.27223	11	9	5	5	4783.64115	10		
4	2	2	3495.93921	6	3488.30125	10	3481.49761	10	9	5	4	4784.66215	4	4760.86383	40
4	3	2	3597.86611	3	3588.98313	9	3581.07543	7	9	6	4	4994.70297	45		
4	3	1	3598.72703	4	3589.86929	20	3581.98441	5	9	6	3	4996.33150	15		
4	4	1	3746.76274	2	3736.40785	9	3727.19625	6	9	7	3	5229.57686	50		
4	4	0	3746.77603	4	3736.42177	25	3727.21062	10	9	7	2	5229.57915	9		
5	0	5	3478.98654	3	3471.68411	9	3465.17074	3	9	8	2	5483.32345	15		
5	1	5	3482.48022	5	3475.05882	40	3468.44193	8	9	8	1	5483.32345	15		
5	1	4	3565.45464	2	3558.19745	15	3551.72501	5	9	9	1	5748.51286	60		
5	2	4	3598.51596	5	3590.54463	25	3583.44122	8	9	9	0	5748.51286	60		
5	2	3	3626.92221	3	3619.27547	10	3612.46369	5	10	0	10	4260.35188	3	4251.26750	300
5	3	3	3719.49292	5	3710.52236	8	3702.53688	11	10	1	10	4260.46692	8	4251.37621	9
5	3	2	3722.73109	4	3713.85137	10	3705.94859	3	10	1	9	4480.39238	8	4462.47736	20
5	4	2	3868.87302	2	3858.43889	35	3849.15618	15	10	2	9	4483.22802	7	4473.60735	40
5	4	1	3868.98701	3	3858.55736	15	3849.27961	6	10	2	8	4644.21708	9		
5	5	1	4050.50393	11	4038.29844	30	4027.44761	40	10	3	8	4669.73608	5	4650.56735	300
5	5	0	4050.51289	11	4038.29961	27	4027.44919	12	10	3	7	4752.73317	9		
6	0	6	3600.05237	4	3592.45943	20	3585.68739	3	10	4	7	4842.13152	10		
6	1	6	3601.85892	2	3594.19274	10	3587.35768	5	10	4	6	4864.37344	15		
6	1	5	3713.08250	3	3705.54385	11	3698.81692	5	10	5	6	5027.07422	8		
6	2	5	3736.17085	5	3727.99455	25	3720.70839	4	10	5	5	5029.81081	12	5016.93455	20
6	2	4	3784.67916	5	3776.97220	40	3770.10488	20	10	6	5	5238.38633	25		
6	3	4	3864.96620	5	3855.87651	27	3847.78449	15	10	6	4	5237.42028	12		
6	3	3	3873.79379	4	3864.93430	40	3857.05163	7	10	7	4	5473.80301	220		
6	4	3	4015.51517	4	4004.98960	30	3995.62744	10	10	7	3	5473.81253	270		
6	4	2	4016.05289	5	4005.55062	13	3996.20955	20	10	8	3	5728.02500	600		
6	5	2	4197.33887	4	4185.03532	50	4174.09656	10	10	8	2	5728.02500	600		
6	5	1	4197.36108	4	4184.94476	50	4174.10525	25	10	9	2	5994.37695	200		
6	6	1	4407.04639	4	4392.82048	35	4379.86781	20	10	9	1	5994.37695	200		
6	6	0	4407.15788	13	4392.67089	35	4380.05315	45	10	10	1	6318.36818	400		
7	0	7	3738.60918	3	3730.69386	10	3723.63477	4	10	10	0	6318.36818	400		
7	1	7	3739.51886	3	3731.56124	20	3724.46591	5	11	0	11	4469.73745	7	4460.19366	50
7	1	6	3879.33628	4	3871.40435	20	3864.32519	8	11	1	11	4469.79655	5	4460.24799	300
7	2	6	3894.16782	3	3885.72495	45	3878.19957	10	11	1	10	4714.81893	11	4695.83585	40
7	2	5	3967.48855	5	3959.63485	30	3952.63451	7	11	2	10	4716.37945	11		
7	3	5	4033.61455	5	4024.25917	120	4016.12198	45	11	2	9	4905.65368	9		
7	3	4	4052.83702	6	4044.03085	25	4036.19767	15	11	3	9	4922.09005	19		
7	4	4	4186.56963	8	4175.93925	40	4166.48450	45	11	3	8	5034.38755	20		
7	4	3	4188.39442	3	4177.83937	30	4168.45415	10	11	4	8	5105.72993	15		
7	5	3	4368.54608	3	4356.10953	300	4345.13890	40	11	4	7	5144.40926	12		
7	5	2	4368.63709	6	4356.23510	50	4345.22003	43	11	5	7	5293.79093	200		
7	6	2	4578.88250	3	4564.51379	300	4552.19560	17	11	5	6	5300.17815	30		
7	6	1	4578.97810	10	4563.77795	8	4551.66218	20	11	6	6	5505.48824	400		
7	7	1	4812.19313	21					11	6	5	5505.17348	50		
7	7	0	4812.19313	21					11	7	5	5741.19043	300		
8	0	8	3894.79901	7	3886.52931	40	3879.15433	30	11	7	4	5741.36145	300		
8	1	8	3895.25304	3	3886.95931	10	3879.56462	20	12	0	12	4696.83433	22	4677.83752	300
8	1	7	4062.83808	8	4054.43257	300	4046.92940	40	12	1	12	4696.86542	9	4677.86534	40
8	2	7	4071.73344	5	4062.95883	25	4055.13678	15	12	1	11	4966.63309	14		
8	2	6	4173.22584	8					12	2	11	4967.49095	12	4947.28958	300
8	3	6	4224.58667	8	4215.11004	15	4206.67214	15	12	2	10	5182.09498	15		
8	3	5	4259.87654	6					12	3	10	5193.88216	15	5173.85749	50

(Table continued)

Table 2. Continued

$J$	$K_a$	$K_c$	$H_2^{16}\text{O}$	$H_2^{17}\text{O}$	$H_2^{18}\text{O}$	$J$	$K_a$	$K_c$	$H_2^{16}\text{O}$	$H_2^{17}\text{O}$	$H_2^{18}\text{O}$	
12	3	9	5336.32707	80		13	3	10	5654.76131	80		
12	4	9	5389.55208	35		13	4	10	5695.67200	800		
12	4	8	5450.88959	300		13	4	9	5781.96170	500		
12	5	8	5587.51879	15		14	0	14	5204.01500	100		
12	5	7	5596.31840	400		14	1	14	5204.01570	60		
12	6	7	5795.73063	400		14	2	12	5786.85327	80		
13	0	13	4941.60570	50	4921.59710	100	14	3	12	5790.43269	40	
13	1	13	4941.62242	60	4921.59900	300	14	4	10	6134.94002	800	
13	1	12	5235.95804	60		14	6	9	6443.79063	800		
13	2	12	5236.01263	830		15	0	15	5483.99625	80		
13	2	11	5477.00637	35		15	1	15	5483.99625	100		
13	3	11	5483.28000	700		15	3	12	6345.92236	15		

<sup>a</sup>Estimated uncertainties given in inverse centimeters times 10<sup>5</sup>.

Table 3. Matrix Elements Used in the Expansion of the Dipole Moment for B-type Transitions of Water Vapor

$j$	$n$	$\langle JK   A'(j)   J'K' \rangle / \langle JK   \Phi(x)   J'K' + \Delta K \rangle, \Delta K = \pm 1$
2	1	$J'(J'+1) + J(J+1)^a$
3	1	$K'^2 + K^2a$
4	1	$K'^2 - K^2a$
5	1	$K'^2 - K^2 - 2m^a$
6	1	$(K'^2 - K^2)(K'^2 - K^2 - 2m)^a$
7	1	$J(J+1) - 2m(m-1) + (2m-1)K\Delta K - K^2 - 1^a$
8	3	$[(J' - K\Delta K - 1)(J' - K\Delta K - 2)(J' + K\Delta K + 2)(J' + K\Delta K + 3)]^{1/2}a$
9	1	$K'^2 J'(J'+1) - K^2 J(J+1)$
10	1	$K^4 - K^4$
11	1	$(K'^2 - K^2)[J'(J'+1) + J(J+1)]$
12	1	$K'^2 (J'^2 + J')^2$
13	1	$K'^6$
14	1	$K'^4$
15	1	$K'^2 J'(J'+1)$
16	1	$K'^6 - K^6$
17	1	$J'(J'+1) \text{ if } m = 0 \text{ and } J = K_c \text{ or } J' = K'_c, \text{ otherwise } 0$
18	1	$J'(J'+1) \text{ if } m = 0 \text{ and } J = K_c \text{ or } J' = K'_c - 1, \text{ otherwise } 0$
19	1	$J'(J'+1) \text{ if } m \neq 0 \text{ and } J = K_c \text{ and } J' = K'_c, \text{ otherwise } 0$

<sup>a</sup>From Ref. 14;  $J' - J = 0, \pm 1$ ;  $m = [J'(J'+1) - J(J+1)]/2$ ;  $K' - K = n\Delta K$ .

energy levels obtained in this study for the (020) states of the three species. Included in the table are estimations of the uncertainties in the values.

## LINE STRENGTHS

The strength  $S$  of an  $\text{H}_2\text{O}$  transition at frequency  $\nu$  may be expressed to good approximation by

$$S = C \left( \frac{\nu}{Q} \right) \left( \frac{g}{T} \right) \left[ 1 - \exp\left(\frac{-\nu}{kt}\right) \right] \exp\left[\frac{-E(L)}{kt}\right] |R(L, U)|^2,$$

where

$$C = 8\pi^3/3hc,$$

$$Q = Q_V Q_R,$$

$$E(L) = E_V(L) + E_R(L), \quad (1)$$

where  $Q$  is the partition function, which can be expressed as the product of the vibrational,  $Q_V$ , and the rotational,  $Q_R$ , partition functions;  $g$  is the degeneracy that is due to the nuclear spin of the lower-state level;  $k$  is the Boltzmann constant;  $T$  is the temperature;  $E(L)$  is the lower-state energy, which is equal to the sum of the lower-state vibrational energy  $E_V(L)$  and the rotational energy  $E_R(L)$ ; and  $R(L, U)$  is the vibration-rotation dipole moment matrix element connecting the lower state  $L$  with the upper state  $U$ . When  $T = 296$  K,  $Q_R$  is 175.0, 175.5, and 176.1 for

$\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{17}\text{O}$ , and  $\text{H}_2^{18}\text{O}$ , respectively, and  $Q_V = 1.0004$  for the three species and for temperatures within 30 K of 300 K,  $Q(T) = Q(296 \text{ K}) (296/T)^{3/2}$ .

Without consideration of near-resonance effects, the vibration-rotation dipole moment element,  $R(L, U)$ , given in Eq. (1), can be expressed as

$$R(L, U) = \sum_j u(j) x(j),$$

$$x(j) = \langle V'', J'', K_a'', K_c'' | A(j) | V', J', K_a', K_c' \rangle, \quad (2)$$

where  $u(j)$  are the dipole moment coefficients,  $A(j)$  are the transformed transition moment operators, and prime and double prime denote upper and lower states, respectively.  $x(1)$  is the matrix element of the direction cosines in which  $A(1) = \Phi_\alpha$  with  $\alpha = z$  for A-type transitions and  $\alpha = x$  for B-type transitions. The asymmetric top wave functions,  $\text{AS}(V, J, K_a, K_c)$ , are expressed as an expansion of the symmetry-adapted wave functions,  $s(J, K, \gamma)$ , as

$$\text{AS}(V, J, K_a, K_c) = \Psi_v C(J, K_a, K_c | J, K, \gamma) s(J, K, \gamma), \quad (3)$$

where the  $C$ 's are coefficients of the wave functions, thus expressing the lower- and the upper-state wave functions in terms of symmetry-adapted rotational wave functions.

The matrix elements involved in  $R(L, U)$  and used in this study are given in Table 3. The elements  $j = 2$  to  $j = 8$  are those given by Flaud and Camy-Peyret,<sup>14</sup> and the following 11 terms ( $j = 9$  to  $j = 19$ ) were empirically derived

and found to be necessary in the  $H_2^{16}O$  analysis<sup>1</sup> of the (010)–(000) band. The analysis of the  $\nu_2$  bands of  $H_2^{17}O$  and  $H_2^{18}O^2$  used as many as 18 matrix elements ( $j = 1$  to and including  $j = 18$ ).

The measured line strengths were least-squares fitted by use of the expressions given in Eqs. (1)–(3) and outlined in Ref. 1. The matrix elements of the direction cosines were computed from the vibration-rotation parameters given in the literature: the (000) and (010) states of  $H_2^{16}O$  from Ref. 1, the (020) state of  $H_2^{16}O$  from Ref. 11, the

(000) and (010) states of  $H_2^{17}O$  and  $H_2^{18}O$  from Ref. 22, and the (020) states of  $H_2^{17}O$  and  $H_2^{18}O$  from Ref. 12. It should be noted that the measured line strengths were normalized to 100% of the isotopic sample, and these normalized values were used in the analyses. Values and associated estimated uncertainties of the matrix elements of the expanded dipole moment derived from the fits are given in Table 4. The lowest two rows for each band and isotopic species list the number of lines fitted and the values of the standard deviation in percent,  $\sigma\%$ , of the line-

**Table 4. Effective Dipole Moment Expansion Coefficients (in debyes) Derived from Least-Squares Fits of  $H_2^{16}O$ ,  $H_2^{17}O$ , and  $H_2^{18}O$  Measured Line Strengths in the (020)–(010) and (020)–(000) Bands<sup>a</sup>**

$j$	$H_2^{16}O$	$H_2^{17}O$	$H_2^{18}O$	$H_2^{16}O^b$
(020)–(010) Bands				
1	0.1990(14)	0.1963(32)	0.1951(12)	0.1807(200)
2	$-1.33(125) \times 10^{-5}$	$-5.31(898) \times 10^{-5}$	$-1.15(309) \times 10^{-5}$	
3	$-1.66(389) \times 10^{-4}$	$3.54(948) \times 10^{-4}$	$2.07(462) \times 10^{-4}$	
4	$-1.266(14) \times 10^{-2}$	$-1.281(62) \times 10^{-2}$	$-1.137(33) \times 10^{-2}$	
5	$-4.69(74) \times 10^{-4}$	$-8.0(147) \times 10^{-5}$	$-5.05(51) \times 10^{-4}$	
6	$-7.08(99) \times 10^{-5}$	$-6.10(347) \times 10^{-5}$	$-2.93(68) \times 10^{-5}$	
7	$3.65(83) \times 10^{-5}$	$1.53(15) \times 10^{-4}$	$2.97(79) \times 10^{-5}$	
8	$-6.49(227) \times 10^{-5}$	$-6.2(115) \times 10^{-5}$	$2.4(301) \times 10^{-6}$	
9	$5.9(143) \times 10^{-6}$	$5.21(481) \times 10^{-5}$	$-5.22(124) \times 10^{-5}$	
10	$1.07(33) \times 10^{-4}$	$1.73(99) \times 10^{-4}$	$9.36(302) \times 10^{-5}$	
11	$-5.98(757) \times 10^{-6}$	$-4.77(237) \times 10^{-5}$	$1.77(71) \times 10^{-5}$	
12	$3.00(219) \times 10^{-8}$	$-6.97(554) \times 10^{-7}$	$2.25(101) \times 10^{-7}$	
13	$5.5(128) \times 10^{-7}$	$5.50(576) \times 10^{-6}$	$4.8(265) \times 10^{-7}$	
14	$-2.18(641) \times 10^{-6}$	$-2.46(245) \times 10^{-4}$	$-9(107) \times 10^{-6}$	
15	$-2.21(435) \times 10^{-6}$	$8.36(565) \times 10^{-5}$	$-2.15(135) \times 10^{-5}$	
16	$-1.31(70) \times 10^{-6}$	$-3.36(163) \times 10^{-6}$	$-1.02(61) \times 10^{-6}$	
17	$1.26(63) \times 10^{-4}$	$1.00(281) \times 10^{-4}$	$2.20(98) \times 10^{-4}$	
18	$4.74(255) \times 10^{-5}$	$8.7(1078) \times 10^{-6}$	$1.44(31) \times 10^{-4}$	
19	$-1.83(473) \times 10^{-5}$	$2.52(219) \times 10^{-4}$	$1.00(64) \times 10^{-4}$	
$N^c$	201	98	141	20
$\sigma\%^d$	3.4	5.5	4.5	6.6
(020)–(000) Bands				
	$H_2^{16}O^e$	$H_2^{17}O^f$	$H_2^{18}O^g$	
1	$7.742(12) \times 10^{-3}$	$7.813(23) \times 10^{-3}$	$7.850(32) \times 10^{-3}$	$7.266(190) \times 10^{-3}$
2	$-2.95(59) \times 10^{-7}$	$6.22(537) \times 10^{-7}$	$-2.01(28) \times 10^{-6}$	$1.94(109) \times 10^{-6}$
3	$1.22(235) \times 10^{-6}$	$-1.42(87) \times 10^{-5}$	$-1.46(96) \times 10^{-5}$	$3.18(170) \times 10^{-6}$
4	$-2.006(15) \times 10^{-4}$	$-1.82(11) \times 10^{-4}$	$-1.701(46) \times 10^{-4}$	$-1.71(26) \times 10^{-4}$
5	$6.942(43) \times 10^{-5}$	$6.83(11) \times 10^{-5}$	$6.660(68) \times 10^{-5}$	$7.22(156) \times 10^{-5}$
6	$1.454(43) \times 10^{-6}$	$1.18(15) \times 10^{-6}$	$9.40(63) \times 10^{-7}$	$-5.04(240) \times 10^{-6}$
7	$-3.483(28) \times 10^{-6}$	$-3.71(20) \times 10^{-6}$	$-3.57(10) \times 10^{-6}$	$-3.71(140) \times 10^{-6}$
8	$7.60(143) \times 10^{-7}$	$1.43(63) \times 10^{-6}$	$1.54(42) \times 10^{-6}$	
9	$-1.941(44) \times 10^{-6}$	$-1.35(23) \times 10^{-6}$	$-1.896(75) \times 10^{-6}$	
10	$4.99(54) \times 10^{-7}$	$-2.36(117) \times 10^{-6}$	$-1.58(61) \times 10^{-6}$	
11	$9.31(23) \times 10^{-7}$	$7.24(135) \times 10^{-7}$	$8.27(41) \times 10^{-7}$	
12	$-1.32(382) \times 10^{-10}$	$6.65(378) \times 10^{-9}$	$7.18(126) \times 10^{-9}$	
13	$8.50(332) \times 10^{-9}$	$-1.46(87) \times 10^{-7}$	$4.1(434) \times 10^{-9}$	
14	$-4.34(245) \times 10^{-7}$	$4.54(243) \times 10^{-6}$	$1.06(185) \times 10^{-6}$	
15	$2.37(547) \times 10^{-8}$	$-7.43(380) \times 10^{-7}$	$-2.51(134) \times 10^{-7}$	
16	$-1.076(72) \times 10^{-8}$	$2.48(325) \times 10^{-8}$	$2.51(120) \times 10^{-8}$	
17	$2.52(39) \times 10^{-6}$	$1.05(178) \times 10^{-6}$	$2.98(128) \times 10^{-6}$	
18	$1.02(19) \times 10^{-6}$	$1.10(65) \times 10^{-6}$	$8.64(390) \times 10^{-7}$	
19	$1.94(25) \times 10^{-6}$	$9.3(140) \times 10^{-7}$	$2.31(86) \times 10^{-6}$	
$N^c$	366	136	252	
$\sigma\%^d$	3.5	2.6	3.9	

<sup>a</sup>Values given within parentheses are uncertainties in the last digit(s).

<sup>b</sup>From Ref. 17; effective constants were computed from the constants given in that study.

<sup>c</sup> $N$  represent the number of line strengths used in the least-squares fit.

<sup>d</sup> $\sigma\%$  is the standard deviation resulting from the least-squares fit in percent;  $\sigma\% = \{\sum[(S_{obs} - S_{cal})/S_{obs}]^2/N\}^{1/2} \times 100$ .

<sup>e</sup>From Ref. 14. Effective constants were computed from the constants given in that study.

<sup>f</sup>From Ref. 15. Effective constants were computed from the constants given in that study.

<sup>g</sup>From Ref. 16. Effective constants were computed from the constants given in that study.

strength fits.  $\sigma\%$  is defined as

$$\sigma\% = 100 \left\{ \sum [S_{\text{obs}} - S_{\text{cal}}]/S_{\text{obs}} \right\}^{1/2}, \quad (4)$$

where  $N$  is the number of lines included in the fit. Measured line strengths of transitions strongly affected by resonance effects were not included in the analyses. Included in Table 4 are values of matrix elements derived in other studies: the (020)–(010) band of  $\text{H}_2^{16}\text{O}$  by Flaud *et al.*,<sup>17</sup> the (020)–(000) band of  $\text{H}_2^{16}\text{O}$  by Flaud and Camy-Peyret,<sup>14</sup> the (020)–(000) band of  $\text{H}_2^{17}\text{O}$  by Camy-Peyret *et al.*,<sup>15</sup> and the (020)–(000) band of  $\text{H}_2^{18}\text{O}$  by Flaud *et al.*<sup>16</sup> Those studies<sup>14–17</sup> took into account the interactions among the three vibrational states (020), (100), and (001). To compare those results with the present values involves uncoupling the Fermi-type interaction between the (020) and (100) states. The method used here to do this is to apply the expressions

$$\begin{aligned} C_{32} &= h_{32}/(E_3 - E_2), \\ C_{23} &= h_{32}/(E_2 - E_3), \\ C_{22} &= C_{33} = (1 - C_{23})^{1/2} \\ \mu_2^0(j) &= C_{22}\mu_2(j) + C_{23}\mu_3(j), \\ \mu_3^0(j) &= C_{33}\mu_3(j) + C_{32}\mu_2(j), \end{aligned} \quad (5)$$

where  $h_{32}$  is the first-order coupling constants between the (100) state (index 3) and (020) state (index 2).  $E_3$  and  $E_2$  are the observed rotationless energy levels for the (100) and (020) vibrational states and  $\mu_n(j)$  are the matrix elements obtained in the other studies.<sup>14–17</sup>  $\mu_n^0(j)$  are the uncoupled constants representing the other studies, and the computed values are included in Table 4. The computed values of  $\mu_n^0(j)$  were derived from Eqs. (5) with the coupling constant,  $h_{32}$ , given in Ref. 11 for  $\text{H}_2^{16}\text{O}$  and from Ref. 12 for  $\text{H}_2^{17}\text{O}$  and  $\text{H}_2^{18}\text{O}$  and the matrix elements,  $\mu_n(j)$ , given in Refs. 14–17. These computed values represent a first approximation to the uncoupled constants. Higher-order terms,  $h_{32}'$ , etc., and more involved expressions than those given in Eqs. (5) are involved in obtaining a higher-order approximation of  $\mu_n^0(j)$ . However, the first-order results given in Table 4 are good approximations.

