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High-Resolution Spectrum of Water Vapor between 30 and 720 cm^{-1}

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The pure rotational spectrum of natural water vapor between 30 and 720 cm^{-1} has been recorded by a double-beam Fourier spectrometer. The maximum resolution achieved was about 0.018 cm^{-1} and the accuracy of the observed line positions was better than ± 0.001 cm^{-1} in favorable conditions. The 550 line positions observed have been compared with the values derived from rotation–vibration spectra. The strongest lines of the isotopic molecules $H_2{}^{18}O$, $H_2{}^{17}O$, and $HD^{16}O$ have been identified and many rotational transitions in the vibrational level (010) have also been assigned.

I. INTRODUCTION

The spectrum of water vapor is most suitable for calibration of spectrometers in the far-infrared region. The reason is that the pure rotational spectrum of H_2O has relatively strong lines over the whole far-infrared spectral region. Further, the sample often involves a small amount of water, so that the strongest water lines are usually present in all spectra. This is more significant in high-resolution work where relatively weak water lines appear in the spectrum, because they are often much narrower than the other absorptions. These originally troublesome lines can, however, be used in providing the wavenumber scale if their frequencies are known with sufficient accuracy.

The pure rotational spectrum of water vapor has previously been measured by, for example, Rao *et al.* (*1*) in the region 260–540 cm^{-1}, Hall and Dowling (*2*) in 5–125 cm^{-1} and (*3*) in 92–250 cm^{-1}, Izatt *et al.* (*4*) in 475–692 cm^{-1}, Sanderson and Scott (*5*) in 20–220 cm^{-1}, Sakai (*6*) in 20–120 cm^{-1}, Winther (*7*) in 100–650 cm^{-1}, and Fleming and Gibson (*8*) in 10–40 cm^{-1}.

There is available no measurement performed by one instrument and extending over the whole far-infrared region with such a high resolution and accuracy that we would have been able to use it for the calibration of our interferometer. These facts have suggested to us that it would be advantageous to record a new absorption spectrum of natural water vapor between 30 and 720 cm^{-1}.

II. EXPERIMENTAL DETAILS

A. *Recording of the Interferograms and Computation of the Spectrum*

The interferograms of water vapor were recorded with a Michelson-type double-beam Fourier spectrometer (*9*) constructed in our laboratory. The sampling points of the interferograms, typically 70 000, were collected into the disk memory of a Hewlett–

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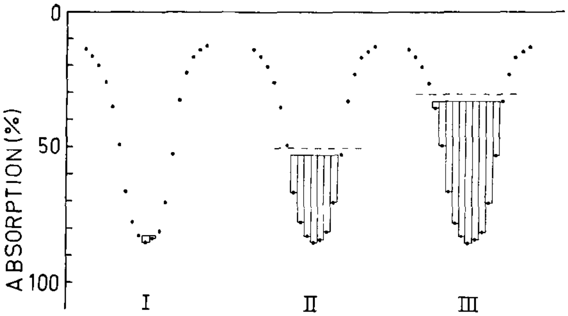

FIG. 1. Illustration of three methods for evaluating the center of the gravity of an absorption line. In the first method the original line is replaced by the line formed by three spectral points, in the second by the line below the 50% absorption level, and in the third by the line below the 30% absorption level.

Packard 21MX computer connected on line to the Fourier spectrometer. The interferograms were recorded out to an optical path difference of 50 cm, which gives a truncation broadening of about 0.012 cm^{-1}. All the interferograms were recorded using a cell with an absorbing path length of 1 m. The pressures of water vapor were between 0.4 and 4 Torr. The spectrum was computed by the fast Fourier transform of 8192 points, using mathematical filtering and phase correction (*10*) simultaneously. Very small errors in the measurement of the optical path difference were also corrected by a computation method (*11*), whenever necessary, before the Fourier transform. The spectra were plotted with the aid of a Hewlett-Packard Graphic Plotter 7210A.

B. Calculations of Line Positions

The line positions were computed directly from the spectral points produced by the fast Fourier transform. In the spectrum for the calculation of the line positions the interval of the adjacent spectral points computed was typically 4×10^{-3} cm^{-1}. The intensity scale of the spectrum was fixed so that the strongest line in each recording had 100% absorption in that scale. The line position was obtained by evaluating the

TABLE I

The Measurement Conditions of the Spectrum Shown in Fig. 2

Range (cm^{-1})	Pressure (Torr)	Thickness of beam splitter (μm)	Filters	Windows of gas cell
30-150	1.4	18	black polyethylene	polyethylene
150-390	1.8	5	black polyethylene	polyethylene
390-720	4.0	3.5	OCLI*, LI3200-9	KBr

* Optical Coating Laboratory, INC.

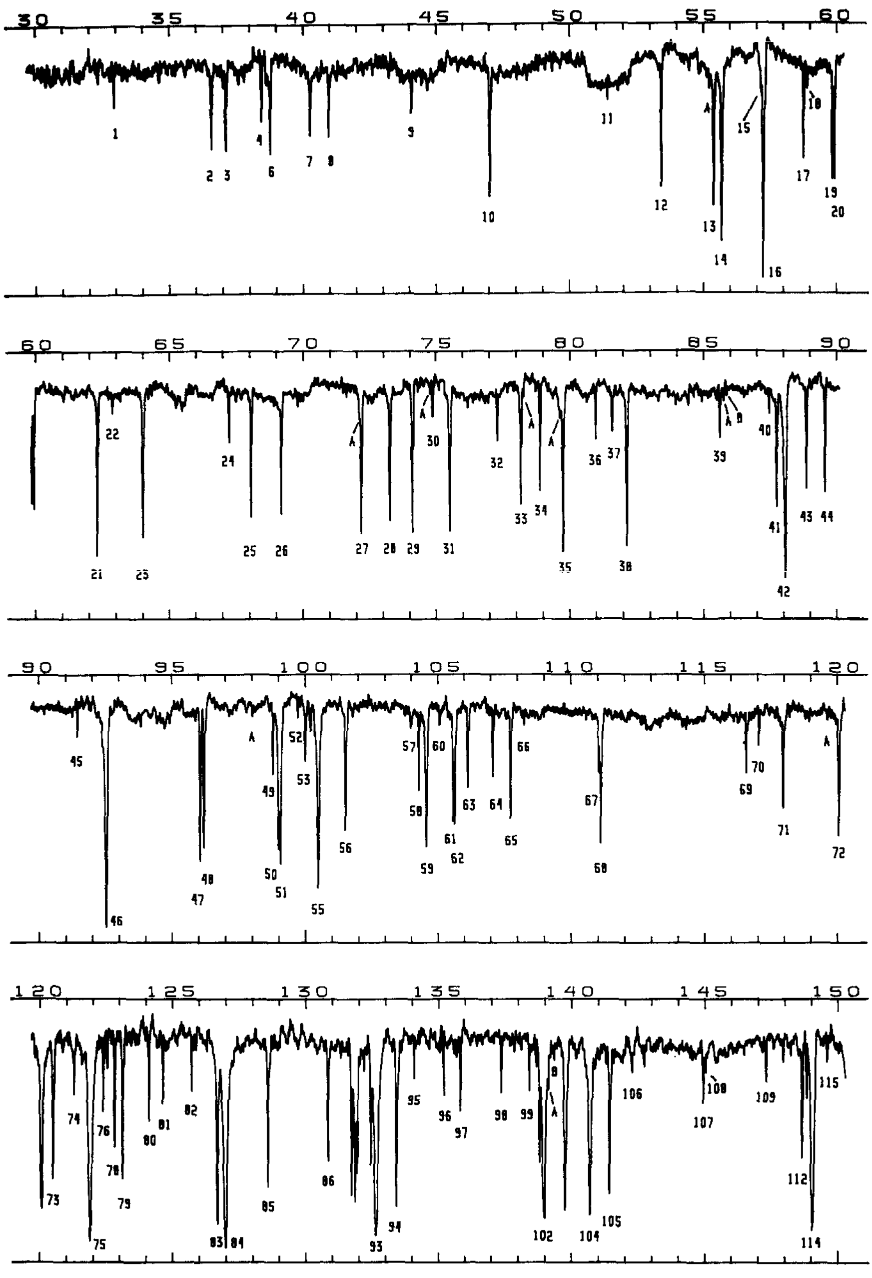

FIG. 2. Pure rotational spectrum of water vapor between 30 and 720 cm^{-1}. The apodized spectrum was recorded in three runs under the measurement conditions listed in Table I. Resolution is about 0.03 cm^{-1}. Absorption is down. The HD^{16}O abundance between 150 and 390 cm^{-1} is greater than in natural water. The unapodized part of this spectrum between 30 and 150 cm^{-1} has been published in IUPAC Tables (*14*).

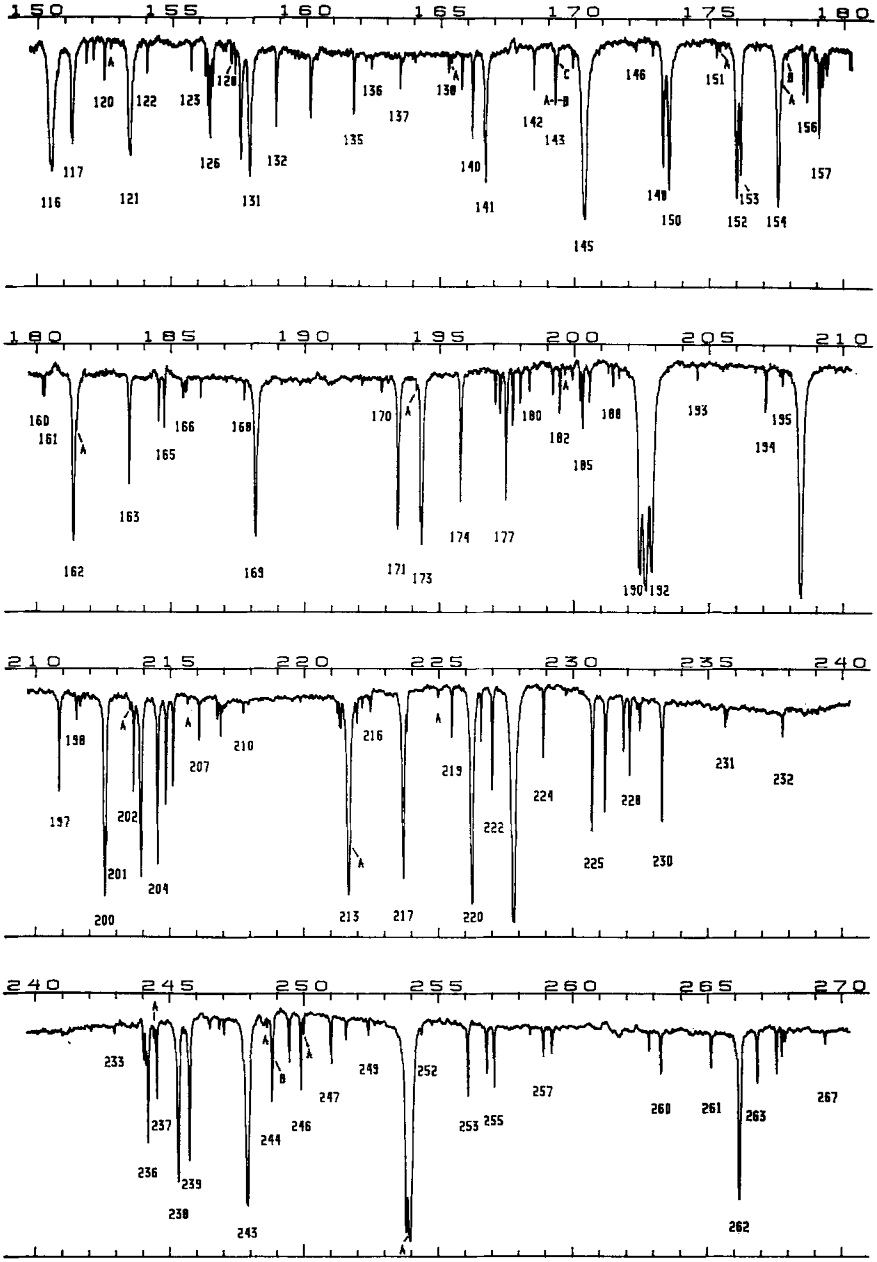

FIGURE 2—*Continued*

center of gravity of the line in three different ways. These methods are illustrated in Fig. 1. The positions of the lines with weaker than 40% absorption were usually taken from the computation by the first method, those of the lines with absorption within 40–70% were computed by the third method, and the positions of the lines with greater

