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Spectrum of $H_2{}^{18}O$ in the 2900 to 3400 cm^{-1} Region [1]

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Measurements of line center positions of $H_2{}^{18}O$ in the 2900 to 3400 cm^{-1} region have been made at high resolution. This region contains absorptions of the (020) band and *P*-branch absorptions of the (100) and (001) bands of $H_2{}^{18}O$. Values of the energy levels of the (020) state were determined in which ground state energy levels derived by Fraley, Rao, and Jones [*J. Mol. Spectrosc.* **29**, 312 (1969)] and Williamson, Rao, and Jones [*J. Mol. Spectrosc.* **40**, 372 (1971)] were used in the analysis. A new set of ground state levels was obtained by an iterative procedure.

INTRODUCTION

A knowledge of the positions and strengths of water vapor vibration–rotation lines in the 2900 to 3400 cm^{-1} region is important for the interpretation of atmospheric spectra obtained for the purpose of detecting air pollutants which may be present in the atmosphere and which have strong dipole transition intensities in this spectral interval (for example HCl, NH_3, NO_2, C_2H_2, C_2H_4, and C_2H_6). High resolution laboratory studies of $H_2{}^{16}O$ line center measurements in the 3 μm region have been done by Pugh and Rao (*1*), Camy-Peyret *et al.* (*2*), and Flaud and Camy-Peyret (*3*). High resolution measurements of strengths and air-broadened widths of $H_2{}^{16}O$ lines in the 2950 to 3400 cm^{-1} region have been reported by Toth (*4*). Comparable measurements of $H_2{}^{18}O$ in the 2900 to 3400 cm^{-1} region are the subject of this study. The present investigation involves line center measurements and the line strengths will be the subject of a forthcoming publication.

The majority of the $H_2{}^{18}O$ lines in the 3.3 μm region are of the (020) band with the band center at 3139.054 cm^{-1}. Also in this spectral interval are several *P*-branch lines of the (100) and (001) bands. Previous laboratory investigations of $H_2{}^{18}O$ line center measurements include an analysis of high resolution spectra of the (100) and (001) bands covering the 3340 to 4030 cm^{-1} region by Fraley *et al.* (*5*). Williamson *et al.* (*6*) observed the (010) band in the 1330 to 1967 cm^{-1} region at high resolution. Calculations of positions and rigid-rotor strengths of $H_2{}^{18}O$ lines in the 2864 to 4435 cm^{-1} region are included in a tabulation of H_2O transitions in the 2.7 μm region reported by Gates *et al.* (*7*). The calculated line positions of the (020) band (*7*) are greater than those obtained in this study; the maximum difference is $\sim$1.6 cm^{-1} for high K_{-1} transitions and the

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minimum difference is on the average 0.04 cm^{-1} for transitions involving upper and lower state K_{-1} equal to 0 or 1.

EXPERIMENTAL DETAILS

The data were obtained with a 1.8 m Jarrel–Ash grating spectrometer with a 300 lines/mm grating blazed at 5.7 μm in first order. Observations were made in first order for the region 2900 to 3240 cm^{-1} at a resolution of $\sim$0.07 cm^{-1}, and in second order for the 3240 to 3400 cm^{-1} region at a resolution of $\sim$0.04 cm^{-1}. The source was a 1000 W quartz-iodine projection lamp and the detector was a PbS element which was cooled to approximately -80°C. A multitraversal cell of 2 m base length was used for all measurements. The foreoptics, source, and detector were housed in a vacuum box which was connected to the vacuum spectrometer and the absorption cell.

The oxygen 18 enriched H_2O sample was obtained from the Bio-Rad Corporation. The stated sample mixture ratio of $H_2{}^{18}O$ to $H_2{}^{16}O$ was 1-to-1 and the $H_2{}^{17}O$ impurity was 0.1% of the sample. Sample pressures were measured with an oil manometer and a capacitance pressure sensor. Sample pressures ranged from 2 to 8 mm Hg and the path lengths ranged from 8 to 40 m with the gas samples at room temperature. The $H_2{}^{18}O$ line positions were calibrated from the known $H_2{}^{16}O$ absorptions (*1*, *2*, *3*).

DATA ANALYSIS

The quantum assignments of the measured $H_2{}^{18}O$ lines were determined in the following manner. Approximate locations of several $H_2{}^{18}O$ absorptions were determined from the listing of Gates *et al.* (*7*). By this procedure, the strongest $H_2{}^{18}O$ absorptions were easily identified in the spectra. Additional methods were employed to assign weaker transitions. These included: (a) determining approximate locations of $H_2{}^{18}O$ lines from a knowledge of the frequency difference between identical transitions of $H_2{}^{16}O$ and $H_2{}^{18}O$, (b) comparing the peak absorption of an $H_2{}^{18}O$ line to that of the same transition of the $H_2{}^{16}O$ molecule, and (c) calculating the line positions of the (100) and (001) bands from the listings given by Fraley *et al.* (*5*). It was determined that the frequency differences between identical transitions of $H_2{}^{16}O$ and $H_2{}^{18}O$ ranged between 8 and 20 cm^{-1} for the (001) and (020) bands and between 2 and 14 cm^{-1} for the (100) band. It is interesting to note that using a gas sample with 50% $H_2{}^{18}O$ and 50% $H_2{}^{16}O$ greatly simplified the task of identifying close lying lines since the intensity of a transition for either isotopic specie is comparable except in a very few cases where resonance effects, which alter the normal transition strengths, are different for the two molecules.

