JOURNAL OF MOLECULAR SPECTROSCOPY 67, 206–218 (1977)

Spectrum of $H_2{}^{18}O$ and $H_2{}^{17}O$ in the 6974 to 7387 cm^{-1} Region[1]

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Measurements of the line center positions of $H_2{}^{18}O$ and $H_2{}^{17}O$ in the 6974 to 7387 cm^{-1} region have been made at a spectral resolution of $\sim$0.07 cm^{-1}. The region contains absorptions of the (101) and (200) bands of $H_2{}^{18}O$ and $H_2{}^{17}O$. *R*-branch transitions of the (021) band of $H_2{}^{18}O$ were also observed. Values of the energy levels in the (101) and (200) states of $H_2{}^{18}O$ were determined from the data and the ground state levels derived by Toth, Flaud, and Camy-Peyret [(*J. Mol. Spectrosc.* 67, 185–205 (1977)]. Seven levels in the (101) state of $H_2{}^{17}O$ were also obtained.

INTRODUCTION

In an earlier study (*1*), the spectrum of water vapor was obtained in the 6900 to 7500 cm^{-1} region which encompasses the vibration–rotation transitions of five bands. Although the quantum assignments for the majority of the absorptions have been determined (*1*, *2*), there still remain a number of weak features in those spectra which have not been assigned or have been assigned incorrectly. These features are due to: (a) weak transitions of the high J and/or K_{-1} lines of $H_2{}^{16}O$; (b) "hot" band transitions of $H_2{}^{16}O$; and (c) transitions of the isotopic species, $H_2{}^{18}O$ and $H_2{}^{17}O$. To simplify the process for the identification of the weak absorptions due to $H_2{}^{16}O$ requires that the spectra of $H_2{}^{18}O$ and $H_2{}^{17}O$ are known. Also, a knowledge of the transition frequencies of the isotopic species is necessary for the interpretation of the telluric spectrum in this spectral interval. For these reasons, the spectra of oxygen-18 enriched water vapor were recorded to determine line center frequencies and values of the upper state levels of $H_2{}^{18}O$ in the 6970 to 7380 cm^{-1} region. From these spectra, it was also possible to identify a number of the strong transitions of $H_2{}^{17}O$ in the (101) band.

The spectral region chosen for this study is where the strongest absorptions of water vapor are located for the bands (120), (021), (200), (101), and (002). The analysis of

[1] This paper presentes the results of one phase of research carried out at the Jet Propulsion Laboratory, California Institute of Technology, under Contract NAS 7-100, sponsored by the National Aeronautics and Space Administration.

ISSN 0022-2852

TABLE 1. ENERGY LEVELS (CM^{-1}) IN THE (101) AND (200) STATES OF $H_2{}^{18}O$ AND $H_2{}^{17}O$

$JK_{-1}K_1$	$H_2{}^{18}O$ (101)	$H_2{}^{18}O$ (200)	$H_2{}^{17}O$ (101)
0 0 0	7228.897	7185.897	7238.725
1 0 1	7252.002	7208.892	
1 1 1	7263.447	7220.750	
1 1 0	7268.727	7226.000	
2 0 2	7296.819	7253.513	
2 1 2	7304.115	7261.525	
2 1 1	7320.598	7277.182	7330.557
2 2 1	7354.346	7312.212	
2 2 0	7355.783	7313.865	
3 0 3	7360.923	7317.485	
3 1 3	7364.759	7321.892	
3 1 2	7396.700	7352.871	
3 2 2	7423.333	7381.165	7433.777
3 2 1	7429.851	7388.133	
3 3 1	7493.691	7453.955	
3 3 0	7493.958	7454.111	
4 0 4	7442.698	7399.140	7452.909
4 1 4	7444.406	7401.204	
4 1 3	7495.589	7451.484	7506.310
4 2 3	7514.212	7471.976	
4 2 2	7530.681	7488.858	7540.886
4 3 2	7588.007	7548.841	
4 3 1	7589.732	7549.895	7600.900
4 4 1	7681.675	7644.166	
4 4 0	7681.750	7644.201	
5 0 5	7541.745	7498.013	
5 1 5	7542.434	7498.883	7552.885
5 1 4	7614.903	7570.683	
5 2 4	7626.140	7583.671	
5 2 3	7656.493	7615.730	
5 3 3	7705.694	7668.202	
5 3 2	7711.818	7671.565	
5 4 2	7799.860		
5 4 1	7800.392		
5 5 1	7917.270		
5 5 0	7917.285		
6 0 6	7658.216	7614.228	
6 1 6	7658.473	7614.579	
6 1 5	7752.298	7708.100	
6 2 5	7758.148	7715.271	
6 2 4	7814.518	7766.958	
6 3 4	7845.510	7802.192	
6 3 3	7861.324		
6 4 3	7940.933		
6 4 2	7943.877		
6 5 2	8059.306		
6 5 1	8059.332		
6 6 1	8198.708		
6 6 0	8198.708		
7 0 7	7792.270	7747.901	
7 1 7	7792.351	7748.050	
7 1 6	7906.524	7862.335	
7 2 6	7909.251		
7 2 5	7988.027		
7 3 5	8008.987		
7 3 4	8037.802		
7 4 4	8109.067		
7 4 3	8113.250		
7 5 3	8225.370		
7 5 2	8225.537		
7 6 2	8361.623		
7 6 1	8361.623		
8 0 8	7943.916	7899.174	
8 1 8	7943.955	7899.220	
8 1 7	8077.510		
8 2 7	8078.734		
8 2 6	8178.731		
8 3 6	8191.036		
8 4 4	8309.696		
8 6 2	8553.805		
9 0 9	8113.180	8067.920.	
9 1 9	8113.257	6067.954	
9 1 8	8265.555		
9 2 8	8266.241		
10 0 10	8299.747		
10 1 10	8299.888		

these spectra did not include the identification of the transitions due to the (120) and (002) bands for $H_2{}^{18}O$ or the determination of the levels in the (021) state. Further measurements covering the regions below 6970 and above 7380 cm^{-1} will be made to complete the analysis of the five bands of $H_2{}^{18}O$.

EXPERIMENT AND ANALYSIS

The spectra were obtained with a 1.8 m Jarrel–Ash spectrometer with the grating blazed at 5.7 μm in first order and the data were recorded in forth order. The $H_2{}^{18}O$

