High-resolution rotational absorption spectra of $H_2{}^{16}O$, $HD^{16}O$, and $D_2{}^{16}O$ between 110 and 500 cm^{-1}

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Received September 19, 1994; revised manuscript received April 18, 1995

Pure rotational spectra of ^{16}O isotopic species of H_2O, HDO, and D_2O were measured with a high-resolution Fourier-transform spectrometer in order to obtain better calibration line positions for high-resolution spectroscopy. The number of assigned lines for HDO was ~380 and for H_2O it was ~310 between 170 and 500 cm^{-1}. For D_2O, ~220 lines in the 110–420-cm^{-1} region were assigned. The calibration was performed with the highly accurate ν_2 band of carbonyl sulfide. © 1995 Optical Society of America

1. INTRODUCTION

The extent of the pure rotational spectrum of water vapor is large, and water vapor lines are almost always present in far-infrared measurements. This makes it feasible to use water vapor in the calibration procedure of far-infrared spectra. However, there is one problem in using H_2O lines for calibration. Water vapor is everywhere in the spectrometer: this causes a small dispersion effect in Fourier spectrometers and H_2O lines are often too strong. In our earlier works with water we found that H_2O line shapes are a bit asymmetric when the phase of a spectrum has been adjusted with absorption lines of a linear molecule by using the method described in Ref. 1. When peak positions in the wave-number scale are calculated, assuming that the lines are symmetrical, there will be errors in H_2O line positions. We started this work with an idea that by using D_2O or HDO lines in calibration one can avoid this problem because these molecules will not be present in a spectrometer tank. However, by carefully examining this measurement, we have found the same kind of differences by comparing symmetries of the line shapes in the D_2O and the HDO spectra with those of the carbonyl sulfide (OCS) ν_2 band. So it seems that the reason for different symmetries cannot be caused by the dispersion effect. It may be typical for a water spectrum. In this paper we cannot give an answer to this question, but we have estimated error limits that are due this effect and, knowing these limits, we can use measured lines for calibration purposes.

A high-resolution Fourier-transform spectrum of pure rotation of natural water was measured by Kauppinen *et al.* in 1978. Later Johns[3] made a more accurate measurement with higher resolution by using isotopically enriched samples, but the spectra were extended for H_2O to 350 cm^{-1} and for D_2O to 220 cm^{-1} only. Kauppinen *et al.* used certain selected water vapor lines to calibrate their spectra. Johns used, in addition to water vapor lines, some lines of diatomic molecules. All the calibration lines used by Johns were below 200 cm^{-1}. Guelachvili and Narahari Rao[4] have included two sections of pure rotational spectra of H_2O in their *Handbook of Infrared Standards*. According to the references given in Ref. 4, the first section is essentially included in the paper by Johns.[3] The second section (lines of $H_2{}^{16}O$ between 500 and 720 cm^{-1}) was recorded by J. Kauppinen and V.-M. Horneman in Oulu and is published in Ref. 4 only.

When accomplishing our recent work[5] on HCCI we observed that, especially in the region above 300 cm^{-1}, line positions of the water vapor spectrum were not known accurately enough to be used in the calibration of modern high-resolution spectrometers. Also, the accurate determination of the band center of the ν_2 band of OCS near 520 cm^{-1} (see Ref. 6) gives a good possibility of transferring the calibration from the higher wave-number side to the water spectrum. In previous water works, the calibration was based on either calculated water-vapor peak positions or on lines in the lower wave-number part of the spectrum.

In an ideal Fourier spectrometer, the calibration of the wave-number scale can be illustrated by a rubber band with one end (the origin) fixed and the other end stretched to give the proper length. Mathematically this is expressed by the determination of the constant k in

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

where ν_c is the calculated wave number and ν is the actual wave number. According to this procedure, wave numbers above the calibration lines are extrapolations, whereas wave numbers below the calibration lines are interpolations. Thus it should be more accurate to select calibration lines that are above the sample spectrum rather than below it.

When this work was started we also planned to perform least-squares fits to derive accurate values for the molecular constants of D_2O and HDO. Recently Toth[7–9] made this calculation by using the spectra of the (010)–(000) bands together with rotational spectra in the literature. Our data set is rather limited (only a part of the rotational spectrum is used), and if we use it alone, we hardly get a better set of molecular constants than those given in the literature. We believe that making a thorough fitting would be a matter of a separate work. Our measurements are more accurate than previous ones, especially in the wave-number region between 300 and 500 cm^{-1}. Therefore it is worth publishing the results without fitting. By doing so we are offering somebody the possibility of making the refitting. At this moment we are not planning to do it ourselves.