## RESULTS

Table 5 lists lines of the transitions observed in the (020)–(010) bands of  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{17}\text{O}$ , and  $\text{H}_2^{18}\text{O}$ . Entries for the table include the observed line position, the observed minus the computed line position ( $\text{o} - \text{c}$ ), rotational quantum assignments, the observed strength, the estimated uncertainty in the measured strength (%), the observed

**Table 5. Line Positions ( $\text{cm}^{-1}$ ) and Strengths ( $\text{cm}^{-2}/\text{atm}^a$  at 296 K) Observed in the (020)–(010) Bands of  $\text{H}_2^{16}\text{O}$ ,  $\text{H}_2^{17}\text{O}$  and  $\text{H}_2^{18}\text{O}^b$**

Observed Position	Upper $J$	$K_a$	$K_c$	Lower $J$	$K_a$	$K_c$	Observed Strength	%s	( $\text{o} - \text{c}$ )%	R	Mol	Observed Position	Upper $J$	$K_a$	$K_c$	Lower $J$	$K_a$	$K_c$	Observed Strength	%s	( $\text{o} - \text{c}$ )%	R	Mol		
1304.2856	-12	6	3	3	7	4	4	6.48E-05	6	-7.7	1.05	6	1414.42225	-2	4	1	3	5	2	4	5.32E-04	2	-0.7	1.18	6
1315.9257	-58	5	2	4	6	3	3	1.61E-04	5	10.2	1.35	6	1418.58218	0	2	1	2	3	2	1	2.17E-03	3	-1.5	1.26	6
1316.12975	13	5	4	1	6	5	2	3.27E-04	2	3.9	1.11	6	1420.97888	4	7	1	7	7	2	6	1.70E-04	2	-5.4	1.44	6
1316.5410	12	5	5	1	6	6	0	6.23E-05	4	2.6	1.11	6	1421.21595	3	6	1	6	7	0	7	1.45E-03	2	3.0	1.14	6
1320.32726	-8	5	3	3	6	4	2	1.64E-04	3	0.7	1.17	6	1426.44056	4	6	2	5	7	1	6	4.53E-04	3	-0.2	1.07	6
1324.4947	-2	5	3	2	6	4	3	5.02E-04	2	1.3	1.18	6	1426.61023	5	3	1	2	4	2	3	2.50E-03	3	2.1	1.24	6
1327.73560	8	4	1	4	5	2	3	4.00E-04	3	4.9	1.37	6	1426.81052	46	9	2	8	9	3	7	3.16E-05	15	13.8	1.65	6
1337.29574	-5	7	2	5	8	3	6	1.15E-04	2	-1.4	1.10	6	1428.87888	3	7	0	7	7	1	6	5.40E-04	2	-6.1	1.41	6
1340.61955	0	4	4	1	5	5	0	6.63E-04	3	-2.4	1.10	6	1436.23315	4	5	0	5	6	1	6	2.42E-03	3	1.8	1.15	6
1340.63498	0	4	4	0	5	5	1	2.21E-04	2	-2.4	1.10	6	1437.80136	-19	7	3	5	8	2	6	2.10E-05	6	8.6	1.07	6
1344.59250	5	10	1	10	11	0	11	5.87E-05	5	-0.6	1.03	6	1440.57280	0	6	1	6	6	2	5	9.88E-04	2	-3.9	1.41	6
1346.00352	-1	4	3	2	5	4	1	1.03E-03	3	0.1	1.18	6	1440.69965	0	5	1	5	6	0	6	7.87E-04	2	0.9	1.13	6
1347.03157	-4	4	3	1	5	4	2	3.48E-04	3	1.1	1.20	6	1441.54075	7	8	2	7	8	3	6	1.98E-04	2	-3.8	1.36	6
1348.5919	-28	5	0	5	5	3	2	2.95E-05	5	-1.2	1.52	6	1441.55834	1	2	1	1	3	2	2	1.12E-03	3	-2.1	1.22	6
1351.57014	-2	4	2	3	5	3	2	1.06E-03	5	-1.1	1.22	6	1444.75223	-4	9	1	8	9	2	7	9.89E-05	2	1.1	1.43	6
1355.20988	3	5	2	3	6	3	4	5.85E-04	2	-3.7	1.14	6	1445.1889	-44	10	3	8	10	4	7	1.59E-05	3	-4.4	1.29	6
1356.03840	-16	10	1	10	10	2	9	4.78E-05	15	12.4	1.94	6	1452.25217	-5	5	2	4	6	1	5	2.27E-04	2	-0.8	1.08	6
1357.2062	49	10	0	10	10	1	9	1.34E-05	10	-5.7	1.62	6	1452.46881	4	4	0	4	5	1	5	1.20E-03	2	2.5	1.19	6
1358.7220	-13	9	1	8	10	2	9	4.40E-05	3	-7.7	0.96	6	1452.60703	3	1	1	1	2	2	0	1.27E-03	4	-1.9	1.26	6
1363.56407	-12	9	0	9	10	1	10	1.65E-04	5	-5.1	1.00	6	1453.61730	-3	9	3	7	9	4	6	1.53E-05	3	-2.2	1.30	6
1363.83430	24	9	1	9	10	0	10	5.44E-05	3	6.8	1.13	6	1453.78864	1	6	0	6	6	1	5	3.81E-04	2	-1.9	1.41	6
1369.53155	12	4	2	2	5	3	3	4.20E-04	3	2.8	1.25	6	1454.21313	-17	7	2	6	7	3	5	1.50E-04	3	-0.6	1.38	6
1370.89231	-9	3	3	1	4	4	0	6.33E-04	2	-0.5	1.20	6	1458.8659	2	10	4	7	10	5	6	7.50E-06	3	-3.3	1.27	6
1371.03946	-2	3	3	0	4	4	1	1.92E-03	4	0.5	1.22	6	1459.60773	2	1	1	0	2	2	1	4.39E-03	3	-1.6	1.25	6
1377.09005	10	3	1	3	4	2	2	3.40E-04	4	2.2	1.32	6	1459.88895	-12	8	3	6	8	4	5	1.18E-04	2	2.2	1.34	6
1378.3371	-29	9	1	9	9	2	8	3.86E-05	5	6.6	1.76	6	1460.93765	-6	4	1	4	5	0	5	3.65E-03	7	7.9	1.24	6
1380.62326	-22	9	0	9	9	1	8	1.10E-04	3	-0.2	1.63	6	1462.10226	-10	8	4	5	8	5	4	4.83E-05	2	-1.8	1.26	6
1381.628	127	3	0	3	3	3	0	1.63E-05	10	2.2	1.52	6	1462.5273	-77	7	4	4	7	5	3	3.85E-05	5	17.7	1.51	6
1381.76344	-11	3	2	2	4	3	1	7.39E-04	3	3.0	1.29	6	1462.65777	-1	6	4	3	6	5	2	1.43E-04	3	-6.3	1.18	6
1382.42319	-2	8	0	8	9	1	9	1.15E-04	4	-3.3	1.04	6	1462.73198	1	5	4	2	5	5	1	5.44E-05	4	0.1	1.26	6
1382.97003	-6	8	1	8	9	0	9	3.59E-04	2	0.8	1.08	6	1462.84380	-2	5	4	1	5	5	0	1.61E-04	2	-1.3	1.25	6
1383.65332	-2	8	2	7	9	1	8	1.10E-04	3	-4.2	1.00	6	1462.9107	-21	8	5	4	8	6	3	1.69E-05	2	-1.3	1.27	6
1384.17029	-2	7	1	6	8	2	7	2.68E-04	3	0.6	1.10	6	1463.1153	1	7	5	3	7	6	2	1.05E-05	4	4.5	1.33	6
1387.93363	1	3	2	1	4	3	2	2.15E-03	6	-4.0	1.19	6	1463.17298	-5	6	4	2	6	5	1	5.02E-05	3	-1.2	1.25	6
1400.08708	1	8	1	8	8	2	7	2.47E-04	3	-2.7	1.54	6	1463.20339	-7	7	5	2	7	6	1	2.78E-05	3	-8.0	1.17	6
1400.94226	1	7	0	7	8	1	8	7.51E-04	3	0.0	1.09	6	1463.2238	-52	8	5	3	8	6	2	5.00E-06	10	-13.2	1.13	6
1402.05544	-1	7	1	7	8	0	8	2.46E-04	2	-1.4	1.07	6	1463.37604	-1	6	5	2	6	6	1	3.71E-05	3	2.9	1.30	6
1404.16854	2	5	1	4	6	2	5	9.54E-04	2	-1.6	1.14	6	1463.39803	0	6	5	1	6	6	0	1.18E-05	3	-1.8	1.25	6
1404.44444	-48	8	0	8	8	1	7	9.50E-05	5	8.4	1.71	6	1463.64686	-10	9	5	4	9	6	3	7.70E-06	3	-1.5	1.28	6
1406.1886	15	8	3	6	9	2	7	2.80E-05	4	-7.2	0.90	6	1464.10649	1	7	3	5	7	4	4	8.20E-05	2	1.0	1.31	6
1408.52956	0	2	2	1	3	3	0	3.56E-03	3	-2.4	1.24	6	1464.22716	0	7	4	3	7	5	2	9.75E-05	2	0.5	1.27	6
1409.75911	-7	2	2	0	3	3	1	1.23E-03	2	0.5	1.27	6	1464.45849	0	6	2	5	6	3	4	8.45E-04	2	-1.9	1.33	6
1410.5015	8	10	2	9	10	3	8	3.03E-05	4	2.1	1.52	6	1464.6143	36	11	2	9	11	3	8	6.86E-06	10	-5.0	1.25	6

(Table continued)

Table 5. Continued

Observed Position	o - c	Upper		Lower		Observed Strength	%s (o - c)%	R	Mol	Observed Position	o - c	Upper		Lower		Observed Strength	%s (o - c)%	R	Mol						
		J	K <sub>a</sub>	K <sub>c</sub>	J	K <sub>a</sub>	K <sub>c</sub>					J	K <sub>a</sub>	K <sub>c</sub>	J	K <sub>a</sub>	K <sub>c</sub>								
P1466.18106	-4	8	4	4	8	5	3	1.10E-05	3	-50.7	1.33	6	1695.34025	5	5	3	3	5	2	4	2.17E-04	10	-10.8	0.95	6
1466.58454	-6	6	3	4	6	4	3	4.32E-04	2	0.3	1.30	6	1695.7761	-9	7	2	5	6	3	4	2.34E-04	5	-0.2	1.31	6
1467.0251	2	8	1	7	8	2	6	8.75E-05	3	-3.9	1.32	6	1697.73825	-4	7	1	7	6	0	6	1.08E-03	3	-2.7	1.20	6
1467.64570	1	3	0	3	4	1	4	4.55E-03	2	0.5	1.18	6	1703.68015	7	6	3	4	6	2	5	4.45E-04	2	4.2	1.10	6
1467.79752	2	5	3	3	5	4	2	2.00E-04	2	-1.3	1.28	6	1714.6101	6	8	1	8	7	0	7	1.91E-03	7	-5.4	1.18	6
1468.26682	-3	4	3	2	4	4	1	5.80E-04	2	-0.7	1.29	6	1715.68791	-1	3	2	1	2	1	2	2.19E-03	5	-0.4	1.05	6
P1468.970	-85	7	6	2	7	7	1	1.76E-06	10	-31.8	1.09	6	1718.05010	-6	7	1	6	6	2	5	1.06E-03	5	7.7	1.32	6
P1469.066	-35	7	6	1	7	7	0	5.20E-06	10	-34.0	1.09	6	1723.04619	-4	5	2	4	4	1	3	7.25E-04	5	-3.7	1.06	6
1470.74848	-22	9	4	5	9	5	4	2.30E-05	4	7.6	1.38	6	1731.03695	-4	9	0	9	8	1	8	1.20E-03	10	9.2	1.38	6
1470.86848	-3	5	3	2	5	4	1	6.10E-04	2	-0.4	1.29	6	1735.3075	-26	6	2	5	5	1	4	1.66E-03	4	2.3	1.14	6
1472.37346	-6	6	3	4	7	2	5	9.82E-05	2	5.5	1.05	6	1757.02465	-8	3	3	1	2	2	0	9.40E-04	6	-5.0	0.97	6
1474.62823	2	6	3	3	6	4	2	1.46E-04	2	-0.4	1.28	6	1758.33307	-1	3	3	0	2	2	1	3.25E-03	10	9.8	1.12	6
1477.24875	-2	4	2	3	4	3	2	1.73E-03	2	-2.1	1.30	6	1778.53099	3	4	3	2	3	2	2	1.93E-03	10	-4.5	0.95	6
1478.12349	4	5	0	5	5	1	4	2.20E-03	4	-0.5	1.38	6	1805.32540	4	5	2	3	4	1	4	4.48E-04	4	-5.7	0.94	6
1480.22927	5	3	2	2	3	3	1	4.97E-04	3	-3.6	1.28	6	1810.99747	5	6	3	4	5	2	3	7.02E-04	3	-2.6	0.94	6
1480.69765	-8	7	3	4	7	4	3	2.62E-04	2	2.7	1.31	6	1814.71469	-2	5	3	2	4	2	3	1.11E-03	4	1.3	0.97	6
1482.47745	2	2	0	2	3	1	3	1.70E-03	3	-0.2	1.20	6	1822.42389	3	7	3	5	6	2	4	1.30E-04	7	0.1	0.97	6
1482.53983	-4	3	1	3	4	0	4	1.35E-03	2	0.2	1.15	6	1831.99401	2	8	3	6	7	2	5	1.93E-04	3	-2.9	0.95	6
1485.13356	0	3	2	1	3	3	0	1.57E-03	3	-0.6	1.30	6	1832.011	-222	6	3	3	6	0	6	4.47E-06	10	-2.0	1.04	6
1486.74365	5	7	1	6	7	2	5	6.90E-04	2	-1.3	1.32	6	1832.9259	-118	11	2	9	10	3	8	1.72E-05	6	5.3	1.26	6
1490.0218	-29	4	2	2	4	3	1	5.25E-04	15	-18.3	1.08	6	1839.14695	-2	4	4	1	3	3	1	1.43E-03	3	1.9	0.97	6
1494.8717	11	9	2	7	9	3	6	8.71E-05	7	-0.2	1.27	6	1839.32443	-15	4	4	0	3	3	1	4.68E-04	7	0.1	0.95	6
1495.03784	-9	9	3	6	9	4	5	5.00E-05	4	-4.0	1.21	6	1841.1283	76	9	3	7	8	2	6	3.26E-05	5	3.1	1.03	6
1495.61167	0	2	1	2	2	2	1	2.57E-03	3	-0.9	1.31	6	1849.64108	1	6	3	3	5	2	4	1.73E-04	3	2.6	0.93	6
1498.37984	-5	1	0	1	2	1	2	5.05E-03	2	-0.2	1.22	6	1851.33775	-11	10	3	8	9	2	7	4.42E-05	4	5.6	1.09	6
1498.5172	32	11	3	8	11	4	7	5.26E-06	6	-0.9	1.24	6	P1854.1889	-10	6	6	1	6	5	2	1.00E-05	4	26.5	1.12	6
1499.82819	6	4	0	4	4	1	3	1.27E-03	2	-1.8	1.31	6	P1854.8108	-4	7	6	1	7	5	2	8.15E-06	4	22.1	1.45	6
1502.08947	-1	6	2	4	6	3	3	3.50E-04	4	-1.0	1.26	6	1855.1722	37	8	6	3	8	5	4	3.40E-06	10	2.0	1.01	6
1502.43622	10	8	2	6	8	3	5	9.10E-05	15	10.8	1.41	6	1861.85017	10	6	6	2	4	5	1	5.45E-05	5	2.1	0.87	6
1502.6598	-56	8	1	8	7	2	5	6.00E-06	10	-1.2	2.43	6	1862.95590	0	5	4	2	4	3	1	2.85E-04	3	1.4	0.93	6
1504.61315	2	7	2	5	7	3	4	5.74E-04	2	1.1	1.27	6	1864.17125	-1	5	4	1	4	3	2	8.45E-04	2	0.3	0.92	6
1506.0207	9	2	1	2	3	0	3	4.00E-03	8	6.9	1.25	6	1865.96936	-3	4	3	2	3	0	3	4.10E-05	4	-4.1	0.87	6
1508.3019	-33	5	3	3	6	2	4	4.00E-05	4	-3.4	0.97	6	1872.1939	-12	7	3	4	7	0	7	4.18E-06	10	-10.9	1.06	6
1511.48584	-2	5	1	4	5	2	3	3.16E-03	2	6.1	1.37	6	1885.02076	-5	6	4	3	5	3	2	4.48E-04	2	-0.9	0.88	6
1511.85960	4	2	1	1	2	2	0	1.18E-03	2	1.9	1.31	6	1891.55097	7	7	3	4	6	2	5	1.98E-04	2	4.6	0.88	6
1515.29144	3	3	1	2	3	2	1	4.80E-03	2	-1.2	1.27	6	1902.0417	2	5	3	3	4	0	4	1.90E-05	3	5.0	0.90	6
1515.67386	3	4	1	3	4	2	2	1.50E-03	3	1.8	1.30	6	1903.97983	-12	7	4	4	6	3	3	7.21E-05	3	0.4	0.86	6
1528.31120	0	2	0	2	2	1	1	2.44E-03	3	0.0	1.27	6	1916.68207	1	7	4	3	6	3	4	2.08E-04	2	-0.5	0.84	6
1531.12875	-3	1	1	1	2	0	2	7.44E-04	2	0.5	1.18	6	1918.86008	-1	8	4	5	7	3	4	9.20E-05	5	-0.5	0.83	6
1534.93548	4	1	0	1	1	1	0	6.33E-03	3	0.3	1.26	6	1920.88517	-5	5	5	1	4	4	0	1.42E-04	2	-2.9	0.87	6
1543.7319	8	2	2	1	3	1	2	3.88E-04	10	-11.8	0.98	6	1920.91334	-29	5	5	0	4	4	1	4.41E-04	2	0.6	0.90	6
1543.8972	-13	4	3	2	5	2	3	1.28E-04	5	-2.7	0.99	6	1924.73505	-7	7	2	5	6	1	6	5.12E-05	2	-4.1	0.73	6
1547.8894	-74	6	1	6	5	2	3	6.11E-05	5	0.9	1.76	6	1929.7078	6	9	4	6	8	3	5	1.16E-05	3	-5.1	0.79	6
1583.3559	-29	1	1	0	1	0	1	5.53E-03	5	-0.8	1.16	6	1937.46111	18	10	4	7	9	3	6	1.43E-05	3	4.6	0.89	6
1586.9943	23	2	0	2	1	1	0	9.42E-04	5	-2.5	1.22	6	1941.33656	4	8	3	5	7	2	6	1.96E-05	3	0.4	0.77	6
1590.3812	-14	2	1	1	2	0	2	2.02E-03	3	-0.7	1.15	6	1944.19954	-7	6	3	4	5	0	5	4.28E-05	2	1.6	0.81	6
1592.3218	90	3	1	2	2	2	1	7.32E-04	3	1.3	1.32	6	1945.47626	-3	6	5	2	5	4	1	2.32E-04	3	-1.3	0.84	6
1601.3467	-33	1	1	1	0	0	0	1.49E-03	4	5.0	1.23	6	1945.66567	1	6	5	1	5	4	2	7.80E-05	3	-0.4	0.85	6
1602.72990	6	3	1	2	3	0	3	4.75E-03	3	4.8	1.21	6	1948.5126	26	12	4	9	11	3	8	1.24E-06	10	-16.1	0.83	6
1619.36015	0	2	1	2	1	0	1	5.69E-03	5	-1.9	1.16	6	1969.38050	-1	7	5	2	6	4	3	3.74E-05	4	-0.6	0.81	6
1620.33590	8	3	2	1	3	1	2	3.54E-03	3	3.8	1.16	6	1970.25548	-1	7	5	2	6	4	3	1.13E-04	2	0.1	0.81	6
1620.4691	-38	4	2	2	4	1	3	9.92E-04	5	-2.1	1.10	6	1974.3505	131	4	4	1	3	1	2	1.60E-06	10	-11.4	0.90	6
1621.12141	35	4	1	3	4	0	4	8.64E-04	3	-0.7															