TABLE 2. MEASUREMENTS AND ASSIGNMENTS OF $H_2{}^{18}O$ AND $H_2{}^{17}O$ IN THE 6975 TO 7387 CM^{-1} SPECTRAL REGION

Line No.	Frequency (CM^{-1}) (Obs.)	Frequency (CM^{-1}) (Calc.)	Upper State $JK_{-1}K_1$	Lower State $JK_{-1}K_1$	Band	Mol.
1	6974.616		7 0 7	6 0 6	21	18
1	6974.616		7 1 7	6 1 6	21	18
2	6976.841		5 1 4	4 1 3	21	18
3	6977.814	6977.828	9 1 8	10 1 9	101	18
4	6977.972	6977.970	9 2 8	10 2 9	101	18
5	6978.285	6978.327	7 5 2	8 5 3	101	18
5	6978.285	6978.290	10 0 10	11 0 11	101	18
6	6978.424	6978.424	10 1 10	11 1 11	101	18
7	6978.884		5 2 4	4 2 3	21	18
8	6978.983	6978.990	7 5 3	8 5 4	101	18
9	6979.838	6979.845	8 3 6	9 3 7	101	18
10	6979.984					
11	6980.415	6980.418	7 1 6	8 2 7	200	18
12	6980.528	6980.521	8 2 6	9 2 7	101	18
13	6980.869					
14	6982.873	6982.877	8 0 8	9 1 9	200	18
15	6982.956	6982.962	8 1 8	9 0 9	200	18
16	6985.465	6985.468	3 1 3	4 3 2	101	18
17	6985.733		4 3 2	3 3 1	21	18
18	6986.398					
19	6986.645		4 3 1	3 3 0	21	18
20	6986.805	6986.807	7 4 3	8 4 4	101	18
21	6988.252		7 2 6	8 1 7	200	18
21	6988.252	6988.261	4 2 2	5 3 3	200	18
22	6988.606		8 0 8	7 0 7	21	18
23	6989.460					
24	6989.597					
25	6989.863	6989.859	4 1 3	5 3 2	101	18
26	6990.010					
27	6990.198					
28	6990.473	6990.471	7 3 4	8 3 5	101	18
29	6992.432	6992.428	7 4 4	8 4 5	101	18
30	6994.532	6994.531	6 6 0	7 6 1	101	18
30	6994.532	6994.538	6 6 1	7 6 2	101	18
31	6996.401		5 2 3	4 2 2	21	18
32	6997.533	6997.539	4 0 4	5 2 3	101	18
33	6997.854		6 1 5	5 1 4	21	18
34	6998.909		6 2 5	5 2 4	21	18
35	7000.465	7000.462	3 2 2	4 3 1	200	18
36	7001.083					
37	7001.504	7001.501	6 1 5	7 2 6	200	18
38	7002.190		9 1 9	8 1 8	21	18
38	7002.190		9 0 9	8 0 8	21	18
39	7002.776	7002.747	8 1 7	9 1 8	101	18
39	7002.776	7002.823	8 2 7	9 2 8	101	18
40	7003.393	7003.395	9 0 9	10 0 10	101	18
41	7003.452	7003.456	9 1 9	10 1 10	101	18
42	7004.751					
43	7006.900	7006.902	7 0 7	8 1 8	200	18
44	7007.131	7007.132	7 1 7	8 0 8	200	18
45	7007.276	7007.276	7 3 5	8 3 6	101	18
46	7007.430	7007.431	3 1 3	4 2 2	200	18
47	7007.520					
48	7007.798	7007.798	7 2 5	8 2 6	101	18
49	7008.125	7008.125	6 5 1	7 5 2	101	18
50	7008.312	7008.312	6 5 2	7 5 3	101	18
51	7008.839	7008.842	3 2 1	4 3 2	200	18
52	7009.065		5 3 3	4 3 2	21	18
53	7011.812		5 3 2	4 3 1	21	18
54	7013.575	7013.576	6 2 5	7 1 6	200	18
55	7014.234		10 1 10	9 1 9	21	18
55	7014.234		10 0 10	9 0 9	21	18
56	7017.221		7 1 6	6 1 5	21	18
57	7017.953		7 2 6	6 2 5	21	18
58	7018.178	7018.173	6 4 2	7 4 3	101	18
59	7019.038	7019.033	6 4 3	7 4 4	101	18
60	7019.665	7019.681	8 0 8	8 1 7	200	18
61	7020.234	7020.230	5 1 4	6 2 5	200	18
62	7021.362		6 2 4	5 2 3	21	18
63	7021.792	7021.736	6 3 4	7 2 5	200	18
63	7021.792	7021.769	6 3 3	7 3 4	101	18
64	7022.300					
65	7022.984					
66	7025.863		11 1 11	10 1 10	21	18
67	7027.031	7027.031	7 1 6	8 1 7	101	18
68	7027.336	7027.334	7 2 6	8 2 7	101	18
69	7027.660	7027.658	8 0 8	9 0 9	101	18
69	7027.660	7027.658	8 1 8	9 1 9	101	18
70	7029.906	7029.906	2 2 1	3 3 0	200	18
71	7030.242	7030.243	6 0 6	7 1 7	200	18
72	7030.794	7030.797	6 1 6	7 0 7	200	18
73	7031.766	7031.770	2 2 0	3 3 1	200	18
74	7032.176		6 3 4	5 3 3	21	18
75	7032.746	7032.744	6 3 4	7 3 5	101	18
76	7033.169					
77	7034.062	7034.062	6 2 4	7 2 5	101	18
78	7035.470		8 1 7	7 1 6	21	18
79	7036.114		8 2 7	7 2 6	21	18
80	7036.726					
81	7037.190	7037.190	5 5 1	6 5 2	101	18
81	7037.190	7037.170	5 5 0	6 5 1	101	18
82	7037.313	7037.314	4 1 3	5 2 4	200	18
82	7037.313	7037.269	9 0 9	9 2 8	101	18
83	7037.540					
84	7037.707		6 3 3	5 3 2	21	18
85	7040.610		5 4 2	4 4 1	21	18
86	7040.740		5 4 1	4 4 0	21	18
87	7042.496	7042.492	5 2 4	6 1 5	200	18
88	7046.205	7046.206	7 0 7	7 1 6	200	18
89	7048.200	7048.201	5 4 1	6 4 2	101	18
90	7048.820	7048.824	5 4 2	6 4 3	101	18
91	7050.605	7050.603	6 1 5	7 1 6	101	18
92	7050.727	7050.725	2 1 2	3 2 1	200	18
93	7051.160	7051.156	6 3 4	6 4 3	200	18
94	7051.352	7051.352	7 1 7	8 1 8	101	18
94	7051.352	7051.352	7 0 7	8 0 8	101	18
95	7051.550	7051.549	6 2 5	7 2 6	101	18
96	7052.665	7052.667	5 0 5	6 1 6	200	18
97	7053.200	7053.209	5 3 2	6 3 3	101	18
98	7053.432					
99	7053.669					
100	7054.032	7054.030	5 1 5	6 0 6	200	18
101	7054.877					

sample, supplied by the Bio-Rad Corp., was a mixture of $H_2{}^{18}O$ (50%) and $H_2{}^{16}O$ (50%) with a 0.1% impurity due to $H_2{}^{17}O$. A multitraversal cell of 2 m base length was used for all of the measurements. The $H_2{}^{18}O$ and $H_2{}^{17}O$ line positions were calibrated from the known $H_2{}^{16}O$ absorptions (*2*). The spectral resolution was $\sim$0.07 cm^{-1}.

The identifications of the $H_2{}^{18}O$ and $H_2{}^{17}O$ absorptions were made by superimposing spectra of $H_2{}^{18}O/H_2{}^{16}O$ with those of $H_2{}^{16}O$ in which the optical densities of $H_2{}^{16}O$ were identical in the two spectra and noting that the $H_2{}^{18}O$ features are much stronger in the former and the $H_2{}^{17}O$ absorptions are approximately five times greater in the former than in the $H_2{}^{16}O$ spectrum. The quantum assignments of the observed $H_2{}^{18}O$ lines were determined from the $H_2{}^{16}O$ absorptions and the $H_2{}^{18}O$ ground state levels given by Toth *et al.* (*3*) in the following manner. The frequency difference between identical transitions