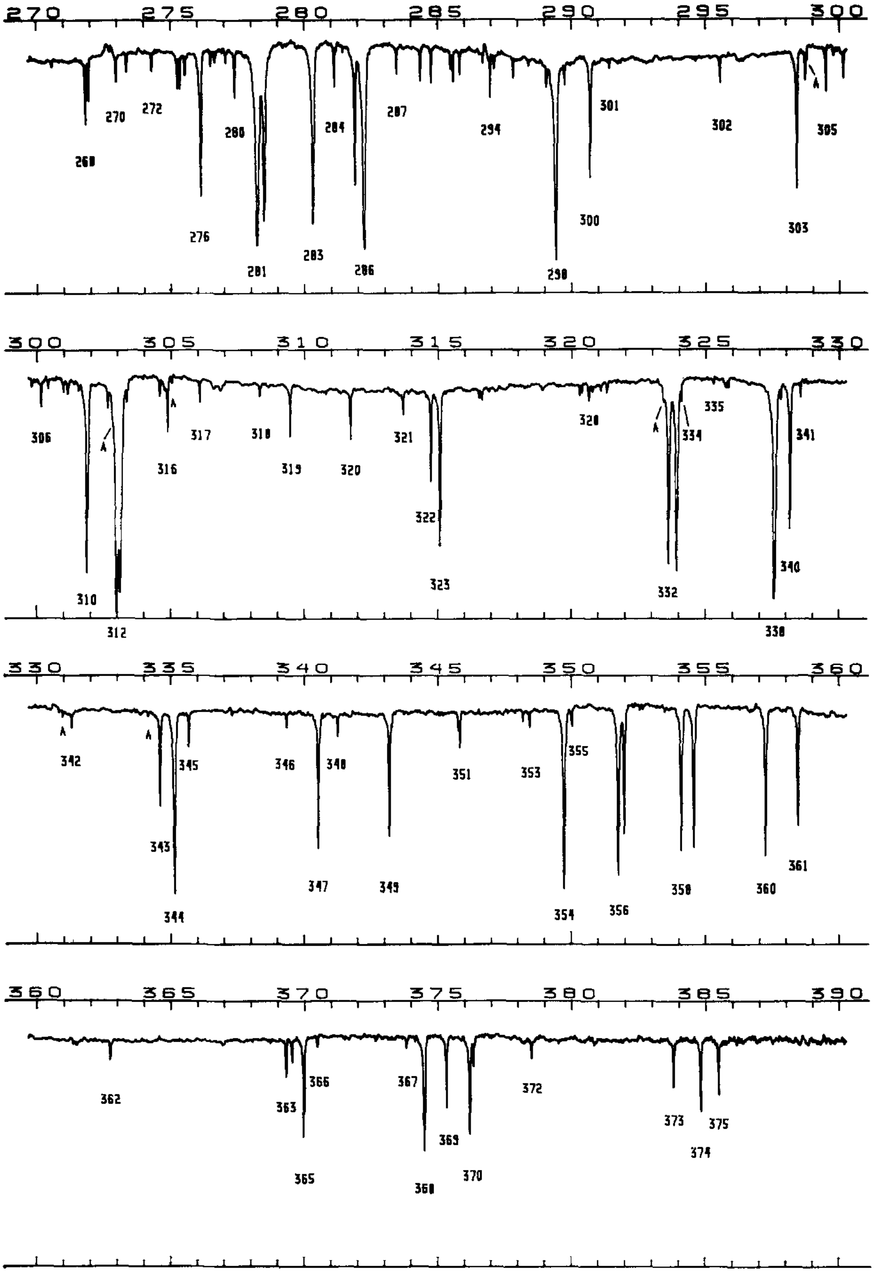

FIGURE 2—*Continued*

than 70% absorption were computed by the second method. The positions of the lines just resolved were taken from the computation accomplished in the first way. If the number of the computed points in the line is sufficient, the error in the line position due to the computation methods shown in Fig. 1 is, in practice, much smaller than the errors caused by the noise in the spectrum.

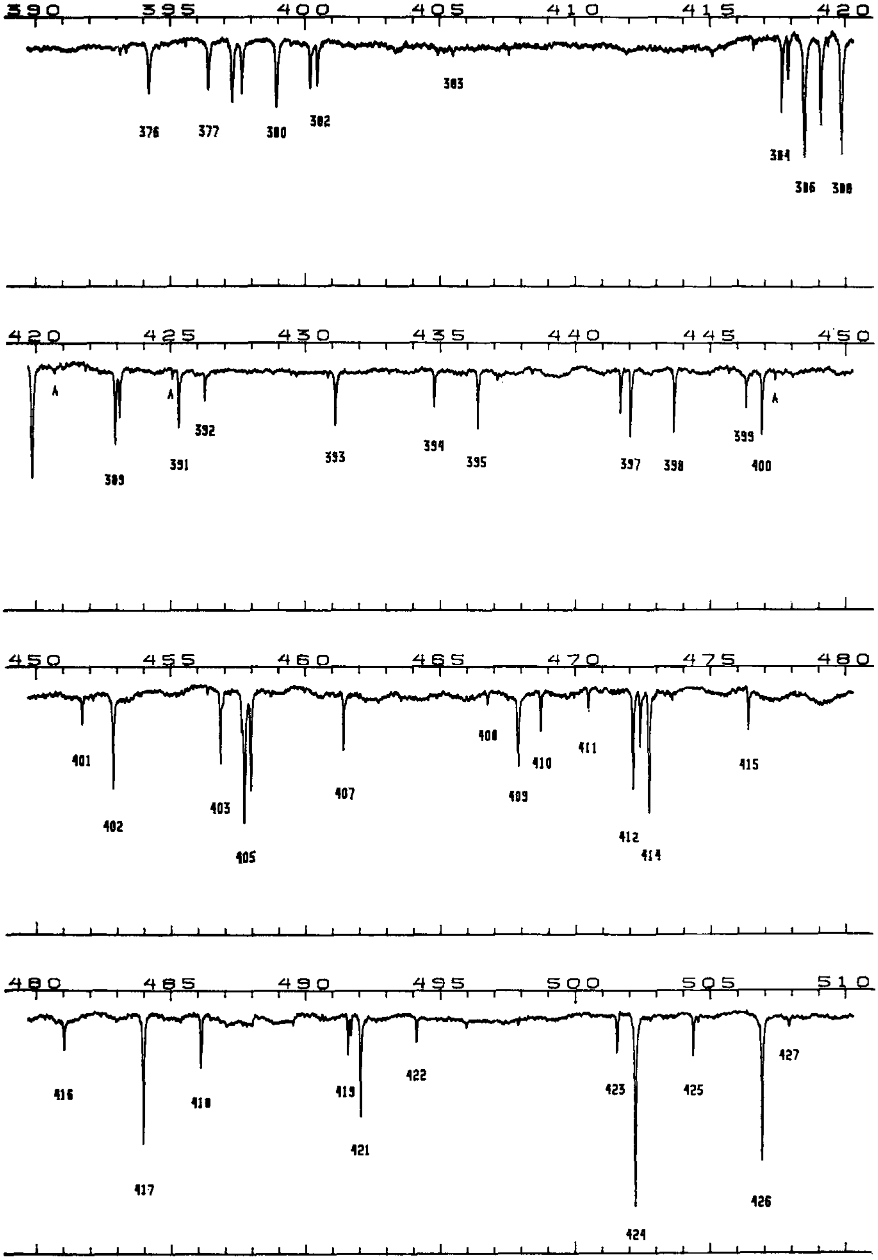

FIGURE 2—*Continued*

C. *Calibration and Accuracy of Wavenumbers*

The wavenumber scale of the spectrum produced by a Fourier spectrometer is always linear, that is

$$\nu = k\nu_c, \tag{1}$$

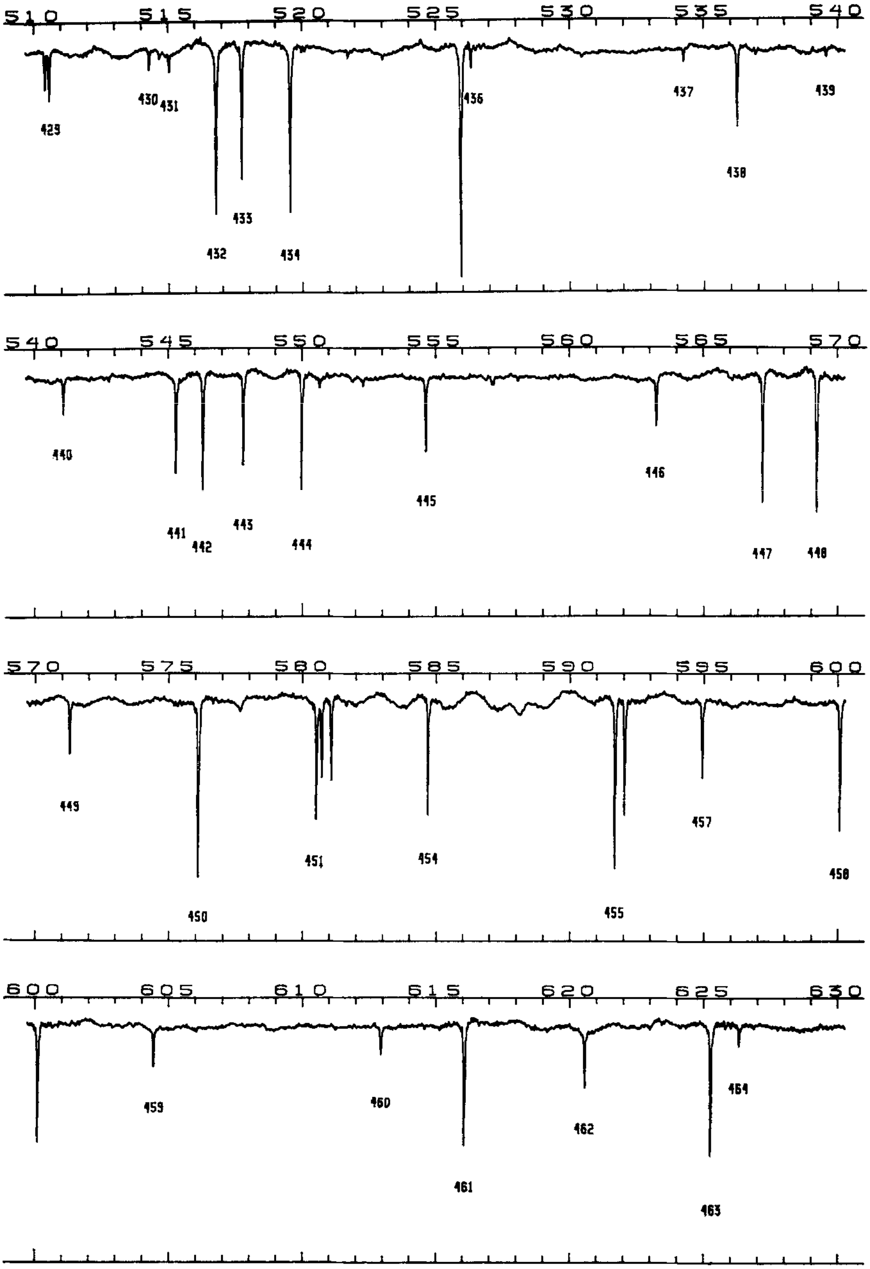

FIGURE 2—*Continued*

where k is constant, ν_c is the calculated wavenumber, and ν is the actual wavenumber. The linearity of the scale of the spectrum means that the Fourier spectrometer only requires one calibration line. In the present instrument it is the He–Ne or argon ion laser line used for the measurement of the position of the moving mirror in the inter-

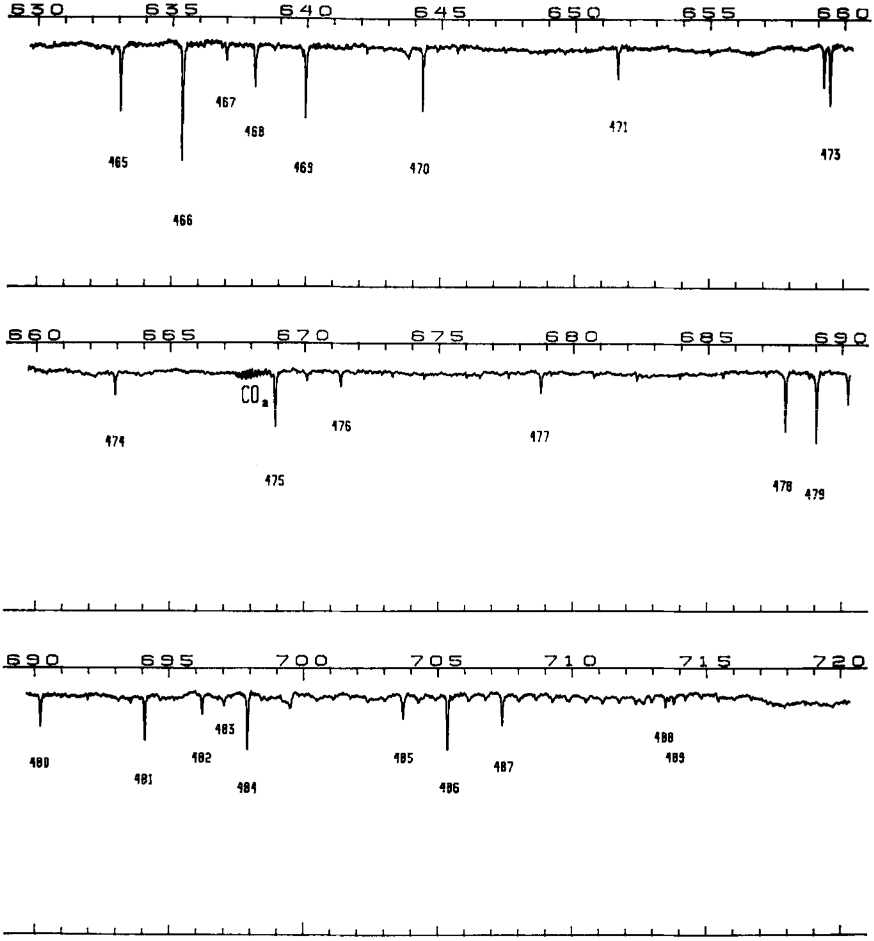

FIGURE 2—*Continued*

ferometer. The constant k in Eq. (1) is determined by the following equation (*12*):

$$k = \frac{\cos\beta}{(1 + a\epsilon\delta\nu)[1 - (\Omega/4\pi)]}, \tag{2}$$

where β is the angle between the laser beam and the infrared beam, Ω is the finite solid angle subtended by the source, $\delta\nu$ is the half-width of an infrared line, ϵ is the linear phase error of the interferogram, and a is the parameter varying within 1.6–2.6, depending on the line shape. The equation is valid for the peak position. The solid angle Ω and the angle β can be estimated with certain accuracy from the dimensions of the interferometer and the linear phase error can be eliminated from the interferogram (*10*). After this we have the relative error of the wavenumber $|\Delta\nu/\nu| < 4 \times 10^{-6}$ (*12*). The accuracy of the wavenumbers can be improved by using some calibration line also in the infrared beam, because with the help of that line the constant k can be measured more