RESULTS AND DISCUSSION

Table 1 is a listing of the line numbers, measured line center positions, upper and lower rotational quantum numbers ($JK_{-1}K_1$), ground state energy levels, relative line strengths, and band assignments. The line numbers pertain to the numbering of the absorptions shown in Fig. 1. The relative line strengths S' given in Table 1 were calculated from the expression;

$$S' = g \cdot \nu \cdot \exp(-E''/kT)/(Q \cdot \nu_0), \tag{1}$$

TABLE 1

MEASUREMENTS AND ASSIGNMENTS OF OXYGEN 18 WATER VAPOR IN THE 2.94 TO 3.45 MICRON SPECTRAL REGION

LINE NUMBER	FREQ -1 CM	ROTATIONAL TRANSITION UPPER STATE			LOWER STATE			E -1 CM	STRENGTH TEMP=295K	BAND
1	2919.56	7	3	4	8	4	5	1116.520	.6923-04	020
2	2921.82	10	1	10	11	0	11	1321.440	.2551-04	020
3	2922.092	7	4	3	8	5	4	1246.369	.3580-04	020
3	2922.092	6	3	4	7	4	3	925.698	.1759-03	020
4	2922.884	4	1	4	5	2	3	445.160	.1833-02	020
5	2924.848	5	2	4	6	3	3	658.023	.2159-03	020
6	2942.535	9	0	9	10	1	10	1109.770	.7215-04	020
7	2942.754	9	1	9	10	0	10	1109.808	.2405-04	020
8	2944.428	6	4	3	7	5	2	1051.210	.9506-04	020
9	2945.220	8	2	6	9	3	7	1211.190	.1468-04	020
9	2945.226	6	4	2	7	5	3	1050.990	.3206-04	020
10	2946.48	10	2	9	11	1	10	1518.550	.9836-05	020
11	2950.343	5	3	3	6	4	2	752.195	.1380-03	020
12	2950.919	7	2	6	8	3	6	1001.709	.1226-03	020
13	2954.909	5	3	2	6	4	3	751.040	.4169-03	020
14	2957.329	6	2	4	7	3	5	812.753	.1025-03	020
15	2957.390	9	1	8	10	2	9	1288.264	.3036-04	020
16	2961.550	4	2	3	5	3	2	565.727	.1383-02	020
17	2962.365	8	0	8	9	1	9	916.300	.6222-04	020
18	2963.15	9	2	8	10	1	9	1287.727	.1017-04	020
19	2963.335	8	1	8	9	0	9	916.250	.1367-03	020
20	2967.077	5	2	3	6	3	4	645.387	.7008-03	020
21	2969.037	5	4	2	6	5	1	980.121	.7439-04	020
22	2969.200	5	4	1	6	5	2	860.079	.2232-03	020
23	2969.924	6	5	2	7	6	1	1204.186	.4594-04	020
23	2969.924	6	5	1	7	6	2	1204.172	.1532-04	020
24	2971.019	8	1	7	8	2	8	1075.920	.2364-04	020
25	2972.139	3	1	3	4	2	2	314.460	.1176-02	020
26	2976.287	4	3	2	5	4	1	504.795	.8569-03	020
27	2977.443	4	3	1	5	4	2	604.550	.2861-03	020
28	2977.54	9	0	9	9	1	8	1074.779	.8659-04	020
29	2980.907	4	2	2	5	3	3	500.595	.4756-03	020
30	2982.421	7	1	6	8	2	7	881.900	.2222-03	020
31	2982.637	7	0	7	8	1	8	741.000	.4419-03	020
32	2983.557	7	1	7	8	0	8	740.930	.1474-03	020
33	2992.219	6	1	5	7	2	6	706.608	.1748-03	020
34	2992.380	3	2	2	4	3	1	380.700	.8569-03	020
35	2993.523	4	4	1	5	5	0	733.678	.4596-03	020
35	2993.523	4	4	0	5	5	1	733.573	.1532-03	020
36	2994.256	5	5	0	6	6	1	1033.195	.1067-03	020
36	2994.256	5	5	1	6	6	0	1033.135	.3555-04	020
37	2997.653	8	1	8	8	2	7	881.900	.2234-03	020
38	2998.706	7	2	6	8	1	7	879.481	.7537-04	020
39	2999.008	3	2	1	4	3	2	379.293	.2594-02	020
40	2999.56	8	0	8	8	1	7	879.481	.7539-04	020
41	3000.89	6	6	1	7	7	0	1378.980	.1979-04	020
42	3001.18	3	3	1	4	4	0	482.660	.5226-03	020
43	3001.29	5	1	4	6	2	5	550.447	.1126-02	020
44	3001.35	3	3	0	4	4	1	482.632	.1568-02	020
45	3001.594	6	0	6	7	1	7	583.972	.3199-03	020
46	3003.578	6	1	6	7	0	7	583.767	.9582-03	020
47	3008.469	8	3	6	9	2	7	1198.190	.4792-04	020
48	3011.010	4	1	3	5	2	4	414.177	.7323-03	020
49	3013.917	2	1	2	3	2	1	210.800	.5930-02	020
50	3017.875	7	1	7	7	2	6	706.608	.1763-03	020
51	3019.010	6	2	5	7	1	6	701.697	.5418-03	020
52	3019.370	2	2	1	3	3	0	282.304	.4192-02	020
53	3019.824	5	0	5	6	1	6	645.355	.1892-02	020
54	3020.683	2	2	0	3	3	1	282.093	.1398-02	020
55	3021.948	7	0	7	7	1	6	701.697	.5423-03	020
56	3022.798	3	1	2	4	2	3	298.629	.3875-02	020
57	3023.593	5	1	5	6	0	6	444.860	.6331-03	020
58	3036.740	4	0	4	5	1	5	325.216	.1140-02	020
59	3036.902	6	1	6	6	2	5	550.447	.1140-02	020
60	3037.476	2	1	1	3	2	2	204.763	.2052-02	020
61	3042.255	5	2	4	6	1	5	541.183	.3982-03	020
62	3043.992	4	1	4	5	0	5	324.044	.3447-02	020
63	3044.501	6	0	6	6	1	5	541.183	.3985-03	020
64	3046.065	9	1	8	9	2	7	1198.190	.4855-04	020
65	3048.224	1	1	1	2	2	0	134.785	.2397-02	020
66	3052.443	3	0	3	4	1	4	223.830	.5636-02	020
67	3053.437	8	2	7	8	3	6	1001.709	.1268-03	020
68	3054.280	5	1	5	5	2	4	414.177	.7428-03	020
69	3055.385	1	1	0	2	2	1	133.480	.8766-02	020
70	3065.368	3	1	3	4	0	4	221.237	.1911-02	020
71	3065.43	7	2	6	7	3	5	812.753	.1067-03	020
72	3066.71	8	1	7	8	2	6	980.230	.4715-04	020
73	3066.813	5	0	5	5	1	4	398.372	.2417-02	020
74	3067.338	6	3	4	7	2	5	780.440	.3749-03	020
75	3067.655	2	0	2	3	1	3	141.577	.2820-02	020
76	3068.911	4	2	3	5	1	4	398.372	.2419-02	020
77	3069.410	4	1	4	4	2	3	298.629	.3935-02	020
78	3075.320	6	2	5	6	3	4	645.387	.7264-03	020
79	3081.944	3	1	3	3	2	2	204.763	.2082-02	020
80	3082.854	5	2	4	5	3	3	500.595	.4919-03	020
81	3083.958	1	0	1	2	1	2	78.395	.1154-01	020
81	3083.958	7	1	6	7	2	5	780.440	.3769-03	020
82	3087.989	4	2	3	4	3	2	379.293	.2671-02	020
83	3088.397	2	1	2	3	0	3	136.344	.8738-02	020
84	3090.047	8	3	6	8	4	5	1115.620	.7327-04	020
85	3090.990	3	2	2	3	3	1	282.093	.1432-02	020
86	3091.247	2	1	2	2	2	1	133.480	.8869-02	020
87	3094.223	7	3	5	7	4	4	921.910	.6323-04	020
88	3096.750	6	3	4	6	4	3	751.040	.4369-03	020
89	3097.580	6	1	5	6	2	4	601.246	.3025-03	020