Table 5. Continued

Observed Position	o - c	Upper $J$	$K_a$	Lower $J$	$K_a$	Observed Strength	%s (o - c)%	R	Mol	Observed Position	o - c	Upper $J$	$K_a$	Lower $J$	$K_a$	Observed Strength	%s (o - c)%	R	Mol						
1381.6782	18	7	1	6	8	2	7	2.88E-04	10	4.5	1.18	7	1806.1648	41	6	3	4	5	2	3	7.84E-04	10	4.4	1.05	7
1385.6420	-23	3	2	1	4	3	2	2.22E-03	5	-4.7	1.23	7	1810.2821	-20	5	3	2	4	2	3	1.17E-03	10	-0.1	1.02	7
1397.2337	72	8	1	8	8	2	7	2.96E-04	10	4.2	1.85	7	1834.2624	-2	4	4	0	3	3	1	4.85E-04	10	5.0	0.98	7
1398.1021	-24	7	0	7	8	1	8	8.16E-04	10	-3.7	1.19	7	1859.0940	-7	5	4	1	4	3	2	9.38E-04	10	3.5	1.02	7
1401.7261	7	5	1	4	6	2	5	1.02E-03	10	2.0	1.22	7	1898.618	274	7	4	4	6	3	3	7.50E-05	10	-4.8	0.89	7
1406.1634	1	2	2	1	3	3	0	3.85E-03	7	3.5	1.34	7	1915.3447	-101	5	5	1	4	4	0	1.52E-04	10	-2.3	0.93	7
1407.4152	-38	2	2	0	3	3	1	1.40E-03	10	11.5	1.44	7	1915.3675	26	5	5	0	4	4	1	4.72E-04	10	1.1	0.97	7
1415.85827	-5	2	1	2	3	2	1	2.25E-03	3	0.2	1.31	7	1939.9009	10	6	5	2	5	4	1	2.82E-04	10	-0.4	1.03	7
1418.25568	35	6	1	6	7	0	7	1.52E-03	3	-2.0	1.20	7	1312.2216	31	5	4	2	6	5	1	1.28E-04	10	-0.3	1.30	8
1422.99515	-26	6	2	5	7	1	6	4.73E-04	10	0.7	1.12	7	1312.3700	6	5	4	1	6	5	2	3.93E-04	10	1.9	1.33	8
1425.69461	-11	7	0	7	7	1	6	6.02E-04	10	-0.2	1.58	7	*1313.0047	-13	5	5	0	6	5	1	3.11E-04	10	-0.7	1.41	8
1433.3589	-12	5	0	5	6	1	6	2.25E-03	10	-12.3	1.07	7	1316.1710	-1	5	3	3	6	4	2	1.60E-04	10	-10.3	1.14	8
1437.66140	34	5	1	5	6	0	6	8.69E-04	10	3.6	1.25	7	1320.4350	-2	5	3	2	6	4	3	5.40E-04	5	-0.2	1.27	8
1437.7213	-2	6	1	6	6	2	5	1.03E-03	10	-5.4	1.47	7	1322.1127	-25	4	1	4	5	2	3	3.39E-04	4	-8.1	1.16	8
1438.9725	-48	2	1	1	3	2	2	1.11E-03	10	-4.5	1.21	7	1333.7129	-27	7	2	5	8	3	6	1.31E-04	10	2.3	1.25	8
1449.5920	-46	4	0	4	5	1	5	1.37E-03	10	11.2	1.36	7	1336.8391	-107	4	4	1	5	5	0	8.58E-04	10	7.6	1.42	8
1449.9455	22	1	1	1	2	2	0	1.35E-03	5	3.2	1.34	7	1341.9183	-5	4	3	2	5	4	1	1.14E-03	4	2.4	1.31	8
1457.80470	3	4	1	4	5	0	5	3.47E-03	3	-2.1	1.18	7	1343.0095	4	4	3	1	5	4	2	3.80E-04	10	2.0	1.31	8
1464.3090	-12	6	3	4	6	4	3	5.04E-04	10	-2.2	1.52	7	1346.8175	-8	4	2	3	5	3	2	1.10E-03	3	0.8	1.27	8
1464.7610	-2	3	0	3	4	1	4	4.60E-03	10	-1.1	1.20	7	1351.2461	-6	5	2	3	6	3	4	6.63E-04	4	4.6	1.29	8
1466.05085	9	4	3	2	4	4	1	6.15E-04	10	-2.7	1.36	7	1358.3313	-14	9	0	9	10	1	10	1.62E-04	10	-5.6	1.12	8
1468.71685	0	5	3	2	5	4	1	7.63E-04	10	8.8	1.61	7	1365.3591	7	4	2	2	5	3	3	3.84E-04	10	-9.0	1.14	8
1470.90920	2	4	1	4	4	2	3	2.50E-03	10	-4.6	1.35	7	1366.9722	9	3	3	0	4	4	1	2.06E-03	3	0.0	1.30	8
1474.7784	-31	4	2	3	4	3	2	1.83E-03	5	-2.8	1.38	7	1377.2125	-55	3	2	2	4	3	1	1.70E-04	5	-2.7	1.23	8
1474.83030	-4	5	0	5	5	1	4	2.27E-03	4	-2.7	1.42	7	1377.6053	4	8	1	8	9	0	9	3.99E-04	10	2.7	1.20	8
1477.3884	17	4	2	3	5	1	4	7.72E-04	10	-8.0	1.03	7	1377.8532	-17	8	2	7	9	1	8	1.18E-04	10	-7.0	1.07	8
1477.8017	-11	3	2	2	3	3	1	5.96E-04	10	11.1	1.53	7	1379.4483	39	7	1	6	8	2	7	2.57E-04	10	-10.0	1.05	8
1478.68585	41	7	3	4	7	4	3	3.00E-04	10	-3.7	1.50	7	1383.59278	-2	3	2	1	4	3	2	2.33E-03	3	2.0	1.29	8
1479.29913	-1	3	1	3	4	0	4	1.52E-03	3	9.1	1.30	7	1395.5685	-25	7	0	7	8	1	8	8.50E-04	7	6.2	1.24	8
1479.5640	4	2	0	2	3	1	3	1.69E-03	6	-2.1	1.19	7	1396.5810	17	7	1	7	8	0	8	2.51E-04	10	-5.7	1.10	8
1482.7765	-7	3	2	1	3	3	0	1.65E-03	10	0.6	1.36	7	1399.54289	0	5	1	4	6	2	5	9.80E-04	5	-1.1	1.17	8
1483.3318	20	7	1	6	7	2	5	7.19E-04	10	-1.7	1.37	7	1404.06481	-1	2	2	1	3	3	0	3.65E-03	4	-1.5	1.27	8
1483.46702	0	3	1	3	3	2	2	1.03E-03	10	-0.6	1.36	7	1405.31886	-13	2	2	0	3	3	1	1.25E-03	3	0.4	1.29	8
1494.09670	6	5	2	3	5	3	2	1.74E-03	4	0.6	1.40	7	1413.42388	-2	2	1	2	3	2	1	2.28E-03	3	5.9	1.33	8
1495.42225	-3	1	0	1	2	1	2	5.16E-03	10	1.8	1.25	7	1413.5440	-15	6	0	6	7	1	7	5.00E-04	3	1.5	1.18	8
1496.5920	-30	4	0	4	4	1	3	1.16E-03	6	-10.0	1.20	7	1415.5606	75	7	1	7	7	2	6	1.70E-04	10	-4.7	1.44	8
1499.6482	-1	6	2	4	6	3	3	3.56E-04	10	-9.3	1.28	7	1415.61710	16	6	1	6	7	0	7	1.49E-03	3	1.3	1.17	8
1512.5656	1	3	1	2	3	2	1	4.54E-03	5	-7.8	1.20	7	1419.9340	-12	6	2	5	7	1	6	5.05E-04	5	4.3	1.20	8
1512.83594	-15	4	1	3	4	2	2	1.60E-03	7	6.6	1.39	7	1421.81073	0	3	1	2	4	2	3	2.56E-03	4	4.9	1.27	8
1513.6656	10	0	0	0	1	1	1	1.28E-03	10	-8.9	1.12	7	1422.8605	0	7	0	7	7	1	6	5.93E-04	10	4.0	1.55	8
1513.68322	0	3	0	3	3	1	2	5.70E-03	5	-3.5	1.24	7	1430.7938	-3	5	0	5	6	1	6	2.44E-03	5	0.2	1.16	8
1525.2369	-5	2	0	2	2	1	1	2.32E-03	4	-3.9	1.21	7	1434.9537	47	5	1	5	6	0	6	8.30E-04	6	3.4	1.20	8
1527.71433	6	1	1	1	2	0	2	7.27E-04	10	-1.8	1.15	7	1435.17559	3	6	1	6	6	2	5	1.06E-03	2	4.2	1.51	8
1531.8972	7	1	0	1	1	1	0	6.40E-03	3	2.6	1.27	7	1436.2158	36	8	2	7	8	3	6	2.39E-04	10	9.6	1.64	8
1579.8958	42	1	1	0	1	0	1	5.77E-03	5	4.8	1.21	7	1445.3526	-3	5	2	4	6	1	5	2.65E-04	10	9.4	1.26	8
1583.9142	-50	2	0	2	1	1	1	1.00E-03	10	5.1	1.29	7	1447.02485	1	4	0	4	5	1	5	1.20E-03	4	1.6	1.19	8
1584.9572	-36	2	1	1	2	0	2	2.10E-03	7	4.3	1.20	7	1447.5673	3	1	1	2	2	0	0	1.33E-03	6	4.7	1.32	8
1589.6172	10	3	1	2	2	2	1	6.91E-04	5	-2.3	1.25	7	1452.9880	3	5	1	5	5	2	4	6.36E-04	5	10.7	1.56	8
1597.84810	-1	1	1	1	0	0	0	1.50E-03	8	7.2	1.24	7	1454.6385	-17	1	0	2	2	2	1	4.10E-03	10	-6.8	1.16	8
1599.38444	6	3	1	2	3	0	3	4.70E-03	3	4.9	1.20	7	1455.0129	-8	4	1	4	5	0	5	3.39E-03	4	-0.9	1.15	8
1609.04007	0	3	0	3	2	1	2	5.44E-03	4	3.0	1.27	7	1458.7182	43	6	4	3	6	5	2	1.51E-04	10	-10.5	1.25	8
1615.82229	4	2	1	2	1	0	1	5.60E-03	10	-2.0	1.15	7	1458.9237	17	5	4	1	5	5	0	1.83E-04	10	1.4	1.42	8
1616.40133	0	3	2	1	3	1	2	3.10E-03	4	-10.1	1.02	7	1459.4908	-6	6	2	5	6	3	4	8.74E-04	4	-1.9	1.38	8
1619.58201	-16	2	2	0	2	1	1	7.54E-04	10	-8.8	1.02	7	1462.18628	6	3	0	3	4	1	4	4.45E-03	4	-1.3	1.16	8
1622.0503	52	4	1	3	3	2	2	4.18E-04	10	-1.6	1.24	7	1462.2708	-12	6										

Table 5. Continued

Observed Position	$\Delta$	Upper $J K_a K_c$	Lower $J K_a K_c$	Observed Strength	%s ( $\Delta - c$ )%	R	Mol	Observed Position	$\Delta$	Upper $J K_a K_c$	Lower $J K_a K_c$	Observed Strength	%s ( $\Delta - c$ )%	R	Mol
1556.7454	40	4 1 4	3 2 1	3.09E-04	10	2.3	1.45 8	1687.0822	-72	5 3 3	5 2 4	2.71E-04	10	1.5	1.18 8
1576.81118	0	1 1 0	1 0 1	5.65E-03	3	1.7	1.19 8	1689.2579	4	7 0 7	6 1 6	3.20E-03	10	-8.1	1.19 8
1581.16602	16	2 0 2	1 1 1	9.55E-04	7	-0.4	1.23 8	1690.97723	2	7 1 7	6 0 6	1.16E-03	5	-0.0	1.29 8
1583.9053	-4	2 1 1	2 0 2	2.05E-03	3	0.6	1.17 8	1691.4169	-8	7 2 5	6 3 4	2.48E-04	10	3.3	1.39 8
1587.20097	-18	3 1 2	2 2 1	7.58E-04	3	4.5	1.37 8	1701.8743	8	4 2 3	3 1 2	2.85E-03	10	-3.5	1.06 8
1594.7293	-4	1 1 1	0 0 0	1.46E-03	5	3.3	1.21 8	1707.0111	1	8 0 8	7 1 7	7.15E-04	5	0.3	1.38 8
1596.4029	12	3 1 2	3 0 3	4.54E-03	3	-0.6	1.16 8	1707.8239	2	8 1 8	7 0 7	2.14E-03	5	-0.0	1.32 8
1606.23627	0	3 0 3	2 1 2	5.50E-03	3	2.8	1.28 8	1712.1433	23	7 1 6	6 2 5	1.05E-03	4	6.5	1.31 8
1612.66848	-3	2 1 2	1 0 1	5.95E-03	4	2.6	1.21 8	1724.25837	-43	9 0 9	8 1 8	1.17E-03	5	-1.2	1.34 8
1612.89803	-3	3 2 1	3 1 2	3.58E-03	2	1.1	1.17 8	1724.6424	-12	9 1 9	8 0 8	3.98E-04	10	0.8	1.36 8
1613.2438	4	4 2 2	4 1 3	1.10E-03	10	4.1	1.22 8	1727.43150	0	6 2 5	5 1 4	1.55E-03	5	-4.4	1.06 8
1614.9925	30	4 1 3	4 0 4	8.15E-04	3	-8.2	1.07 8	1728.8245	-46	5 4 1	5 3 2	3.54E-04	10	10.9	1.32 8
1616.0387	26	2 2 0	2 1 1	8.65E-04	4	1.0	1.17 8	1738.0231	-24	8 1 7	7 2 6	2.06E-04	10	2.4	1.23 8
1617.7603	-8	5 2 3	4 3 2	3.06E-04	10	-4.8	1.32 8	1741.1290	-8	10 0 10	9 1 9	1.85E-04	10	-6.9	1.30 8
1619.18678	-2	5 2 3	5 1 4	2.08E-03	3	1.5	1.20 8	1741.31288	14	10 1 10	9 0 9	5.94E-04	6	1.4	1.40 8
1619.6027	-11	4 1 3	3 2 2	4.46E-04	10	2.1	1.32 8	1748.40805	12	3 3 1	2 2 0	9.60E-04	4	-9.9	0.99 8
1628.26481	1	3 1 3	3 2 0	2.25E-03	5	-1.3	1.18 8	1749.7621	2	3 3 0	2 2 1	3.06E-03	6	-3.3	1.06 8
1629.6956	1	4 0 4	3 1 3	2.20E-03	6	0.9	1.26 8	1754.3625	-1	8 2 7	7 1 6	6.12E-04	3	-1.0	1.13 8
1631.6368	-15	2 2 1	2 1 2	1.94E-03	4	3.7	1.19 8	1757.6911	4	11 0 11	10 1 10	2.88E-04	10	5.7	1.54 8
1638.70238	1	5 1 4	5 0 5	1.30E-03	10	-3.1	1.11 8	1761.3855	76	9 1 8	8 2 7	3.07E-04	10	-4.5	1.16 8
1640.8202	-21	3 2 2	3 1 3	6.50E-04	10	-6.5	1.07 8	1769.78478	-3	4 3 2	3 2 1	2.18E-03	3	3.6	1.07 8
1643.01874	1	4 1 4	3 0 3	7.45E-03	3	4.7	1.28 8	1776.4078	10	4 3 1	3 2 2	6.42E-04	10	-4.9	0.98 8
1651.08358	0	5 0 5	4 1 4	6.41E-03	3	2.6	1.30 8	1787.6560	3	5 3 3	4 2 2	4.38E-04	10	3.5	1.03 8
1652.1160	-7	5 1 4	4 2 3	1.40E-03	10	-7.8	1.18 8	1788.2920	-14	5 5 0	5 4 1	7.96E-05	10	-2.6	1.43 8
1658.2546	-1	5 1 5	4 0 4	2.15E-03	5	0.4	1.25 8	1798.3760	-53	5 2 3	4 1 4	4.20E-04	10	-2.7	0.88 8
1660.0260	8	5 3 2	5 2 3	9.62E-04	5	5.2	1.18 8	1801.8622	38	6 3 4	5 2 3	7.27E-04	4	1.7	0.98 8
1665.3282	-2	6 1 5	6 0 6	2.01E-04	10	-3.9	1.10 8	1806.3396	-5	5 3 2	4 2 3	1.18E-03	5	7.4	1.03 8
1667.1038	30	4 3 1	4 2 2	4.18E-04	10	10.5	1.27 8	1829.5689	-11	4 4 1	3 3 0	1.55E-03	4	-0.2	1.05 8
1668.0397	35	2 2 1	1 1 0	3.80E-03	10	-8.4	1.04 8	1829.7576	-20	4 4 0	3 3 1	4.88E-04	5	-5.9	0.99 8
1670.75385	-2	6 0 6	5 1 5	1.71E-03	7	2.7	1.32 8	1853.2859	-15	5 4 2	4 3 1	3.06E-04	10	4.9	1.00 8
1674.33498	-6	6 1 6	5 0 5	4.95E-03	3	-1.8	1.25 8	1854.57636	6	5 4 1	4 3 2	8.88E-04	4	1.8	0.97 8
1674.7116	-15	2 2 0	1 1 1	1.24E-03	4	3.9	1.16 8	1875.1726	-19	6 4 3	5 3 2	4.50E-04	5	2.1	0.88 8
1678.2685	-46	3 3 1	3 2 2	3.09E-04	5	-6.4	1.11 8	1884.0157	15	7 3 4	6 2 5	1.76E-04	10	4.6	0.78 8
1683.3627	-26	6 1 5	5 2 4	4.50E-04	10	-0.1	1.24 8	1910.4178	-10	5 5 1	4 4 0	1.60E-04	10	-2.7	0.98 8
1686.3315	2	6 2 5	6 1 6	5.11E-04	5	-5.5	1.07 8	1910.4407	0	5 5 0	4 4 1	5.10E-04	8	3.3	1.05 8
1686.34978	-3	3 2 2	2 1 1	1.23E-03	6	2.7	1.15 8	1934.9394	-11	6 5 2	5 4 1	2.39E-04	10	1.4	0.87 8

<sup>a</sup>1 atm = 760 Torr.

<sup>b</sup> $\Delta - c$ , Observed minus computed line positions ( $\text{cm}^{-1} \times 10^5$ ). Computed values are derived from the energy levels given in Table 2 and the lower state, (010), levels given in Ref. 1 for  $\text{H}_2^{16}\text{O}$  and Ref. 2 for  $\text{H}_2^{17}\text{O}$  and  $\text{H}_2^{18}\text{O}$ . %s, Estimated uncertainties in the measured line strengths given in percent. ( $\Delta - c$ ), Percent difference between the observed and computed line strengths. R, Ratio of the observed line strength derived in this study to the computed value given in Refs. 17–19. Mol, Isotopic species in which 6 represents  $\text{H}_2^{16}\text{O}$ , 7 represents  $\text{H}_2^{17}\text{O}$ , and 8 represents  $\text{H}_2^{18}\text{O}$ . An asterisk denotes a doubled absorption with the quantum assignment given for the stronger transition. The strength given represents the sum of the strengths of the two comparable transitions. P denotes that the transition is strongly perturbed.

minus the computed line strength in percent [ $(\Delta - c)\%$ ], the ratio R of the observed line strength to that given for  $\text{H}_2^{16}\text{O}$  in the tabulation by Flaud *et al.*<sup>17</sup> (and in the 1992 edition of the HITRAN database<sup>19</sup> and Ref. 18), and the molecular species (6 denotes  $\text{H}_2^{16}\text{O}$ ; 7,  $\text{H}_2^{17}\text{O}$ ; and 8,  $\text{H}_2^{18}\text{O}$ ). The values for the line strengths are normalized to 100% of the isotopic species in units of inverse square centimeters per atmosphere (1 atm = 760 Torr), whereas the values given in Refs. 17–19 are given in  $\text{cm}^{-1}/(\text{mol cm}^{-2})$  and reduced by the normal isotopic abundances ( $3.7 \times 10^{-4}$  for  $\text{H}_2^{17}\text{O}$  and  $2.04 \times 10^{-3}$  for  $\text{H}_2^{18}\text{O}$ ). Therefore values from Refs. 17–19 were converted into square inverse centimeters per atmosphere by application of the factor  $2.48 \times 10^{19}$  (at 296 K) and division of the result by the proper isotopic abundance in natural water to determine the values of R given in Table 5. The experimental line strengths are presented in the table for a temperature of 296 K, whereas the sample temperatures of several of the spectra from which the strengths were determined were slightly different than 296 K. These values were converted to those for  $T = 296$  K with the use of Eqs. (1) and the  $v_2$  rotational levels given in Refs. 1 and 2.

The observed positions are given to three, four, or five decimal places in Table 5, which indicates the accuracy of these measurements. Obviously the most accurate estimates are given with five significant figures past the deci-

mal, and, as was reported in Refs. 1 and 2, the absolute uncertainty for these measurements is  $\pm 6 \times 10^{-5} \text{ cm}^{-1}$ . The computed line positions were derived from the rotational energies given in Table 2 for the (020) states and the levels given for the (010) states given in Ref. 1 for  $\text{H}_2^{16}\text{O}$  and Ref. 2 for  $\text{H}_2^{17}\text{O}$  and  $\text{H}_2^{18}\text{O}$ . An asterisk next to the line-position value denotes a doubled absorption for which two transitions were not adequately resolved in the spectra. The quantum assignments given for these features are for the stronger of the two, and the values of the observed and the computed strengths represent the sum of the strengths of the two comparable transitions.

The computed line strengths were derived from the dipole moment expansion coefficients given in Table 4 and Eqs. (1)–(3). Not all the line-strength measurements given in Table 5 were included in the least-squares analyses. Entries with %s = 15% were not included because these transitions resulted in averaged values with uncertainties of as much as 60% to possibly less than 10%. This range of uncertainty for each of these transitions arises for one or more of the following reasons: (a) blending, (b) weakness of transition intensity, and (c) poor agreement between values derived from the various spectra. Other entries not included in the line-strength analyses were those labeled P in Table 5. These transitions are strongly perturbed owing to resonance interactions,

and the computed strengths derived for these transitions and used to obtain values of  $(o - c)\%$  in Table 5 represent the unperturbed values.