TABLE II

Pure Rotational Transitions of Natural Water Vapor between 30 and 720 cm^{-1a}

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
1		2(0, 2)- 1(1, 1)	32.95373	.9554	-17	0.928 -2
			.9539		-15	
2		3(1, 2)- 3(0, 3)	36.60408	.6056	-15	0.618 -1
			.6037		-19	
3		1(1, 1)- 0(0, 0)	37.13728	.1371	+2	0.184 -1
			.1369		-2	
4		3(1, 2)- 2(2, 1)	38.46404	.4661	-21	0.960 -2
			.4632		-29	
5		6(3, 4)- 5(4, 1)	38.63742	.6378	-4	0.881 -3
			.6380		+2	
6		3(2, 1)- 3(1, 2)	38.79063	.7905	+1	0.656 -1
			.7909		+4	
7		4(2, 2)- 4(1, 3)	40.28242	.2827	-3	0.205 -1
			.2823		-4	
8		2(2, 0)- 2(1, 1)	40.98819	.9894	-12	0.178 -1
			.9880		-14	
9		6(2, 5)- 5(3, 2)	44.09947	.0996	-1	0.216 -2
			.0995		-1	
10		5(2, 3)- 5(1, 4)	47.05323	.0548	-16	0.538 -1
			.0532		-16	
11		6(3, 3)- 5(4, 2)	51.43429	.4347	-4	0.600 -3
			.4349		+2	
12		4(1, 3)- 4(0, 4)	53.44422	.4454	-12	0.268 -1
			.4447		-7	
13A	18	2(1, 2)- 1(0, 1)	55.239	.2327	+63	0.325 -3
13		2(2, 1)- 2(1, 2)	55.40538	.4064	-10	0.671 -1
			.4061		-3	
14		2(1, 2)- 1(0, 1)	55.70214	.7045	-24	0.159 0
			.7016		-29	
15		4(3, 2)- 5(0, 5)	57.16877	.1724	-36	0.278 -3
			.1688		-36	
16		3(0, 3)- 2(1, 2)	57.26534	.2676	-23	0.148 0
			.2656		-20	
17		6(3, 3)- 6(2, 4)	58.77530	.7744	+9	0.114 -1
			.7750		+6	
18		7(3, 5)- 6(4, 2)	58.91364	.9157	-21	0.493 -3
			.9139		-18	
19		6(2, 4)- 6(1, 5)	59.86800	.8682	-2	0.147 -1
			.8679		-3	
20		7(3, 4)- 7(2, 5)	59.94676	.9464	+4	0.186 -1
			.9470		+6	
21		5(3, 2)- 5(2, 3)	62.30150	.3021	-6	0.591 -1
			.3014		-7	
22		8(4, 5)- 7(5, 2)	62.87330	.8741	-8	0.397 -3
			.8737		-4	
23		5(2, 3)- 4(3, 2)	63.99390	SH		0.116 -1
			.9941			
		3(2, 2)- 3(1, 3)	64.02288	.0226	+3	0.338 -1
			.0228		+2	
24		8(3, 5)- 8(2, 6)	67.24547	.2454	+1	0.330 -2
			.2454		0	
25		4(3, 1)- 4(2, 2)	68.06315	.0635	-4	0.281 -1
			.0632		-3	
26		4(1, 3)- 3(2, 2)	69.19560	.1955	+1	0.190 -1
			.1957		+2	
27A		8(4, 4)- 7(5, 3)	72.12884	.1289	-1	0.195 -3
			.1291		+2	
27		3(1, 3)- 2(0, 2)	72.18789	.1888	-9	0.990 -1
			.1877		-11	
28		3(3, 0)- 3(2, 1)	73.26248	.2627	-2	0.798 -1
			.2626		-1	

accurately than from the dimensions of the interferometer. Hence, in practice, we often use water vapor lines for the calibration of the wavenumber scale.

In this work we used six water vapor lines to fix the constant *k*. The wavenumbers

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I	
29		5(1, 4)- 5(0, 5)	74.10944 .1097	.1093	+1 +4	0.845	-1
30A	18	4(2, 3)- 4(1, 4)	74.799	.7919	+71	0.229	-3
30		8(3, 6)- 7(4, 3)	74.87900 .8787	.8781	+9 +6	0.124	-2
31		4(2, 3)- 4(1, 4)	75.52416 .5242	.5252	-10 -10	0.112	0
32		9(4, 5)- 9(3, 6)	77.31620 .3164	.3156	+6 +8	0.322	-2
33		7(2, 5)- 7(1, 6)	78.19591 .1957	.1953	+6 +4	0.322	-1
33A		10(4, 6)-10(3, 7)	78.30309 .3018	.3055	-24 -37	0.382	-3
34		3(3, 1)- 3(2, 2)	78.91783 .9181	.9178	0 +3	0.293	-1
35A	18	4(0, 4)- 3(1, 3)	79.660	.6619	-19	0.225	-3
35		4(0, 4)- 3(1, 3)	79.77426 .7738	.7758	-15 -20	0.110	0
36		9(3, 6)- 9(2, 7)	80.99792 .9977	.9966	+13 +11	0.500	-2
37		8(4, 4)- 8(3, 5)	81.61863 .6184	.6169	+17 +15	0.291	-2
38		4(3, 2)- 4(2, 3)	82.15440 .1542	.1564	-20 -22	0.107	0
39		7(3, 4)- 6(4, 3)	85.63180 .6322	.6311	+7 +11	0.432	-2
39A		11(4, 7)-11(3, 8)	85.78445 .7843	.7849	-5 -6	0.399	-3
39B		10(3, 8)- 9(4, 5)	85.89281 .8929	.8938	-10 -9	0.191	-3
40	18	4(1, 4)- 3(0, 3)	87.486	.4908	-48	0.884	-3
41		5(3, 3)- 5(2, 4)	87.75941 .7592	.7589	+5 +3	0.312	-1
42		4(1, 4)- 3(0, 3)	88.07673 .0766	.0757	+10 +9	0.432	0
43		7(4, 3)- 7(3, 4)	88.88044 .8804	.8804	0 0	0.216	-1
44		5(2, 4)- 5(1, 5)	89.58352 .5837	.5838	-3 -1	0.346	-1
45	18	2(2, 1)- 1(1, 0)	91.456	.4533	+27	0.757	-3
46		2(2, 1)- 1(1, 0)	92.53014 .5305	.5312	-11 -7	0.370	0
47		6(3, 4)- 6(2, 5)	96.06703 .0672	.0686	-16 -14	0.684	-1
48		6(1, 5)- 6(0, 6)	96.20913 .2089	.2194		0.244	-1
		6(4, 2)- 6(3, 3)	96.23163 .2316			0.146	-1
49A	18	2(2, 0)- 1(1, 1)	98.035	.0300	+50	0.241	-3
49		6(2, 4)- 5(3, 3)	98.80532 .8057	.8057	-4 0	0.943	-2
50		2(2, 0)- 1(1, 1)	99.02705 .0270	.0274	-4 -4	0.118	0
51		5(1, 4)- 4(2, 3)	99.09507 .0951	.0957	-6 -6	0.133	0
52	18	5(1, 4)- 4(2, 3)	99.743	.7378	+52	0.272	-3

of these lines, 73.26248, 107.74633, 183.46417, 245.75529, 483.98489, and 616.07312 cm^{-1}, were derived from the energy levels of Flaud and Camy-Peyret (*13*). These lines were selected in such a way that at least two of them occur in every recording. It was also required that their accuracy be of the order of 0.001 cm^{-1} as determined by the error limits in Flaud and Camy-Peyret's work (*13*). In each recording the constant *k* was

TABLE II—*Continued*

NO	MO	$J'(K'_a,K'_c)-J''(K''_a,K''_c)$	FREQ	OBS	DIFF	I
53		8(2, 6)- 8(1, 7)	100.02140	.0215	-1	0.676 -2
			.0213		-2	
54A		10(3, 7)-10(2, 8)	100.18106	.1804	+7	0.763 -3
			.1809		+5	
54	18	5(0, 5)- 4(1, 4)	100.214	.2166	-26	0.953 -3
55A	17	5(0, 5)- 4(1, 4)	100.356	.3715	-155	0.173 -3
55		5(0, 5)- 4(1, 4)	100.50979	.5104	-6	0.466 0
			.5096		-8	
56		5(4, 1)- 5(3, 2)	101.52908	.5294	-3	0.666 -1
			.5287		-7	
57A	18	5(1, 5)- 4(0, 4)	103.979	.9811	-21	0.352 -3
57B		10(4, 7)- 9(5, 4)	104.03850	.0359	+26	0.225 -3
			.0389		+30	
58		4(4, 0)- 4(3, 1)	104.29178	.2915	+3	0.220 -1
			.2916		+1	
59		5(1, 5)- 4(0, 4)	104.57256	.5735	-9	0.172 0
			.5728		-7	
60		9(4, 5)- 8(5, 4)	105.06856	.0661	+25	0.722 -3
			.0690		+29	
61		4(4, 1)- 4(3, 2)	105.59106	.5912	-1	0.672 -1
			.5911		-1	
62		6(2, 5)- 6(1, 6)	105.65929	.6588	+5	0.820 -1
			.6591		+3	
63		5(4, 2)- 5(3, 3)	106.14633	.1463	0	0.236 -1
			.1458		-5	
64		7(3, 5)- 7(2, 6)	107.08602	.0869	-9	0.146 -1
			.0856		-13	
65		6(4, 3)- 6(3, 4)	107.74633	.7460	+3	0.515 -1
			.7460		0	
66		10(5, 5)-10(4, 6)	108.25284	.2522	+6	0.373 -3
			.2553		+31	
67		7(4, 4)- 7(3, 5)	111.05005	.0505	-5	0.102 -1
			.0501		-4	
68		3(2, 2)- 2(1, 1)	111.12564	.1259	-3	0.148 0
			.1254		-5	
59		8(4, 5)- 8(3, 6)	116.59265	.5923	+4	0.159 -1
			.5930		+7	
70		9(5, 4)- 9(4, 5)	117.06213	.0626	-5	0.364 -2
			.0617		-9	
71		7(1, 6)- 7(0, 7)	117.97064	.9702	+4	0.534 -1
			.9710		+8	
72A	18	6(0, 6)- 5(1, 5)	119.644	.6348	+92	0.340 -3
72		6(0, 6)- 5(1, 5)	120.07112	.0715	-4	0.166 0
			.0718		+3	
73		8(3, 6)- 8(2, 7)	120.51584	.5168	-10	0.247 -1
			.5156		-12	
74	18	6(1, 6)- 5(0, 5)	121.311	.3038	+72	0.106 -2
75		6(1, 6)- 5(0, 5)	121.90435	.9039	+5	0.518 0
			.9047		+8	
76		8(3, 5)- 7(4, 4)	122.41306	.4144	-13	0.199 -2
			.4135		-9	
77		11(3, 8)-11(2, 9)	122.55888	.5623	-34	0.930 -3
			.5583		-40	
78		9(2, 7)- 9(1, 8)	122.84167	.8423	-6	0.110 -1
			.8417		-6	
79		7(2, 6)- 7(1, 7)	123.12886	.1296	-7	0.188 -1
			.1294		-2	

adjusted so that the spectrum gave the best attainable agreement with the calibration values. Now, we must bear in mind that the constant *k* is not the same in all the recordings, because Ω and β may change during the adjustments needed in the selection of the wavenumber region. For example, in the spectrum of 150–390 cm^{-1} seen in Fig. 2 the