TABLE 1 (CONT.)

LINE NUMBER	FREQ cm^{-1}	ROTATIONAL TRANSITION UPPER STATE			LOWER STATE			E cm^{-1}	STRENGTH TEMP=295K	BAND
90	3097.994	5	3	3	5	4	2	604.550	.2377-03	020
91	3098.287	3	2	2	4	1	3	274.733	.1487-02	020
92	3098.437	4	3	2	4	4	1	482.632	.1619-02	020
93	3099.326	4	3	1	4	4	0	482.560	.5397-03	020
94	3100.792	4	2	2	4	3	1	380.700	.8879-03	020
95	3101.30	5	3	3	6	2	4	601.246	.3028-03	020
96	3102.305	0	0	0	1	1	1	36.750	.4756-02	020
97	3103.392	3	0	3	3	1	2	172.988	.7347-02	020
98	3103.585	9	2	7	9	3	6	1279.800	.3320-04	020
99	3104.372	6	3	3	6	4	2	752.195	.1452-03	020
100	3106.568	5	1	4	5	2	3	445.160	.1949-02	020
101	3106.735	5	2	3	5	3	2	505.727	.1450-02	020
102	3107.454	2	1	1	2	2	0	134.785	.2953-02	020
103	3110.529	3	1	2	3	2	1	210.800	.6121-02	020
104	3110.720	4	1	3	4	2	2	314.460	.1230-02	020
105	3111.493	6	2	4	6	3	3	653.623	.2297-03	020
106	3113.078	1	1	1	2	0	2	69.930	.4059-02	020
106	3113.078	7	2	5	7	3	4	339.561	.2352-03	020
107	3115.040	8	4	5	8	5	4	1246.369	.3923-04	020
108	3115.48	7	4	4	7	5	3	1050.990	.3392-04	020
108	3115.48	5	4	2	5	5	1	733.673	.1595-03	020
109	3115.57	5	4	1	5	5	0	733.678	.4784-03	020
109	3115.57	6	4	3	6	5	2	880.079	.2342-03	020
110	3116.11	6	4	2	6	5	1	880.121	.7307-04	020
111	3117.251	7	4	3	7	5	2	1051.210	.1017-03	020
112	3120.903	1	0	1	1	1	0	42.024	.1399-01	020
113	3121.971	9	3	6	9	4	5	1355.190	.2312-04	020
114	3128.792	2	2	1	3	2	1	210.800	.6156-02	020
115	3135.912	4	3	2	5	2	3	445.160	.1967-02	020
116	3140.914	6	5	2	6	5	1	1033.195	.1119-03	020
116	3140.914	6	5	1	6	6	0	1033.195	.3730-04	020
117	3150.452	6	3	3	7	2	6	706.608	.1840-03	020
118	3151.818	3	1	3	2	2	0	134.785	.2995-02	020
119	3154.283	7	3	4	8	2	7	981.900	.2350-03	020
120	3154.474	3	2	1	4	1	4	223.830	.5825-02	020
121	3155.503	5	3	2	6	2	5	550.447	.1134-02	020
122	3156.078	6	4	3	7	3	4	839.561	.2891-03	020
123	3156.302	4	2	2	5	1	5	325.216	.1185-02	020
124	3157.243	4	1	4	3	2	1	210.800	.6212-02	020
125	3161.202	2	2	0	3	1	3	141.577	.2906-02	020
126	3165.098	1	1	0	1	0	1	23.756	.1551-01	020
127	3166.733	7	4	3	8	3	6	1001.709	.1315-03	020
128	3167.120	5	2	3	6	1	6	445.355	.1985-02	020
129	3167.90	4	3	1	5	2	4	314.177	.7704-03	020
130	3169.39	3	3	1	4	2	2	314.460	.1254-02	020
131	3170.44	7	2	5	8	5	4	1246.369	.3434-04	100
132	3170.89	9	2	8	10	3	7	1534.368	.2809-05	100
133	3172.311	2	1	1	2	0	2	63.930	.4136-02	020
134	3172.474	2	0	2	1	1	1	36.750	.4863-02	020
135	3178.344	8	1	8	9	2	7	1198.190	.4354-04	100
136	3183.000	1	1	1	0	0	0	.000	.5838-02	020
137	3183.45	6	4	2	7	3	5	812.753	.1108-03	020
138	3184.97	4	2	3	3	3	0	282.304	.4421-02	020
139	3185.087	3	1	2	3	0	3	136.344	.9011-02	020
140	3185.36	3	3	0	4	2	3	298.629	.4034-02	020
141	3185.911	8	7	1	9	8	2	1800.000	.7725-06	100
142	3187.348	3	1	2	2	2	1	133.480	.9146-02	020
143	3197.282	3	0	3	2	1	2	78.995	.1197-01	020
144	3200.558	2	1	2	1	0	1	23.756	.1568-01	020
145	3202.75	5	2	4	4	3	1	380.700	.9171-03	020
146	3203.04	9	1	9	10	3	8	1440.295	.1314-04	001
147	3203.943	5	4	1	6	3	4	645.387	.7568-03	020
147	3203.943	4	1	3	4	0	4	221.237	.1397-02	020
148	3205.415	3	2	1	3	1	2	172.888	.7588-02	020
149	3206.701	4	2	2	4	1	3	274.793	.1539-02	020
150	3207.982	2	2	0	2	1	1	94.790	.3705-02	020
151	3214.381	6	2	5	5	3	2	505.727	.1501-02	020
152	3216.664	3	1	3	2	0	2	69.930	.4194-02	020
153	3220.561	7	0	7	8	3	6	1301.709	.1151-03	100
154	3221.469	4	4	1	5	3	2	505.727	.1504-02	020
155	3221.883	7	1	6	8	4	5	1116.620	.6571-04	100
156	3222.684	2	2	1	2	1	2	78.995	.1206-01	020
157	3224.657	9	2	8	10	4	7	1574.435	.5376-05	001
158	3227.669	5	1	4	5	0	5	324.044	.3655-02	020
159	3228.918	6	2	4	6	1	5	541.183	.4226-03	020
160	3231.506	3	2	2	3	1	3	141.577	.2971-02	020
161	3231.700	4	1	4	3	0	3	136.344	.9143-02	020
162	3233.167	5	2	3	4	3	2	379.293	.2797-02	020
163	3235.148	8	2	7	9	3	6	1273.800	.2377-04	100
164	3241.348	5	0	5	4	1	4	223.830	.5965-02	020
165	3242.313	7	1	7	8	2	6	980.230	.4288-04	100
166	3243.442	4	2	3	4	1	4	223.830	.5989-02	020
167	3247.213	5	1	5	4	0	4	221.237	.2224-02	020
168	3248.40	6	5	2	7	4	3	925.698	.1955-03	020
169	3250.940	7	2	5	7	1	6	701.897	.5834-03	020
170	3252.337	8	5	4	9	6	3	1620.138	.5689-05	100
170	3252.337	8	5	3	9	6	4	1620.000	.1898-05	100
171	3252.52	6	3	3	5	4	2	604.550	.3125-03	020
172	3253.103	5	1	4	4	2	3	298.629	.4170-02	020
173	3253.641	6	0	6	7	4	3	925.698	.1643-03	001
174	3253.970	6	1	5	6	0	6	944.960	.6814-03	020
175	3259.312	6	1	5	7	4	4	921.910	.5728-04	100
176	3259.548	2	2	1	1	1	0	42.024	.1461-01	020
177	3260.791	5	3	2	5	2	3	445.160	.2045-02	020
178	3266.500	6	4	3	7	5	2	1204.172	.1413-04	001
179	3267.524	4	3	1	4	2	2	314.460	.1293-02	020
180	3268.314	6	4	2	7	5	1	1204.186	.4241-04	001
181	3269.503	6	2	4	5	3	3	500.595	.5217-03	020