The values of  $R$  for  $H_2^{17}O$  and  $H_2^{18}O$  given in Table 5 were inferred from the  $H_2^{16}O$  values given by Flaud *et al.*<sup>17</sup> Measurements of the strengths of  $H_2^{17}O$  and  $H_2^{18}O$  transitions have not been reported in the literature for the (020)–(010) bands, and therefore values for them given in Refs. 18 and 19 were computed from the transition moment constants of  $H_2^{16}O$  given by Flaud *et al.*<sup>17</sup>

Table 6 is a listing comparable in content with that of Table 5. This table lists the measurements and computations for the (020)–(000) band of  $H_2^{16}O$ . An added feature for this table is that the computed line-strength values are given in place of the percent differences in the column for  $(o - c)\%$  if the magnitude of  $(o - c)\%$  is 14% or greater. The majority of these entries are of transitions that are moderately to strongly perturbed. Also included in Table 6 are two transitions, located at 4077.72 and 4106.87  $\text{cm}^{-1}$ , of which the computed strengths given by

**Table 6. Line Positions ( $\text{cm}^{-1}$ ) and Strengths ( $\text{cm}^{-2}/\text{atm}^a$  at 296 K) Observed in the (020)–(000) Band of  $H_2^{16}O$**

Observed Position	$o - c$	Upper $J$	$K_a$	$K_c$	Lower $J$	$K_a$	$K_c$	Observed Strength	%s	$(o - c)\%$	$R$	Observed Position	$o - c$	Upper $J$	$K_a$	$K_c$	Lower $J$	$K_a$	$K_c$	Observed Strength	%s	$(o - c)\%$	$R$
2622.5753	-15	9	0	9	10	3	8	3.10E-06	10	1.3	1.06	2966.0063	12	5	3	2	6	4	3	4.14E-03	2	1.8	1.11
2670.0044	-3	10	2	9	11	3	8	1.88E-06	5	-12.7	0.90	2966.83284	12	10	1	10	10	2	9	1.53E-04	4	-2.3	1.09
2681.8148	58	9	1	8	10	4	7	3.54E-06	7	1.5	1.03	2967.33362	4	10	0	10	10	1	9	5.25E-05	3	-0.2	1.11
2693.3318	41	8	1	8	9	2	7	1.35E-05	4	-0.4	1.05	2967.98477	-1	6	2	4	7	3	5	8.15E-04	2	0.7	1.11
2730.089	-228	9	2	8	10	3	7	3.60E-06	10	5.3	1.09	2969.51627	-2	9	1	8	10	2	9	6.50E-04	2	1.5	1.08
2732.49271	-41	7	0	7	8	3	6	2.68E-05	4	-7.0	0.99	2970.1744	0	5	0	5	5	3	2	6.75E-05	5	8.5	1.17
2788.8142	3	8	2	7	9	3	6	5.04E-05	8	6.1	1.12	2973.25241	3	4	2	3	5	3	2	7.00E-03	4	-1.4	1.10
2819.44924	25	6	1	6	7	2	5	1.66E-04	3	-3.7	1.05	2974.58888	4	8	0	8	9	1	9	1.43E-03	2	0.3	1.12
2820.48697	-39	9	3	7	10	4	6	1.00E-05	10	0.5	1.04	2974.8280	-45	12	4	9	13	3	10	6.50E-06	8	3.01E-06	1.27
2830.00743	-34	5	0	5	6	3	4	1.36E-04	3	2.5	1.11	2975.08458	5	8	1	8	9	0	9	4.29E-03	5	0.3	1.11
2844.0105	45	7	2	6	8	3	5	7.10E-05	4	3.1	1.10	2975.22271	6	9	2	8	10	1	9	2.16E-04	2	-1.3	1.05
2864.35029	-84	8	3	6	9	4	5	1.31E-04	3	-4.6	1.00	*2975.2944	-68	9	7	2	10	8	3	1.76E-05	2	1.5	0.93
2871.3305	84	4	0	4	5	3	3	6.00E-05	10	1.2	1.11	2977.94343	-1	5	2	3	6	3	4	4.95E-03	2	1.3	1.12
2879.70636	-36	5	1	5	6	2	4	1.98E-04	5	0.8	1.11	2979.07153	5	10	3	8	11	2	9	9.09E-05	2	2.6	1.06
2883.027	-66	10	5	6	11	6	5	1.31E-05	10	9.0	1.21	2980.24024	1	5	4	2	6	5	1	1.03E-03	2	-0.5	1.05
2890.1627	14	12	0	12	13	1	13	3.43E-05	7	0.3	1.09	2980.38811	-4	5	4	1	6	5	2	3.08E-03	2	-1.0	1.04
2890.19489	-28	12	1	12	13	0	13	1.10E-04	6	7.0	1.16	2981.14415	-5	6	5	2	7	6	1	9.13E-04	2	1.0	1.03
2893.07588	6	9	4	5	10	5	6	5.55E-05	2	-3.8	0.99	2981.17111	-4	6	5	1	7	6	2	3.08E-04	3	2.1	1.04
2893.81418	4	6	2	5	7	3	4	8.11E-04	2	0.2	1.09	2982.45252	-5	8	1	7	9	2	8	4.85E-04	2	-0.3	1.07
2904.43818	19	8	4	5	9	5	4	1.74E-04	2	0.6	1.04	2984.21159	5	3	1	3	4	2	2	1.88E-03	2	1.6	1.15
2906.72554	-9	3	0	3	4	3	2	1.45E-04	2	2.6	1.14	2987.52481	1	4	3	2	5	4	1	8.06E-03	3	-1.0	1.08
2909.4350	-90	11	3	8	12	4	9	9.70E-06	10	10.6	1.13	2988.19165	3	7	6	2	8	7	1	7.13E-05	2	0.8	1.01
2909.68935	46	9	5	4	10	6	5	4.10E-05	4	5.1	1.05	2988.28775	-1	7	6	1	8	7	2	2.08E-04	2	-2.0	1.00
2911.33232	8	8	4	4	9	5	5	4.75E-05	3	4.02E-05	1.13	2988.54570	10	9	1	9	9	2	8	1.39E-04	2	-3.7	1.09
2911.88958	2	11	0	11	12	1	12	2.95E-04	3	-5.7	1.06	2988.61258	6	4	3	1	5	4	2	2.74E-03	2	-0.2	1.10
2911.95194	1	11	1	11	12	0	12	9.90E-05	5	-4.7	1.07	2989.62427	4	9	0	9	9	1	8	4.27E-04	2	-3.2	1.09
2912.46818	2	9	3	6	10	4	7	8.70E-05	2	-1.6	1.03	2991.45528	-4	4	0	4	4	3	1	3.17E-05	3	4.5	1.15
2918.99160	10	8	3	5	9	4	6	8.57E-05	2	-0.8	1.05	2991.9710	-1	4	2	2	5	3	3	3.08E-03	2	0.3	1.12
2922.1143	22	12	1	12	12	2	11	1.54E-05	10	7.6	1.08	2992.65373	-2	8	2	7	9	1	8	1.53E-03	3	0.8	1.09
2924.2591	16	12	1	11	13	2	12	1.00E-05	6	7.0	1.10	2993.73595	0	7	1	6	8	2	7	2.95E-03	2	-0.1	1.09
2930.12835	-1	7	3	4	8	4	5	7.16E-04	2	0.7	1.08	2994.64644	2	7	0	7	8	1	8	8.70E-03	4	3.1	1.15
2930.65783	-10	7	4	4	8	5	3	1.76E-04	2	1.1	1.05	2995.45513	1	7	1	7	8	0	8	2.85E-03	2	1.0	1.13
2932.65156	-6	8	5	4	9	6	3	1.27E-04	3	2.0	1.02	2998.97188	0	9	3	7	10	2	8	7.83E-05	2	1.0	1.06
2933.1213	26	8	5	3	9	6	4	4.10E-05	4	-1.6	0.99	*2999.15758	-18	8	7	2	9	8	1	5.45E-05	4	-2.9	0.92
2933.35685	9	10	1	10	11	0	11	8.28E-04	3	2.6	1.13	2999.8623	54	11	4	8	12	3	9	3.22E-06	4	-4.1	0.88
2933.72895	1	6	3	4	7	4	3	1.53E-03	3	-2.4	1.05	3003.47424	-2	6	1	5	7	2	6	1.83E-03	2	2.9	1.14
2934.028	-222	12	2	10	13	3	11	4.10E-06	10	2.86E-06	1.10	3004.6868	46	4	4	1	5	5	0	6.30E-03	4	0.3	1.07
2935.19362	2	4	1	4	5	2	3	1.92E-03	2	0.7	1.13	3004.7025	-38	4	4	0	5	5	1	2.10E-03	4	0.2	1.07
2936.7416	-19	2	0	2	3	3	1	1.72E-05	4	2.6	1.15	3004.98381	-2	12	2	11	12	3	10	1.15E-05	3	-9.2	0.95
2936.96703	4	5	2	4	6	3	3	8.90E-04	2	-0.4	1.10	3005.4456	17	5	5	1	6	6	0	7.25E-04	5	6.1	1.09
2940.06758	-1	11	1	10	12	2	11	8.87E-05	2	0.7	1.05	3005.4544	-40	5	5	0	6	6	1	2.18E-03	5	6.4	1.10
2941.76294	-2	11	2	10	12	1	11	3.02E-05	5	2.0	1.06	3006.42575	0	12	1	11	12	2	10	4.52E-06	3	7.8	1.08
2941.9863	28	9	6	3	10	7	4	1.10E-05	4	4.14E-05	1.03	3009.65271	16	8	1	8	8	2	7	1.10E-03	3	1.0	1.14
2943.1464	-16	11	2	9	12	3	10	2.77E-05	5	0.8	1.01	3010.2322	-26	3	2	1	4	3	2	1.58E-02	3	-1.6	1.11
2944.6606	24	11	1	11	11	2	10	1.74E-05	3	1.1	1.12	3011.27736	1	7	2	6	8	1	7	1.05E-03	3	1.3	1.10
2946.0497	-8	6	3	3	7	4	4	5.95E-04	4	-0.3	1.08	3011.90863	9	8	0	8	8	1	7	3.73E-04	2	-1.2	1.12
2949.1483	8	10	2	8	11	3	9	2.66E-05	5	0.0	1.04	*3012.0683	16	9	8	1	10	9	2	1.07E-05	7	8.9	0.93
2951.536	-156	10	7	4	11	8	3	5.18E-06	4	3.73E-06	1.27	3012.2320	-1	6	6	1	7	7	0	4.55E-04	4	4.84E-04	0.95
2951.553	190	10	7	3	11	8	4	1.73E-06	4	1.24E-06	1.27	3012.34352	-3	6	6	0	7	7	1	1.78E-04	3	-0.8	0.99
2953.41383	11	9	2	7	10	3	8	2.07E-04	4	-1.2	1.05	3012.37684	1	3	3	1	4	4	0	4.90E-03	2	-0.9	1.09
2954.15386	-1	9	0	9	10	1	10	1.93E-03	2	-1.2	1.09	3013.57316	0	6	0	6	6	7	1	4.98E-03	5	0.5	1.13
2954.39855	-14	9	1	9	10	0	10	6.81E-04	3	5.8	1.15	3015.61527	-1	6	1	6	7	0	7	1.56E-02	3	4.0	1.17
2955.1132	-13	5	1	4	5	4	1	9.55E-06	5	24.5	1.23	3021.31066	7	11	2	10	11	3	9	1.47E-05	3	2.2	1.03
2955.25618	-1	10	1	9	11	2	10	8.40E-05	3	0.6	1.06	*3021.549											

Table 6. Continued

Observed Position	o - c	Upper	$J$	$K_a$	$K_c$	Lower	$J$	$K_a$	$K_c$	Observed Strength	%s	(o - c)%	R	Observed Position	o - c	Upper	$J$	$K_a$	$K_c$	Lower	$J$	$K_a$	$K_c$	Observed Strength	%s	(o - c)%	R
3034.26407	-17	3	1	2	4	2	3	1.81E-02	3	-2.3	1.11	3125.13178	-6	7	2	5	7	3	4	4.00E-03	2	-0.3	1.08				
3034.39503	-2	7	0	7	7	1	6	2.63E-03	2	-2.0	1.12	3125.51643	-2	9	4	6	9	5	5	5.00E-05	3	-5.1	0.94				
3035.78362	-3	5	1	5	6	0	6	7.85E-03	2	0.0	1.13	3126.00249	-8	1	1	1	2	0	2	6.55E-03	2	2.3	1.18				
3037.09961	6	10	2	9	10	3	8	1.48E-04	2	2.3	1.07	3126.5686	-4	8	4	5	8	5	4	3.85E-04	2	2.1	1.03				
3042.42387	15	10	1	9	10	2	8	5.27E-05	2	-1.7	1.03	3126.7852	-5	2	0	2	2	1	1	1.58E-02	3	-0.2	1.16				
*3046.6235	0	9	9	0	10	10	1	6.60E-06	5	5.64E-06	0.87	3127.42006	-4	6	4	2	6	5	1	4.02E-04	2	0.9	1.05				
3048.67233	-2	4	0	4	5	1	5	1.06E-02	3	-0.4	1.13	3128.06590	-2	10	5	6	11	4	7	1.37E-05	4	1.07E-05	0.96				
3048.94745	-1	6	1	6	6	2	5	4.98E-03	3	-2.0	1.12	3128.10084	-5	8	3	5	8	4	4	3.17E-04	2	-0.4	1.04				
3049.0445	0	2	1	1	3	2	2	8.04E-03	2	-0.9	1.14	3128.55876	-6	7	4	3	7	5	7	2.71E-04	2	0.0	1.02				
3050.70281	3	7	3	5	8	2	6	3.29E-04	2	-2.1	1.06	3133.06957	-3	1	0	1	1	1	0	4.20E-02	2	-0.2	1.16				
3052.00952	1	9	2	8	9	3	7	1.42E-04	3	-0.4	1.06	3133.56880	-9	9	3	6	9	4	5	4.03E-04	2	1.3	1.04				
3055.61013	-1	5	2	4	6	1	5	2.73E-03	2	0.3	1.12	3134.4975	16	9	4	5	9	5	4	1.77E-04	5	4.5	1.04				
3056.35632	-4	4	1	4	5	0	5	3.30E-02	2	2.1	1.16	3135.37910	-11	11	3	8	11	4	7	3.90E-05	2	2.7	0.99				
3057.14658	3	6	0	6	6	1	5	1.95E-03	3	-0.8	1.14	3136.27988	-11	10	3	7	10	4	6	4.36E-05	2	-3.5	0.97				
3059.92945	-3	1	1	1	2	2	0	8.27E-03	3	-0.7	1.15	3136.41190	4	7	4	4	8	3	5	1.05E-04	3	-0.4	1.03				
3061.22892	8	9	1	8	9	2	7	5.10E-04	2	-1.1	1.06	3136.74535	-1	7	1	7	6	2	4	1.06E-05	3	8.1	1.21				
3062.2831	36	13	2	11	13	3	10	2.05E-06	10	-4.4	0.89	3139.6678	2	10	4	6	10	5	5	2.05E-05	3	-3.0	0.94				
3062.34785	6	9	4	6	10	3	7	2.45E-05	3	-0.9	1.00	3142.77956	-1	2	2	1	3	1	2	4.95E-03	3	2.6	1.17				
3064.40416	1	3	0	3	4	1	4	3.80E-02	2	-0.6	1.13	3145.41371	-2	11	4	7	11	5	6	2.05E-05	3	0.4	0.95				
3065.61738	0	8	2	7	8	3	6	1.14E-03	2	1.2	1.10	3151.35542	1	4	3	2	5	2	3	2.18E-03	2	-0.8	1.10				
3066.27142	-4	5	1	5	5	2	4	3.07E-03	2	0.4	1.16	3152.10094	-2	10	5	6	10	6	5	2.58E-05	3	4.4	0.96				
3067.01176	1	1	1	0	2	2	1	3.03E-02	3	0.7	1.16	3152.28080	-2	6	5	2	6	6	1	3.17E-04	3	-0.8	0.98				
3068.9305	-1	12	3	10	12	4	9	7.10E-06	7	7.92E-06	0.93	3152.3025	-8	6	5	1	6	6	0	1.06E-04	3	-0.5	0.98				
3076.2266	-21	12	2	10	12	3	9	2.40E-06	6	2.34E-06	0.88	3152.35617	2	7	5	3	7	6	2	8.60E-05	3	-2.5	0.95				
3077.47344	0	7	2	6	7	3	5	8.65E-04	2	-0.3	1.10	3152.3950	-52	9	5	5	9	6	4	2.09E-05	2	-5.2	0.89				
3077.93830	-5	3	1	3	4	0	4	1.23E-02	3	-1.0	1.13	3152.42329	8	8	5	4	8	6	3	1.48E-04	3	0.0	0.95				
3079.0601	-14	11	3	9	11	4	8	9.70E-06	3	-3.5	0.93	3152.44235	-7	7	5	2	7	6	1	2.56E-04	2	-3.4	0.94				
3079.52895	-5	5	0	5	5	1	4	1.21E-02	3	0.2	1.15	3152.627	0	13	4	9	13	5	8	1.16E-06	5	-10.1	0.80				
3079.6827	0	2	0	2	3	1	3	1.33E-02	2	-0.6	1.15	3152.72461	0	8	5	3	8	6	2	4.95E-05	3	0.1	0.96				
3079.92632	1	8	1	7	8	2	6	4.98E-04	2	-2.6	1.06	3153.27893	-1	9	5	4	9	6	3	6.83E-05	2	2.7	0.97				
3081.34196	-2	4	1	4	4	2	3	1.37E-02	3	-3.7	1.11	3154.3484	-46	10	5	5	10	6	4	9.03E-06	3	7.7	0.97				
3082.55629	2	6	3	4	7	2	5	1.61E-03	3	0.1	1.09	3155.34825	3	6	1	6	5	2	3	1.33E-04	2	1.8	1.17				
3082.60700	2	4	2	3	5	1	4	9.55E-03	2	-1.0	1.11	3156.1317	11	11	5	6	11	6	5	7.90E-06	5	-3.3	0.87				
3087.19210	2	6	2	5	6	3	4	5.05E-03	2	-2.2	1.09	3163.82721	0	3	1	3	2	2	0	5.22E-04	3	1.6	1.18				
3088.1380	4	11	5	7	12	4	8	2.10E-06	10	1.61E-06	1.09	3164.18558	3	6	3	3	7	2	6	2.84E-04	2	1.6	1.08				
3088.39982	1	10	3	8	10	4	7	1.01E-04	3	-0.6	0.99	3165.66644	5	9	4	5	10	3	8	5.64E-05	3	0.0	1.00				
3089.6306	19	7	0	7	6	3	4	6.45E-06	8	20.9	1.23	3166.70071	6	5	1	5	4	2	2	1.56E-04	2	-0.5	1.15				
3090.0783	-17	4	0	4	3	3	1	3.40E-06	4	-2.4	1.09	3167.1882	23	9	5	5	10	4	6	1.18E-05	6	9.73E-06	0.98				
3092.43016	7	11	2	9	11	3	8	4.25E-05	2	0.0	0.98	3167.23672	3	7	3	4	8	2	7	3.54E-04	3	-0.7	1.02				
3093.68955	-12	3	1	3	3	2	2	6.01E-03	2	0.5	1.16	3167.9111	12	3	2	1	4	1	4	2.63E-03	2	0.7	1.13				
3094.54785	9	5	2	4	5	3	3	2.83E-03	2	-0.7	1.12	3169.31353	-17	4	2	2	5	1	5	5.53E-04	4	3.5	1.14				
3095.94468	0	1	0	1	2	1	2	3.70E-02	4	-0.8	1.15	3169.54796	1	4	1	4	3	2	1	1.21E-03	2	1.8	1.19				
3096.0554	-10	9	3	7	9	4	6	1.02E-04	3	1.9	1.04	3169.81962	-1	5	3	2	6	2	5	1.50E-03	2	-0.9	1.07				
3096.085	83	6	0	6	5	3	3	3.94E-06	10	-2.0	1.03	3170.08176	-5	8	4	4	9	3	7	1.54E-04	2	3.28E-05	1.01				
3096.4696	-3	5	0	5	4	3	2	1.78E-05	2	5.8	1.16	3173.15850	4	6	4	5	3	7	3	5.08E-04	2	-1.3	1.03				
3096.92638	3	7	1	6	7	2	5	4.17E-03	2	0.1	1.11	3174.93228	13	2	2	0	3	1	3	8.32E-04	2	2.2	1.15				
3098.81641	17	8	4	5	9	3	6	1.69E-04	3	2.9	1.06	3175.22688	30	11	5	6	12	4	9	4.50E-06	6	12.8	0.91				
3099.54760	-1	4	2	3	4	3	2	1.08E-02	2	-3.4	1.09	3178.11896	-6	1	1	0	1	0	1	4.42E-02	3	1.2	1.17				
3099.80083	3	4	0	4	4	1	3	7.68E-03	2	-1.2	1.14	3179.49101	-2	8	3	5	9	2	8	4.08E-05	2	-2.7	0.95				
3101.15571	3	2	1	2	3	0	3	3.34E-02	3	0.1	1.15	3179.66986	4	5	2	3	6	1	6	7.47E-04	3	-0.4	1.08				
3101.87788	-13	8	3	6	8	4	5	7.75E-04	2	1.2	1.06	3181.9027	56	11	4	7	12	3	10	5.60E-06	6	4.55E-06	0.99				
*3102.174	0	10	10	1	11	11	0	6.90E-07	15	-29.3	0.74	3182.27837	1	7	4	3	8	3	6	3.35E-04	2	2.6	1.01				
3103.01575	4	2	1	2	2	2	1	1.59E-02	3	0.7	1.17	3182.51832	5	4	3	1	5	2	4	6.42E-04	2	-0.2	1.09				
3105.87046	-8	7	3	5	7	4	4	5.60E-04	2	1.3	1.07	3183.0510	-34	10	6	4	10	7	3	2.86E-06	10	3.15E-06	0.82				
3106.06741	0	10	2	8	10	3	7	5.52E-05	2	-0.4	1.01	3183.2679	50	11	6	5	11	7	4	2.85E-06	5	-9.4	0.76				
3107.33075	-3	3	2	1	3	3	0	1.01E-02	2	-3.2	1.10	3183.675	0	11	6	6	11	7	5	8.70E-07	10	1.04E-06	0.76				
3108.24122	-7	6	3	4	6	4	3	2.96E-03	2	-0.5	1.08	3184.041	15	10	6	5	10	7	4	9.11E-06	4						