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
80		8(5, 3)- 8(4, 4)	124.13567	.1363	-6	0.320 -2
			.1364		+1	
81		9(4, 6)- 9(3, 7)	124.65361	.6530	+6	0.244 -2
			.6532		+2	
82	18	4(2, 3)- 3(1, 2)	125.741	.7391	+19	0.935 -3
83		6(1, 5)- 5(2, 4)	126.69673	.6970	-3	0.630 -1
			.6970		0	
84		4(2, 3)- 3(1, 2)	126.99681	.9969	-1	0.457 0
			.9971		+2	
85		7(5, 2)- 7(4, 3)	128.59835	.5993	-10	0.199 -1
			.5980		-13	
86		6(5, 1)- 6(4, 2)	130.85210	.8523	-2	0.106 -1
			.8519		-4	
87		5(5, 0)- 5(4, 1)	131.73526	.7351	+2	0.341 -1
			.7354		+3	
88	18	3(2,1)- 2(1, 2)	131.805	.8166	-116	0.749 -3
89		6(5, 2)- 6(4, 3)	131.87396	.8748	-8	0.321 -1
			.8741		-7	
		7(5, 3)- 7(4, 4)	131.90285			0.682 -2
			.9028			
90		5(5, 1)- 5(4, 2)	131.95876	.9595	-7	0.114 -1
			.9594		-1	
91	17	3(2, 1)- 2(1, 2)	132.208	.2074	+6	0.136 -3
92		8(5, 4)- 8(4, 5)	132.45817	.4575	+7	0.105 -1
			.4578		+3	
93		3(2, 1)- 2(1, 2)	132.66005	.6602	-2	0.366 0
			.6602		0	
94		7(2, 5)- 6(3, 4)	133.43137	.4314	0	0.405 -1
			.4312		-2	
95		9(5, 5) -9(4, 6)	134.09585	.0968	-10	0.152 -2
			.0956		-12	
96		10(4, 7)-10(3, 8)	135.20782	.2080	-2	0.303 -2
			.2077		-3	
97		9(3, 7)- 9(2, 8)	135.84574	.8460	-3	0.414 -2
			.8468		+8	
98		10(5, 6)-10(4, 7)	137.38325	.3836	-4	0.174 -2
			.3822		-14	
99	18	7(0, 7)- 6(1, 6)	138.412	.4244	-124	0.892 -3
100	17	7(0, 7)- 6(1, 6)	138.698	.6931	+49	0.162 -3
101		8(1, 7)- 8(0, 8)	138.82676	.8274	-6	0.111 -1
			.8269		-5	
102		7(0, 7)- 6(1, 6)	138.99114	.9906	+5	0.436 0
			.9908		+2	
102A	18	7(1, 7)- 6(0, 6)	139.112	.1384	-264	0.303 -3
102B	18	5(2, 4)- 4(1, 3)	139.384	.3708	+132	0.284 -3
103		7(1, 7)- 6(0, 6)	139.78282	.7815	+13	0.148 0
			.7823		+8	
104		5(2, 4)- 4(1, 3)	140.71186	.7123	-4	0.139 0
			.7118		-5	
105		8(2, 7)- 8(1, 8)	141.43790	.4387	-8	0.342 -1
			.4374		-13	
106	010	3(2, 1)- 2(1, 2)	142.275	.2781	-31	0.174 -3
107		10(2, 8)-10(1, 9)	144.95032	.9504	-1	0.174 -2
			.9499		-5	

calibration altered the constant k so that $\Delta k/k$ was 3×10^{-6}, which means a correction of 0.0006 cm^{-1} at 200 cm^{-1} and, correspondingly, in the spectrum of 390–720 cm^{-1} $\Delta k/k$ was -1×10^{-6}. In this way we achieve a wavenumber accuracy of ± 0.001 cm^{-1}.

TABLE II—*Continued*

NO	MO	$J'(K'_a,K'_c)-J''(K''_a,K''_c)$	FREQ	OBS	DIFF	I
108		11(6, 5)-11(5, 6)	145.05313	.0526	+5	0.299 -3
			.0517		-9	
109	18	3(3, 1)- 2(2, 0)	147.308	.3116	-36	0.591 -3
110		11(4, 8)-11(3, 9)	147.95963	.9570	+26	0.376 -3
			.9592		+22	
111	17	3(3, 1)- 2(2, 0)	148.129	.2550	-1260	0.107 -3
112		3(3, 0)- 3(0, 3)	148.65719	.6582	-10	0.570 -2
			.6572		-10	
113	18	3(3, 0)- 2(2, 1)	148.824	.8315	-75	0.179 -2
114		3(3, 1)- 2(2, 0)	149.05528	.0545	+8	0.289 0
			.0555		+10	
115	17	3(3, 0)- 2(2, 1)	149.621	.6229	-19	0.324 -3
116		3(3, 0)- 2(2, 1)	150.51715	.5175	-4	0.874 0
			.5167		-8	
116A		10(6, 4)-10(5, 5)	150.75249	.7523	+2	0.329 -3
			.7570		+47	
117		7(1, 6)- 6(2, 5)	151.30249	.3026	-1	0.190 0
			.3027		+1	
118	HDO	5(3, 3)- 4(2, 2)	151.830	.8302	-2	0.648 -4
119	18	6(2, 5)- 5(1, 4)	152.075	.0876	-126	0.693 -3
120		10(3, 8)-10(2, 9)	152.49407	.4943	-2	0.557 -2
			.4944		+1	
120A	17	6(2, 5)- 5(1, 4)	152.733	.7260	+70	0.126 -3
121		6(2, 5)- 5(1, 4)	153.45420	.4542	0	0.339 0
			.4541		-1	
122		9(6, 3)- 9(5, 4)	154.08575	.0857	+1	0.265 -2
			.0866		+9	
123		8(6, 2)- 8(5, 3)	155.72598	.7291	-31	0.196 -2
			.7341		+50	
124		10(6, 5)-10(5, 6)	156.25393	.2599		0.102 -2
			.2550			
		9(6, 4)- 9(5, 5)	156.26030			0.892 -3
			.2698			
125		7(6, 1)- 7(5, 2)	156.35851	.3589	-4	0.103 -1
			.3583		-6	
126		6(6, 0)- 6(5, 1)	156.42613	.4457		0.408 -2
			.4265			
		8(6, 3)- 8(5, 4)	156.44496			0.589 -2
			.4455			
		6(6, 1)- 6(5, 2)	156.45913			0.122 -1
			.4590			
127		7(6, 2)- 7(5, 3)	156.53828	.5402	-19	0.345 -2
			.5419		+17	
128A		11(6, 6)-11(5, 7)	156.84731*	.8143	+330	0.112 -3
			.8097		-46	
128B	HDO	11(1,10)-10(2, 9)	156.901	.8987	+23	0.730 -5
128C	18	8(0, 8)- 7(1, 7)	156.958	.9282	+298	0.221 -3
128D	010	8(1, 8)- 7(0, 7)	157.025	.0242	+8	0.155 -3
128	18	8(1, 8)- 7(0, 7)	157.233	.2230	+100	0.669 -3
129	HDO	5(3, 2)- 4(2, 3)	157.368	.3674	+6	0.667 -4

III. RESULTS

The results are mainly given in Table II and in the spectra shown in Figs. 2–4.

Figure 2 shows an overall view of the apodized spectrum recorded in three runs under the measurement conditions listed in Table I. Each range was computed from a single

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I	
130		8(0, 8)- 7(1, 7)	157.58436 .5850	.5846	-2 +4	0.108	0
131		8(1, 8)- 7(0, 7)	157.91901 .9198	.9203	-13 -5	0.327	0
132		9(1, 8)- 9(0, 9)	158.91136 .9109	.9112	+2 -3	0.181	-1
133		9(2, 8)- 9(1, 9)	160.17573 .1744	.1774	-17 -30	0.611	-2
134		9(3, 6)- 8(4, 5)	160.21053 .2104	.2114	-9 -10	0.568	-2
135		4(3, 1)- 4(0, 4)	161.78979 .7902	.7902	-4 0	0.395	-2
136		12(4, 9)-12(3,10)	162.44536 .4447	.4460	-6 -13	0.379	-3
137	HDO	6(3, 4)- 5(2, 3)	163.520	.5190	+10	0.506	-4
138	010	3(3, 0)- 2(2, 1)	165.310	.3096	+4	0.415	-3
138A	18	7(2, 6)- 6(1, 5)	165.425	.4189	+61	0.171	-3
139		11(2, 9)-11(1,10)	165.81617 .8161	.8161	+1 0	0.216	-2
140		8(2, 6)- 7(3, 5)	166.21764 .2182	.2180	-4 +2	0.135	-1
141		7(2, 6)- 6(1, 5)	166.70255 .7028	.7025	+1 +3	0.834	-1
142	18	4(3, 2)- 3(2, 1)	168.493	.4923	+7	0.150	-2
143A	HDO	4(4, 1)- 3(3, 0)	169.278	.2777	+3	0.101	-3
143B	HDO	4(4, 0)- 3(3, 1)	169.307	.3078	-8	0.101	-3
143C	17	4(3, 2)- 3(2, 1)	169.370	.3704	-4	0.272	-3
144		11(3, 9)-11(2,10)	169.93275 .9338	.9337	-10 +1	0.746	-3
145		4(3, 2)- 3(2, 1)	170.36058 .3604	.3622	-16 -18	0.733	0
146	HDO	13(1,13)-13(0,12)	172.278	.2735	+45	0.588	-5
147	18	8(1, 7)- 7(2, 6)	172.873	.8922		0.100	-3
	18	4(2, 2)- 3(1, 3)	172.883			0.198	-3
148		8(1, 7)- 7(2, 6)	173.28226 .2825	.2832	-9 -7	0.489	-1
149	HDO	7(3, 5)- 6(2, 4)	173.356	.3542	+18	0.360	-4
150		4(2, 2)- 3(1, 3)	173.50090 .5008	.5020	-11 -12	0.968	-1
151	18	9(0, 9)- 8(1, 8)	175.250	.2589	-89	0.432	-3
151A	18	9(1, 9)- 8(0, 8)	175.370	.3817	-117	0.144	-3
152		9(0, 9)- 8(1, 8)	176.00597 .0061	.0066	-6 -5	0.211	0
153		9(1, 9)- 8(0, 8)	176.14636 .1470	.1464	0 +6	0.705	-1
154		4(3, 1)- 3(2, 2)	177.54117 .5412	.5406	+6 +6	0.248	0
154A	HDO	6(2, 4)- 5(1, 5)	177.684	.6807	+33	0.190	-4

interferogram. In this spectrum resolution is only 0.03 cm^{-1} owing to the apodization. Within 150–390 cm^{-1} the $HD^{16}O$ abundance is greater than in natural water. The spectrum was computed in parts of 30 cm^{-1} using mathematical filtering. Each part consists of about 8000 computed points. The ranges 30–150, 150–390, and 390–720 cm^{-1} were individually scaled. The line strengths are comparable with each other only within

TABLE II—*Continued*

NO	MO	$J'(K'_a,K'_c)-J''(K''_a,K''_c)$	FREQ	OBS	DIFF	I
154B		11(7, 4)-11(6, 5)	177.84724* .8576	.8575	-103 +1	0.175 -3
155		10(1, 9)-10(0,10)	178.48581 .4855	.4860	-2 -5	0.291 -2
156		7(7, 0)- 7(6, 1)	178.62220 .6202	.6227		0.323 -2
		7(7, 1)- 7(6, 2)	178.62874 .6248			0.108 -2
157A		10(7, 3)-10(6, 4)	178.90858* .9045	.9088	-2 -43	0.170 -3
157B		8(7, 1)- 8(6, 2)	179.05198 .0442	.0517	+3 -75	0.816 -3
157		8(7, 2)- 8(6, 3)	179.07940 .0780	.0834		0.245 -2
		10(2, 9)-10(1,10)	179.08438 .0847		+10 +13	0.877 -2
158		9(7, 2)- 9(6, 3)	179.20608 .2045	.2049	+12 -4	0.125 -2
159A		9(7, 3)- 9(6, 4)	179.34670 .3330	.3383	+84 -53	0.417 -3
159B		10(7, 4)-10(6, 5)	179.37319 .3743	.3700	+32 +43	0.510 -3
160	18	8(2, 7)- 7(1, 6)	180.203	.2193	-163	0.340 -3
161		11(4, 7)-10(5, 6)	180.28862 .2893	.2888	-2 +5	0.414 -3
162		8(2, 7)- 7(1, 6)	181.38627 .3862	.3860	+3 +2	0.166 0
162A	HDO	8(3, 6)- 7(2, 5)	181.498	.4925	+55	0.238 -4
163		5(3, 2)- 5(0, 5)	183.46417 .4643	.4645	-3 -2	0.126 -1
164	HDO	5(4, 2)- 4(3, 1)	184.565	.5641	+9	0.854 -4
165	HDO	5(4, 1)- 4(3, 2)	184.772	.7701	+19	0.858 -4
166A	010	4(3, 2)- 3(2, 1)	185.477	.4808	-38	0.348 -3
166B		12(2,10)-12(1,11)	185.59724 .5889	.5897	+75 -8	0.264 -3
167	18	5(3, 3)- 4(2, 2)	186.136	.1347	+13	0.362 -3
168		12(3,10)-12(2,11)	187.75500 .7563	.7552	-2 +11	0.806 -3
169		5(3, 3)- 4(2, 2)	188.18885 .1887	.1876	+13 +11	0.177 0
170	18	9(1, 8)- 8(2, 7)	192.879	.8515	+275	0.190 -3
171		9(1, 8)- 8(2, 7)	193.47943 .4796	.4797	-3 -1	0.929 -1
172A	HDO	10(3, 8)- 9(2, 7)	194.152	.1478	+42	0.858 -5
172		10(0,10)- 9(1, 9)	194.32263 .3228	.3223	+3 +5	0.402 -1
173		10(1,10)- 9(0, 9)	194.38151 .3805	.3805	+10 0	0.121 0
174		9(2, 7)- 8(3, 6)	195.80526 .8057	.8058	-5 -1	0.307 -1
175	HDO	7(3, 4)- 6(2, 5)	197.087	.0858	+12	0.360 -4
176		10(3, 7)- 9(4, 6)	197.26474 .2647	.2641	+6 +6	0.136 -2

a narrow region, because the background spectrum is not constant over the whole working range. Some of the line numbers used in Table II are also marked in Fig. 2. Many weak lines or shoulders around a certain strong line have been indicated by letters: A, B, C, and D.