2. EXPERIMENTAL DETAILS

A Fourier spectrometer, IFS 120 HR, made by Bruker, was used for the measurements. A White-type cell that gives an absorption path length of 3.2 m was filled with a mixture of H_2O, D_2O, and HDO to a total pressure of 50 Pa (0.35 Torr), and then 50 Pa (0.35 Torr) of OCS was added for calibration. It is difficult to give the exact partial pressures of the isotopomers $H_2{}^{16}O$, $D_2{}^{16}O$, and $HD{}^{16}O$ because there is always some residual amount of natural water present in the cell. The cell with white polyethylene windows was at room temperature (295 K). Experimental conditions were kept constant, and a total number of 370 scans were recorded to get the signal-to-noise ratio as high as possible. When a bolometer detector is used, a measuring period of ~2 weeks is needed. Parts of the H_2O lines in our spectrum are too strong, but this was not taken to be a serious problem because the emphasis was on D_2O and HDO lines. The lower wave-number limit was set to ~100 cm^{-1} by the 3.5-μm Mylar beam splitter that was used. The upper limit, ~600 cm^{-1}, was due to the bolometer cold filter. Lines above the Q branch of the ν_2 band of OCS were not taken into consideration.

Interferograms were collected in six packages, which were transformed separately into spectra, and then the sum spectrum was calculated and calibrated by the use of the lines of OCS. In the calibration more than 100 lines were used to determine the calibration constant k in Eq. (1). The signal-to-noise ratio in the best part of the spectrum was ~100 with a spectral resolution of ~0.0025 cm^{-1}. Two small sections of the spectra are shown in Fig. 1. The isotopic species responsible for each line is shown, but no detailed assignments are given. A second spectrum with a different ratio between the pressures of H_2O and D_2O was measured to verify the isotopic assignments.

3. LINE ASSIGNMENTS

The energy levels tabulated by Toth[7–9] were used to calculate the wave numbers for the allowed transitions. Selection rules used for the C_{2v} species were[10]

$$\Delta J = 0,\ \pm 1; \qquad \Delta K_a = \pm 1,\ \pm 3, \ldots ; \\ \Delta K_c = \pm 1,\ \pm 3, \ldots . \tag{2}$$

For HDO an additional class of transitions is possible according to

$$\Delta J = 0,\ \pm 1; \qquad \Delta K_a = 0,\ \pm 2, \ldots ; \\ \Delta K_c = \pm 1,\ \pm 3, \ldots . \tag{3}$$

Although the species that contain the isotopes ^{18}O and ^{17}O are not considered in this work, the wave numbers for the allowed transitions were calculated for $D_2{}^{18}O$, $HD^{18}O$, and $HD^{17}O$ from the energy levels given by Toth[8,9] and for $H_2{}^{18}O$ and $H_2{}^{17}O$ given in Ref. 11. These data were used only to verify the assignments, and no tables for observed peak positions are given.

Standard Bruker's procedures were used to calculate the peak positions in the experimental spectrum, and a computer program was written to pick the peaks that corresponded to allowed transitions. Only a few lines were left unassigned in the spectrum. These were expected to belong mainly to the rotational transition in the excited vibrational states.

4. RESULTS AND DISCUSSION

Peak positions of the observed transitions of $H_2{}^{16}O$, $HD^{16}O$, and $D_2{}^{16}O$ are given in Tables 1, 2, and 3, respectively. Also given are the assignments, the values for the calculated transitions, and the differences between the observed and the calculated values. The values measured by Johns,[3] or in some cases those of Kauppinen *et al.*,[2] with the differences between the present values, are given for comparison.

For $H_2{}^{16}O$ and $HD^{16}O$, Tables 1 and 2 cover the region from 170 to 520 cm^{-1}. The lines below 170 cm^{-1} are not tabulated because our results did not differ significantly from the results of Johns.[3] The situation is the same with the $H_2{}^{16}O$ lines above 500 cm^{-1}, which are given in Ref. 4. For $D_2{}^{16}O$ the observations of Johns[3] end near 200 cm^{-1}, and to provide reasonable overlapping, Table 3 was extended as low as 110 cm^{-1}. More than 80 new transitions were assigned to $D_2{}^{16}O$, mostly above 220 cm^{-1}. For HDO the amount of new lines was even higher, ~300. This is due to the fact that the sample cell used by Johns[3] was only 15 cm long, and he did not even try to record weak lines.