TABLE 2—*Continued*

Line No.	Frequency (CM^{-1}) (Obs.)	Frequency (CM^{-1}) (Calc.)	Upper State $JK_{-1}K_1$	Lower State $JK_{-1}K_1$	Band	Mol.
102	7055.257	7055.255	5 2 3	6 2 4	101	18
103	7060.309	7060.309	5 3 3	6 3 4	101	18
104	7060.798					
105	7062.001	7061.999	8 0 8	8 2 7	101	18
106	7062.088	7062.092	8 2 6	8 4 5	101	18
107	7063.772					
108	7064.130	7064.126	6 1 6	6 2 5	200	18
109	7064.461	7064.462	8 1 8	8 1 7	101	18
110	7064.725		6 4 2	5 4 1	21	18
111	7065.722					
112	7066.194	7066.195	4 3 2	4 4 1	200	18
112	7066.194	7066.127	7 2 5	7 4 4	101	18
113	7066.770	7066.771	5 3 2	5 4 1	200	18
114	7066.964	7066.964	5 3 3	6 2 4	200	18
115	7068.023	7068.031	9 2 8	9 2 7	101	18
116	7069.700					
117	7069.890	7069.886	6 2 5	6 3 4	200	18
118	7072.423	7072.424	2 1 1	3 2 2	200	18
119	7073.050	7073.049	6 0 6	6 1 5	200	18
120	7073.609	7073.615	4 2 3	5 1 4	200	18
121	7073.731	7073.724	5 1 4	6 1 5	101	18
122	7073.923	7073.924	4 0 4	5 1 5	200	18
123	7074.462	7074.488	6 1 6	7 1 7	101	16
123	7074.462	7074.434	6 0 6	7 0 7	101	18
124	7075.692	7075.687	5 2 4	6 2 5	101	18
125	7075.802	7075.799	8 1 7	8 3 6	101	18
126	7076.959	7076.956	4 4 0	5 4 1	101	18
127	7077.150	7077.157	4 1 4	5 0 5	200	18
127	7077.150	7077.128	4 4 1	5 4 2	101	18
128	7081.883	7081.879	7 1 6	7 2 5	200	18
129	7082.441					
130	7083.074	7083.074	5 2 4	5 3 3	200	18
131	7084.002	7084.002	4 3 1	5 3 2	101	18
132	7084.712	7084.713	5 1 5	5 2 4	200	18
133	7085.523	7085.522	4 2 2	5 2 3	101	18
134	7085.993	7085.965	1 1 1	2 2 0	200	18
134	7085.993	7086.019	2 0 2	3 2 1	101	18
135	7087.413	7087.410	4 3 2	5 3 3	101	18
136	7090.656	7090.656	7 1 7	7 1 6	101	18
137	7092.684	7092.685	4 2 3	4 3 2	200	18
138	7093.658	7093.717	4 3 1	5 3 2	101	17
138	7093.658	7093.656	3 0 3	4 1 4	200	18
139	7094.951					
140	7095.097	7095.099	4 2 2	5 2 3	101	17
141	7096.894	7096.892	5 0 5	6 0 6	101	18
142	7097.084	7097.088	5 1 5	6 1 6	101	18
143	7097.224	7097.228	4 1 3	5 1 4	101	18
144	7098.512	7098.505	8 2 7	8 2 6	101	18
145	7099.063	7099.070	3 2 2	3 3 1	200	18
146	7099.363					
147	7099.461					
148	7099.654	7099.652	5 0 5	5 1 4	200	18
149	7100.045	7100.042	4 2 3	5 2 4	101	18
150	7100.660	7100.658	3 1 3	4 0 4	200	18
151	7102.586	7102.583	4 1 4	4 2 3	200	18
152	7103.682	7103.682	4 3 2	5 2 3	200	18
153	7104.138					
154	7106.468					
155	7106.635	7106.635	5 1 5	6 1 6	101	17
156	7106.851	7106.862	6 1 5	6 2 4	200	18
156	7106.851	7106.913	6 1 5	6 3 4	101	18
157	7107.438	7107.436	4 1 3	5 1 4	101	17
158	7107.742	7107.763	6 0 6	6 2 5	101	18
159	7108.152	7108.155	4 2 2	4 3 1	200	18
160	7108.344	7108.349	6 2 4	6 3 3	200	18
161	7110.001	7110.000	5 2 3	5 3 2	200	18
162	7111.603					
163	7111.948	7111.945	2 0 2	3 1 3	200	18
164	7113.240	7113.255	3 3 0	4 3 1	101	18
165	7113.690					
166	7114.308	7114.306	5 1 4	5 3 3	101	18
167	7114.394	7114.400	3 3 1	4 3 2	101	18
168	7115.390	7115.390	3 2 1	4 2 2	101	18
169	7117.129	7117.134	3 1 3	3 2 2	200	18
170	7118.651	7118.651	4 0 4	5 0 5	101	18
171	7119.190	7119.190	4 1 4	5 1 5	101	18
172	7121.116	7121.112	5 3 2	6 2 5	200	18
173	7121.892	7121.897	3 1 2	4 1 3	101	18
174	7124.334	7124.337	4 0 4	4 1 3	200	18
175	7124.709	7124.712	3 2 2	4 2 3	101	18
176	7125.187	7125.187	2 1 2	3 0 3	200	18
177	7125.523	7125.524	5 1 4	5 2 3	200	18
178	7127.568	7127.575	5 0 5	5 2 4	101	18
179	7128.028	7128.048	2 1 2	2 2 1	200	18
180	7128.245	7128.249	4 0 4	5 0 5	101	17
181	7128.794	7128.795	7 2 6	7 2 5	101	18
182	7129.904	7129.902	1 0 1	2 1 2	200	18
183	7131.575					
184	7134.339	7134.343	3 2 2	4 2 3	101	17
185	7135.725	7135.725	4 3 1	5 2 4	200	18
186	7137.022	7137.023	4 1 3	4 2 2	200	18
187	7138.436	7138.436	4 4 1	5 3 2	200	18
188	7139.319	7139.328	2 2 1	3 1 2	200	18
189	7139.488	7139.494	3 3 1	4 2 2	200	18
190	7139.688	7139.689	3 0 3	4 0 4	101	18
191	7140.926	7140.930	3 1 3	4 1 4	101	18
192	7142.073	7142.071	3 1 2	3 2 1	200	18
193	7142.398	7142.397	2 1 1	2 2 0	200	18
194	7144.074	7144.073	5 1 5	5 1 4	101	18
194	7144.074	7144.077	4 0 4	4 2 3	101	18
195	7144.602	7144.601	3 0 3	3 1 2	200	18
196	7144.984	7144.983	2 2 0	3 2 1	101	18
197	7147.715	7147.714	2 1 1	3 1 2	101	18
198	7149.147	7149.147	0 0 0	1 1 1	200	18
199	7149.589	7149.588	2 2 1	3 2 2	101	18
200	7150.822	7150.822	1 1 1	2 0 2	200	18
201	7154.360	7154.368	8 6 2	8 6 3	101	18
201	7154.360	6900.417	8 6 3	8 6 2	101	18
202	7154.773		2 2 0	3 2 1	101	17
203	7155.488	7155.490	3 3 0	4 2 3	200	18
204	7156.164	7156.165	3 0 3	3 2 2	101	18
205	7157.446	7157.446	7 6 2	7 6 1	101	18
205	7157.446	7157.453	7 6 1	7 6 2	101	18
205	7157.446	7157.450	2 1 1	3 1 2	101	17

of $H_2{}^{16}O$ and $H_2{}^{18}O$ range between 12 and 25 cm^{-1} and the peak absorptions for the same transitions in the two molecules are approximately equal. Also the ground state levels of $H_2{}^{18}O$ (*3*) were used to calculate upper state levels from identified $H_2{}^{18}O$ features and then the positions of other transitions could be determined. The $H_2{}^{17}O$ assignments were obtained by noting that their transition frequencies lie in a region midway between the positions of identical transitions of $H_2{}^{16}O$ and $H_2{}^{18}O$.