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
177		9(2, 8)- 8(1, 7)	197.49533 .4945	.4955	-2 -10	0.327 -1
178		11(1,10)-11(0,11)	197.73877 .7397	.7385	+3 +12	0.375 -2
179		11(2,10)-11(1,11)	198.01877 .0182	.0195	-7 -13	0.125 -2
180		8(8, 1)- 8(7, 2)	198.35297 .3510	.3524	+6 -14	0.646 -3
		8(8, 0)- 8(7, 1)	198.35571 .3504			0.215 -3
181		9(8, 1)- 9(7, 2)	199.21589 .2161	.2166	-7 -5	0.439 -3
		9(8, 2)- 9(7, 3)	199.21824 .2206			0.146 -3
182	HDO	6(4, 3)- 5(3, 2)	199.481	.4791	+19	0.663 -4
182A	HDO	11(3, 9)-10(2, 8)	199.664	.6600	+40	0.476 -5
183		10(8, 3)-10(7, 4)	199.93800 .9354	.9380	0 -26	0.201 -3
184	18	6(3, 4)- 5(2, 3)	200.227	.2238	+32	0.695 -3
185A	HDO	6(4, 2)- 5(3, 3)	200.305	.3045	+5	0.667 -4
185	18	4(4, 1)- 3(3, 0)	200.328	.3354	-74	0.205 -2
186	18	4(4, 0)- 3(3, 1)	200.567	.5772	-102	0.683 -3
187	17	6(3, 4)- 5(2, 3)	201.282	.2769	+51	0.126 -3
188	17	4(4, 1)- 3(3, 0)	201.444	.4417	+23	0.371 -3
189	17	4(4, 0)- 3(3, 1)	201.678	.6750	+30	0.124 -3
190		6(3, 4)- 5(2, 3)	202.46800 .4681	.4678	+2 +3	0.340 0
191		4(4, 1)- 3(3, 0)	202.68916 .6889	.6888	+4 +1	0.000 0
192		4(4, 0)- 3(3, 1)	202.91512 .9147	.9155	-4 -8	0.334 0
193		13(2,11)-13(1,12)	204.55913* .5760	.5726	-135 +34	0.259 -3
194	18	5(3, 2)- 4(2, 3)	207.098	.0950	+30	0.109 -2
195	17	5(3-, 2)- 4(2, 3)	207.738	.7357	+23	0.197 -3
196		5(3, 2)- 4(2, 3)	208.44980 .4497	.4491	+7 +6	0.531 0
197		5(4, 1)- 5(1, 4)	210.88381 .8833	.8838	0 -5	0.563 -2
198	18	7(3, 5)- 6(2, 4)	211.507	.5083	-13	0.135 -3
	HDO	7(2, 5)- 6(1, 6)	211.508			0.121 -4
199	18	11(0,11)-10(1,10)	211.670	.6517	+183	0.126 -3
200		11(0,11)-10(1,10)	212.55987 .5599	.5752		0.614 -1
		11(1,11)-10(0,10)	212.58470 .5852			0.205 -1

Figure 3 shows some parts of the spectrum unapodized and extended, in order to make clear the regions where the lines are close together. The resolution is 0.018 cm^{-1} defined as the half-width of the line. Figure 4 verifies the achieved maximum resolution of 0.018 cm^{-1} and the symmetrical line shape. The half-width of a weak line number 123

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
201		10(1, 9)- 9(2, 8)	212.63271 .6339	.6313	+14 +26	0.168 -1
		4(4, 0)- 4(1, 3)	212.63735 .6371			0.851 -3
202A	18	10(2, 9)- 9(1, 8)	213.485	.5040	-190	0.105 -3
202	HDO	5(5, 1)- 4(4, 0)	213.638	.6453		0.831 -4
	HDO	5(5, 0)- 4(4, 1)	213.640			0.831 -4
	HDO	7(4, 4)- 6(3, 3)	213.661			0.468 -4
203		7(3, 5)- 6(2, 4)	213.92057 .9205	.9207	-1 -2	0.661 -1
204		10(2, 9)- 9(1, 8)	214.55453 .5543	.5540	+5 +3	0.515 -1
205		6(3, 3)- 6(0, 6)	214.85243 .8518	.8619		0.284 -2
		6(4, 2)- 6(1, 5)	214.87493 .8745			0.221 -2
206		3(3, 1)- 2(0, 2)	215.12860 .1286	.1280	+6 +6	0.452 -2
206A		9(9, 0)- 9(8, 1)	215.64497* .6635	.6647	-197 -12	0.101 -3
		9(9, 1)- 9(8, 2)	215.73955* .6636			0.336 -4
207	HDO	7(4, 3)- 6(3, 4)	216.097	.0944	+26	0.476 -4
208		12(1,11)-12(0,12)	216.77014 .7747	.7714	-13 +33	0.483 -3
209		12(2,11)-12(1,12)	216.90078 .9020	.9019	-11 +1	0.145 -2
210	010	6(3, 4)- 5(2, 3)	217.744	.7428	+12	0.162 -3
211	18	8(3, 6)- 7(2, 5)	221.269	.2522	+168	0.217 -3
212A	18	5(2, 3)- 4(1, 4)	221.330	.3308	-8	0.387 -3
212B	HDO	8(3, 5)- 7(2, 6)	221.369	.3662	+28	0.218 -4
213		5(2, 3)- 4(1, 4)	221.67246 .6725	.6725	0 0	0.189 0
213A		10(2, 8)- 9(3, 7)	221.73729 .7370	.7371	+2 -1	0.612 -2
214	010	4(4, 1)- 3(3, 0)	221.983	.9830	0	0.475 -3
215	010	4(4, 0)- 3(3, 1)	222.167	.1663	+7	0.159 -3
216	010	5(3, 2)- 4(2, 3)	222.477	.4764	+6	0.252 -3
217		8(3, 6)- 7(2, 5)	223.70620 .7061	.7060	+2 +1	0.106 0
218	18	5(4, 2)- 4(3, 1)	223.850	.8386	+114	0.489 -3
219A	17	5(4, 2)- 4(3, 1)	224.991	.9835	+75	0.887 -4
219	18	5(4, 1)- 4(3, 2)	225.503	.5010	+20	0.147 -2
220		5(4, 2)- 4(3, 1)	226.27203 .2713	.2722	-2 -9	0.239 0
221	17	5(4, 1)- 4(3, 2)	226.599	.5966	+24	0.267 -3
	HDO	8(4, 5)- 7(3, 4)	226.603			0.297 -4

at 155.7291 cm^{-1} is smaller than 0.018 cm^{-1}. The separation of the doublet components number 143 around 169.3 cm^{-1} is 0.030 cm^{-1} and the spacing in the doublet number 159 around 179.35 is 0.032 cm^{-1}. The resolution is very near to the theoretical one

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
222		7(4, 3)- 7(1, 6)	227.02311 .0231	.0230	+1 +1	0.565 -2
223		5(4, 1)- 4(3, 2)	227.82448 .8242	.8234	+11 +8	0.720 0
224	HDO	6(5, 2)- 5(4, 1)	228.909	.9168		0.629 -4
	HDO	6(5, 1)- 5(4, 2)	228.926			0.629 -4
225		12(0,12)-11(1,11)	230.72336 .7252	.7332		0.930 -2
		12(1,12)-11(0,11)	230.74179 .7402			0.279 -1
226		11(1,10)-10(2, 9)	231.21426 .2149	.2131	+12 +18	0.239 -1
227		11(3, 8)-10(4, 7)	231.88742 .8872	.8878	-4 -6	0.233 -2
228		11(2,10)-10(1, 9)	232.11766 .1179	.1178	-1 +1	0.803 -2
229	HDO	8(4, 4)- 7(3, 5)	232.490	.4868	+32	0.307 -4
230		9(3, 7)- 8(2, 6)	233.31967 .3200	.3188	+9 +12	0.176 -1
231		13(1,12)-13(0,13)	235.64320 .6398	.6399	+33 -1	0.505 -3
231A		13(2,12)-13(1,13)	235.69403 .7011	.7005	-65 +6	0.168 -3
232	HDO	9(4, 6)- 8(3, 5)	237.785	.7794	+56	0.170 -4
233	18	4(3, 2)- 3(0, 3)	242.949	.9561	-71	0.830 -4
234	HDO	7(5, 3)- 6(4, 2)	244.038	.0355	+25	0.442 -4
235	HDO	7(5, 2)- 6(4, 3)	244.125	.1219	+31	0.442 -4
236		10(3, 8)- 9(2, 7)	244.20693 .2070	.2067	+2 +3	0.243 -1
237A	18	6(3, 3)- 5(2, 4)	244.447	.4455	+15	0.215 -3
237		11(2, 9)-10(3, 8)	244.53636 .5366	.5363	+1 +3	0.897 -2
238		6(3, 3)- 5(2, 4)	245.34003 .3399	.3403	-3 -4	0.105 0
	18	6(4, 3)- 5(3, 2)	245.313			0.900 -3
239		4(3, 2)- 3(0, 3)	245.75529 .7550	.7550	+3 0	0.406 -1
240	17	6(4, 3)- 5(3, 2)	246.538	.5291	+89	0.163 -3
241	HDO	10(4, 7)- 9(3, 6)	246.877	.8718	+52	0.891 -5
242	010	5(4, 1)- 4(3, 2)	247.046	.0479	-19	0.342 -3
243		6(4, 3)- 5(3, 2)	247.91283 .9127	.9113	+15 +14	0.440 0
244A	HDO	8(2, 6)- 7(1, 7)	248.644	.6420	+20	0.712 -5
244		13(0,13)-12(1,12)	248.81727 .8222	.8238		0.114 -1
		13(1,13)-12(0,12)	248.83570 .8290			0.380 -2
244B		8(4, 4)- 8(1, 7)	248.88550 .8851	.8842	+13 +9	0.115 -2
245A	HDO	9(3, 6)- 8(2, 7)	249.448	.4427	+53	0.116 -4

determined by the half-width of the instrument profile, i.e., the convolution of the truncation and the aperture broadening (*12*).

In Table II the observed wavenumbers are partly the average values of several

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
245		12(1,11)-11(2,10)	249.47473 .4817	.4789	-42 +28	0.335 -2
246		12(2,11)-11(1,10)	249.90380 .9025	.9034	+4 -9	0.101 -1
246A	HDO	9(4, 5)- 8(3, 6)	250.019	.0120	+70	0.180 -4
247A	18	5(5, 1)- 4(4, 0)	251.014	.0058	+82	0.479 -3
247	18	5(5, 0)- 4(4, 1)	251.046	.0377	+83	0.143 -2
248	18	6(4, 2)- 5(3, 3)	251.599	.5909	+81	0.305 -3
249A	17	5(5, 1)- 4(4, 0)	252.392	.3749	+171	0.868 -4
249B	17	5(5, 0)- 4(4, 1)	252.423	.4158	+72	0.260 -3
249C	17	6(4, 2)- 5(3, 3)	252.640	.6300	+100	0.553 -4
250		6(4, 2)- 5(3, 3)	253.81225 .8123	.8113	+10 +10	0.149 0
251A		5(5, 1)- 4(4, 0)	253.93901 .9391	.9361	+29 +30	0.234 0
251		5(5, 0)- 4(4, 1)	253.96868 .9685	.9700	-13 -15	0.701 0
252		14(1,13)-14(0,14)	254.37886 .3732	.3974		0.527 -4
		14(2,13)-14(1,14)	254.39270* .3954		-47 -20	0.160 -3
253		7(3, 4)- 7(0, 7)	256.11331 .1137	.1134	-1 +3	0.402 -2
254	HDO	6(6, 1)- 5(5, 0)	256.822	.8187	+33	0.479 -4
	HDO	6(6, 0)- 5(5, 1)	256.822		+33	0.479 -4
255		11(3, 9)-10(2, 8)	257.10009 .1018	.1005	-4 +13	0.344 -2
256	010	6(3, 3)- 5(2, 4)	258.441	.4288		0.499 -4
		13(4, 9)-12(5, 8)	258.40478* .4203			0.835 -4
257	HDO	8(5, 4)- 7(4, 3)	258.926	.9205	+55	0.284 -4
258	HDO	8(5, 3)- 7(4, 4)	259.242	.2352	+68	0.285 -4
259		12(3, 9)-11(4, 8)	262.83844* .8456	.8373	+11 +83	0.365 -3
260		4(4, 1)- 4(1, 4)	263.26962 .2695	.2721	-25 -26	0.666 -3
	18	7(4, 4)- 6(3, 3)	263.286			0.158 -3
261		12(2,10)-11(3, 9)	265.13922 .1368	.1375	+17 -7	0.124 -2
262		7(4, 4)- 6(3, 3)	266.19532 .1956	.1953	0 +3	0.773 -1
263		14(0,14)-13(1,13)	266.83330 .8446	.8444		0.140 -2
		14(1,14)-13(0,13)	266.85173 .8468			0.420 -2
264		13(1,12)-12(2,11)	267.55969 .5600	.5592	+5 +8	0.378 -2
265		13(2,12)-12(1,11)	267.75959 .7554	.7569	+27 -15	0.126 -2

recordings. The typical rms deviation in the position of the line, e.g., at 519.5893 cm^{-1}, was 2×10^{-4} cm^{-1} as derived from seven different recordings. In Table II the observed wavenumbers of $H_2{}^{16}O$ lines have been compared with two frequencies. The first value