TABLE 1 (CONT.)

LINE NUMBER	FREQ -1 CM	ROTATIONAL TRANSITION UPPER STATE			LOWER STATE			E -1 CM	STRENGTH TEMP=295K	BAND
182	3273.180	3	3	0	3	2	1	210.800	.6440-02	020
183	3274.083	8	4	5	9	5	4	1468.567	.1200-04	100
184	3275.359	6	2	5	6	1	6	445.355	.2053-02	020
185	3277.093	8	3	6	9	4	5	1355.190	.2087-04	100
186	3278.295	7	0	7	6	1	6	445.355	.2054-02	020
186	3278.295	3	2	2	2	1	1	94.790	.3786-02	020
187	3279.361	6	6	1	7	7	0	1378.980	.1860-04	100
187	3279.361	6	6	0	7	7	1	1378.980	.6200-05	100
188	3279.620	7	5	2	8	6	3	1399.740	.1681-04	100
188	3279.620	7	1	7	6	0	6	444.860	.6867-03	020
189	3280.550	7	1	6	7	0	7	583.767	.1047-02	020
190	3282.453	4	3	2	4	2	3	298.629	.4208-02	020
191	3284.647	6	1	5	5	2	4	414.177	.7988-03	020
192	3285.166	7	3	4	6	4	3	751.040	.4635-03	020
193	3288.370	7	4	3	6	5	2	880.079	.2472-03	020
193	3288.370	5	3	3	5	2	4	414.177	.7997-03	020
194	3289.848	7	3	5	8	5	4	1246.369	.3476-04	001
195	3290.075	5	1	4	6	4	3	751.040	.3992-03	100
196	3292.77	5	4	2	6	6	1	1033.195	.9841-04	001
197	3294.392	4	2	3	3	1	2	172.888	.7799-02	020
198	3295.180	8	0	8	7	1	7	583.972	.3501-03	020
199	3295.559	7	2	6	8	3	5	1047.317	.3142-04	100
200	3295.789	8	1	8	7	0	7	583.767	.1051-02	020
201	3297.331	6	3	4	6	2	5	550.447	.1238-02	020
202	3299.310	3	2	1	2	1	2	78.995	.1235-01	020
203	3302.980	7	4	4	8	5	3	1247.200	.1188-04	100
204	3306.01	8	1	7	8	0	8	740.930	.1633-03	020
205	3306.080	6	1	6	7	2	5	780.440	.3476-03	100
206	3306.277	6	5	2	7	6	1	1204.186	.4399-04	100
206	3306.277	6	5	1	7	6	2	1204.172	.1466-04	100
207	3307.249	7	2	5	6	3	4	645.387	.7812-03	020
208	3308.65	9	2	7	9	1	8	1074.779	.9522-04	020
208	3308.65	5	2	4	4	1	3	274.793	.1588-02	020
209	3309.522	7	3	5	7	2	6	706.608	.1933-03	020
210	3311.322	9	0	9	8	1	8	781.000	.4906-03	020
211	3311.614	9	1	9	8	0	8	780.930	.1636-03	020
212	3312.498	7	4	3	8	5	4	1246.369	.3588-04	100
213	3313.878	7	1	6	6	2	5	550.447	.1248-02	020
214	3314.141	8	2	7	8	1	8	781.000	.4910-03	020
215	3314.462	7	1	7	8	3	6	1001.709	.1155-03	001
216	3318.693	7	2	6	8	4	5	1116.620	.6602-04	001
217	3319.694	6	3	4	7	5	3	1050.990	.3032-04	001
218	3320.141	7	3	5	8	4	4	1126.480	.2151-04	100
219	3322.262	5	0	5	6	3	4	645.387	.6749-03	100
220	3322.348	6	2	5	5	1	4	398.372	.2618-02	020
221	3324.759	8	3	6	8	2	7	981.900	.2477-03	020
222	3326.871	10	0	10	9	1	9	916.300	.6987-04	020
223	3327.011	10	1	10	9	0	9	916.250	.2097-03	020
224	3328.663	6	6	1	7	5	2	1051.210	.1086-03	020
224	3328.663	9	3	6	10	4	7	1574.435	.7277-05	100
225	3328.902	7	4	3	7	3	4	839.561	.3050-03	020
226	3330.004	9	1	8	9	0	9	916.250	.2099-03	020
227	3332.695	5	5	1	6	6	0	1033.195	.3404-04	100
227	3332.695	5	5	0	6	6	1	1033.195	.1021-03	100
228	3335.635	7	0	7	8	2	6	980.230	.4303-04	001
229	3337.005	7	2	6	6	1	5	541.183	.4368-03	020
230	3337.593	6	4	2	6	3	3	658.623	.2466-03	020
231	3339.926	4	2	2	3	1	3	141.577	.3070-02	020
232	3340.446	6	3	3	7	5	2	1051.210	.9143-04	001
233	3341.879	11	0	11	10	1	10	1109.770	.8194-04	020
234	3341.947	11	1	11	10	0	10	1109.808	.2731-04	020
235	3343.551	5	4	1	5	3	2	505.727	.1561-02	020
236	3344.715	8	3	5	9	4	6	1338.580	.7849-05	100
237	3346.508	4	4	0	4	3	1	380.700	.9583-03	020
238	3347.646	3	3	0	3	0	3	136.344	.9471-02	020
239	3347.767	5	3	3	6	5	2	880.079	.2112-03	001
240	3347.910	4	4	1	4	3	2	379.293	.2096-02	020
241	3348.563	5	4	2	5	3	3	500.595	.5343-03	020
242	3349.065	3	3	1	2	2	0	134.785	.3183-02	020
243	3350.047	6	2	5	7	3	4	839.561	.2640-03	100
244	3350.246	6	4	3	6	3	4	645.387	.7913-03	020
245	3350.507	3	3	0	2	2	1	133.480	.9613-02	020
246	3352.597	8	2	6	9	4	5	1355.190	.2083-04	001
246	3352.697	5	3	2	6	5	1	880.121	.7047-04	001
247	3353.440	8	2	7	7	1	6	701.697	.6018-03	020
248	3353.718	7	4	4	7	3	5	812.753	.1167-03	020
249	3356.668	4	0	4	5	4	1	509.796	.8103-03	001
250	3356.285	6	3	4	7	4	3	925.698	.1737-03	100
251	3358.084	7	3	4	8	4	5	1116.620	.6849-04	100
252	3358.945	6	2	5	7	4	4	921.910	.5758-04	001
253	3359.697	8	4	5	8	3	6	1001.709	.1395-03	020
254	3362.211	5	4	1	6	5	2	880.079	.2174-03	100
255	3362.873	5	4	2	6	5	1	880.121	.7247-04	100
256	3366.238	4	0	4	5	3	3	500.595	.4619-03	100
257	3366.889	6	1	6	7	3	5	812.753	.9831-04	001
258	3367.454	5	1	5	6	2	4	601.246	.2828-03	100
259	3370.277	4	3	2	3	2	1	210.800	.6631-02	020
260	3370.804	12	1	12	13	0	13	1800.000	.2452-05	100
261	3371.400	9	2	8	8	1	7	879.481	.8473-04	020
262	3372.211	11	1	10	12	2	11	1767.000	.2882-05	100
263	3374.744	4	3	2	5	5	1	733.673	.1449-03	001
264	3375.112	6	3	3	7	4	4	921.910	.5932-04	100
265	3376.289	4	3	1	5	5	0	733.678	.4369-03	001
266	3377.229	4	3	1	3	2	2	204.763	.2281-02	020
267	3381.668	9	2	7	8	3	6	1001.709	.1405-03	020
268	3381.900	5	3	2	5	0	5	324.044	.3830-02	020
269	3384.771	7	1	6	8	3	5	1047.317	.3147-04	001
270	3385.131	7	2	5	8	4	4	1126.480	.2139-04	001

TABLE 1 (CONT.)