RESULTS

Values of the levels for the (101) and (200) states of $H_2{}^{18}O$ and seven levels of the (101) state of $H_2{}^{17}O$ are listed in Table 1. These values were determined from the measurements and the ground state levels of $H_2{}^{18}O$ and $H_2{}^{17}O$ given by Toth *et al.* (*3*).

TABLE 2—*Continued*

Line No.	Frequency (CM^{-1}) (Obs.)	(Calc.)	Upper State $JK_{-1}K_1$	Lower State $JK_{-1}K_1$	Band	Mol.
205	7157.446	7157.450	2 1 1	3 1 2	101	17
206	7158.727	7158.724	2 0 2	2 1 1	200	18
207	7159.245					
208	7160.482	7160.481	2 0 2	3 0 3	101	18
209	7162.546	7162.547	2 1 2	3 1 3	101	18
210	7163.109					
211	7163.341	7163.342	2 0 2	2 2 1	101	18
212	7163.643	7163.642	4 2 2	5 1 5	200	18
213	7164.310	7164.304	3 2 1	4 1 4	200	18
214	7165.512	7165.513	6 6 0	6 6 1	101	18
214	7165.512	7165.513	6 6 1	6 6 0	101	18
215	7166.867	7166.868	1 0 1	1 1 0	200	18
216	7169.437	7169.432	7 3 5	7 3 4	101	18
217	7169.602	7169.603	4 1 4	4 1 3	101	18
218	7169.895		8 5 3	8 5 4	101	18
219	7171.511					
220	7171.646					
221	7172.176					
222	7172.714					
223	7173.938	7173.938	1 1 0	2 1 1	101	18
224	7174.540	7174.543	7 5 2	7 5 3	101	18
225	7179.236	7179.191	6 5 2	6 5 1	101	18
225	7179.236	7179.252	6 5 1	6 5 2	101	18
226	7180.978	7180.981	5 2 4	5 2 3	101	18
227	7182.080	7182.074	1 0 1	2 0 2	101	18
228	7183.364	7183.363	7 4 4	7 4 3	101	18
229	7183.585	7183.585	5 5 1	5 5 0	101	18
229	7183.585	7183.604	5 5 0	5 5 1	101	18
230	7184.455	7184.457	1 1 1	2 1 2	101	18
230	7184.455	7184.422	5 1 5	4 2 2	200	18
231	7186.896	7186.901	6 3 4	6 3 3	101	18
232	7187.112	7187.107	3 1 3	2 2 0	200	18
233	7188.749	7188.742	6 4 3	6 4 2	101	18
234	7191.352	7191.350	7 4 3	7 4 4	101	18
235	7191.459		6 5 2	6 3 3	21	18
236	7191.877	7191.875	3 1 3	3 1 2	101	18
237	7192.681					
238	7192.835	7192.841	6 4 2	6 4 3	101	18
239	7193.046	7193.057	8 4 4	8 4 5	101	18
240	7195.063	7195.066	5 4 2	5 4 1	101	18
241	7195.845	7195.845	5 4 1	5 4 2	101	18
242	7198.999	7198.999	4 4 1	4 4 0	101	18
243	7199.101	7199.104	4 4 0	4 4 1	101	18
244	7199.747	7199.751	4 2 3	4 2 2	101	18
245	7199.969	7199.964	5 3 3	5 3 2	101	18
246	7201.140		5 5 1	5 3 2	21	18
247	7202.245	7202.244	1 1 0	1 0 1	200	18
248	7205.141	7205.141	0 0 0	1 0 1	101	18
249	7207.290	7207.254	2 1 1	2 0 2	200	18
249	7207.290	7207.304	4 3 2	4 3 1	101	18
250	7209.324	7209.326	2 1 2	2 1 1	101	18
251	7209.731					
252	7210.446	7210.441	4 3 1	4 3 2	101	18
253	7211.222	7211.221	5 3 2	5 3 3	101	18
254	7211.391	7211.385	3 3 1	3 3 0	101	18
255	7211.863	7211.863	3 3 0	3 3 1	101	18
256	7212.536	7212.533	3 2 2	3 2 1	101	18
257	7213.290					
258	7214.056	7214.055	4 2 2	4 1 3	200	18
259	7214.950	7214.950	0 0 0	1 0 1	101	17
260	7215.246	7215.249	3 2 1	3 1 2	200	18
261	7215.775					
262	7215.939	7215.939	6 3 3	6 3 4	101	18
263	7216.532	7216.533	3 1 2	3 0 3	200	18
264	7216.758	7216.763	2 0 2	1 1 1	200	18
265	7217.012					
266	7217.363	7217.369	5 2 3	5 1 4	200	18
267	7219.079	7219.076	2 2 0	2 1 1	200	18
268	7219.560	7219.561	2 2 1	2 2 0	101	18
269	7220.087	7220.087	4 3 1	4 3 2	101	17
270	7221.113		6 3 3	6 2 4	200	18
271	7221.425	7221.423	1 1 1	1 1 0	101	18
272	7222.305	7222.342	3 2 2	3 2 1	101	17
272	7222.305	7222.306	2 2 0	2 2 1	101	18
273	7224.792					
274	7225.093	7225.036	7 3 4	7 3 5	101	18
274	7225.093	7225.093	3 2 1	3 2 2	101	18
275	7225.783	7225.779	6 2 4	6 1 5	200	18
276	7226.403	7226.406	5 3 2	5 2 3	200	18
277	7230.251	7230.250	4 1 3	4 0 4	200	18
278	7231.970	7231.977	1 1 0	1 1 1	101	18
279	7235.434	7235.434	4 3 1	4 2 2	200	18
280	7237.768	7237.769	2 1 2	1 0 1	200	18
281	7238.491	7238.495	3 0 3	2 1 2	200	18
282	7239.601	7239.597	3 2 2	3 1 3	200	18
283	7241.608	7241.608	2 1 1	2 1 2	101	18
284	7241.923					
285	7243.315	7243.311	3 3 0	3 2 1	200	18
286	7246.638	7246.636	5 1 4	5 0 5	200	18
287	7246.729	7246.726	4 1 3	3 2 2	200	18
288	7247.789					
289	7248.153	7248.147	4 2 3	4 1 4	200	18
290	7249.198	7249.197	3 3 1	3 2 2	200	18
291	7250.220	7250.220	4 3 2	4 2 3	200	18
292	7251.323	7251.321	2 1 1	2 1 2	101	17
293	7251.996	7251.964	3 1 3	2 0 2	200	18
293	7251.996	7252.002	1 0 1	0 0 0	101	18
294	7255.138	7255.132	3 1 2	3 1 3	101	18
295	7257.285		6 4 3	6 3 4	200	18
296	7257.577	7257.572	4 0 4	3 1 3	200	18
297	7258.456	7258.455	5 2 4	5 1 5	200	18
298	7258.760					
299	7258.932					
300	7259.892		5 4 1	5 3 2	200	18
301	7262.161					
302	7263.245	7263.247	6 1 5	6 0 6	200	18
303	7263.497	7263.498	4 4 0	4 3 1	200	18
304	7264.063	7264.065	6 2 4	6 2 5	101	18
305	7264.863	7264.875	4 4 1	4 3 2	200	18
305	7264.863	7264.866	4 1 4	3 0 3	200	18
306	7265.540		5 4 2	5 3 3	200	18
307	7265.935					
308	7267.368	7267.365	2 1 2	1 1 1	101	18
309	7269.920	7269.925	6 2 5	6 1 6	200	18