Table 6. Continued

Observed Position	o - c	Upper J K <sub>a</sub> K <sub>c</sub>	Lower J K <sub>a</sub> K <sub>c</sub>	Observed Strength	%s	(o - c)%	R	Observed Position	o - c	Upper J K <sub>a</sub> K <sub>c</sub>	Lower J K <sub>a</sub> K <sub>c</sub>	Observed Strength	%s	(o - c)%	R
3218.0840	82	9 2 8	8 3 5	4.20E-06	3	5.1	1.07	3303.28418	2	5 3 3	5 2 4	3.06E-03	3	2.7	1.11
3218.929	0	11 7 5	11 8 4	3.50E-07	15	-9.7	0.75	3303.67912	-4	7 4 4	8 1 7	2.77E-05	5	7.2	0.87
3219.38352	-5	3 2 1	3 1 2	2.98E-02	3	-2.7	1.10	3304.41822	6	8 3 6	9 0 9	5.26E-05	2	4.59E-05	0.85
*3219.515	-394	10 7 4	10 8 3	4.00E-06	10	-10.6	0.77	3305.1650	11	9 3 7	8 4 4	1.43E-05	2	-1.1	0.96
*3219.7740	10	9 7 2	9 8 1	9.30E-06	10	-9.7	0.79	3307.4793	14	9 4 6	10 1 9	9.50E-06	8	7.36E-06	0.79
*3219.9198	14	8 7 2	8 8 1	1.44E-05	6	-9.9	0.82	3307.68855	-6	7 2 6	7 1 7	9.52E-04	2	2.5	1.10
3220.00824	0	5 4 1	6 3 4	6.83E-04	3	-0.8	1.03	3308.31966	-14	8 0 8	7 1 7	3.50E-03	3	-2.6	1.08
3220.44214	-1	4 2 2	4 1 3	8.72E-03	3	-0.9	1.11	3308.69870	-2	4 2 3	3 1 2	2.28E-02	3	-0.3	1.10
3222.03471	1	2 2 0	2 1 1	7.76E-03	3	1.1	1.15	3309.00939	-1	8 1 8	7 0 7	1.10E-02	3	1.6	1.13
3223.32582	3	7 2 5	8 1 8	1.24E-04	2	-2.9	0.95	3311.3012	16	6 4 3	7 1 6	9.57E-05	2	1.1	0.88
3223.4815	-13	8 5 3	9 4 6	2.46E-05	5	-4.0	0.95	3312.0547	-4	6 3 4	6 2 5	5.30E-03	3	0.9	1.08
3227.3588	9	6 2 5	5 3 2	6.20E-04	4	-6.0	1.04	3313.25298	-3	3 2 1	2 1 2	2.00E-02	2	1.6	1.12
3227.46465	-2	5 2 3	5 1 4	1.59E-02	3	-3.7	1.07	3314.46457	6	10 3 7	10 2 8	3.48E-05	3	0.8	1.00
3227.596	-98	10 3 7	11 2 10	4.00E-06	10	0.0	0.77	3317.0992	-9	10 2 8	11 1 11	4.60E-06	10	2.81E-06	0.82
3229.37672	-1	8 2 7	7 3 4	6.15E-05	3	-1.9	1.04	3318.50978	0	7 2 5	6 3 4	1.37E-03	2	0.2	1.06
3229.90022	-8	3 1 3	2 0 2	1.51E-02	2	-1.5	1.14	3318.77414	-20	8 1 7	8 0 8	4.17E-04	2	2.3	1.07
3231.35855	-9	5 3 3	4 4 0	1.03E-04	2	-1.8	1.06	3320.46258	8	9 2 7	9 1 8	4.23E-04	2	2.8	1.05
3232.27355	0	4 1 3	3 2 2	2.66E-03	3	0.4	1.14	3321.8997	-21	8 4 5	7 5 2	5.85E-05	3	-3.7	0.90
3232.61891	6	7 2 6	6 3 3	8.16E-05	2	-0.4	1.08	3322.4082	8	9 3 7	10 0 10	9.57E-06	3	6.95E-06	0.81
3233.01935	-3	4 0 4	3 1 3	1.32E-02	2	-0.1	1.15	3323.01890	0	5 2 4	4 1 3	5.73E-03	6	2.5	1.11
3234.62320	-8	5 3 2	4 4 1	3.25E-04	2	-0.2	1.08	3323.4875	-8	7 5 3	6 6 0	5.00E-06	10	-1.8	0.88
3236.64897	-4	2 2 1	2 1 2	1.75E-02	3	-0.7	1.12	3323.5798	80	7 5 2	6 6 1	1.53E-05	3	6.5	0.89
3236.7705	7	7 5 3	8 4 4	4.72E-05	3	8.9	0.95	3323.8112	-3	7 6 1	8 5 4	1.25E-05	3	4.14E-05	1.29
3237.95050	-10	4 4 1	5 3 2	4.95E-04	3	-1.0	1.04	3324.00634	3	7 3 5	7 2 6	8.88E-04	2	3.0	1.09
3240.10670	0	5 1 4	5 0 5	1.13E-02	3	1.0	1.13	3324.5411	-6	9 0 9	8 1 8	5.65E-03	2	0.2	1.09
3241.77341	7	6 2 4	6 1 5	2.74E-03	3	3.1	1.13	3324.86730	-7	9 1 9	8 0 8	1.90E-03	2	0.9	1.10
3242.80789	6	4 4 0	5 3 3	1.69E-04	2	-1.4	1.04	3326.2242	43	10 4 6	10 3 7	2.81E-05	10	7.8	1.10
3244.40529	-1	5 2 3	4 3 2	1.77E-03	3	-1.5	1.10	3326.42480	-2	7 1 6	6 2 5	5.80E-03	3	-1.2	1.05
3244.94259	-6	4 1 4	3 0 3	4.49E-02	2	-0.6	1.14	3326.6671	65	8 4 4	7 5 3	1.30E-05	5	1.38E-05	0.87
3245.40216	-3	3 2 2	3 1 3	6.70E-03	4	1.3	1.14	3326.8470	0	13 3 10	14 2 13	1.95E-05	4	2.22E-07	0.85
3245.92850	7	7 5 2	8 4 5	1.24E-04	3	-10.7	0.93	3327.57072	4	8 2 7	8 1 8	1.29E-03	5	3.6	1.08
3251.63510	-6	10 6 4	11 5 7	1.32E-05	4	1.76E-06	0.93	3328.87554	-5	9 4 5	9 3 6	2.45E-04	2	3.3	1.01
3253.0155	-17	8 2 6	9 1 9	1.74E-05	2	0.5	0.87	3331.184	-167	11 4 7	11 3 8	2.00E-05	10	-2.9	0.96
3254.14814	-1	5 0 5	4 1 4	3.59E-02	2	-1.4	1.13	3332.1323	-23	8 3 5	7 4 4	8.10E-05	4	10.7	1.12
3254.62489	0	6 3 4	5 4 1	3.87E-04	2	0.5	1.07	3336.1554	-8	8 4 4	8 3 5	9.20E-05	3	1.41E-04	1.02
3257.22613	0	4 2 3	4 1 4	1.54E-02	2	-1.4	1.10	3336.4086	-102	10 5 6	11 2 9	1.50E-05	8	4.97E-06	0.95
*3257.8527	-115	9 8 1	9 9 0	2.40E-06	5	-8.8	0.82	3336.71326	-5	6 2 5	5 1 4	1.14E-02	2	0.0	1.07
3260.42739	-7	5 1 5	4 0 4	1.29E-02	3	0.5	1.14	3338.98627	-7	8 3 6	8 2 7	1.08E-03	3	-2.0	1.02
3263.27440	-2	7 2 5	7 1 6	3.37E-03	2	4.4	1.12	3340.14170	-1	10 0 10	9 1 9	8.85E-04	2	0.0	1.08
3263.67922	-6	6 3 3	5 4 2	1.39E-04	2	-2.2	1.04	3340.29838	-3	10 1 10	9 0 9	2.68E-03	4	0.9	1.09
3265.09233	1	5 1 4	4 2 3	8.68E-03	2	-5.4	1.06	3340.63360	-9	12 5 8	13 2 11	2.61E-05	3	3.75E-07	1.02
3266.1019	29	6 5 2	7 4 3	2.10E-04	8	1.80E-04	1.00	3342.62633	38	10 3 8	11 0 11	1.80E-05	10	8.62E-06	0.82
3266.38590	-3	6 1 5	6 0 6	1.95E-03	3	2.9	1.13	3342.98188	-10	9 1 8	9 0 9	5.10E-04	3	2.3	1.05
3269.61705	-2	6 5 1	7 4 4	5.29E-05	2	6.18E-05	0.95	3343.7227	-25	11 3 8	11 2 9	2.75E-05	4	5.7	1.05
3270.42704	-5	7 3 4	7 2 5	2.98E-03	2	2.0	1.08	3344.5857	-6	9 4 6	8 5 3	9.27E-06	2	-7.6	0.84
3271.02026	-3	6 3 3	6 2 4	2.03E-03	3	4.1	1.12	3345.6725	1	9 5 5	10 2 8	5.86E-06	2	3.36E-06	0.75
3271.89035	-10	5 2 4	5 1 5	3.42E-03	3	1.9	1.12	3346.03775	4	7 4 3	7 3 4	1.47E-03	3	-1.1	1.03
3272.5182	3	4 3 2	5 0 5	2.04E-04	2	-1.5	1.02	3347.2107	-9	6 6 1	7 5 2	2.89E-05	2	3.29E-05	0.69
3272.7964	5	5 3 3	6 0 6	6.84E-05	3	-3.2	0.96	3347.2416	30	12 4 9	13 1 12	4.30E-05	3	9.08E-07	1.00
3273.42679	-7	6 0 6	5 1 5	9.33E-03	3	0.5	1.14	3347.3060	80	4 4 1	5 1 4	2.72E-05	5	5.7	0.98
3273.4389	13	6 4 3	5 5 0	8.40E-05	10	8.4	1.08	3347.5109	-18	6 6 0	7 5 3	4.00E-06	4	1.22E-05	1.26
3273.77370	7	2 2 1	1 1 0	3.60E-02	4	2.0	1.14	3347.8058	1	11 2 9	12 1 12	1.12E-05	4	3.17E-06	0.85
3273.9801	36	6 4 2	5 5 1	2.60E-05	5	0.5	1.00	3347.84030	14	8 5 4	7 6 1	1.40E-05	3	1.60E-05	0.75
3275.8342	-6	7 3 5	6 4 2	8.75E-05	3	-2.7	1.01	3348.03064	-14	9 2 8	9 1 9	1.69E-04	3	0.4	1.02
3276.22039	0	5 3 2	5 2 3	9.60E-03	3	2.0	1.11	3351.19876	-2	10 2 8	10 1 9	4.55E-05	3	1.5	1.02
3276.51097	-1	6 1 6	5 0 5	2.82E-02	3	-1.2	1.12	3351.26201	1	7 2 6	6 1 5	2.43E-03	3	3.6	1.08
3276.96471	-6	8 3 5	8 2 6	4.16E-04	2	7.3	1.12	3353.22984	0	8 1 7	7 2 6	1.17E-03	2	-0.2	1.03
3277.6127	24	9 6 3	10 5 6	1.86E-04	3	1.42E-05	1.08	3353.66080	7	4 2 2	3 1 3	3.43E-03	3	2.0	1.09
3278.4585	15	3 3 1	4 0 4	3.28E-05	2	-5.9	1.00	3354.50397	5	6 4 2	6 3 3	9.45E-04	2	-1.9	1.02
3278.72262	6	6 3 4	7 0 7	1.51E-04	2	-2.0	0.92	3354.6059	1	9 7 2	10 6 5	2.15E-06	5	1.60E-06	0.56
3280.07350	-1	2 2 0	1 1 1	1.06E-02	3	1.8	1.14	3355.18740	0	11 0 11	10 1 10	1.10E-03	5	-2.7	1.03
3280.7110	4	6 2 4	5 3 3	5.95E-04	2	0.9	1.10	3355.26415	2	11 1 11	10 0 10	3.77E-04	3	-3.2	1.06
3282.94743	-3	4 3 1	4 2 2	4.11E-03	2	1.6	1.11	3356.53135	-11	8 2 6	7 3 5	2.85E-04	2	-3.3	0.99
3284.9922	6	9 2 7	10 1 10	2.80E-05	8	2.12E-05	0.94	3356.55521	18	9 3 7	9 2 8	1.37E-04	2	-0.7	1.01
3288.48261	22	3 3 0	3 2 1	1.12E-02	3	2.1	1.13	3356.6282	21	9 4 5	8 5 4	3.22E-05	2	-6.0	0.85
3288.91839	-7	6 2 5	6 1 6	5.78E-03	2	2.9	1.12	3360.17503	16	5 4 1	5 3 2	4.37E-03	2	-2.6	1.03
3289.5503	-51	7 3 5	8 0 8	3.30E-05	8	9.0	0.94	3362.11312	-6	8 5 4	9 2 7	2.27E-05	2	1.53E-05	0.76
3291.35674	-5	7 0 7	6 1 6	1.79E-02	3	-2.9	1.09	3362.93345	-4	4 4 0	4 3 1	1.51E-03	3	-2.5	1.03
3291.88285	7	9 3 6	9 2 7	3.89E-04	4	3.8	1.06	3363.87708	-1	3 3 0	3 0 3				

Table 6. Continued

Observed Position	o - c	Upper $J K_a K_c$	Lower $J K_a K_c$	Observed Strength	%s	(o - c)%	R	Observed Position	o - c	Upper $J K_a K_c$	Lower $J K_a K_c$	Observed Strength	%s	(o - c)%	R
3373.0506	7	9 5 4	8 6 3	9.22E-06	2	-8.5	0.76	3519.23568	-2	7 6 2	7 5 3	1.55E-04	3	9.80E-05	0.79
3375.42330	9	12 2 10	13 1 13	1.03E-04	2	2.63E-07	1.01	3519.6378	-31	8 6 3	8 5 4	2.93E-04	2	1.53E-04	0.88
3375.61936	-9	8 4 5	8 3 6	7.08E-04	2	0.2	1.02	3519.66745	16	10 6 5	10 5 6	4.15E-05	3	2.14E-05	0.79
3376.10188	0	10 3 8	10 2 9	1.35E-04	2	-3.0	0.99	3519.7214	-56	9 6 4	9 5 5	4.17E-05	4	2.09E-05	0.86
3376.6746	33	4 3 1	4 0 4	2.58E-04	3	-0.7	1.03	3520.23623	7	7 2 5	6 1 6	6.56E-04	2	5.4	0.93
3377.55017	1	9 1 8	8 2 7	1.84E-03	2	2.5	1.02	3525.02075	9	7 4 4	6 3 3	7.52E-04	2	-2.5	0.87
3379.992	140	8 6 3	7 7 0	2.52E-06	4	-1.5	0.81	3528.7247	-3	7 6 2	8 3 5	2.08E-04	3	4.81E-07	0.70
3380.80555	-6	11 2 9	11 1 10	3.63E-05	3	4.08E-05	0.94	3532.7152	3	9 4 5	9 1 8	5.85E-05	3	4.40E-05	0.81
3383.7578	-1	13 0 13	12 1 12	1.47E-04	3	-4.1	0.98	3537.2554	-25	10 4 6	11 1 11	5.64E-06	10	2.81E-07	0.64
3383.7778	0	13 1 13	12 0 12	5.10E-05	3	1.9	1.02	3539.37888	8	8 4 5	7 3 4	9.33E-04	2	3.1	0.88
3384.2658	-22	9 4 6	9 3 7	8.42E-05	3	-4.6	0.97	3539.4155	-15	7 4 3	6 3 4	2.50E-03	4	5.0	0.93
3385.35048	0	9 2 8	8 1 7	6.60E-04	4	5.1	1.04	3539.61824	-2	6 3 4	5 0 5	7.25E-04	3	4.0	0.92
3385.70981	5	4 3 2	3 2 1	1.97E-02	2	-4.1	1.01	3542.24751	0	5 4 2	5 1 5	1.55E-05	5	-2.6	0.82
3387.21188	-13	12 3 10	13 0 13	3.03E-05	3	1.14E-06	1.10	3542.3515	8	10 6 4	11 3 9	1.37E-05	4	2.14E-07	1.26
3389.2617	4	11 2 10	11 1 11	1.96E-05	3	-6.0	0.94	3550.20331	28	9 6 3	10 3 8	9.05E-04	3	7.44E-07	1.04
3392.42560	1	4 3 1	3 2 2	6.92E-03	2	1.5	1.06	3550.26825	-5	8 3 5	7 2 6	2.20E-04	2	5.5	0.89
3393.42608	-5	9 2 7	8 3 6	4.79E-04	2	-1.2	0.97	3550.3400	31	9 4 6	8 3 5	1.25E-04	6	1.09E-04	0.94
3393.5280	-10	15 3 12	16 2 15	1.36E-05	4	1.34E-08	1.10	3558.85727	30	8 6 2	9 3 7	2.03E-04	2	5.24E-07	0.93
3396.00305	0	10 4 7	10 3 8	7.90E-05	4	-8.3	0.95	3559.21243	18	10 4 7	9 3 6	1.14E-04	6	2.8	0.80
*3397.3455	5	14 1 14	13 0 13	6.82E-05	6	4.4	1.04	3562.3695	-15	5 5 1	4 4 0	2.56E-03	2	1.5	0.90
3397.38318	3	5 3 2	5 0 5	7.24E-04	2	0.7	1.02	3562.40485	-23	5 5 0	4 4 1	7.50E-03	5	-0.9	0.90
3400.00681	-6	10 1 9	9 2 8	2.68E-04	3	0.7	0.96	3564.6897	2	6 6 1	7 3 4	3.50E-02	5	5.46E-07	0.85
3401.1693	-51	11 5 6	11 4 7	1.15E-05	7	5.0	1.06	3572.86206	2	7 6 1	8 3 6	6.74E-04	3	1.38E-06	0.86
3402.08377	-5	5 2 3	4 1 4	4.54E-03	2	4.0	1.07	3573.3972	26	4 4 1	3 1 2	6.11E-05	2	-3.5	0.85
3403.7131	-25	5 3 3	4 2 2	4.02E-03	3	1.4	1.05	3576.327	-149	12 4 9	11 3 8	8.70E-06	10	1.05E-05	0.64
3404.14825	-8	10 2 9	9 1 8	8.53E-04	2	4.3	0.99	3581.4540	-90	8 5 3	8 2 6	1.73E-05	4	1.16E-05	0.59
*3410.4805	0	15 0 15	14 1 14	2.00E-05	7	4.5	1.02	3586.2272	4	7 5 2	7 2 5	9.80E-05	3	3.81E-05	0.77
3414.9284	-54	6 5 2	7 2 5	1.70E-05	5	1.08E-05	0.58	3586.9975	-6	6 5 2	5 4 1	3.90E-03	4	5.4	0.89
3418.45555	5	6 3 4	5 2 3	6.12E-03	3	-4.4	0.96	3587.24662	5	6 5 1	5 4 2	1.23E-03	2	-0.3	0.85
3419.1315	68	12 3 10	12 1 11	3.22E-05	3	1.15E-05	0.87	3590.46368	18	6 6 0	7 3 5	2.31E-04	2	2.07E-07	0.86
3421.18462	-11	11 1 10	10 2 9	3.22E-04	2	2.4	0.94	3591.8418	-35	10 5 5	10 2 8	3.60E-06	10	8.4	0.29
3422.36882	5	5 3 2	4 2 3	1.14E-02	3	1.5	1.03	3596.58785	27	6 5 1	6 2 4	5.27E-05	2	9.38E-06	0.79
3423.36084	-31	11 2 10	10 1 9	1.10E-04	10	3.8	0.95	*3595.999	54	7 7 0	7 6 1	8.50E-05	10	-12.4	0.58
3424.42662	1	9 5 4	9 4 5	1.29E-04	3	2.3	0.96	3604.00231	12	5 5 0	5 2 3	8.44E-04	2	1.16E-05	0.83
3427.0974	18	6 3 3	6 0 6	1.33E-04	3	-2.8	0.96	3604.4976	5	4 4 0	3 1 3	1.14E-05	2	1.02E-05	0.93
3427.9850	-64	10 2 8	9 3 7	7.50E-05	6	-0.7	0.92	3605.6791	30	9 4 5	8 3 6	3.15E-04	10	9.6	0.83
3430.4203	0	3 3 1	2 0 2	1.11E-04	5	5.9	1.09	3608.20424	12	9 3 6	8 2 7	1.73E-04	2	0.0	0.74
3430.8411	5	7 3 5	6 2 4	1.11E-03	3	2.7	1.01	3610.76596	17	7 5 3	6 4 2	5.48E-04	2	2.6	0.82
3432.5910	-2	8 5 3	8 4 4	1.10E-04	4	-3.4	0.92	3611.094	-123	6 5 2	7 0 7	1.45E-05	4	6.15E-07	0.44
3437.3999	7	7 5 2	7 4 3	7.50E-04	3	-1.3	0.94	3611.91220	2	7 5 2	6 4 3	1.71E-03	4	5.9	0.85
3439.58102	23	6 5 1	6 4 2	4.20E-04	3	-4.2	0.91	3616.0580	37	6 4 3	5 1 4	2.45E-04	4	-1.9	0.80
3440.17156	-2	5 5 0	5 4 1	1.57E-03	2	3.9	0.94	3632.79782	25	8 5 4	7 4 3	6.09E-04	2	-0.4	0.74
3440.3892	-22	5 5 1	5 4 2	4.98E-04	3	-1.2	0.98	3636.622	-66	8 5 3	7 4 4	1.96E-04	10	-5.6	0.71
3440.61402	6	6 5 2	6 4 3	1.26E-03	2	-5.0	0.96	3637.5728	5	8 4 5	8 1 8	1.56E-05	5	-5.9	0.62
3440.80205	-2	7 5 3	7 4 4	2.45E-04	3	-5.7	0.95	3638.3429	-13	8 3 6	7 0 7	1.67E-04	4	0.5	0.74
3441.3263	13	8 5 4	8 4 5	3.28E-04	3	-9.9	0.92	3643.66389	8	7 4 4	6 1 5	7.50E-05	3	-1.6	0.75
3441.4978	90	12 1 11	11 2 10	3.51E-05	10	-4.9	0.83	3644.14686	6	5 4 1	4 1 4	5.26E-05	2	-2.1	0.77
3442.17688	14	8 3 6	7 2 5	1.59E-03	3	2.7	0.98	3648.14195	-5	10 4 6	9 3 7	2.47E-05	2	-1.5	0.64
3442.64330	12	12 2 11	11 1 10	1.10E-04	4	-1.1	0.87	3651.86548	-2	9 5 5	8 4 4	7.16E-05	2	5.1	0.73
3442.757	89	9 5 5	9 4 6	4.05E-05	5	4.68E-05	0.92	3655.37942	-1	9 2 7	8 1 8	6.90E-05	4	-3.0	0.66
3444.2325	84	7 4 3	8 1 8	3.21E-05	10	1.03E-05	0.84	3658.9384	56	7 5 3	7 2 6	7.93E-06	3	6.37E-06	0.67
3445.7389	95	10 5 6	10 4 7	3.21E-05	10	4.64E-05	0.83	3661.9535	1	9 5 4	8 4 5	2.13E-04	2	1.3	0.70
3454.02827	-50	9 3 7	8 2 6	2.37E-04	2	3.1	0.95	3666.96995	-4	6 6 1	5 5 0	1.63E-03	3	2.03E-03	0.76
3457.58502	-1	6 3 3	5 2 4	1.76E-03	2	2.3	0.99	3665.08455	-18	6 6 0	5 5 1	6.53E-04	3	-3.4	0.73
3458.05361	-4	6 2 4	5 1 5	6.04E-04	3	6.5	1.03	3666.8387	2	10 5 6	9 4 5	6.12E-05	3	1.9	0.66
3461.10447	1	4 3 2	3 0 3	8.42E-04	3	3.7	1.03	3672.3474	-26	10 3 7	9 2 8	1.59E-05	4	1.41E-05	0.71
3461.34413	-2	4 4 1	3 3 0	1.92E-02	4	0.5	1.01	3678.4344	-10	8 5 4	8 2 7	1.60E-05	8	1.32E-05	0.56
3461.55660	-4	4 4 0	3 3 1	6.20E-03	3	-2.8	0.97	3689.4278	42	6 4 2	5 1 5	1.57E-05	3	-3.0	0.68
3466.10313	5	8 4 4	9 1 9	4.58E-03	3	1.24E-06	1.07	3692.87666	-14	9 3 7	8 0 8	1.98E-05	3	-3.3	0.62
3466.5935	12	7 3 4	7 0 7	1.56E-04	2	1.67E-04	0.87	3698.2810	21	11 4 7	10 3 8	1.70E-05	2	5.0	0.60
3467.81442	-1	10 3 8	9 2 7	2.82E-04	4	0.7	0.89	3702.8324	14	6 6 1	7 1 6	1.13E-04	5	7.02E-08	0.88
3469.52962	15	5 4 1	5 1 4	2.01E-04	3	-4.9	0.92	3714.96935	-5	8 6 3	7 5 2	2.87E-04	3	-8.0	0.65
3471.2782	-77	4 4 0	4 1 3	2.17E-05	10	2.51E-05	0.83	3715.44167	6	8 6 2	7 5 3	9.92E-05	3	-4.4	0.62
3473.1472	13	6 4 2	6 1 5	8.00E-05	6	9.39E-05	0.83	3717.6073	31	9 4 6	8 1 7	1.95E-05	3	-4.6	0.59
3484.18026	-3	7 4 3	7 1 6	2.10E-04	8	-7.5	0.95	3724.0072	29	10 2 8	9 1 9	4.60E-06	3	7.07E-06	0.37
3485.03049	1	5 4 2	4 3 1	3.56E-03	3	-0.3	0.96	3725.16493	-2	5 5 0	5 0 5	2.75E-04	3	7.27E-07	0.90
3486.47012	2	5 4 1	4 3 2	1.08E-02	3	0.1	0.96	3745.6091	19	6 6 0	6 3 3	3.20E-04	3	6.57E-07	0.83
3497.44032	16	5 3 3	4 0 4	3.26E-04	3	2.8	0.97	3750.15064	7	5 5 0	4 2 3	7.70E-05	3	1.04E-05	0.99
3497.60126	-17	5 5 0													