LINE NUMBER	FREQ cm^{-1}	ROTATIONAL TRANSITION UPPER STATE			LOWER STATE			E cm^{-1}	STRENGTH TEMP=295K	BAND
271	3386.348	9	2	7	10	3	8	1440.295	.1424-04	100
272	3387.374	5	3	3	6	4	2	752.195	.1362-03	100
273	3387.638	4	4	0	5	5	1	733.673	.1491-03	100
274	3387.711	4	4	1	5	5	0	733.679	.4474-03	100
275	3388.081	5	3	3	4	2	2	314.460	.1340-02	020
276	3388.538	5	2	3	4	1	4	223.830	.6257-02	020
277	3390.264	10	2	9	9	1	8	1074.772	.9860-04	020
278	3391.439	5	3	2	6	4	3	751.040	.4115-03	100
279	3394.374	10	1	9	11	2	10	1518.750	.3245-05	100
280	3394.595	11	0	11	12	1	12	1551.190	.8312-05	100
280	3394.695	11	1	11	12	0	12	1551.190	.2771-05	100
281	3395.105	10	2	9	11	1	10	1518.550	.9748-05	100
282	3397.141	5	2	4	6	3	3	656.623	.2157-03	100
283	3398.875	6	0	6	7	2	5	780.440	.3485-03	001
284	3399.219	5	2	4	6	4	3	751.040	.4023-03	001
285	3401.705	8	2	6	9	3	7	1211.190	.1458-04	100
286	3402.626	6	3	4	5	2	3	445.160	.2134-02	020
287	3404.294	3	0	3	4	3	2	379.203	.2533-02	100
288	3407.329	5	3	2	4	2	3	298.629	.4368-02	020

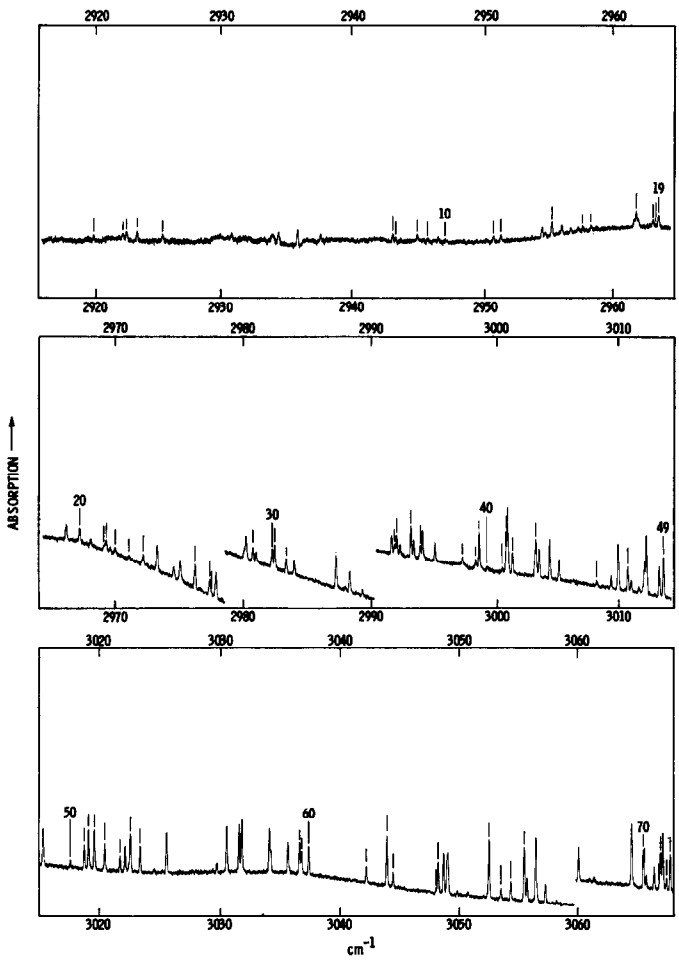

FIG. 1. Scan of the 2920 to 3407 cm^{-1} region of $H_2{}^{18}O$ and $H_2{}^{16}O$. The sample pressure was 4.7 mm Hg and the path was 40 m. The isotopic ratio of the water vapor sample was 1-to-1 for $H_2{}^{18}O$ to $H_2{}^{16}O$. The stroke marks denote the $H_2{}^{18}O$ lines and only these are numbered.