Table 2 is a listing of the line numbers, measured and calculated line center frequencies, upper and lower state rotational quantum numbers, band and isotopic species. The line numbers pertain to the numbering of the absorptions shown in Fig. 1 where the unnumbered features are due to $H_2{}^{16}O$. The calculated frequencies given in Table 2 were determined from the upper state levels given in Table 1 and the ground state levels given by Toth *et al.* (*3*). Tentative quantum assignments were made for several of the measured lines in Table 2 for which values of the upper state levels were not included in Table I and therefore no calculated positions were determined (for example, line numbers 1, 2, 7, 17, 19, 21, 22, etc.). The majority of these lines are in the (021) band. Several other measured positions given in Table 2 do not have quantum assignments (for example, line numbers 10, 13, 18, 23, 24, 26, 27, etc.) and they are due to either

TABLE 2—*Continued*

Line No.	Frequency (CM^{-1}) (Obs.)	Frequency (CM^{-1}) (Calc.)	Upper State $JK_{-1}K_1$	Lower State $JK_{-1}K_1$	Band	Mol.
310	7270.192	7270.188	2 2 1	1 1 0	200	18
311	7271.759	7271.760	4 1 3	4 1 4	101	18
312	7272.060	7272.062	5 1 4	4 2 3	200	18
313	7272.738					
314	7273.034	7273.063	2 0 2	1 0 1	101	18
315	7273.675		6 5 2	6 4 3	200	18
316	7274.185	7274.184	5 0 5	4 1 4	200	18
317	7277.115	7277.115	2 2 0	1 1 1	200	18
318	7277.642	7277.649	5 1 5	4 0 4	200	18
319	7277.759		5 5 0	5 4 1	200	18
319	7277.759		5 5 1	5 4 2	200	18
320	7278.569	7278.553	7 1 6	7 0 7	200	18
320	7278.569	7278.574	2 1 1	1 1 0	101	18
321	7281.431	7281.428	7 2 5	7 2 6	101	18
322	7282.003	7282.005	4 1 3	4 1 4	101	17
323	7284.105					
324	7284.416	7284.418	2 2 1	2 0 2	101	18
325	7285.772	7285.769	3 1 3	2 1 2	101	18
326	7286.374	7286.376	3 2 2	2 1 1	200	18
327	7287.207					
328	7288.375	7288.367	2 1 1	1 1 0	101	17
329	7289.012	7289.012	6 0 6	5 1 5	200	18
330	7289.685	7289.687	5 1 4	5 1 5	101	18
331	7289.855	7289.856	3 2 2	2 2 1	101	18
332	7290.531	7290.532	6 1 6	5 0 5	200	18
333	7290.998	7290.995	3 0 3	2 0 2	101	18
334	7292.981	7292.978	4 2 3	4 0 4	101	18
335	7295.067	7295.066	3 2 1	2 2 0	101	18
336	7295.637		3 1 3	2 1 2	101	17
337	7299.092	7299.092	4 2 3	3 1 2	200	18
338	7299.640	7299.636	3 2 2	2 2 1	101	17
339	7300.958					
340	7301.910	7301.911	3 1 2	2 1 1	101	18
341	7302.090	7302.093	5 2 4	5 0 5	101	18
342	7302.560	7302.555	7 0 7	6 1 6	200	18
343	7302.840	7302.838	4 1 4	3 1 3	101	18
344	7304.328	7304.331	6 3 4	6 1 5	101	18
345	7305.910	7305.912	4 3 2	3 3 1	101	18
346	7306.362	7306.360	4 0 4	3 0 3	101	18
347	7307.422	7307.426	4 3 1	3 3 0	101	18
348	7308.865	7308.868	5 2 4	4 1 3	200	18
349	7309.452	7309.454	4 2 3	3 2 2	101	18
350	7310.874					
351	7311.886					
352	7313.295	7313.295	6 2 5	6 0 6	101	18
353	7315.192	7315.189	8 0 8	7 1 7	200	18
354	7315.445	7315.438	8 1 8	7 0 7	200	18
355	7316.373	7316.369	4 0 4	3 0 3	101	17
356	7316.925	7316.910	6 2 5	5 1 4	200	18
357	7317.218	7317.214	5 4 2	4 4 1	101	18
358	7317.718	7317.716	5 4 1	4 4 0	101	18
359	7318.609	7318.605	5 1 5	4 1 4	101	18
360	7319.172	7319.170	3 3 1	2 2 0	200	18
361	7319.880	7319.881	4 2 2	3 2 1	101	18
362	7320.516	7320.511	5 0 5	4 0 4	101	18
363	7320.629	7320.634	3 3 0	2 2 1	200	18
364	7322.710	7322.705	4 1 3	3 1 2	101	18
365	7324.700					
366	7324.881					
367	7325.470	7325.469	7 2 6	7 0 7	101	18
368	7325.636	7325.625	6 5 2	5 5 1	101	18
368	7325.636	7325.647	6 5 1	5 5 0	101	18
369	7326.398	7326.403	5 3 3	4 3 2	101	18
370	7326.921	7326.921	9 0 9	8 1 8	200	18
371	7327.036	7327.036	9 1 9	8 0 8	200	18
372	7327.520	7327.519	5 2 4	4 2 3	101	18
373	7328.607	7328.580	5 1 5	4 1 4	101	17
373	7328.607	7328.611	7 4 4	7 2 5	101	18
374	7329.454	7329.451	4 2 2	3 2 1	101	17
375	7330.552					
376	7331.117	7331.115	5 3 2	4 3 1	101	18
377	7332.027	7332.027	2 2 0	1 0 1	101	18
378	7332.644					
379	7332.833					
380	7333.257	7333.203	4 1 3	3 1 2	101	17
380	7333.257	7333.257	6 1 6	5 1 5	101	18
381	7334.169	7334.169	6 0 6	5 0 5	101	18
382	7336.384	7336.386	6 4 3	5 4 2	101	18
383	7336.507	7336.511	8 1 7	8 1 8	101	18
384	7337.333					
385	7339.083	7339.083	6 4 2	5 4 1	101	18
386	7340.100	7340.100	5 1 4	4 1 3	101	18
387	7342.030	7342.032	5 2 3	4 2 2	101	18
388	7343.970	7343.978	6 2 5	5 2 4	101	18
389	7344.917	7344.913	6 3 4	5 3 3	101	18
390	7345.297	7345.290	7 5 3	6 5 2	101	18
391	7345.426	7345.422	7 5 2	6 5 1	101	18
392	7346.265					
393	7347.417	7347.417	7 0 7	6 0 6	101	18
394	7349.465		6 5 2	5 3 3	21	18
395	7349.634	7349.628	8 6 2	7 6 1	101	18
395	7349.634	7095.718	8 6 3	7 6 2	101	18
396	7353.740	7353.741	5 3 3	4 2 2	200	18
397	7353.936	7353.937	6 1 5	5 1 4	101	18
398	7357.029	7357.033	6 3 4	5 2 3	200	18
399	7358.028	7358.031	7 4 4	6 4 3	101	18
400	7358.798	7358.798	7 2 6	6 2 5	101	18
401	7359.945	7359.970	8 1 8	7 1 7	101	18
401	7359.945	7359.923	3 2 1	2 0 2	101	18
402	7360.128	7360.134	8 0 8	7 0 7	101	18
403	7361.059	7361.059	7 4 3	6 4 2	101	18
404	7361.860	7361.860	4 4 1	3 3 0	200	18
405	7362.108	7362.106	4 4 0	3 3 1	200	18
405	7362.108		8 5 4	7 5 3	101	18
406	7363.599	7363.602	7 3 5	6 3 4	101	18
407	7365.373	7365.345	7 1 6	6 1 5	101	18
408	7369.362	7369.359	6 2 4	5 2 3	101	18
409	7372.129	7372.135	8 2 7	7 2 6	101	18
410	7372.265	7372.258	9 1 9	8 1 8	101	18
410	7372.265	7372.262	9 0 9	8 0 8	101	18
411	7375.805	7375.815	8 1 7	7 1 6	101	18
412	7378.278	7378.270	8 3 6	7 3 5	101	18
413	7379.190	7379.193	7 3 4	6 3 3	101	18
414	7382.830					
415	7383.494	7383.489	10 0 10	9 0 9	101	18
416	7384.004	7383.992	8 4 4	7 4 3	101	18
417	7384.331	7384.324	9 2 8	8 2 7	101	18
418	7386.069	7386.062	9 1 8	8 1 7	101	18
419	7386.786	7386.789	7 2 5	6 2 4	101	18

unidentified transitions of $H_2{}^{18}O$ or $H_2{}^{17}O$ in the five bands (101), (200), (021), (120), and (002) or "hot" band transitions of $H_2{}^{18}O$.