Table 6. Continued

Observed Position	o - c	Upper $J K_a K_c$	Lower $J K_a K_c$	Observed Strength	%s	(o - c)%	R	Observed Position	o - c	Upper $J K_a K_c$	Lower $J K_a K_c$	Observed Strength	%s	(o - c)%	R
*3892.6331	-1	9 8 1	8 7 2	3.46E-05	6	1.44E-05	0.76	4006.544	5	11 5 6	10 2 9	2.65E-06	6	3.04E-08	0.21
3898.2343	5	6 6 1	5 3 2	7.40E-02	3	1.40E-06	0.84	4007.5890	15	6 6 1	5 1 4	6.35E-03	2	1.78E-08	0.75
3903.18980	12	6 6 0	5 3 3	3.50E-04	2	4.60E-07	0.75	4018.00805	0	15 3 12	14 2 13	1.14E-04	2	9.02E-11	0.97
3915.27836	-3	10 5 5	10 0 10	1.90E-05	4	6.82E-08	0.43	4021.1890	16	10 6 4	9 3 7	4.46E-05	3	4.28E-09	1.68
3929.99945	12	7 6 1	6 3 4	1.37E-03	3	1.54E-06	0.76	4035.97683	15	7 6 2	6 1 5	8.73E-05	3	7.50E-09	0.71
3932.4485	23	8 6 3	7 3 4	3.20E-04	6	1.19E-06	0.74	4070.5912	35	8 6 3	7 1 6	6.83E-05	2	1.04E-09	0.63
3944.1634	13	10 4 6	9 1 9	2.34E-05	3	1.36E-07	0.45	4077.72	-575	8 7 2	7 4 3	2.90E-07	UL	3.10E-09	0.07
3949.42522	-8	10 5 5	9 2 8	4.95E-04	3	1.89E-07	0.36	4106.87	-49	9 7 2	8 4 5	3.20E-07	UL	5.98E-08	0.08
3955.4666	-46	10 6 5	9 3 6	1.30E-05	10	2.54E-07	0.80	4131.7260	29	7 6 1	6 1 6	1.32E-05	4	8.96E-10	0.80
3958.39407	4	8 6 2	7 3 5	5.12E-04	2	2.83E-07	0.83	4159.3060	-64	10 6 5	9 1 8	9.30E-06	10	8.31E-08	0.52
3959.7943	30	6 6 1	6 1 6	1.19E-04	3	1.42E-08	0.81	4188.6099	70	8 6 2	7 1 7	2.20E-06	5	4.20E-09	0.67
3980.1815	0	14 2 12	13 1 13	1.55E-05	4	4.12E-09	1.55	4252.1690	26	9 6 3	8 1 8	4.80E-06	10	3.84E-08	0.58
3983.76244	0	14 3 12	13 0 13	1.06E-04	2	1.11E-08	1.29	4260.40872	9	12 5 8	11 0 11	3.95E-05	3	5.43E-08	1.11

<sup>a</sup>1 atm = 760 Torr.

<sup>b</sup>o - c, Observed minus computed line positions ( $\text{cm}^{-1} \times 10^5$ ). Computed values are derived from the energy levels given in Table 2 and the ground-state levels given in Ref. 1. %s, Estimated uncertainties in the measured line strengths given in percent. (o - c)%, Percent difference between the observed and the computed line strengths or the value of the computed strength if the difference between the observed and the computed values is  $\approx \pm 14\%$  or larger in magnitude. R, Ratio of the observed line strength derived in this study to the computed value given in Refs. 18 and 19. UL, upper limit; there were no apparent absorption features in any of the spectra within  $\pm 0.015 \text{ cm}^{-1}$  of the listed frequency. The observed strength given represents the maximum strength that the transition can have, with nearby absorption features of other transitions and also the signal-to-noise ratio of the spectra taken into consideration. An asterisk denotes a doubled absorption with the quantum assignment given for the stronger transition. The strength given represents the sum of the strengths of the two comparable transitions.

Table 7. Line Positions ( $\text{cm}^{-1}$ ) and Strengths ( $\text{cm}^{-2}/\text{atm}^a$  at 296 K) Observed in the (020)-(000) Band of  $\text{H}_2^{17}\text{O}^b$ 

Observed Position	o - c	Upper $J K_a K_c$	Lower $J K_a K_c$	Observed Strength	%s	(o - c)%	R	Observed Position	o - c	Upper $J K_a K_c$	Lower $J K_a K_c$	Observed Strength	%s	(o - c)%	R
2927.3410	32	7 4 3	8 5 4	5.60E-04	10	3.8		3042.9350	-23	2 1 1	3 2 2	8.10E-03	2	0.5	1.24
2927.5810	36	6 3 4	7 4 3	1.50E-03	10	-4.1	1.12	3048.5478	0	5 2 4	6 1 5	2.68E-03	2	-1.5	1.16
2930.5584	56	5 2 4	6 3 3	7.99E-04	10	-8.7	1.08	3049.8176	34	4 1 4	5 0 5	3.29E-02	2	1.4	1.23
2948.0040	-17	9 0 9	10 1 10	1.92E-03	2	-3.0	1.12	3050.463	40	6 0 6	6 1 5	2.02E-03	5	3.3	1.29
2948.2350	19	9 1 9	10 0 10	6.87E-04	5	4.0		3053.74258	0	1 1 1	2 2 0	8.47E-03	4	2.7	1.28
2949.7345	20	6 4 3	7 5 2	1.40E-03	10	0.2	1.17	3058.08305	-13	3 0 3	4 1 4	3.87E-02	2	0.6	1.24
2955.7105	-5	5 3 3	6 4 2	1.27E-03	3	-2.9	1.15	3059.1772	-30	8 2 7	8 3 6	1.10E-03	5	-4.1	1.15
2955.8535	-2	7 2 5	8 3 6	1.16E-03	3	1.9	1.17	3060.8654	17	1 1 0	2 2 1	3.08E-02	3	3.0	1.28
2960.1463	3	5 3 2	6 4 3	4.15E-03	3	1.0	1.20	3071.2902	-8	3 1 3	4 0 4	1.23E-02	3	-1.4	1.21
2962.3611	-35	6 2 4	7 3 5	8.34E-04	10	3.5	1.21	3072.8047	-1	5 0 5	5 1 4	1.19E-02	3	-1.4	1.24
2963.428	105	9 1 8	10 2 9	6.77E-04	10	3.5		3073.32730	0	2 0 2	3 1 3	1.37E-02	3	1.8	1.27
2967.0677	9	4 2 3	5 3 2	6.90E-03	3	-1.2	1.18	3074.4990	-24	6 3 4	7 2 5	1.53E-03	3	-4.9	1.09
2968.3892	39	8 0 8	9 1 9	1.44E-03	4	0.2	1.16	3075.03925	-8	4 1 4	4 2 3	1.43E-02	2	2.1	1.27
2968.8573	-1	8 1 8	9 0 9	4.60E-03	10	6.3	1.24	3075.36258	-2	4 2 3	5 1 4	9.70E-03	3	0.5	1.20
2972.2035	23	5 2 3	6 3 4	4.86E-03	4	0.2	1.18	3080.92261	26	6 2 5	6 3 4	5.17E-03	2	-0.2	1.21
2974.3245	-49	5 4 2	6 5 1	1.10E-03	3	1.4	1.23	3087.4293	3	3 1 3	3 2 2	6.00E-03	2	1.6	1.27
2974.4798	23	5 4 1	6 5 2	3.25E-03	3	-0.3	1.20	3089.54250	-3	1 0 1	2 1 2	3.78E-02	2	0.9	1.26
2977.8327	10	3 1 3	4 2 2	1.83E-03	6	1.4	1.24	3090.0273	22	7 1 6	7 2 5	4.40E-03	7	2.7	1.28
2981.5858	7	4 3 2	5 4 1	8.10E-03	5	-2.5	1.18	3093.11650	-21	4 0 4	4 1 3	7.35E-03	3	-3.2	1.23
2982.7100	0	4 3 1	5 4 2	2.85E-03	4	1.8	1.23	3093.4361	3	4 2 3	4 3 2	1.15E-02	2	3.0	1.27
2986.1218	23	4 2 2	5 3 3	3.05E-03	3	0.1	1.20	3094.3997	-5	2 1 2	3 0 3	3.44E-02	2	2.4	1.26
2986.1579	6	8 2 7	9 1 8	1.60E-03	10	4.4	1.19	3095.6222	19	8 3 6	8 4 5	8.00E-04	10	-1.0	1.18
2987.7522	-24	7 1 6	8 2 7	3.15E-03	4	5.8	1.22	3096.4000	50	3 2 2	3 3 1	3.27E-03	3	-0.6	1.23
2988.2029	-11	7 0 7	8 1 8	8.70E-03	5	2.5	1.20	3096.79208	-2	2 1 2	2 2 1	1.57E-02	2	0.4	1.26
2989.1625	-17	7 1 7	8 0 8	2.80E-03	4	-1.3	1.16	3099.719	136	7 3 5	7 4 4	5.81E-04	10	1.0	
2997.52760	11	6 1 5	7 2 6	1.90E-03	4	6.3	1.24	3101.3375	-26	3 2 1	3 3 0	1.01E-02	3	-3.3	1.20
2997.7850	-17	3 2 2	4 3 1	5.00E-03	3	2.5	1.24	3102.1712	-21	6 3 4	6 4 3	3.10E-03	5	0.8	1.23
2998.7838	10	4 4 1	5 5 0	6.13E-03	5	-8.2	1.14	3103.3627	-37	5 3 3	5 4 2	1.40E-03	5	-3.6	1.19
2998.802	84	4 4 0	5 5 1	2.00E-03	5	-10.9	1.11	3103.58282	-25	6 1 5	6 2 4	3.30E-03	5	-2.1	1.22
*2999.5344	18	5 5 0	6 6 1	2.68E-03	4	-0.2	1.11	3103.77398	-12	4 3 2	4 4 1	4.27E-03	4	1.9	1.27
3004.2996	1	3 2 1	4 3 2	1.62E-02	2	1.6	1.23	3104.6324	-5	4 3 1	4 4 0	1.42E-03	3	0.9	1.26
3004.6257	-22	7 2 6	8 1 7	1.00E-03	10	-4.0	1.11	3104.8306	-1	3 2 2	4 1 3	2.82E-03	3	-1.7	1.18
3006.4576	31	3 3 1	4 4 0	4.75E-03	6	-6.9	1.16	3106.1251	-16	4 2 2	4 3 1	4.54E-03	4	4.8	1.28
3006.5880	-7	5 1 4	6 2 5	8.77E-03	3	0.4	1.19	3106.45393	-4	5 3 2	5 4 1	4.47E-03	2	-0.2	1.22
3006.61685	-15	3 3 0	4 4 1	1.50E-02	2	-1.9	1.21	3108.0493	-10	0 0 0	1 1 1	1.00E-02	5	0.8	1.28
3007.2977	21	6 0 6	7 1 7	5.02E-03	3	0.7	1.20	3108.5615	-6	5 3 3	6 2 4	7.00E-04	10	-1.1	
3009.2520	15	6 1 6	7 0 7	1.50E-02	2	-0.4	1.18	3109.27735	3	3 0 3	3 1 2	3.68E-02	3	-1.0	1.26
3016.3655	-33	4 1 3	5 2 4	4.36E-03	4	-0.5	1.20	3109.735	-85	9 2 7	9 3 6	5.50E-04	6	-10.0	
3019.50149	-10	2 1 2	3 2 1	1.33E-02	2	0.7	1.24	3110.1230	51	6 3 3	6 4 2	1.06E-03	6	-3.7	1.16
3024.72450	-8	2 2 1	3 3 0	2.56E-02	5	2.4	1.26	3112.4039	-11	5 1 4	5 2 3	1.95E-02	3	-1.1	1.23
3025.1088	22	6 2 5	7 1 6	5.52E-03	4	0.1	1.16	3112.9860	13	2 1 1	2 2 0	7.75E-03	3	0.1	1.25
3025.4393	15	5 0 5	6 1 6	2.36E-02	4	0.9	1.21	3115.7351	12	7 3 4	7 4 3	2.04E-03	4	2.6	1.23
3026.01336	9	2 2 0	3 3 1	8.40E-03	3	-0.8	1.22	3116.20892	6	3 1 2	3 2 1	3.35E-02	3	1.1	1.26
3027.8084	51	7 0 7	7 1 6	2.68E-03	3	1.2	1.25	3116.4150	-36	4 1 3	4 2 2	9.75E-03	2	-2.5	1.21
3028.20585	13	3 1 2	4 2 3	1.83E-02	3	-0.8	1.20	3116.9851	-31	6 2 4	6 3 3	2.55E-03	4	-1.0	1.19
3029.3396	0	5 1 5	6 0 6	7.65E-03	5	-3.0	1.16	3118.7700	2	7 2 5	7 3 4	3.87E-03	4	-6.4	1.13
3042.3669	-13	4 0 4	5 1 5	1.05E-02	3	-2.0	1.20	3119.1696	51	1 1 1	2 0 2	7.10E-03	6	9.6	1.37
3042.5832	-16	6 1 6	6 2 5	5.05E-03	3	1.5	1.24	3120.25917	0	2 0 2	2 1 1	1.59E-02	3	0.0	1.26

(Table continued)