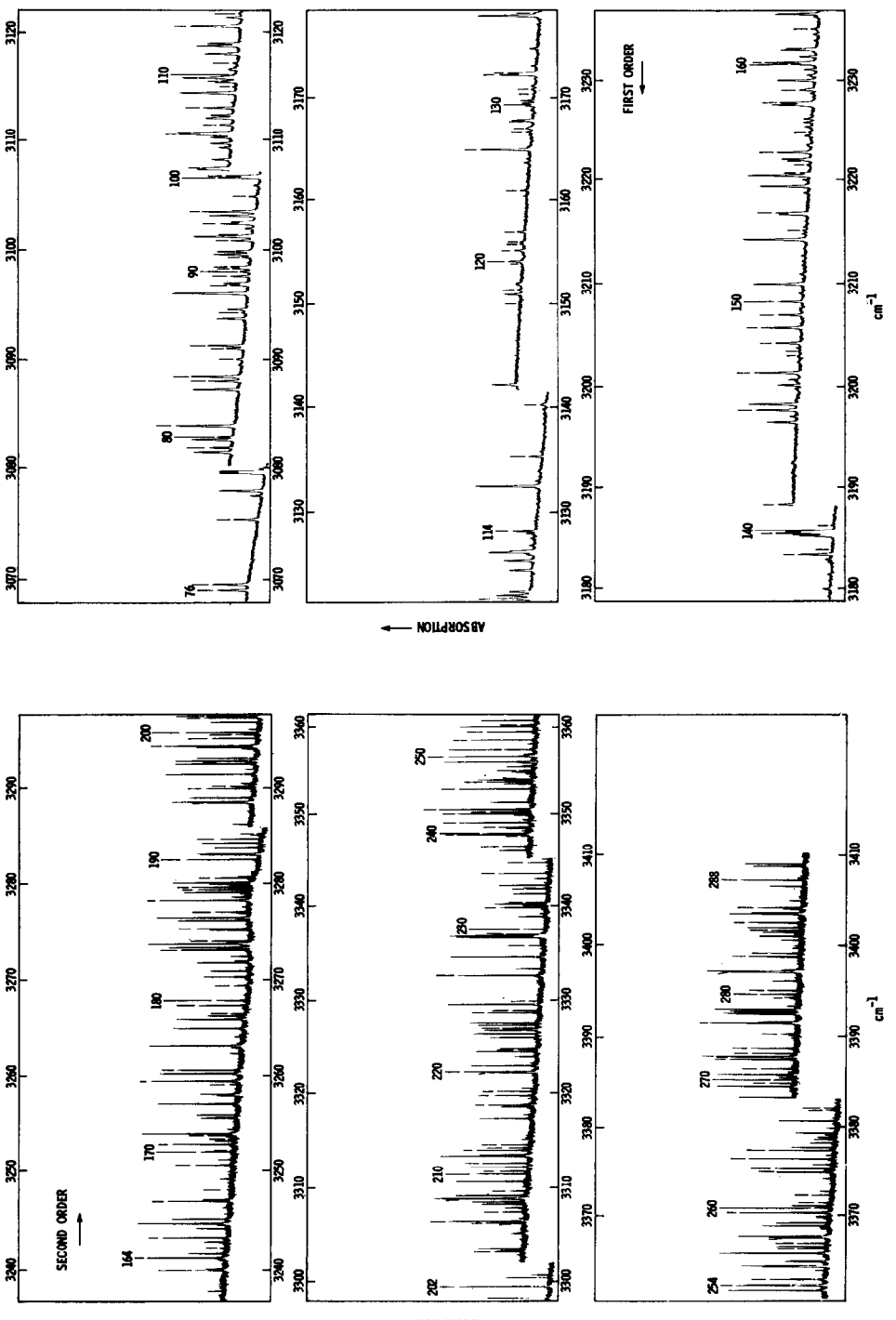

FIG. 1. (*Continued*)

TABLE 2

Energy Levels (cm^{-1}) of the Ground State (000) and the (020) State of $H_2{}^{18}O$

J	K_{-1}	K_1	000 This Work	000 Fraley et al[a]	000 Williamson et al[b]	020 This Work
0	0	0	0	0	0	3139.054
1	0	1	23.756	23.756	23.759	3162.823
1	1	1	36.750	36.751	36.747	3183.004
1	1	0	42.024	42.024	42.023	3188.860
2	0	2	69.930	69.932	69.944	3209.228
2	1	2	78.995	78.995	78.988	3224.719
2	1	1	94.790	94.790	94.790	3242.240
2	2	1	133.480	133.479	133.482	3301.676
2	2	0	134.785	134.785	134.784	3302.776
3	0	3	136.344	136.344	136.344	3276.274
3	1	3	141.577	141.576	141.581	3286.604
3	1	2	172.888	172.887	172.891	3321.429
3	2	2	204.763	204.762	204.764	3373.081
3	2	1	210.800	210.800	210.799	3378.303
3	3	1	282.093	282.093	282.093	3483.850
3	3	0	282.304	282.304	282.305	3483.985
4	0	4	221.237	221.237	221.234	3361.95
4	1	4	223.830	223.830	223.833	3368.041
4	1	3	274.793	274.811	274.793	3425.183
4	2	3	298.629	298.629	298.622	3467.278
4	2	2	314.460	314.460	314.461	3481.497
4	3	2	379.293	379.293	379.293	3581.077
4	3	1	380.700	380.700	380.702	3581.986
4	4	1	482.632	482.632	482.638	3727.199
4	4	0	482.660	482.660	482.672	3727.208
5	0	5	324.044	324.026	324.034	3465.180
5	1	5	325.216	325.194	325.216	3468.454
5	1	4	398.372	398.371	398.384	3551.730
5	2	4	414.177	414.177	414.176	3583.445
5	2	3	445.160	445.160	445.155	3612.465
5	3	3	500.595	500.604	500.594	3702.541
5	3	2	505.727	505.726	505.745	3705.950
5	4	2	604.550	604.549	604.564	3849.157
5	4	1	604.796	604.796	604.797	3849.277
5	5	1	733.673	733.708		4027.45
5	5	0	733.678	733.712		4027.45
6	0	6	444.860	444.848	444.861	3585.675
6	1	6	445.355	445.354	445.364	3587.347
6	1	5	541.183	541.183	541.169	3698.827
6	2	5	550.447	550.447	550.456	3720.710