Table 2 also contains lines which were incorrectly identified as transitions due to $H_2{}^{16}O$ in an earlier study by Toth and Margolis (*1*). These lines (in Table 2, numbers 56, 170, 175, 223, 283, 289, 320, etc.) were observed as weak absorptions in the $H_2{}^{16}O$ spectra (*1*) and essentially do not reflect errors in the determination of several of the upper state levels given in Ref. (*1*) for high J or K_{-1} levels in the states (200), (021),

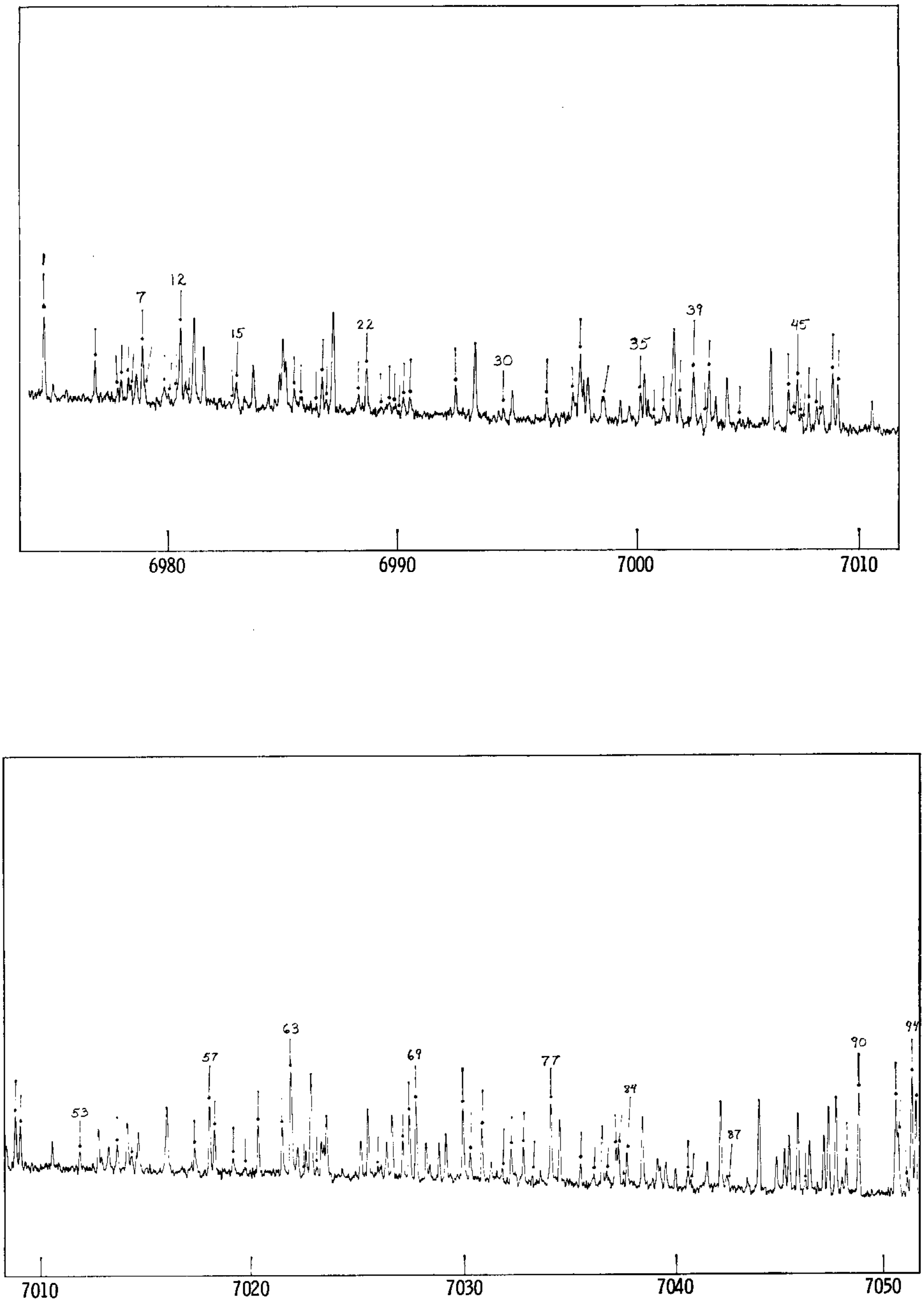
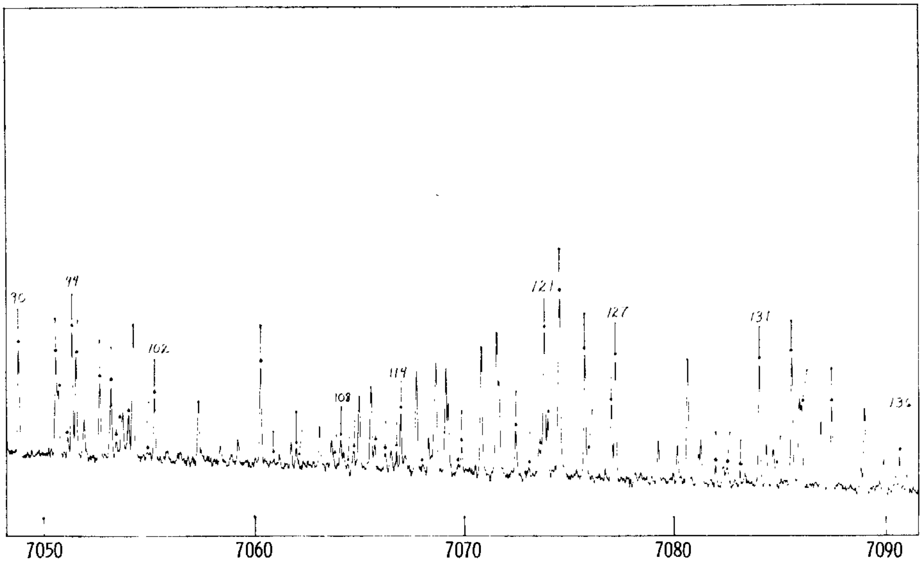


Fig. 1. Scan of the 6974 to 7387 cm^{-1} region of $H_2{}^{18}O$, $H_2{}^{16}O$, and $H_2{}^{17}O$. The sample pressure was 2.3 Torr and the path was 24 m. The isotopic ratio of the water vapor sample was 50, 50 and 0.1% for $H_2{}^{18}O$, $H_2{}^{16}O$, and $H_2{}^{17}O$ respectively. The stroke marks denote the $H_2{}^{18}O$ and $H_2{}^{17}O$ lines and only these are numbered.