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
266	010	6(4, 3)- 5(3, 2)	267.887	.8840	+30	0.209 -3
267	HDO	10(4, 6)- 9(3, 7)	269.398	.3887	+93	0.948 -5
268		12(3,10)-11(2, 9)	271.84263 .8427	.8411	+15 +16	0.397 -2
269	HDO	7(6, 2)- 6(5, 1)	271.963	.9577		0.330 -4
	HDO	7(6, 1)- 6(5, 2)	271.964			0.330 -4
270		8(5, 3)- 8(2, 6)	272.99977 273.0002	.9981	+17 +21	0.431 -3
271	HDO	9(5, 5)- 8(4, 4)	273.397	.3901	+69	0.168 -4
272	HDO	9(5, 4)- 8(4, 5)	274.329	.3196	+94	0.169 -4
273	18	6(5, 2)- 5(4, 1)	275.283	.2843	-13	0.890 -3
274		9(5, 4)- 9(2, 7)	275.37625 .3758	.3742	+21 +16	0.817 -3
275	18	6(5, 1)- 5(4, 2)	275.571	.5702	+8	0.297 -3
276		6(2, 4)- 5(1, 5)	276.14825 .1486	.1484	-2 +2	0.360 -1
277	010	5(5, 1)- 4(4, 0)	276.523	.5388		0.111 -3
	010	5(5, 0)- 4(4, 1)	276.544			0.333 -3
278	17	6(5, 2)- 5(4, 1)	276.701	.6790	+220	0.161 -3
279	18	8(4, 5)- 7(3, 4)	277.059	.0844	-254	0.217 -3
280		7(5, 2)- 7(2, 5)	277.42555 .4254	.4251	+5 +3	0.184 -2
281		6(5, 2)- 5(4, 1)	278.25771 .2581	.2577	0 +4	0.435 0
282		6(5, 1)- 5(4, 2)	278.51802 .5184	.5180	0 +4	0.145 0
283		8(4, 5)- 7(3, 4)	280.35209 .3521	.3523	-2 -2	0.106 0
	18	7(4, 3)- 6(3, 4)	280.311			0.489 -3
284		9(4, 5)- 9(1, 8)	281.15579 .1558	.1553	+5 +5	0.149 -2
285		5(3, 3)- 4(0, 4)	281.91549 .9157	.9153	+2 +4	0.200 -1
286		7(4, 3)- 6(3, 4)	282.25857 .2586	.2581	+5 +5	0.239 0
287		5(4, 2)- 5(1, 5)	283.48926 .4887	.4894	-1 -7	0.458 -3
288		13(2,11)-12(3,10)	284.36382* .3797	.3761	-123 +36	0.131 -2
289		15(0,15)-14(1,14)	284.78001 .7857	.7861	-61 -4	0.140 -2
		15(1,15)-14(0,14)	284.79844 .7867			0.466 -3
290		14(1,13)-13(2,12)	285.51813 .5167	.5094	+87 +73	0.428 -3
291		14(2,13)-13(1,12)	285.60123* .6024	.6024	-12 0	0.128 -2
292		6(5, 1)- 6(2, 4)	285.85903 .8585	.8590	0 -5	0.597 -3

has been calculated from the energy levels reported by Flaud and Camy-Peyret (*13*) and completed with the levels at higher *J* values reported by Pugh and Rao (*15*). The other calculated wavenumbers have been derived from the energy levels evaluated from

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
293		10(5, 5)-10(2, 8)	286.73699 .7380	.7339	+31 +41	0.143 -3
294A	010	7(4, 4)- 6(3, 3)	286.918	.9203	-23	0.367 -4
294	HDO	8(6, 3)- 7(5, 2)	286.995	.9915		0.210 -4
	HDO	8(6, 2)- 7(5, 3)	287.003			0.210 -4
295	HDO	10(5, 6)- 9(4, 5)	287.167	.1563	+107	0.903 -5
	18	9(4, 6)- 8(3, 5)	287.363			0.299 -4
296		13(3,11)-12(2,10)	287.86935* .8590	.8578	+116 +12	0.459 -3
297	18	7(3, 4)- 6(2, 5)	289.114	.0965	+175	0.317 -3
298		7(3, 4)- 6(2, 5)	289.44516 .4454	.4454	-2 0	0.155 0
299		13(3,10)-12(4, 9)	289.74976* .7726	.7714	-216 +12	0.416 -3
300		9(4, 6)- 8(3, 5)	290.72781 .7278	.7277	+1 +1	0.146 -1
301		16(1,15)-16(0,16)	- 291.4393	.4426		0.398 -5
		16(2,15)-16(1,16)	- 291.4463			0.119 -4
	HDO	11(4, 7)-10(3, 8)	291.454			0.446 -5
302		5(5, 0)- 5(2, 3)	295.56584 .5655	.5658	0 -3	0.768 -3
303		10(4, 7)- 9(3, 6)	298.41683 .4170	.4171	-3 -1	0.164 -1
304	HDO	7(7, 1)- 6(6, 0)	298.738	.7403	-23	0.203 -4
	HDO	7(7, 0)- 6(6, 1)	298.738		-23	0.203 -4
304A	18	7(5, 3)- 6(4, 2)	298.795	.8004	-54	0.160 -3
305	18	6(6, 1)- 5(5, 0)	299.517	.5127	+43	0.683 -3
	18	6(6, 0)- 5(5, 1)	299.521			0.227 -3
306	18	7(5, 2)- 6(4, 3)	300.170	.1694	+6	0.483 -3
307	010	7(4, 3)- 6(3, 4)	300.428	.4279	+1	0.114 -3
308	010	6(5, 2)- 5(4, 1)	300.995	.9958	-8	0.207 -3
309	17	6(6, 1)- 5(5, 0)	301.302	.1404	+1616	0.124 -3
	17	6(6, 0)- 5(5, 1)	301.305			0.412 -4
310		7(5, 3)- 6(4, 2)	301.86654 .8668	.8664	+1 +4	0.784 -1
311		16(0,16)-15(1,15)	- 302.6450	.6452		0.141 -3
		16(1,16)-15(0,15)	- 302.6455		 +3	0.427 -3
312A		14(2,12)-13(3,11)	302.85080& .8156	.8264	+244 -108	0.144 -3
312		6(6, 1)- 5(5, 0)	302.98158 .9817	.9850		0.334 0
		6(6, 0)- 5(5, 1)	302.98539 .9855			0.111 0

absorption and emission spectra by Flaud *et al.* (*16*). In that work the emission spectrum of hot water vapor gives naturally more accurate results to the higher energy levels, as it can be clearly seen from Table II by comparing the two calculated wavenumbers

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
313		7(5, 2)- 6(4, 3)	303.11059 .1106	.1100	+6 +6	0.236 0
314		15(1,14)-14(2,13)	303.31940& .3577	.3517	-323 +60	0.393 -3
315		14(3,12)-13(2,11)	304.66430& 304.5988	.5985	+658 +3	0.432 -3
316		11(4, 8)-10(3, 7)	304.87866 .8801	.8790	-3 +11	0.191 -2
316A	HDO	11(5, 6)-10(4, 7)	305.068	.0566	+114	0.453 -5
317		8(3, 5)- 8(0, 8)	306.09363 .0936	.0931	+5 +5	0.499 -3
318		11(5, 6)-11(2, 9)	308.33088 .3303	.3314	-5 -11	0.168 -3
319		6(4, 3)- 6(1, 6)	309.47265 .4723	.4723	+4 0	0.142 -2
320		12(4, 9)-11(3, 8)	311.72911 .7291	.7287	+4 +4	0.187 -2
321	HDO	8(7, 2)- 7(6, 1)	313.714	.7049		0.128 -4
	HDO	8(7, 1)- 7(6, 2)	313.714			0.128 -4
	18	8(4, 4)- 7(3, 5)	313.727			0.747 -4
322		4(4, 1)- 3(1, 2)	314.74227 .7424	.7422	+1 +2	0.645 -2
323		8(4, 4)- 7(3, 5)	315.08174 .0820	.0818	-1 +2	0.365 -1
324	HDO	10(6, 5)- 9(5, 4)	316.575	.5637	+113	0.670 -5
325	HDO	10(6, 4)- 9(5, 5)	316.687	.6749	+121	0.670 -5
326		13(4,10)-12(3, 9)	320.45780& .3189	.3285	+1293 -96	0.185 -3
327		17(0,17)-16(1,16)	- 320.4131	.4121		0.385 -4
		17(1,17)-16(0,16)	- 320.4134			0.389 -4
328	18	8(5, 4)- 7(4, 3)	320.671	.6691	+19	0.227 -3
329		15(2,13)-14(3,12)	- 320.7911	.7943	 -32	0.124 -3
330		16(1,15)-15(2,14)	- 321.1074	.1194		0.366 -4
		16(2,15)-15(1,14)	- 321.1244			0.108 -3
331	18	6(3, 4)- 5(0, 5)	321.343	.3390	+40	0.120 -3
332A		10(4, 6)-10(1, 9)	323.43447 .4326	.4360	-15 -34	0.160 -3
332		6(3, 4)- 5(0, 5)	323.63067 .6310	.6307	0 +3	0.586 -1
333		8(5, 4)- 7(4, 3)	323.92982 .9295	.9300	-2 -5	0.111 0
334A	18	7(6, 2)- 6(5,1)	324.051	.0550	-40	0.123 -3
334	18	7(6, 1)- 6(5, 2)	324.107	.0974	+96	0.370 -3
335	18	8(5, 3)- 7(4, 4)	325.290	.3102	-202	0.757 -4
336	010	7(5, 2)- 6(4, 3)	325.784	.7859	-19	0.112 -3

with the observed ones at high J and K_a values. That is also the main reason for using two calculated values for $H_2{}^{16}O$ line positions in Table II.

The calculated wavenumbers of $H_2{}^{18}O$ lines were derived from the energy levels given by Toth and Margolis (*17*). The calculated positions of $H_2{}^{17}O$ lines were obtained from the results reported by De Lucia and Helminger (*18*). The calculated frequencies and

TABLE II—*Continued*

NO	MO	$J'(K'_a,K'_c)-J''(K''_a,K''_c)$	FREQ	OBS	DIFF	I
337		5(5, 1)- 5(2, 4)	325.86450 .8644	.8663		0.130 -3
338		7(6, 2)- 6(5, 1)	327.55272 .5568	.5820		0.602 -1
		7(6, 1)- 6(5, 2)	327.59514 .5948			0.181 0
339	010	6(6, 1)- 5(5, 0)	327.820	.8177	+23	0.159 -3
	010	6(6, 0)- 5(5, 1)	327.823			0.527 -4
340		8(5, 3)- 7(4, 4)	328.16736 .1683	.1676	-2 +7	0.370 -1
341	HDO	9(7, 3)- 8(6, 2)	328.581	.5670	+140	0.745 -5
	HDO	9(7, 2)- 8(6, 3)	328.581		+140	0.745 -5
342A	HDO	11(6, 6)-10(5, 5)	330.987	.9728	+142	0.334 -5
342		14(4,11)-13(3,10)	331.38870& .2991	.3024	+863 -33	0.151 -3
343A		15(3,12)-14(4,11)	334.12230& .1562	.1596	-373 -34	0.398 -4
343		5(4, 2)- 4(1, 3)	334.61760 .6168	.6175	+1 -7	0.662 -2
344	18	7(2, 5)- 6(1, 6)	335.085	.1577		0.117 -3
		7(2, 5)- 6(1, 6)	335.15769 .1575		0 -2	0.572 -1
345		6(5, 2)- 6(2, 5)	335.68732 .6873	.6876	-3 -3	0.740 -3
346	HDO	8(8, 1)- 7(7, 0)	339.334	.3462	-122	0.659 -5
	HDO	8(8, 0)- 7(7, 1)	339.334		-122	0.659 -5
347		8(3, 5)- 7(2, 6)	340.54913 .5492	.5497	-6 -5	0.218 -1
348		7(4, 4)- 7(1, 7)	341.26493 .2651	.2646	+3 +5	0.357 -3
349		9(5, 5)- 8(4, 4)	343.20503 .2050	.2055	-5 -5	0.150 -1
350	18	7(7, 1)- 6(6, 0)	345.785	.7900	-50	0.781 -4
	18	7(7, 0)- 6(6, 1)	345.785		-50	0.235 -3
351		4(4, 0)- 3(1, 3)	345.85583 .8556	.8550	+8 +6	0.717 -3
352	18	8(6, 3)- 7(5, 2)	348.530	.2237	+3063	0.176 -3
353		9(6, 3)- 9(3, 6)	348.46408 .4647	.4675		0.288 -3
	18	8(6, 2)- 7(5, 3)	348.660$			0.587 -4
354		7(7, 1)- 6(6, 0)	349.75533 .7551	.7565		0.382 -1
		7(7, 0)- 6(6, 1)	349.75821 .7560		+17 -5	0.115 0
355		7(5, 3)- 7(2, 6)	350.03892 .0385	.0374	+15 +11	0.257 -3
356		8(6, 3)- 7(5, 2)	351.77643 .7770	.7772	-8 -2	0.861 -1
357		8(6, 2)- 7(5, 3)	351.99049 .9996	.9950	-45 +46	0.287 -1
358		9(4, 5)- 8(3, 6)	354.11938 .1198	.1205	-11 -7	0.427 -1