6	2	4	601.246	601.246	601.252	3770.096
6	3	4	645.387	645.377	645.377	3847.785
6	3	3	658.623	658.601	658.623	3857.064
6	4	3	751.040	751.031	751.046	3995.637
6	4	2	752.195	752.195	752.214	3996.206
6	5	2	880.079	880.100	880.079	4174.10
6	5	1	880.121	880.146	880.121	4174.11
6	6	1	1033.195	1033.548	1033.495	4379.87
6	6	0	1033.195	1033.548	1033.495	
7	0	7	583.767	583.767	583.757	3723.643
7	1	7	583.972	583.972	583.972	3724.485
7	1	6	701.697	701.697	701.692	3864.321
7	2	6	706.608	706.608	706.608	3878.187
7	2	5	780.440	780.428	780.441	3952.637
7	3	5	812.753	812.753	812.746	4016.130
7	3	4	839.561	839.561	839.564	4036.200
7	4	4	921.910	921.908	921.927	4166.471
7	4	3	925.698	925.698	925.688	4168.458
7	5	3	1050.990	1051.036	1051.010	
7	5	2	1051.210	1051.334	1051.308	
7	6	2	1204.172			
7	6	1	1204.186			
7	7	1	1378.98			
7	7	0	1378.98			
8	0	8	740.930	740.940	740.947	3879.159
8	1	8	741.000	741.013	741.009	3879.557
8	1	7	879.481	879.481	879.482	4046.945
8	2	7	881.900	881.902	881.895	4055.141
8	2	6	980.230	980.230	980.227	
8	3	6	1001.709	1001.718	1001.709	4206.661
8	3	5	1047.317	1047.317	1047.314	
8	4	5	1116.620	1116.635	1116.620	4361.408
8	4	4	1126.480	1126.433	1126.437	
8	5	4	1246.369	1246.319		
8	5	3	1247.20	1247.234		
8	6	3	1399.74			
9	0	9	916.250		916.261	4052.315
9	1	9	916.300		916.341	4052.55
9	1	8	1074.779	1074.779	1074.777	4246.259
9	2	8	1075.920	1075.932	1075.922	4250.89
9	2	7	1198.190	1198.194	1198.187	4383.38
9	3	7			1211.190	
9	3	6	1279.800	1279.822	1279.830	4477.16
9	4	6	1334.68			
9	4	5	1355.19			
10	0	10	1109.808			4243.17
10	1	10	1109.770			4243.270
10	1	9	1287.727			
10	2	9	1288.264			4465.043
10	2	8	1433.061			
10	3	8	1440.295			
10	3	7	1534.368			
11	0	11	1321.44			4451.65
11	1	11				4451.76
11	1	10	1518.55			
12	1	12	1551.19			4677.85