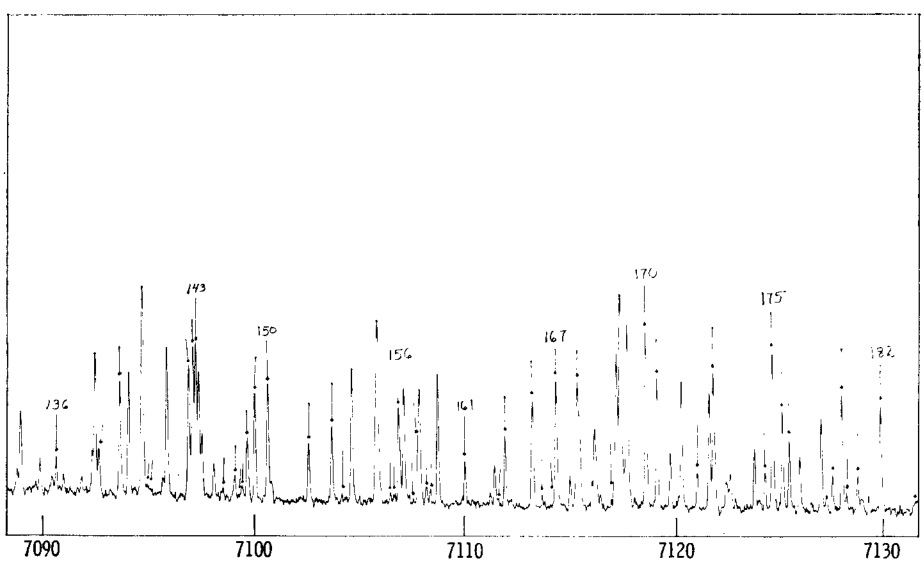
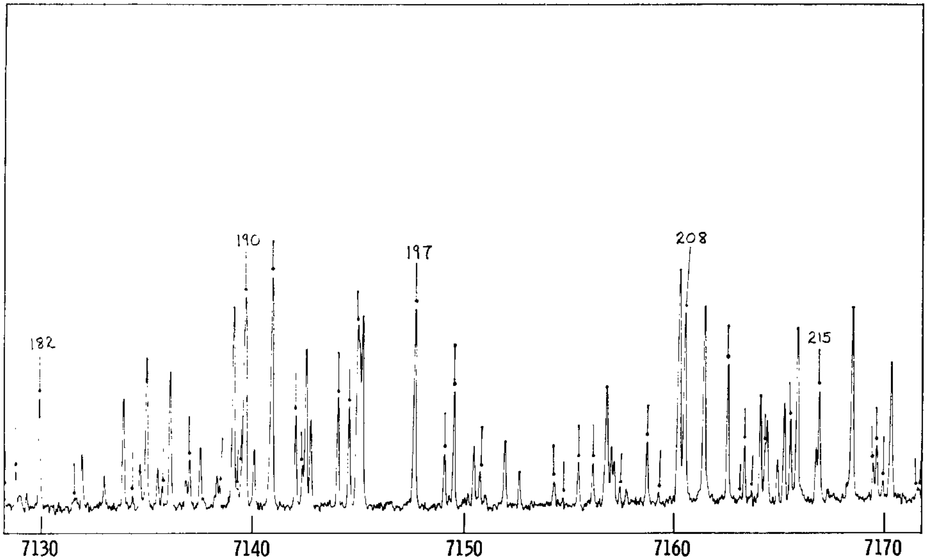


FIG. 1.—*Continued*



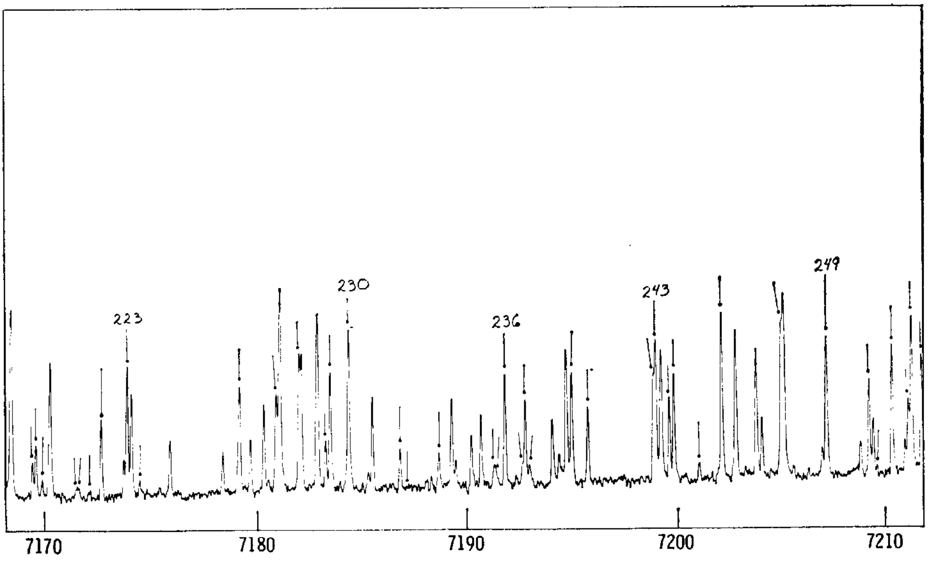
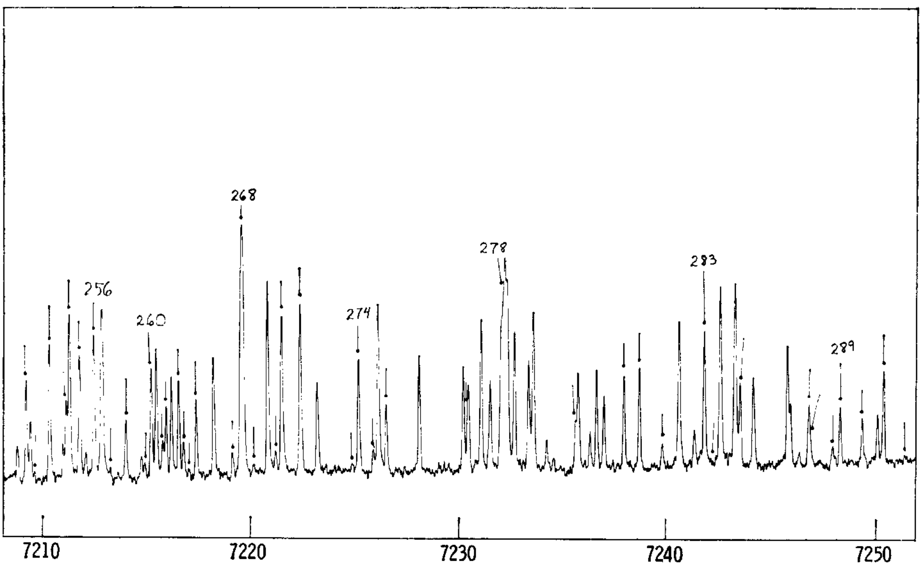