Table 7. Continued

Observed Position	$\text{o} - \text{c}$	Upper $J/K_a K_c$	Lower $J/K_a K_c$	Observed Strength	%s	(o - c)%	R	Observed Position	$\text{o} - \text{c}$	Upper $J/K_a K_c$	Lower $J/K_a K_c$	Observed Strength	%s	(o - c)%	R
3120.475	-89	8 4 5	8 5 4	4.20E-04	10	-1.3		3315.4143	22	5 2 4	4 1 3	5.87E-03	4	2.3	1.23
3120.9115	-31	6 4 3	6 5 2	1.47E-03	10	12.2	1.41	3316.342	-81	7 3 5	7 2 6	9.32E-04	4	8.4	1.22
3120.932	-121	5 4 1	5 5 0	1.30E-03	8	-5.4	1.18	3317.5542	-28	9 0 9	8 1 8	5.97E-03	3	2.3	1.23
3126.5830	7	1 0 1	1 1 0	4.22E-02	2	-0.1	1.26	3317.8611	-13	9 1 9	8 0 8	2.11E-03	3	7.9	1.30
3135.3826	35	2 2 1	3 1 2	4.95E-03	3	2.1	1.24	3319.7950	3	7 1 6	6 2 5	6.40E-03	10	5.8	1.24
3143.1903	61	4 3 2	5 2 3	2.22E-03	5	0.5	1.19	3329.11495	-20	6 2 5	5 1 4	1.15E-02	3	-2.1	1.15
3156.919	106	6 3 3	7 2 6	2.74E-04	10	-0.0		3331.4580	-13	8 3 6	8 2 7	1.10E-03	2	-0.3	1.11
3157.484	409	3 1 3	2 2 0	4.83E-04	10	-4.5		3333.127	0	10 0 10	9 1 9	9.00E-04	10	-3.3	1.16
3160.8014	11	3 2 1	4 1 4	2.57E-03	3	-1.1	1.19	3333.2743	9	10 1 10	9 0 9	2.70E-03	5	-3.4	1.15
3162.2421	11	5 3 2	6 2 5	1.56E-03	7	3.9	1.20	3336.122	-148	9 1 8	9 0 9	5.21E-04	10.	1.7	
3162.418	-302	4 2 2	5 1 5	4.96E-04	10	-5.4		3336.9745	0	7 4 3	7 3 4	1.47E-03	5	2.6	1.11
3167.6720	-52	2 2 0	3 1 3	8.59E-04	5	5.0	1.28	3343.7275	-62	7 2 6	6 1 5	2.41E-03	3	-1.0	1.15
3171.2372	21	1 1 0	1 0 1	4.36E-02	4	-1.4	1.24	3345.5637	-13	6 4 2	6 3 3	9.10E-04	3	-1.7	1.07
3173.030	-51	5 2 3	6 1 6	7.26E-04	10	1.0		3348.1525	0	11 0 11	10 1 10	1.15E-03	6	-5.6	1.13
3174.742	73	4 3 1	5 2 4	6.65E-04	5	3.2		3351.3826	-37	5 4 1	5 3 2	4.40E-03	4	1.5	1.11
3176.620	436	3 3 1	4 2 2	4.65E-04	10	-5.8		3354.2460	22	4 4 0	4 3 1	1.52E-03	5	0.3	1.12
3178.29860	0	2 0 2	1 1 1	6.22E-03	2	-0.5	1.26	3355.6020	8	4 4 1	4 3 2	4.50E-03	3	-1.8	1.10
3178.41238	0	2 1 1	2 0 2	1.57E-02	2	-2.5	1.23	3357.6808	4	3 3 0	2 2 1	3.27E-02	2	-0.2	1.18
3189.1738	4	1 1 1	0 0 0	1.06E-02	3	-1.0	1.26	3357.9177	30	6 4 3	6 3 4	2.92E-03	2	0.1	1.07
3190.474	-24	4 2 3	3 3 0	9.00E-04	10	-5.3	1.18	3360.0730	14	8 2 7	7 1 6	4.07E-03	3	0.1	1.14
3191.10688	-14	3 1 2	3 0 3	3.50E-02	3	-2.8	1.22	3361.3285	0	7 4 4	7 3 5	5.54E-04	10	8.5	
3193.49930	-7	3 1 2	2 2 1	4.50E-03	3	1.5	1.27	3362.700	0	12 1 12	11 0 11	4.97E-04	10	2.1	
3203.1602	13	3 0 3	2 1 2	3.43E-02	3	1.2	1.28	3367.195	175	8 4 5	8 3 6	7.66E-04	10	13.3	
3207.16385	-1	2 1 2	2 1 0	4.25E-02	3	1.9	1.29	3370.5574	43	9 1 8	8 2 7	1.90E-03	10	-1.4	1.12
3209.87327	23	4 1 3	4 0 4	7.18E-03	5	0.6	1.26	3377.54735	0	4 3 2	3 2 1	2.08E-02	4	-0.4	1.16
3211.99541	-2	3 2 1	3 1 2	3.10E-02	3	-0.2	1.23	3377.9722	0	9 2 8	8 1 7	7.00E-04	10	3.4	
3213.1707	0	4 2 2	4 1 3	8.85E-03	2	-1.3	1.21	3389.192	162	5 3 2	5 0 5	7.14E-04	10	7.1	
3214.6042	-19	2 2 0	0 2 1	8.10E-03	4	4.1	1.29	3394.97120	-4	5 2 3	4 1 4	4.52E-03	3	1.8	1.16
3220.8196	-56	6 2 5	5 3 2	6.47E-04	6	1.8		3395.44395	8	5 3 3	4 2 2	3.95E-03	4	-2.4	1.11
3222.90650	8	3 1 3	2 0 2	1.55E-02	3	-0.4	1.26	3410.0833	23	6 3 4	5 2 3	6.56E-03	2	-0.2	1.11
3226.0120	-3	4 1 3	3 2 2	2.50E-03	7	-6.5	1.16	3414.41235	-10	5 3 2	4 2 3	1.14E-02	2	-0.2	1.12
3226.34500	15	4 0 4	3 1 3	1.35E-02	3	0.9	1.27	3422.399	63	7 3 5	6 2 4	1.14E-03	10	1.5	1.11
3229.2651	10	2 2 1	2 1 2	1.78E-02	2	0.0	1.24	3430.9022	-1	5 5 0	5 4 1	1.50E-03	10	1.25E-03	1.10
3233.53650	4	5 1 4	5 0 5	1.13E-02	4	-1.5	1.21	3431.139	-15	5 5 1	5 4 2	5.00E-04	10	4.16E-04	
3234.9759	53	6 2 4	6 1 5	2.72E-03	3	-1.0	1.21	3431.3297	-52	6 5 2	6 4 3	1.23E-03	10	1.08E-03	1.01
3237.94060	-3	4 1 4	3 0 3	4.57E-02	3	-0.4	1.25	3433.732	-77	8 3 6	7 2 5	1.53E-03	3	-7.0	1.01
3238.0587	-5	3 2 2	3 1 3	6.65E-03	3	-0.2	1.22	3449.8060	-28	6 3 3	5 2 4	1.66E-03	6	-5.6	1.01
3238.4700	46	5 2 3	4 3 2	1.70E-03	4	-5.6	1.15	3451.092	3	6 2 4	5 1 5	5.68E-04	7	-0.9	
3247.37984	-4	5 0 5	4 1 4	3.58E-02	3	-3.0	1.21	3452.4452	-31	4 3 2	3 0 3	7.60E-04	10	-5.2	0.98
3256.7495	62	7 2 5	7 1 6	3.28E-03	3	-2.6	1.18	3452.64003	-6	4 4 1	3 3 0	1.92E-02	4	0.8	1.08
3258.75817	-36	5 1 4	4 2 3	9.58E-03	4	3.3	1.25	3452.8599	-21	4 4 0	3 3 1	6.50E-03	3	2.3	1.10
3259.8246	-3	6 1 5	6 0 6	2.15E-03	10	10.3	1.34	3476.2629	0	5 4 2	4 3 1	3.59E-03	2	1.5	1.05
3262.65353	-5	7 3 4	7 2 5	3.07E-03	3	3.3	1.19	3476.9284	0	6 5 1	7 2 6	3.60E-03	10	1.06E-06	1.19
3262.9735	0	6 3 3	6 2 4	1.90E-03	6	-3.4	1.12	3477.75143	0	5 4 1	4 3 2	1.10E-02	3	-3.0	1.06
3264.6639	-50	5 2 4	5 1 5	3.38E-03	4	0.4	1.19	3492.4212	-27	7 3 4	6 2 5	1.96E-03	10	-2.8	0.98
3266.30544	4	2 2 1	1 1 0	3.55E-02	3	-1.1	1.22	3497.8150	-21	6 4 3	5 3 2	5.22E-03	3	-0.6	0.98
3266.5792	0	6 0 6	5 1 5	9.38E-03	3	-0.5	1.23	3503.3710	6	6 4 2	5 3 3	1.90E-03	10	6.3	1.05
3268.05806	13	5 3 2	5 2 3	9.42E-03	3	-0.2	1.17	3508.7420	-69	6 6 1	6 5 2	6.30E-04	2	1.37E-04	
3269.53175	0	6 1 6	5 0 5	2.90E-02	3	-0.1	1.24	3513.3892	-69	7 2 5	6 1 6	7.50E-04	6	6.27E-04	
3272.64375	-7	2 2 0	1 1 1	1.07E-02	2	1.1	1.25	3515.952	-46	7 4 4	6 3 3	7.46E-04	10	-3.2	0.93
3274.79105	25	4 3 1	4 2 2	4.60E-03	10	12.4	1.34	3531.218	248	6 3 4	5 0 5	7.34E-04	10	8.5	0.99
3280.39036	11	3 3 0	3 2 1	1.12E-02	4	1.4	1.21	3545.8357	-34	8 6 2	9 3 7	7.29E-04	10	7.68E-10	1.05
3281.7498	21	6 2 5	6 1 6	5.80E-03	5	3.2	1.21	3551.954	-161	6 6 1	7 3 4	2.40E-03	10	3.90E-09	0.94
3284.44890	0	7 0 7	6 1 6	1.85E-02	3	-1.6	1.21	3553.0616	0	5 5 1	4 4 0	2.57E-03	4	2.04E-03	0.98
3284.9907	8	3 2 2	2 1 1	1.02E-02	2	2.7	1.26	3553.0904	-18	5 5 0	4 4 1	7.60E-03	5	6.12E-03	0.96
3285.8422	18	7 1 7	6 0 6	6.30E-03	4	-0.5	1.22	3557.6376	-32	6 5 2	5 4 1	4.00E-03	2	2.92E-03	0.99
3286.2120	-31	3 3 1	3 2 2	3.50E-03	4	-6.0	1.13	3557.782	-347	6 5 1	5 4 2	1.15E-03	6	9.75E-04	0.97
3286.4631	-36	7 1 6	7 0 7	2.73E-03	3	-2.3	1.14	3578.0600	-14	6 6 0	7 3 5	3.09E-03	3	1.86E-13	1.11
3289.5439	-31	4 3 2	4 2 3	1.19E-02	4	-1.6	1.17	3602.5300	0	7 5 2	6 4 3	1.70E-03	5	1.26E-03	0.91
3295.3940	-34	5 3 3	5 2 4	2.80E-03	4	-5.7	1.10	3623.2740	0	8 5 4	7 4 3	6.51E-04	10	4.82E-04	0.84
3300.5637	69	7 2 6	7 1 7	9.51E-04	2	2.4	1.17	3655.1960	-33	6 6 1	5 5 0	2.03E-03	3	3.77E-04	0.86
3301.1320	9	4 2 3	3 1 2	2.39E-02	2	2.2	1.24	3679.706	584	7 6 1	6 5 2	6.20E-04	2	1.29E-04	0.90
3301.3670	-37	8 0 8	7 1 7	3.50E-03	4	-5.1	1.15	3710.7410	-21	8 6 2	8 3 5	8.10E-04	4	2.31E-08	1.05
3302.01842	0	8 1 8	7 0 7	1.12E-02	3	0.8	1.22	3732.6840	-10	6 6 0	6 3 3	3.00E-03	2	6.85E-08	1.03
3304.2670	-13	6 3 4	6 2 5	5.28E-03	3	1.3	1.16	3860.89204	6	7 6 1	7 1 6	2.70E-03	4	6.87E-07	1.21
3305.8784	22	3 2 1	2 1 2	2.00E-02	3	-0.3	1.21	3890.4918	59	6 6 0	5 3 3	4.68E-03	5	1.82E-06	1.13
3312.034	0	8 1 7	8 0 8	4.00E-04	10	-3.8		3916.7057	-5	7 6 1	6 3 4	2.71E-02	3	1.17E-05	1.16
3312.5625	-15	7 2 5	6 3 4	1.30E-03	10	-6.4	1.08	3938.91423	0	10 5 5	9 2 8	1.62E-02	3	6.88E-09	1.25
3313.2791	-16	7 6 1	8 5 4	1.70E-03	10	1.52E-05	1.15	3944.7885	90	8 6 2	7 3 5	2.08E-03	5	4.72E-06	1.39

<sup>a</sup>1 atm = 760 Torr.

<sup>b</sup> $\text{o} - \text{c}$ , Observed minus computed line positions

**Table 8. Line Positions ( $\text{cm}^{-1}$ ) and Strengths ( $\text{cm}^{-2}/\text{atm}^a$  at 296 K) Observed in the (020)–(000) Band of  $\text{H}_2^{18}\text{O}^b$**

Observed Position	o – c	Upper		Lower		Observed Strength	%%	(o – c)%	R	Observed Position	o – c	Upper		Lower		Observed Strength	%%	(o – c)%	R				
		J	$K_a$	$K_c$	J	$K_a$	$K_c$					J	$K_a$	$K_c$	J	$K_a$	$K_c$						
2892.7945	-62	8	4	5	9	5	4	1.65E-04	10	-9.4	1.09	3053.43097	5	8	2	7	8	3	6	1.08E-03	4	1.8	1.17
2900.47948	0	11	0	11	12	1	12	2.76E-04	2	-5.2	0.99	3054.27365	-9	5	1	5	5	2	4	2.90E-03	3	-1.6	1.23
2900.5349	124	11	1	11	12	0	12	9.26E-05	4	-4.6		3055.38135	-4	1	1	0	2	2	1	3.00E-02	2	1.3	1.29
2908.8325	64	8	3	5	9	4	6	7.91E-05	10	-9.0		3065.36470	1	3	1	3	4	0	4	1.22E-02	2	-0.7	1.22
2919.5619	46	7	3	4	8	4	5	7.20E-04	3	3.1	1.19	3065.4381	29	7	2	6	7	3	5	8.09E-04	7	-1.7	1.15
2921.7095	11	10	0	10	11	1	11	2.60E-04	4	1.2	1.07	3066.7670	-2	8	1	7	8	2	6	4.50E-04	3	-7.2	1.09
2921.8179	14	10	1	10	11	0	11	7.73E-04	2	0.2	1.06	3066.81020	-2	5	0	5	5	1	4	1.14E-02	2	-3.4	1.24
2922.87729	25	4	1	4	5	2	3	1.67E-03	4	-6.3	1.14	3067.3320	37	6	3	4	7	2	5	1.60E-03	3	4.0	1.13
2924.8314	28	5	2	4	6	3	3	8.00E-04	3	-5.3	1.14	3067.65815	-3	2	0	2	3	1	3	1.32E-02	3	-1.0	1.26
2935.1557	-3	6	3	3	7	4	4	5.55E-04	3	-4.3	1.11	3068.91174	3	4	2	3	5	1	4	9.56E-03	2	2.2	1.18
2942.52322	51	9	0	9	10	1	10	1.85E-03	2	-0.7	1.06	3069.41540	-4	4	1	4	4	2	3	1.37E-02	2	-0.8	1.26
2942.7410	48	9	1	9	10	0	10	6.30E-04	3	1.3	1.09	3075.32588	12	6	2	5	6	3	4	5.00E-03	3	1.4	1.21
2944.42395	-23	6	4	3	7	5	2	1.31E-03	2	-3.5	1.11	3081.84274	-5	3	1	3	3	2	2	5.80E-03	3	-0.7	1.27
2945.2189	-35	6	4	2	7	5	3	4.40E-04	4	-3.5	1.11	3082.8452	25	5	2	4	5	3	3	2.77E-03	2	1.3	1.22
2945.7920	3	7	5	2	8	6	3	3.85E-04	5	2.4	1.20	3083.83172	0	1	0	1	2	1	2	3.78E-02	2	1.3	1.30
2946.48584	-8	10	2	9	11	1	10	2.70E-04	3	5.5	1.13	3083.87235	2	7	1	6	7	2	5	4.00E-03	6	0.0	1.21
2946.6749	14	8	2	6	9	3	7	1.70E-04	7	2.9	1.13	3087.1551	-5	4	0	4	4	1	3	7.30E-03	2	-2.4	1.27
2950.3492	-16	5	3	3	6	4	2	1.30E-03	5	3.8	1.22	3087.98053	-8	4	2	3	4	3	2	1.10E-02	2	2.0	1.24
2950.92868	3	7	2	5	8	3	6	1.14E-03	3	3.3	1.16	3088.37779	-6	2	1	2	3	0	3	3.36E-02	2	1.0	1.26
2954.91560	2	5	3	2	6	4	3	3.90E-03	3	-0.8	1.15	3090.03533	-58	8	3	6	8	4	5	7.60E-04	3	2.7	1.14
2955.0047	-5	10	1	10	10	2	9	1.50E-04	10	7.3	1.21	3090.98865	5	3	2	2	3	3	1	3.30E-03	4	3.4	1.27
2957.3428	-32	6	2	4	7	3	5	7.50E-04	3	-3.8	1.10	3091.23865	-7	2	1	2	2	2	1	1.55E-02	2	-0.1	1.28
2957.99467	0	9	1	8	10	2	9	5.95E-04	3	-4.9	1.02	3094.22255	-58	7	3	5	7	4	4	5.41E-04	4	1.7	1.15
2961.5434	1	4	2	3	5	3	2	6.80E-03	3	0.4	1.21	3095.98890	-8	3	2	1	3	3	0	1.05E-02	2	3.5	1.27
2962.8610	27	8	0	8	9	1	9	1.40E-03	2	2.7	1.13	3096.7515	2	6	3	4	6	4	3	2.90E-03	2	1.4	1.16
2963.30698	15	8	1	8	9	0	9	4.18E-03	2	2.0	1.12	3097.57910	4	6	1	5	6	2	4	3.15E-03	4	-1.8	1.21
2967.08095	-11	5	2	3	6	3	4	4.70E-03	2	0.0	1.17	3097.9922	-46	5	3	3	5	4	2	1.42E-03	4	4.6	1.21
2969.0414	-15	5	4	2	6	5	1	1.03E-03	2	0.6	1.16	3098.2800	3	3	2	4	4	1	3	2.83E-03	5	1.2	1.20
2969.20320	-5	5	4	1	6	5	2	3.10E-03	2	0.7	1.16	3098.4318	-6	4	3	2	4	4	1	4.02E-03	3	2.5	1.20
2969.9217	10	6	5	2	7	6	1	9.00E-04	5	-3.1	1.11	3099.3116	-19	4	3	1	4	4	0	1.35E-03	3	2.4	1.21
2969.935	-74	6	5	1	7	6	2	3.00E-04	5	-3.1	1.11	3100.79536	27	4	2	2	4	3	1	4.25E-03	3	1.2	1.22
2971.01988	0	8	1	7	9	2	8	4.76E-04	10	1.5	1.10	3101.2991	8	5	3	3	6	2	4	6.80E-04	5	0.9	1.11
2972.1395	26	3	1	3	4	2	2	1.76E-03	3	-0.2	1.25	3102.30135	30	0	0	0	1	1	1	9.73E-03	3	-1.9	1.28
2976.2824	-9	4	3	2	5	4	1	7.85E-03	2	-0.3	1.17	3103.39048	1	3	0	3	3	1	2	3.65E-02	2	-1.0	1.29
2976.6182	12	9	1	9	9	2	8	1.41E-03	3	6.9		3104.8641	-1	6	3	3	6	4	2	1.05E-03	6	2.2	1.17
2976.78392	0	7	6	1	8	7	2	2.54E-04	10	8.0	1.24	3106.56644	1	5	1	5	4	2	3	1.88E-02	3	-1.4	1.23
2977.4403	11	4	3	1	5	4	2	2.62E-03	2	-1.4	1.16	3106.7348	-5	5	2	3	5	3	2	1.12E-02	2	2.3	1.22
2977.5618	6	9	0	9	9	1	8	4.12E-04	3	2.3	1.19	3107.45610	-2	2	1	1	2	2	0	7.60E-03	2	-0.9	1.26
2980.3742	50	8	2	7	9	1	8	1.55E-03	7	5.8	1.14	3110.4975	-34	7	3	4	7	4	3	1.85E-03	3	0.3	1.13
2980.9013	-4	4	2	2	5	3	3	2.95E-03	4	-0.3	1.19	3110.5318	-7	8	2	6	8	3	5	5.50E-04	8	2.4	1.17
2982.4110	-4	7	1	6	8	2	7	2.87E-03	3	1.2	1.11	3110.62040	1	3	1	2	3	2	1	3.30E-02	2	1.0	1.27
2982.63603	0	7	0	7	8	1	8	8.10E-03	2	-0.0	1.13	3110.7200	-6	4	1	3	4	2	2	9.65E-03	3	-1.3	1.24
2983.55350	-6	7	1	7	8	0	8	2.74E-03	4	1.0	1.14	3111.4945	-28	6	2	4	6	3	3	2.48E-03	5	0.7	1.19
2982.21910	1	6	1	5	7	2	6	1.70E-03	5	-0.7	1.12	3114.43770	11	2	0	2	1	1	1	1.60E-02	2	1.0	1.32
2992.38050	-16	3	2	2	4	3	1	4.71E-03	4	-0.6	1.21	3115.0383	-38	8	4	5	8	5	4	3.87E-04	3	2.5	1.13
2993.51315	0	4	4	1	5	5	0	6.20E-03	3	-0.1	1.16	3115.4772	41	5	4	2	5	5	1	4.32E-04	5	3.4	1.16
2993.55313	7	4	4	0	5	5	1	2.10E-03	4	1.4	1.17	3115.55058	-28	6	4	3	6	5	2	1.14E-03	5	-2.4	1.09
*2994.2545	-55	5	5	0	6	6	1	2.80E-03	5	1.3	1.15	3115.5963	-21	5	4	1	5	5	1	1.25E-03	2	-0.3	1.13
2997.65047	0	8	1	8	8	2	7	1.02E-03	3	0.7	1.20	3116.09426	-66	6	4	2	6	5	1	3.93E-04	5	0.6	1.12
2998.7045	-20	7	2	6	8	1	7	9.70E-04	3	-2.4	1.07	3116.8722	15	8	3	5	8	4	4	2.90E-04	10	-6.6	1.04
2999.00447	2	3	2	1	4	3	2	1.56E-02	3	0.6	1.22	3117.25090	1	7	4	3	7	5	2	7.71E-04	10	2.6	1.13
2999.65912	-34	8	0	8	8	1	7	3.33E-04	3	-5.4	1.14	3120.79695	1	0	1	1	1	0	1	4.25E-02	2	0.6	1.32
3000.8810	-38	6	6	1	7	7	0	4.80E-04	10	-14.3	1.13	3121.9745	67	9	3	6	9	4	5	3.88E-04	4	0.3	1.10
3001.0663	-42	6	6	0	7	7	1	1.85E-04	10	8.0	1.11	3128.79120	5	2	2	1	3	1	2	4.77E-03	3	0.1	1.21
3001.17300	-5	3	3	1	4	4	0	4.90E-03	2	2.1	1.21	3135.9170	15	4	3	2	5	2	3	2.10E-03	2	-0.3	1.12
3001.2742	4	5	1	4	6	2	5	8.50E-03	3	0.7	1.17	*3140.904	158	6	5	2</							