$ Reference (19)

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
359		9(5, 4)- 8(4, 5)	354.58886 .5885	.5897	-8 -12	0.456 -1
360		6(4, 3)- 5(1, 4)	357.26756 .2673	.2679	-3 -6	0.296 -1
361		10(5, 6)- 9(4, 5)	358.48388 .4828	.4840	-1 -12	0.158 -1
362		9(3, 6)- 9(0, 9)	362.75095 .7503	.7503	+7 0	0.489 -3
363		11(5, 7)-10(4, 6)	369.33380 .3356	.3338	0 +18	0.163 -2
364		8(5, 4)- 8(2, 7)	369.56666 .5664	.5663	+4 +1	0.572 -3
365		7(3, 5)- 6(0, 6)	369.99770 .9973	.9978	-1 -5	0.143 -1
366	18	8(7, 2)- 7(6, 1)	370.720$	.5089	+2111	0.111 -3
	18	8(7, 1)- 7(6, 2)	-			0.370 -4
367		7(6, 1)- 7(3, 4)	373.83730 .8367	.8371	+2 -4	0.283 -3
368		8(7, 2)- 7(6, 1)	374.49732 .4967	.4982		0.544 -1
		8(7, 1)- 7(6, 2)	374.50419 .5019			0.181 -1
369		9(6, 4)- 8(5, 3)	375.32966 .3384	.3353	-56 +31	0.120 -1
370		9(6, 3)- 8(5, 4)	376.21644 .2173	.2160	+4 +13	0.360 -1
371		12(5, 8)-11(4, 7)	376.36464 .3651	.3651	-5 0	0.136 -2
372		8(4, 5)- 8(1, 8)	378.54639 .5460	.5460	+4 0	0.619 -3
373		10(5, 5)- 9(4, 6)	383.82067 .8218	.8210	-3 +8	0.547 -2
374		7(4, 4)- 6(1, 5)	384.83862 .8385	.8388	-2 -3	0.101 -1
375		5(4, 1)- 4(1, 4)	385.50304 .5026	.5043	-13 -17	0.445 -2
376		8(8, 1)- 7(7, 0)	394.22809 .2275	.2295		0.295 -1
		8(8, 0)- 7(7, 1)	394.23116 .2275			0.983 -2
377		8(2, 6)- 7(1, 7)	396.43252 .4332	.4356	-31 -24	0.960 -2
378		9(3, 6)- 8(2, 7)	397.31902 .3190	.3201	-11 -11	0.251 -1
379		10(6, 5)- 9(5, 4)	397.67568 .6761	.6752	+5 +9	0.132 -1
380		9(7, 3)- 8(6, 2)	398.95038 .9373	.9663		0.762 -2
		9(7, 2)- 8(6, 3)	398.97756 .9763			0.229 -1
381		10(4, 6)- 9(3, 7)	400.22144 .2197	.2225	-11 -28	0.472 -2
382		10(6, 4)- 9(5, 5)	400.47731 .4832	.4823	-50 +9	0.437 -2
383		8(6, 3)- 8(3, 6)	405.49578 .4963	.4969	-11 -6	0.217 -3
384		11(5, 6)-10(4, 7)	417.65942 .6592	.6599	-5 -7	0.513 -2
385		11(6, 6)-10(5, 5)	417.92827* .8900	.8934	+349 -34	0.141 -2
386		8(4, 5)- 7(1, 6)	418.49476 .4948	.4949	-1 -1	0.235 -1

$ Reference (19)

TABLE II—*Continued*

NO	MO	$J'(K'_a,K'_c)-J''(K''_a,K''_c)$	FREQ	OBS	DIFF	I
387		9(8, 1)- 8(7, 2)	419.11405 .1144	.1137		0.123 -1
		9(8, 2)- 8(7, 1)	419.11664 .1137			0.411 -2
387A	HDO	12(4, 9)-11(1,10)	419.372	.3579	+141	0.633 -6
388		8(3, 6)- 7(0, 7)	419.87275 .8728	.8737	-10 -9	0.257 -1
388A		9(4, 6)- 9(1, 9)	420.67508 .6744	.6750	+1 -6	0.957 -4
389		10(7, 4)- 9(6, 3)	422.96312 .9638	.9630	+1 +8	0.848 -2
390		10(7, 3)- 9(6, 4)	423.12559* .1179	.1245	+11 -66	0.283 -2
391A		10(5, 6)-10(2, 9)	425.08514 .0843	.0867	-16 -24	0.151 -3
391		11(6, 5)-10(5, 6)	425.32930 .3287	.3282	+11 +5	0.421 -2
392		5(5, 1)- 4(2, 2)	426.29394 .2939	.2944	-5 -5	0.756 -3
393		6(4, 2)- 5(1, 5)	431.15518 .1552	.1552	0 0	0.163 -2
394		12(6, 7)-11(5, 6)	434.80787* .8074	.8044	+35 +30	0.118 -2
395		9(9, 0)- 8(8, 1)	436.50605* .4269	.4261	+800 +8	0.586 -2
		9(9, 1)- 8(8, 0)	436.50048* .4269			0.195 -2
396		5(5, 0)- 4(2, 3)	441.71414 .7138	.7142	-1 -4	0.156 -2
397		6(5, 2)- 5(2, 3)	442.08829 .0882	.0884	-1 -2	0.628 -2
398		10(8, 3)- 9(7, 2)	443.69504 .6947	.6975		0.458 -2
		10(8, 2)- 9(7, 3)	443.77569* .7000			0.153 -2
399		11(7, 5)-10(6, 4)	446.34278* .3500	.3526	-98 -26	0.924 -3
400		11(7, 4)-10(6, 5)	446.92261* .9313	.9314	-88 -1	0.276 -2
400A		13(6, 8)-12(5, 7)	447.50340& .4166	.4128	+906 +38	0.945 -4
401		12(6, 6)-11(5, 7)	451.83671* .7132	.7177	+1190 -45	0.399 -3
402		11(4, 7)-10(3, 8)	452.87969 .8792	.8800	-3 -8	0.412 -2
403		7(5, 3)- 6(2, 4)	456.87347 .8734	.8739	-4 -5	0.304 -2
404		12(5, 7)-11(4, 8)	457.64544* .6589	.6574	-120 +15	0.457 -3
405		9(2, 7)- 8(1, 8)	457.75900 .7587	.7606	-16 -19	0.137 -1
		10(3, 7)- 9(2, 8)	457.76409 .7647			0.301 -2
406		9(4, 6)- 8(1, 7)	457.99468 .9945	.9944	+3 +1	0.471 -2
407		10(9, 2)- 9(8, 1)	- 461.4489	.4496	-7	0.216 -2
		10(9, 1)- 9(8, 2)	- 461.4490			0.720 -3
408		10(4, 7)-10(1,10)	466.78627 .7868	.7856	+7 +12	0.115 -3

intensities of $HD^{16}O$ lines were taken from the work in Ref. (*19*) and the calculated wavenumbers of the lines due to the rotational transitions in the vibration level (010) were derived from the results of Camy-Peyret and Flaud (*20*).

The calculation of the relative intensities, with the exception of the $HD^{16}O$ lines, is

TABLE II—*Continued*

NO	MO	$J'(K_a',K_c')-J''(K_a'',K_c'')$	FREQ	OBS	DIFF	I
409		11(8, 4)-10(7, 3)	467.89350& .8939	.9134		0.502 -3
		11(8, 3)-10(7, 4)	467.92832* .9187			0.150 -2
410		12(7, 6)-11(6, 5)	468.63414* .7541	.7539	-1198 +2	0.801 -3
411		12(7, 5)-11(6, 6)	470.30560& .5065	.5071	-2015 -6	0.264 -3
412		9(3, 7)- 8(0, 8)	472.16783 .1682	.1671	+7 +11	0.441 -2
413		6(5, 1)- 5(2, 4)	472.42376 .4234	.4246	-8 -12	0.102 -2
414		8(5, 4)- 7(2, 5)	472.75702 .7569	.7567	+3 +2	0.821 -2
415		10(10, 1)- 9(9, 0)	- 476.4223	.4206	+17	0.918 -3
		10(10, 0)- 9(9, 1)	- 476.4223		+17	0.306 -3
416		13(6, 7)-12(5, 8)	481.04928* .0445	.0440	+53 +5	0.195 -3
417		7(4, 3)- 6(1, 6)	483.98489 .9849	.9849	0 0	0.371 -2
418		11(9, 3)-10(8, 2)	485.91140& 486.1363	.1368		0.236 -3
		11(9, 2)-10(8, 3)	486.18922* .1371		+524 +3	0.708 -3
419		12(8, 5)-11(7, 4)	491.59330& .6097	.6079	-146 +18	0.439 -3
420		12(8, 4)-11(7, 5)	491.80780& .7182	.7153	+925 +29	0.146 -3
421		9(5, 5)- 8(2, 6)	492.06913 .0688	.0696	-5 -8	0.187 -2
422		13(7, 6)-12(6, 7)	494.18480& .1359	.1422	+426 -63	0.205 -3
423		11(10, 2)-10(9, 1)	- 501.5707	.5736	-29	0.996 -4
		11(10, 1)-10(9, 2)	- 501.5707		-29	0.299 -3
424		10(4, 7)- 9(1, 8)	502.25642 .2564	.2568	-4 -4	0.683 -2
425		13(5, 8)-12(4, 9)	504.38876* .3839	.3847	+41 -8	0.271 -3
426		7(5, 2)- 6(2, 5)	506.92395 9238	.9244	-5 -6	0.325 -2
427		14(7, 8)-13(6, 7)	507.88630& .9205	.8984	-121 +221	0.388 -4
428		12(9, 4)-11(8, 3)	- 510.4236	.4257	-21	0.207 -3
		12(9, 3)-11(8, 4)	- 510.4280			0.689 -4
429		12(4, 8)-11(3, 9)	510.59687* .5811	.5853	+116 -42	0.364 -3
430		11(11, 0)-10(10, 1)	- 514.2945	.3032	-87	0.116 -3
		11(11, 1)-10(10, 0)	- 514.2945		-87	0.385 -4
431		13(8, 5)-12(7, 6)	- 515.0605	.0633	-28	0.112 -3
432		10(5, 6)- 9(2, 7)	516.79800 .7969	.7970	+10 -1	0.327 -2
433		10(2, 8)- 9(1, 9)	517.75876 .7582	.7581	+7 +1	0.202 -2

based on the well-known formula

$$I \sim [\exp(-E_i/kT) - \exp(-E_j/kT)]\nu_{ij}S_{ij}g_i, \tag{3}$$

where E_i and E_j are lower- and upper-state energies, respectively, ν_{ij} is the transition frequency, S_{ij} is the transition strength, and g_i is the lower-state statistical weight.