FIG. 1.—*Continued*



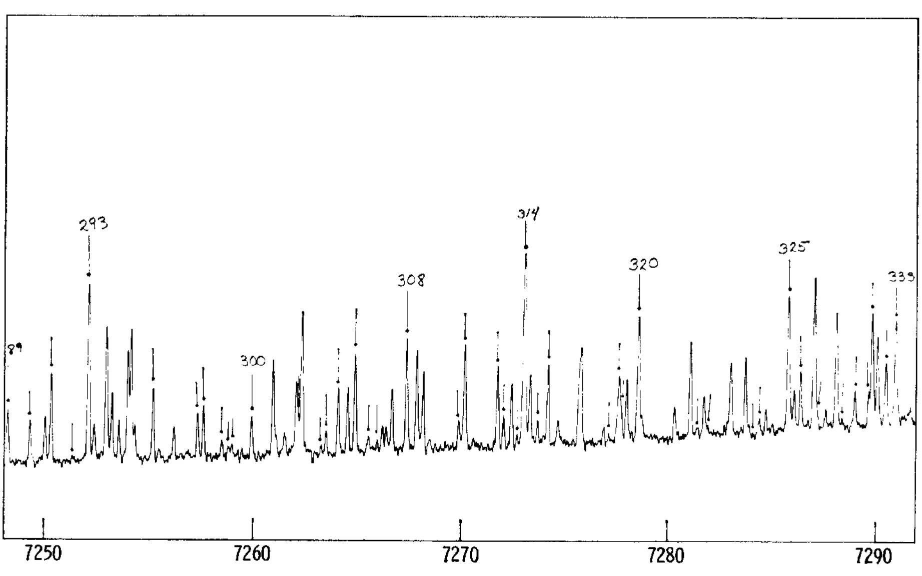
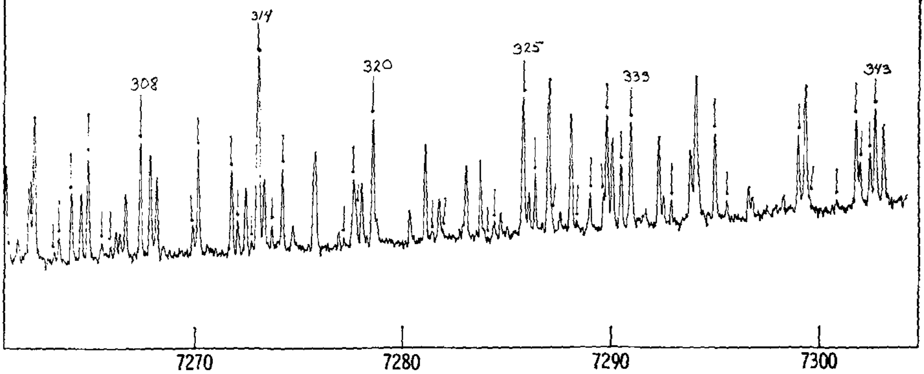


FIG. 1.—*Continued*



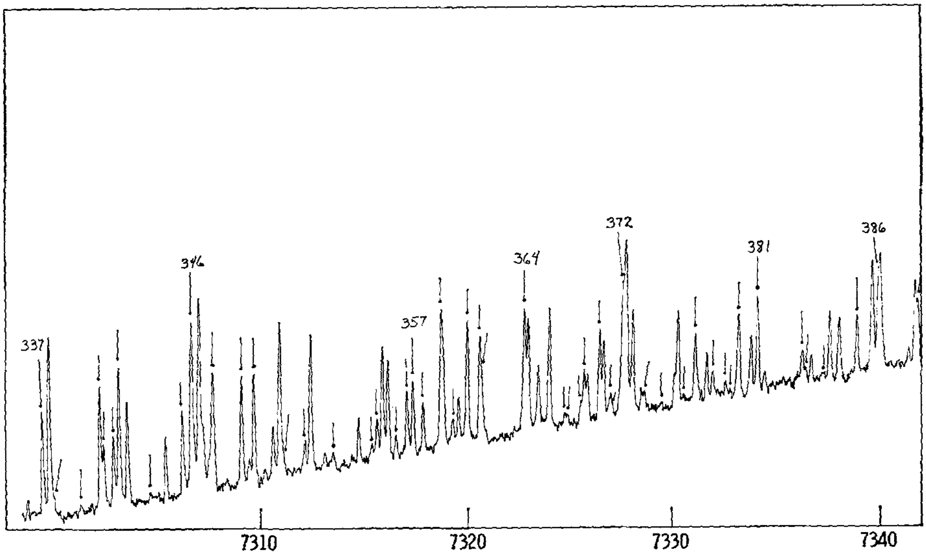
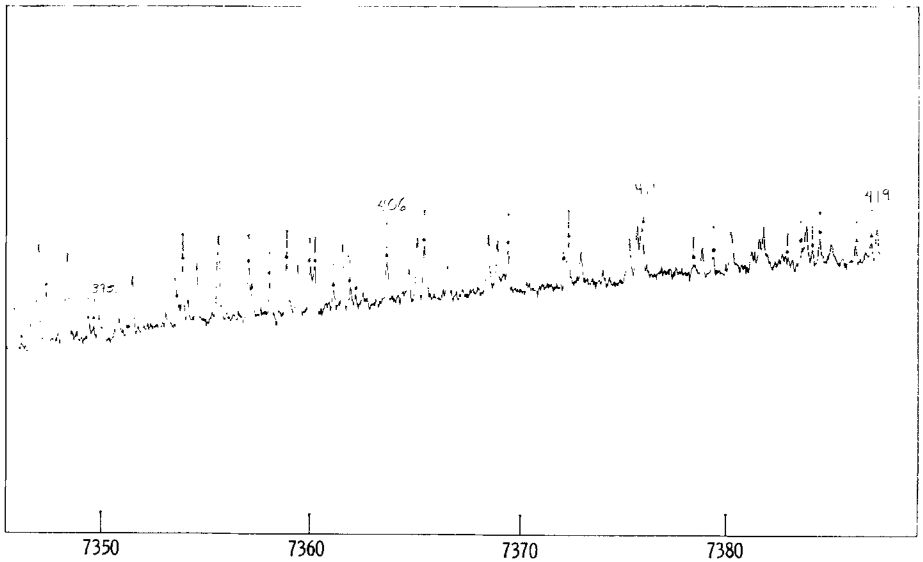


FIG. 1.—*Continued*



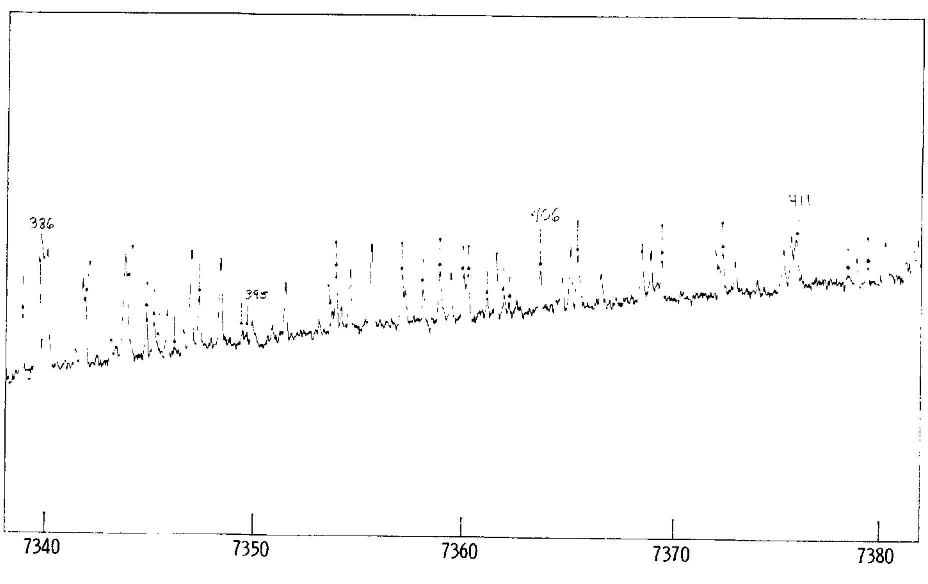


FIG. 1.—*Continued*

(210), and (002). Also in that earlier paper, several of the measured positions were not assigned and many of those lines are due to $H_2{}^{18}O$.

RECEIVED: February 7, 1977

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