a. See Ref (5)

b. See Ref (6)

where g is the statistical weighting factor for the ground state level (same as $H_2{}^{16}O$), ν is the line center frequency, E'' is the ground state energy level, k is Boltzmann's constant, Q is the rotational partition function and ν_0 is the band center frequency. Values of S' are of little value for the purpose of analyzing atmospheric spectra but they were included in Table 1 because they are required in determining the vibrational band

TABLE 3

Positions (cm^{-1}) of $H_2{}^{18}O$ and $H_2{}^{16}O$ Lines which were Blended in the Spectral Data

$H_2{}^{16}O$						$H_2{}^{18}O$					
	Upper		Lower				Upper		Lower		
Position[a]	J	$K_{-1}K_1$	J	$K_{-1}K_1$	Band	Position[b]	J	$K_{-1}K_1$	J	$K_{-1}K_1$	Band
2935.193	4	1 4	5	2 3	020	2935.154	6	3 3	7	4 4	020
2980.387	5	4 1	6	5 2	020	2980.362	8	2 7	9	1 8	020
3087.192	6	2 5	6	3 4	020	3087.16	4	0 4	4	1 3	020
3095.945	1	0 1	2	1 2	020	3095.999	3	2 1	3	3 0	020
3101.156	2	1 2	3	0 3	020	3101.154	5	3 2	5	4 1	020
3110.594	4	3 1	4	4 0	020	3110.502	7	3 4	7	4 3	020
3114.493	0	0 0	1	1 1	020	3114.438	2	0 2	2	1 1	020
3199.359	6	4 2	7	3 5	020	3199.404	4	2 2	3	3 1	020
3214.123	2	1 2	1	0 1	020	3214.093	5	2 3	5	1 4	020
3220.442	4	2 2	4	1 3	020	3220.37	4	0 4	3	1 3	020
						3220.420	4	1 3	3	2 2	020
3223.326	7	2 5	8	1 8	020	3223.318	5	3 2	4	4 1	020
3260.427	5	1 5	4	0 4	020	3260.459	6	0 6	5	1 5	020
3262.517	6	1 5	7	4 4	100	3262.533	6	4 2	5	5 1	020
3263.275	7	2 5	7	1 6	020	3263.303	6	1 6	5	0 5	020
3266.101	6	5 2	7	4 3	020	3266.026	2	2 0	1	1 1	020
3266.086	8	3 6	9	5 5	001						
3272.518	4	3 2	5	0 5	020	3272.518	8	0 8	9	2 7	001
3278.841	9	1 8	10	3 7	001	3278.81	6	6 1	7	7 0	100
3293.093	7	1 6	7	0 7	020	3293.089	5	4 1	6	6 0	001
3294.210	3	3 1	3	2 2	020	3294.215	7	2 6	7	1 7	020
3326.797	7	1 7	8	3 6	001	3326.827	8	1 7	9	3 6	001
3329.644	7	2 6	8	4 5	001	3329.680	6	4 3	7	5 2	100
3336.897	9	3 6	10	4 7	100	3336.926	6	4 2	7	5 3	100
3340.298	10	1 10	9	0 9	020	3340.337	8	1 7	7	2 6	020
3364.347	3	3 1	2	2 0	020	3364.359	9	1 8	8	2 7	020

a. See Ref. (3)

b. Calculated from energy levels given in this work and in Ref (5)

strength S_v, and F, a factor which accounts for the vibration–rotation effects, from laboratory spectra used to determine values of the absolute line strength S. S is expressed as

$$S = S_v \cdot S' \cdot F \cdot L, \tag{2}$$

where L is the rigid-rotor transition intensity. Values of E'' given in Table 1 were determined from the analysis of the present data which is the subject of the following discussion.

Values of the energy levels of the ground state and the (020) state are presented in Table 2. Also included in Table 2 are values of E'' reported in the work of Fraley *et al.* (*5*) and Williamson *et al.* (*6*). Values given in the first and last columns of Table 2 were determined by the method of combination differences using ground state levels given

in Refs. (*5*) and (*6*) as an initial set of E'' and therefore deriving an initial set of energy levels for the (020) state from the measured line positions. The initial set of upper state levels were then used to determine new values for the ground state levels. This process was repeated several times. This technique was used for the (020) band having 2 or more observed lines with identical upper state quantum numbers. For levels of the (020) state which are involved in only one observed transition, such as the $000 \leftarrow 111$ transition, the upper level was calculated from the measured line frequency and the ground state level, obtained by the method given above. The same procedure was used to determine ground state levels which were involved in only one observed transition. For a few observed lines, it was not possible to determine values of either the upper state or lower state levels such as those listed as line numbers 141, 260, and 262 in Table 1. For these lines an approximate value of E'' was entered in Table 1. The ground state levels obtained in this work are, on the average, in good agreement with those given in Refs. (*5*) and (*6*) with the exceptions being the levels 660, 661, and 752.

Several $H_2{}^{18}O$ lines were blended with $H_2{}^{16}O$ lines in the spectra to an extent that these line positions could not be measured with very much accuracy. Table 3 is a listing of these lines for both isotopic species along with their quantum and band assignments. The $H_2{}^{16}O$ frequencies are those given by Flaud and Camy-Peyret (*3*) and the $H_2{}^{18}O$ values were calculated from the levels of the ground and (020) states derived in this work (given in Table 2), and also from the (001) and (100) levels given by Fraley *et al.* (*5*).

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