Table 8. Continued

Observed Position	o - c	Upper $J$	$K_a$	$K_c$	Lower $J$	$K_a$	$K_c$	Observed Strength	%s	(o - c)%	R	Observed Position	o - c	Upper $J$	$K_a$	$K_c$	Lower $J$	$K_a$	$K_c$	Observed Strength	%s	(o - c)%	R	
3199.4026	-43	4	2	2	3	3	1	3.77E-04	3	0.1	1.20	3334.6027	-80	9	2	8	9	1	9	1.80E-04	10	9.4	1.19	
3200.95970	8	2	1	2	4	1	0	1	4.14E-02	2	-1.2	1.31	3337.01940	0	7	2	6	6	1	5	2.32E-03	4	-0.0	1.14
3202.7394	70	5	2	4	4	3	1	3.35E-04	4	-1.8	1.15	3337.59936	-9	6	4	2	6	3	3	9.20E-04	3	-0.4	1.09	
3203.8970	2	5	4	1	6	3	4	6.60E-04	10	0.9	1.04	3339.92960	5	4	2	2	3	1	3	3.30E-03	4	-2.8	1.20	
3203.9456	9	4	1	3	4	0	4	6.75E-03	3	-5.0	1.24	3340.33205	48	8	1	7	7	2	6	1.19E-03	3	2.6	1.13	
3205.41310	-6	3	2	1	3	1	2	3.13E-02	2	1.8	1.28	3341.8821	-23	11	0	11	10	1	10	1.11E-03	3	-1.6	1.10	
3206.69440	0	4	2	2	4	1	3	8.90E-03	3	1.1	1.26	3341.94870	0	11	1	11	10	0	10	3.59E-04	2	-4.6	1.06	
3207.98334	18	2	2	0	2	1	1	7.73E-03	2	-0.0	1.26	3342.5628	27	9	3	7	9	2	8	1.33E-04	10	-1.0	1.08	
3214.10320	3	5	2	3	5	1	4	1.67E-02	4	1.6	1.26	3343.55076	-1	5	4	1	5	3	2	4.40E-03	3	2.4	1.12	
3214.97960	5	6	2	5	5	3	2	6.03E-04	3	0.1	1.15	3345.0989	14	8	2	6	7	3	5	2.86E-04	4	-3.5	1.06	
3216.67145	19	3	1	3	2	0	2	1.56E-02	2	0.2	1.31	3346.5080	-10	4	4	0	4	3	1	1.47E-03	3	-1.6	1.09	
3220.3904	10	4	0	4	3	1	3	1.33E-02	2	0.3	1.29	3347.6440	7	3	3	0	3	0	3	3.70E-04	3	3.5	1.08	
3221.4673	-11	4	4	1	5	3	2	4.53E-04	5	-5.2	1.01	3347.90460	-3	4	4	1	4	3	2	4.50E-03	3	-0.4	1.10	
3222.68544	3	2	2	1	2	1	2	1.79E-02	2	0.7	1.28	3349.06255	0	3	3	1	2	2	0	1.07E-02	2	0.2	1.20	
3223.3047	-32	5	3	2	4	4	1	3.15E-04	5	-0.6	1.14	3350.2449	9	6	4	3	6	3	4	2.95E-03	3	0.9	1.09	
3227.67810	-16	5	1	4	5	0	5	1.10E-02	2	-2.7	1.24	3350.50475	-5	3	3	0	2	2	1	3.24E-02	2	0.9	1.20	
3228.92495	24	6	2	4	6	1	5	2.54E-03	2	-3.5	1.19	3353.44260	15	8	2	7	7	1	6	3.85E-03	3	0.1	1.11	
3231.51515	3	3	2	3	3	1	3	6.45E-03	6	-2.9	1.22	3353.2262	-19	10	2	9	10	1	10	2.03E-04	10	9.4	1.17	
3231.69895	0	4	1	4	3	0	3	4.60E-02	4	0.8	1.30	3356.377	0	12	0	12	11	1	11	1.50E-04	10	0.6	1.11	
3233.1720	-7	5	2	3	4	3	2	1.68E-03	4	-2.7	1.14	3356.4110	0	12	1	12	11	0	11	4.40E-04	3	-1.6	1.09	
3241.34224	6	5	0	5	4	1	4	3.68E-02	2	1.2	1.29	3359.7014	-7	8	4	5	8	3	6	6.70E-04	3	-3.8	1.05	
3242.9916	5	6	3	4	5	4	1	3.70E-04	5	-1.7	1.11	3360.7510	60	4	3	1	4	0	1	2.34E-04	2	-1.7	1.00	
3243.44385	18	4	2	3	4	1	4	1.56E-02	2	-0.1	1.25	3362.300	0	10	3	8	10	2	9	1.44E-04	10	2.5	1.15	
3247.20800	8	5	1	5	4	0	4	1.29E-02	3	0.3	1.28	3370.2761	-5	4	3	2	3	2	1	2.05E-02	2	0.6	1.18	
3248.398	127	6	5	2	7	4	3	1.90E-04	10	5.5	1.00	*3370.3922	6	13	0	13	12	1	12	2.03E-04	10	-7.4	1.03	
3250.9402	2	7	2	5	7	1	6	3.15E-03	4	-0.6	1.19	3371.4027	47	9	2	8	8	1	7	6.36E-04	3	-0.3	1.08	
3253.1049	7	5	1	4	4	2	3	9.30E-03	5	3.4	1.24	3374.8920	0	12	3	10	13	0	13	3.50E-04	10	2.56E-06	1.30	
3253.9707	1	6	1	5	6	0	6	1.83E-03	2	-3.5	1.19	3377.22850	0	4	3	1	3	2	2	6.71E-03	2	-0.7	1.16	
3255.74470	-11	7	3	4	7	2	5	2.86E-03	3	0.5	1.15	3381.6706	-10	9	2	7	8	3	6	4.90E-04	3	-4.9	1.04	
3255.8137	-7	6	3	3	6	2	4	1.83E-03	5	-3.7	1.12	3381.90185	1	5	3	2	5	0	5	7.00E-04	10	8.8	1.07	
3257.0290	32	4	3	2	5	0	5	2.10E-04	10	11.4	1.09	3386.56784	0	10	1	9	9	2	8	3.20E-04	3	12.4	1.23	
3258.22546	-2	5	2	4	5	1	5	3.34E-03	5	0.3	1.22	3388.0775	8	5	3	3	4	2	2	3.99E-03	2	1.7	1.17	
3259.65062	-1	2	2	1	1	1	0	3.57E-02	2	-0.5	1.28	3388.63520	7	5	2	3	4	1	4	4.25E-03	3	-2.5	1.15	
3260.47164	-1	6	0	6	5	1	5	9.25E-03	2	0.4	1.25	3390.26550	8	10	2	9	9	1	8	8.55E-04	2	-1.8	1.06	
3260.79000	-1	5	3	2	5	2	3	9.60E-03	4	4.4	1.22	3402.6260	9	6	3	4	5	2	3	6.40E-03	3	1.0	1.13	
3263.08876	-7	8	3	5	8	2	6	3.75E-04	5	-0.8	1.13	3407.3284	-1	5	3	2	4	2	3	1.11E-02	3	0.2	1.14	
3263.31095	2	6	1	6	5	0	5	2.90E-02	3	2.2	1.28	3407.5685	0	11	1	10	10	2	9	3.50E-04	10	-3.3	1.07	
3263.9344	-6	7	3	5	6	4	2	8.54E-05	10	-5.3	1.24	3414.88455	43	7	3	5	6	2	4	1.02E-03	5	-5.8	1.03	
3266.02315	-1	2	2	0	1	1	1	1.03E-02	2	-2.8	1.25	3419.522	180	7	5	2	7	4	3	8.00E-04	4	2.2	1.02	
3267.52495	0	4	3	1	4	2	2	4.03E-03	2	1.7	1.20	3421.9175	-23	6	5	1	6	4	2	3.95E-04	2	-11.2	1.01	
3269.5086	-1	6	2	4	5	3	3	5.60E-04	4	-1.5	1.12	3422.65654	15	5	5	0	5	4	1	1.45E-03	3	-4.6	1.03	
3273.1813	-2	3	3	0	3	2	1	1.09E-02	3	0.9	1.20	3422.9039	51	5	5	1	5	4	2	5.05E-04	3	-0.4	1.07	
3275.36212	-4	6	2	5	6	1	6	5.55E-03	5	0.4	1.19	3423.06355	0	6	5	2	6	4	3	1.25E-03	3	-6.7	1.01	
3276.4161	-8	5	5	0	6	4	3	1.63E-04	4	9.7	1.01	3423.7344	0	8	5	4	8	4	5	3.65E-04	10	-7.0	1.10	
3278.3655	-15	8	2	6	8	1	7	3.85E-04	6	-0.0	1.15	3426.21928	0	8	3	6	7	2	5	1.55E-03	2	-2.5	1.05	
3278.9730	-44	9	3	6	9	2	7	3.70E-04	3	0.7	1.14	3442.88345	1	6	3	3	5	2	4	1.66E-03	2	-2.1	1.06	
3279.61970	2	7	1	7	6	0	6	6.33E-03	3	3.3	1.26	3444.7383	-46	4	3	2	3	0	3	8.00E-04	3	4.2	1.05	
3280.54717	-22	7	1	6	7	0	7	2.75E-03	4	1.8	1.20	3444.8893	14	4	4	1	3	3	0	1.92E-02	6	2.1	1.11	
3282.45531	6	4	3	2	4	2	3	1.19E-02	3	1.1	1.19	3445.11605	1	4	4	0	3	3	1	6.30E-03	3	0.4	1.10	
3284.64686	-13	6	1	5	5	2	4	2.65E-03	4	-0.3	1.17	3450.918	-109	5	4	1	5	1	4	1.78E-04	10	-3.2	0.83	
3285.16477	11	7	3	4	6	4	3	3.40E-04	3	-2.8	1.09	3466.760	18	7	4	3	7	1	6	2.05E-04	4	3.1	0.95	
3288.3688	11	5	3	3	5	2	4	3.00E-03	5	4.1	1.21	3468.45360	-6	5	4	2	4	3	1	3.50E-03	2	-0.1	1.06	
3294.38920	-12	4	2	3	3	1	2	2.31E-02	3	0.1	1.25	3469.98793	-6	5	4	1	3	2	1.08E-02	2	2.1	1.08		
3295.16780	0	8	0	8	7	1	7	3.60E-03	2	2.1	1.21	3481.3026	-27	5	3	3	4	0	4	3.51E-04	10	17.1	1.15	
3295.78664	-18	8	1	8	7	0	7	1.08E-02	2	1.6	1.21	3489.89860	0	6	4	3	5	3	2	5.20E-03	2	-0.9	1.02	
3297.33351	-13	6	3	4	6	2	5	5.10E-03	2	1.1	1.15	3495.6129	-38	6	4	2	5	3	3	1.83E-03	3	2.6	1.05	
3299.30740	-2	3	2	1	2	1	2	1.96E-02	3	-1.9	1.25	3499.7910	-45	6	6	1	6	5	6	3.85E-04	3	4.63E-04	1.34	
3304.98927	-17	7	6	2	8	5	3	6.90E-04	3															

**Table 9. Observed<sup>a</sup> and Computed Frequencies (cm<sup>-1</sup>) of Transitions in the (000)–(000), (010)–(010) and (020)–(020) Bands of H<sub>2</sub><sup>16</sup>O<sup>b</sup>**

J	K <sub>a</sub>	K <sub>c</sub>	J	K <sub>a</sub>	K <sub>c</sub>	Band	Observed	Computed <sup>b</sup>	un <sup>c</sup>	Δ <sup>d</sup>
13	6	8	14	3	11	(000)–(000)	8.671080	8.67149	25	-41
14	6	9	15	3	12	(000)–(000)	4.657032	4.65794	30	-91
14	4	10	15	3	13	(000)–(000)	8.253713	8.26239	65	-868
15	6	10	16	3	13	(000)–(000)	5.914661	5.90778	300	688
16	6	11	17	3	14	(000)–(000)	11.309290	11.30540	425	389
5	5	1	6	4	2	(010)–(010)	6.975438	6.97547	6	-3
6	6	1	7	5	2	(010)–(010)	9.795591	9.79556	5	3
6	6	0	7	5	3	(010)–(010)	9.921501	9.92149	7	1
7	4	3	6	5	2	(010)–(010)	19.281922	19.28190	5	2
7	7	0	8	6	3	(010)–(010)	8.787791	8.78783	10	-4
7	7	1	8	6	2	(010)–(010)	8.769325	8.76930	8	3
9	2	8	8	3	5	(010)–(010)	19.803984	19.80400	4	-2
9	6	3	8	7	2	(010)–(010)	14.718144	14.71812	6	2
9	6	4	8	7	1	(010)–(010)	14.634263	14.63431	7	5
10	7	4	9	8	1	(010)–(010)	18.295137	18.29522	13	-8
14	3	12	13	4	9	(010)–(010)	10.792600	10.79264	7	-4
3	2	1	4	1	4	(020)–(020)	11.045102	11.04507	7	3
4	2	2	5	1	5	(020)–(020)	13.459058	13.45899	8	7
6	2	5	5	3	2	(020)–(020)	13.439784	13.43976	6	2
6	5	2	7	4	3	(020)–(020)	8.944492	8.94445	5	4
6	5	1	7	4	4	(020)–(020)	10.791625	10.79145	9	18
7	3	5	6	4	2	(020)–(020)	17.561721	17.56166	7	6

<sup>a</sup>From Ref. 20.<sup>b</sup>The computed values for the (000)–(000) and (010)–(010) bands were derived from rotational energy levels given in Ref. 1, and those for the (020)–(020) band were calculated from levels given in Table 2 of the present study.<sup>c</sup>un, Uncertainty of computed frequencies derived from estimated uncertainties given in Ref. 1 and this study; values × 10<sup>5</sup>.<sup>d</sup>Δ, Observed minus computed frequencies × 10<sup>5</sup>.

Flaud *et al.*<sup>18</sup> (and included in the HITRAN listing<sup>19</sup>) were much larger than estimated in this study. In fact there were no apparent absorption features in any of the spectra within ±0.015 cm<sup>-1</sup> of the listed frequencies, and the observed line-strength values represent upper-limit values.

Values of R given in Table 6 were derived from computed line-strength values given in Refs. 18 and 19. It should be noted that the computed values derived by Flaud and Camy-Peyret<sup>14</sup> several years ago differ somewhat from those reported in Refs. 18 and 19. The computed strengths given in Ref. 18 were derived from an analysis or unreported measurements obtained, for the most part, with a grating spectrometer with a spectral resolution of 0.03–0.05 cm<sup>-1</sup>, and these same values were incorporated into the HITRAN database.<sup>19</sup>

Tables 7 and 8 are listings for the (020)–(000) bands of H<sub>2</sub><sup>17</sup>O and H<sub>2</sub><sup>18</sup>O, respectively, and they are similar in content to that of Table 6. The line-strength values are normalized to 100% of the isotopic species. The previous computed values of line strengths used to determine values of R in the two tables were taken from the studies by Camy-Peyret *et al.*<sup>15</sup> for H<sub>2</sub><sup>17</sup>O and Flaud *et al.*<sup>16</sup> for H<sub>2</sub><sup>18</sup>O, and these values are also given in the HITRAN database.<sup>19</sup> A few of the transitions given in the tables do not have entries for R, which means that those transitions were not included in the previous calculations.<sup>15,16</sup> This is because Refs. 15 and 16 used an intensity cutoff criterion that included the isotopic abundance.

The high-accuracy measurements of H<sub>2</sub><sup>16</sup>O pure rotational frequencies obtained by Pearson *et al.*<sup>20</sup> are presented in Table 9 for their observations in the (000)–(000), (010)–(010), and (020)–(020) bands. Included in this

table are computed frequencies derived from rotational energy levels given in this study and listed in Table 2 and from the energy-level values for the (000) and (010) states given in my recent paper.<sup>1</sup> The table lists the rotational quantum assignments, band, measured frequency given by Pearson *et al.*<sup>20</sup> (converted from megahertz to inverse centimeters with the speed of light as 2.99792458 × 10<sup>10</sup> cm/s), the computed frequencies from my previous work, the uncertainty (un) of the computed frequency, and the difference (Δ) between the measured and the computed frequencies. In the analysis of the ν<sub>2</sub> band,<sup>1</sup> I incorrectly gave the value of the energy for the 14 3 11 rotational level of the ground state as 2739.45102(15) cm<sup>-1</sup>, whereas the corrected value used to compute the frequency of the first entry in Table 9 is 2739.42853(20) cm<sup>-1</sup>. The values of un are based on the estimated uncertainties of the two rotational level energies involved in a transition and are computed from the expression

$$un = (un_1^2 + un_2^2)^{1/2}, \quad (6)$$

where un<sub>1</sub> and un<sub>2</sub> are the uncertainties of the two involved rotational energies. Inspection of the values of un and Δ shows that there is good agreement, on average, between the measured and the computed frequencies within the limits placed on the computed values.

## DISCUSSION AND CONCLUSION

More than 1600 transitions frequencies measured in this study were determined to an absolute accuracy of 0.0001 cm<sup>-1</sup> (3 MHz) or better for the majority of the lines.

The experimental line strengths were fitted by least squares to a model that included 19 dipole moment expansion coefficients. The fitting technique did not take into account the interactions between the vibrational states (020), (100), and (001), and therefore the computed strengths derived in this study represent unperturbed values. The experimental results for the (100)–(010), (001)–(010), (100)–(000), and (001)–(000) bands of  $H_2^{16}O$  will be featured in a forthcoming publication,<sup>23</sup> and measurements in the (100)–(000) and (001)–(000) bands of  $H_2^{17}O$  and  $H_2^{18}O$  are under way. These results, including those of the present study, will be fitted to a theoretical model that includes interactions between the three interacting vibrational states.

## ACKNOWLEDGMENTS

The author thanks the Kitt Peak National Observatory for the use of the FTS and J. Wagner and C. Plymate for their assistance in obtaining the  $H_2O$  spectra. The Atmospheric Trace Molecule Spectroscopy (ATMOS) dedicated Computer Facility was used in the analysis of the experimental data. The research described in this paper was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contract with the National Aeronautics and Space Administration.

## REFERENCES

- R. A. Toth, “ $\nu_2$  band of  $H_2^{16}O$ : line strengths and transition frequencies,” *J. Opt. Soc. Am. B* **8**, 2236–2255 (1991).
- R. A. Toth, “Transition frequencies and absolute strengths of  $H_2^{17}O$  and  $H_2^{18}O$  in the 6.2- $\mu\text{m}$  region,” *J. Opt. Soc. Am. B* **9**, 462–482 (1992).
- D. M. Gates, R. F. Calfee, D. W. Hansen, and W. S. Benedict, “Line parameters and computed spectra for water vapor bands at 2.7  $\mu$ ,” *Natl. Bur. Stand. (U.S.) Monogr.* **71** (August 3, 1964).
- W. S. Benedict and R. F. Calfee, “Line parameters for the 1.9 and 6.3 micron water vapor bands,” U.S. Department of Commerce Environmental Science Services Administration professional paper (Government Printing Office, Washington, D.C., June 2, 1967).
- G. Guelachvili, “Experimental Doppler-limited spectra of the  $\nu_2$  bands of  $H_2^{16}O$ ,  $H_2^{17}O$ ,  $H_2^{18}O$  and HDO by Fourier-transform spectroscopy: secondary wave-number standards between 1066 and 2296  $\text{cm}^{-1}$ ,” *J. Opt. Soc. Am. B* **73**, 137–150 (1983).
- L. A. Pugh and K. Narahari Rao, “Spectrum of water vapor in the 1.9 and 2.7  $\mu$  regions,” *J. Mol. Spectrosc.* **47**, 403–408 (1973).
- L. A. Pugh, “A detailed study of the near-infrared spectrum of water vapor,” Ph.D. dissertation (Ohio State University, Columbus, Ohio, 1972; microfilm 72-21,005, University Microfilms, Ann Arbor, Michigan).
- C. Camy-Peyret, J.-M. Flaud, G. Guelachvili, and C. Amiot, “High resolution Fourier transform spectrum of water between 2930 and 4255  $\text{cm}^{-1}$ ,” *Mol. Phys.* **26**, 825–855 (1973).
- J.-M. Flaud and C. Camy-Peyret, “The  $2\nu_2$ ,  $\nu_1$ , and  $\nu_3$  bands of  $H_2^{16}O$  rotational study of the (000) and (020) states,” *Mol. Phys.* **4**, 811–823 (1973).
- R. A. Toth and J. S. Margolis, “Spectrum of  $H_2^{18}O$  in the 2900 to 3400  $\text{cm}^{-1}$  region,” *J. Mol. Spectrosc.* **57**, 236–245 (1975).
- J.-M. Flaud and C. Camy-Peyret, “The interacting states (020), (100), and (001) of  $H_2^{16}O$ ,” *J. Mol. Spectrosc.* **51**, 142–150 (1974).
- C. Camy-Peyret, J.-M. Flaud, and R. A. Toth, “The interacting states (020), (100), and (001) of  $H_2^{17}O$  and  $H_2^{18}O$ ,” *J. Mol. Spectrosc.* **87**, 233–241 (1981).
- R. A. Toth, “Strengths and air-broadened widths of  $H_2O$  lines in the 2950–3400  $\text{cm}^{-1}$  region,” *J. Quantum Spectrosc. Radiat. Transfer* **13**, 1127–1142 (1973).
- J.-M. Flaud and C. Camy-Peyret, “Vibration-rotation intensities in  $H_2O$ -type molecules application to the  $2\nu_2$ ,  $\nu_1$ , and  $\nu_3$  bands of  $H_2^{16}O$ ,” *J. Mol. Spectrosc.* **55**, 278–310 (1975).
- C. Camy-Peyret, J.-M. Flaud, and R. A. Toth, “Line positions and intensities for the  $2\nu_2$ ,  $\nu_1$  and  $\nu_3$  bands of  $H_2^{17}O$ ,” *Mol. Phys.* **42**, 595–604 (1981).
- J.-M. Flaud, C. Camy-Peyret, and R. A. Toth, “Line positions and intensities for the  $2\nu_2$ ,  $\nu_1$ , and  $\nu_3$  bands of  $H_2^{18}O$ ,” *Can. J. Phys.* **58**, 1748–1757 (1980).
- J.-M. Flaud, C. Camy-Peyret, J.-Y. Mandin, and G. Guelachvili, “ $H_2^{16}O$  hot bands in the 6.3  $\mu\text{m}$  region,” *Mol. Phys.* **2**, 413–426 (1977).
- J.-M. Flaud, C. Camy-Peyret, and R. A. Toth, *Water Vapour Line Parameters from Microwave to Medium Infrared* (Pergamon, London, 1981).
- L. S. Rothman, R. R. Gamache, R. H. Tipping, C. P. Rinsland, M. A. H. Smith, D. C. Benner, V. M. Devi, J.-M. Flaud, C. Camy-Peyret, A. Perrin, A. Goldman, S. T. Massie, L. R. Brown, and R. A. Toth, “The HITRAN molecular database: editions of 1991 and 1992,” *J. Quantum Spectrosc. Radiat. Transfer* **48**, 469–507 (1993).
- J. C. Pearson, T. Anderson, E. Herbst, F. C. De Lucia, and P. Helminger, “Millimeter- and submillimeter-wave spectrum of highly excited states of water,” *Astrophys. J.* **379**, L41–L43 (1991).
- R. A. Toth, “Line-frequency measurements and analysis of  $N_2O$  between 900 and 4700  $\text{cm}^{-1}$ ,” *Appl. Opt.* **30**, 5289–5315 (1991).
- C. Camy-Peyret, J.-M. Flaud, and N. Papineau, “La bande  $\nu_2$  des espèces isotopiques  $H_2^{17}O$  et  $H_2^{18}O$ ,” *C. R. Acad. Sci. Paris B* **290**, 537–540 (1980).
- R. A. Toth, “ $\nu_1-\nu_2$ ,  $\nu_3-\nu_2$ ,  $\nu_2$ , and  $\nu_3$  bands of  $H_2^{16}O$ : line positions and strengths,” *J. Opt. Soc. Am. B* (to be published).