TABLE II—*Continued*

NO	MO	$J'(K'_a,K'_c)-J''(K''_a,K''_c)$	FREQ	OBS	DIFF	I
434		11(3, 8)-10(2, 9)	519.58931 .5893	.5893	0 0	0.311 -2
435		10(3, 8)- 9(0, 9)	525.95996 .9596	.9593	+7 +3	0.603 -2
436		12(10, 3)-11(9, 2)	- 526.3413	.3416	 -3	0.867 -4
		12(10, 2)-11(9, 3)	- 526.3414			0.289 -4
437		13(9, 5)-12(8, 4)	- 534.2441	.2694		0.178 -4
		13(9, 4)-12(8, 5)	- 534.2655		 -39	0.534 -4
438		6(6, 1)- 5(3, 2)	536.24592 .2458	.2466	-7 -8	0.710 -3
439		12(11, 2)-11(10, 1)	- 539.5770	.5800	 -30	0.332 -4
		12(11, 1)-11(10, 2)	- 539.5770		 -30	0.111 -4
440		6(6, 0)- 5(3, 3)	541.09048 .0907	.0904	+1 +3	0.213 -3
441		8(4, 4)- 7(1, 7)	545.29662 .2970	.2968	-2 +2	0.683 -3
442		8(5, 3)- 7(2, 6)	546.30343 .3040	.3034	0 +6	0.823 -3
443		11(5, 7)-10(2, 8)	547.81795 .8183	.8167	+13 +16	0.532 -3
444		11(4, 8)-10(1, 9)	550.01004 .0109	.0116	-16 -7	0.925 -3
445		7(6, 2)- 6(3, 3)	554.63645 .6403	.6414	-50 -11	0.528 -3
446		6(5, 2)- 5(0, 5)	563.25096 .2511	.2513	-3 -2	0.230 -3
447		7(6, 1)- 6(3, 4)	567.21543 .2149	.2156	-2 -7	0.117 -2
448		8(6, 3)- 7(3, 4)	569.25522 .2554	.2548	+4 +6	0.212 -2
449		13(4, 9)-12(3,10)	571.27012* .2853	.2867	-166 -14	0.282 -3
450		11(2, 9)-10(1,10)	576.11481 .1157	.1141	+7 +16	0.247 -2
451		11(3, 9)-10(0,10)	580.53622 .5372	.5372	-10 0	0.823 -3
452		12(3, 9)-11(2,10)	580.73082* .7386	.7321	-13 +65	0.340 -3
453		9(6, 4)- 8(3, 5)	581.08396 .0932	.0889	-49 +43	0.634 -3
454		12(5, 8)-11(2, 9)	584.70797 .7077	.7078	+2 -1	0.636 -3
455		9(5, 4)- 8(2, 7)	591.69735 .6971	.6970	+4 +1	0.148 -2
456		10(6, 5)- 9(3, 6)	592.05401 .0542	.0542	-2 0	0.114 -2
457		8(6, 2)- 7(3, 5)	594.94339 .9525	.9479	-45 +46	0.380 -3
458		12(4, 9)-11(1,10)	600.10416 .1035	.1042	0 -7	0.984 -3
459		11(6, 6)-10(3, 7)	604.48420* .4471	.4503	+339 -32	0.176 -3
460		7(5, 3)- 6(0, 6)	612.95060 .9502	.9519	-13 -17	0.871 -4
461		9(4, 5)- 8(1, 8)	616.07312 .0728	.0733	-2 -5	0.843 -3

The transition strength S_{ij} were approximately derived from Appendix V in Ref. (*21*). Accordingly, the relative intensities in Table II only give rough estimates, especially for the transitions with high J values. The intensity of the strongest line at 202.689 cm^{-1} was set equal to unity. In estimating the intensities of $H_2{}^{18}O$ and $H_2{}^{17}O$ lines the natural abundances of 0.204 and 0.037%, respectively, were used.

TABLE II—*Continued*

NO	MO	$J'(K'_a,K'_c)-J''(K''_a,K''_c)$	FREQ	OBS	DIFF	I
462		12(6, 7)-11(3, 8)	620.57987* .5794	.5787	+12 +7	0.218 -3
463		9(6, 3)- 8(3, 6)	625.26726 .2681	.2679	-6 +2	0.787 -3
464		13(5, 9)-12(2,10)	626.38895* .3206	.3247	+643 -41	0.609 -4
465		12(2,10)-11(1,11)	633.09074 .0888	.0906	+1 -18	0.305 -3
466		12(3,10)-11(0,11)	635.39757 .3985	.3975	+1 +10	0.916 -3
467		7(7, 1)- 6(4, 2)	637.03356 .0335	.0336	0 -1	0.652 -4
468		7(7, 0)- 6(4, 3)	638.09130 .0891	.0904	+9 -13	0.189 -3
469		13(3,10)-12(2,11)	639.95012* .9736	.9734	-233 +2	0.286 -3
470		10(5, 5)- 9(2, 8)	644.32002 3218	.3216	-16 +2	0.233 -3
471		13(4,10)-12(1,11)	651.71389* .5758	.5823	+1316 -65	0.106 -3
472		10(6, 4)- 9(3, 7)	659.22677 .2320	.2325	-57 -5	0.143 -3
473		8(7, 2)- 7(4, 3)	659.45418 .4530	.4548	-6 -18	0.347 -3
474		8(7, 1)- 7(4, 4)	662.94532 .9466	.9480	-27 -14	0.104 -3
475		8(5, 4)- 7(0, 7)	668.92357 .9236	.9235	+1 +1	0.207 -3
476		14(5,10)-13(2,11)	671.39378& .3560	.3646	+291 -86	0.492 -4
477		9(7, 3)- 8(4, 4)	678.81203 .8078	.8100	+20 -22	0.127 -3
478		9(7, 2)- 8(4, 5)	687.88069 .8796	.8806	+1 -10	0.282 -3
479		13(2,11)-12(1,12)	689.01960* .0380	.0387	-191 -7	0.984 -4
480		13(3,11)-12(0,12)	690.23673* .2226	.2213	+154 +13	0.103 -3
481		10(7, 4)- 9(4, 5)	694.11100 .1121	.1117	-7 +4	0.323 -3
482		10(4, 6)- 9(1, 9)	696.24291 .2409	.2437	-8 -28	0.855 -4
483		14(3,11)-13(2,12)	697.06010* .0711	.0604	-3 +107	0.245 -5
484		11(6, 5)-10(3, 8)	697.92037 9186	.9197	+7 -11	0.201 -3
485		14(4,11)-13(1,12)	703.77913* .7127	.7143	+648 -16	0.854 -4
486		11(5, 6)-10(2, 9)	705.36131 .3613	.3615	-2 -2	0.254 -3
		11(7, 5)-10(4, 6)	705.34811* .3623			0.666 -4
487		8(6, 3)- 7(1, 6)	707.39789 .3981	.3994	-15 -13	0.118 -3
488		10(7, 3)- 9(4, 6)	713.48174* .4833	.4847	-30 -14	0.593 -4
489		12(7, 6)-11(4, 7)	713.67482* .7935	.7950	-1202 -15	0.861 -4

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[a] The meanings of different columns are as follows: NO: line number; MO: molecule; $J'(K'_a, K'_c) - J''(K''_a, K''_c)$: rotational quantum numbers of the upper and lower levels in the rotational transition; FREQ: calculated wavenumbers in cm^{-1}; OBS: observed wavenumber in cm^{-1}; DIFF: calculated wavenumber − observed wavenumber in $10^{-4}\ \mathrm{cm}^{-1}$; I: calculated relative intensity.

In the column MO the empty space = $H_2{}^{16}O$, 18 = $H_2{}^{18}O$, 17 = $H_2{}^{17}O$, HDO = $HD^{16}O$, and 010 = the rotational transition at the (010) level. In the column FREQ the upper wavenumber of $H_2{}^{16}O$ was mainly derived from Ref. (*13*). An asterisk at the end of the upper wavenumber indicates that one of the energy levels was obtained from Ref. (*13*) and the other from Ref. (*15*), and & indicates that both energy levels were taken from Ref. (*15*). The lower wavenumber of $H_2{}^{16}O$ was derived from Ref. (*16*). In the column OBS SH = shoulder.

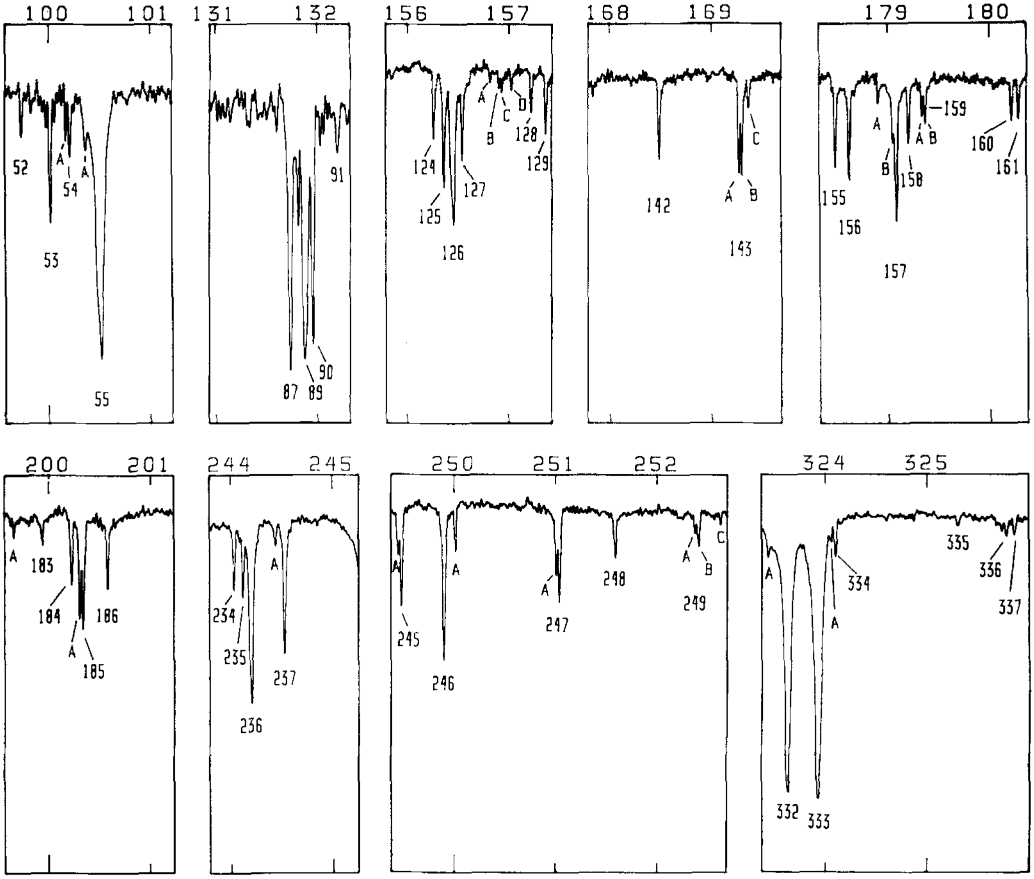

FIG. 3. Some parts of an unapodized water spectrum transformed from the same interferogram as in Fig. 2. Resolution is 0.018 cm^{-1}, pressure 1.8 Torr, and absorption path length 1 m.

IV. DISCUSSION

From Table II we clearly see that at lower J values the line positions of the pure rotational $H_2{}^{16}O$ spectrum agree very well with the wavenumbers calculated from the rotation–vibration spectra. At higher J and K_a values our line positions for $H_2{}^{16}O$ are more reliable for many lines than the calculated ones. We further see that the rotational levels of the isotopic species $H_2{}^{18}O$, $H_2{}^{17}O$, and $HD^{16}O$ are less accurate than those of $H_2{}^{16}O$. In interferometers similar to ours the only way to make a very accurate calibration of the wavenumbers is to use an absorption line in an infrared beam besides the laser line, for it is only then that the radiation used for calibration follows exactly the same path through the interferometer as that under study. With the help of the results of this work, it is easy to select the proper calibration lines as far as 700 cm^{-1}.

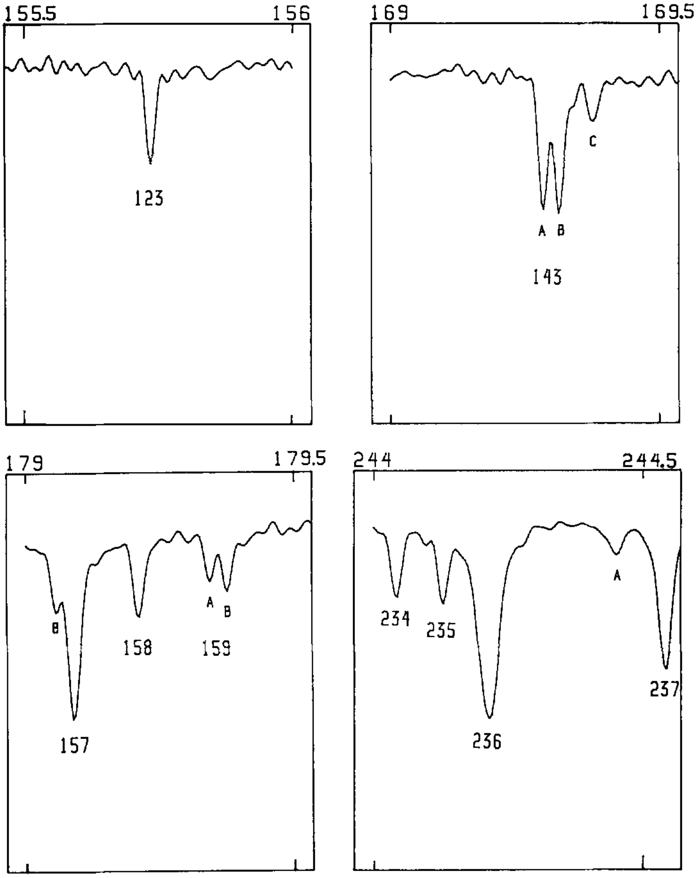

FIG. 4. More extended details of the unapodized spectrum. The splitting of doublet 143 is 0.030 cm^{-1} and that of doublet 159 is 0.032 cm^{-1}. The half-width of weak line 123 is smaller than 0.018 cm^{-1}.

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