Figure 2 illustrates the compatibility of the observed line positions (O) and those calculated (C) from the energy levels given by Toth.[7] The average of the O − C values is not 0. When data that differed by more than 0.001 cm^{-1} were rejected, the average of 236 observations was 0.00011 cm^{-1} and the rms value was 0.00027 cm^{-1}. As can be seen from Fig. 2 the deviation from 0 tends to

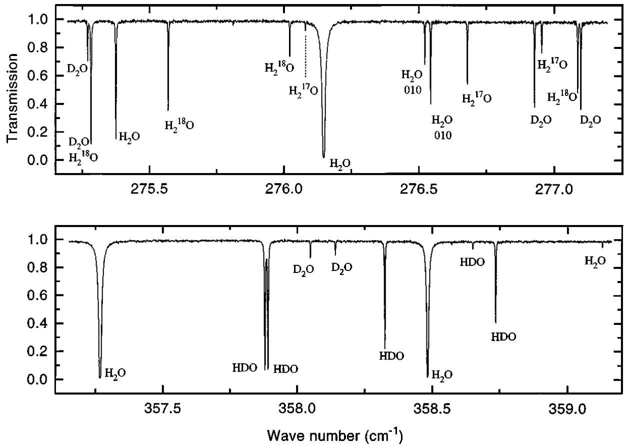

Fig. 1. Two sections of the experimental spectra. Experimental conditions: absorption path length, 3.2 m; sample pressure, 50 Pa (0.35 Torr) for a mixture of H_2O, D_2O, and HDO and 50 Pa (0.35 Torr) of OCS; room temperature, 295 K. Isotopic species that produced the various absorption lines are shown. O without a superscript means ^{16}O and 010 means the rotational transition in the excited vibrational state $\nu_2 = 1$.

Table 1. Absorption Peaks (in Reciprocal Centimeters) Assigned to the Pure Rotational Transitions[a] of $H_2{}^{16}O$ Between 170 and 520 cm^{-1}

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
4	3	2	3	2	1	170.36056			0.36056	
8	1	7	7	2	6	173.28223			0.28212	
4	2	2	3	1	3	173.50109			0.50106	
9	0	9	8	1	8	176.00575			0.00575	
9	1	9	8	0	8	176.14643			0.14627	
4	3	1	3	2	2	177.54110			0.54103	
11	7	4	11	6	5	177.85952	177.859389	-131		
13	4	10	13	3	11	178.13167	178.132081	410		
10	1	9	10	0	10	178.48588	178.485860	-20	0.48587	-10
7	7	0	7	6	1	178.61971	178.619658	-52	0.61983	-172
7	7	1	7	6	2	178.62440	178.624325	-75		
10	7	3	10	6	4	178.90699	178.906829	-161		
12	7	6	12	6	7	178.99932	178.999260	-60		
8	7	1	8	6	2	179.04882	179.048776	-44	0.04874	36
8	7	2	8	6	3	179.07872	179.078630	-90	0.07982	-1190
10	2	9	10	1	10	179.08415	179.084081	-68	0.08424	-159
9	7	2	9	6	3	179.20490	179.204866	-33	0.20474	126
11	7	5	11	6	6	179.21534	179.215737	396		
9	7	3	9	6	4	179.33792	179.337783	-136		
10	7	4	10	6	5	179.37222	179.372227	7	0.37238	-153
11	4	7	10	5	6	180.28930	180.289346	45	0.28915	196
7	6	2	7	5	3	181.38923		-		
8	2	7	7	1	6	181.38620		-	0.38626	
5	3	2	5	0	5	183.46420	183.463595	-605	0.46411	-515
12	2	10	12	1	11	185.59085	185.591095	245		
7	4	3	8	1	8	187.07450	187.074506	6		
12	3	10	12	2	11	187.75578	187.755776	-3	0.75593	-154
5	3	3	4	2	2	188.18863			0.18867	
9	1	8	8	2	7	193.47936			0.47937	
10	0	10	9	1	9	194.32225	194.321374	-876	0.32229	-916
10	1	10	9	0	9	194.38154			0.38154	
9	2	7	8	3	6	195.80559			0.80563	
10	3	7	9	4	6	197.26463	197.265043	412	0.26473	313
9	2	8	8	1	7	197.49504			0.49514	
11	1	10	11	0	11	197.73791	197.737883	-26	0.73804	-157
11	2	10	11	1	11	198.01840	198.018360	-40	0.0183	60
8	8	0	8	7	1	198.35284	198.352543	-296		
8	8	1	8	7	2	198.35301	198.352543	-467	0.35279	-247
9	8	1	9	7	2	199.21714	199.217138	-1	0.21706	78
9	8	2	9	7	3	199.22154	199.221737	196		
10	8	2	10	7	3	199.91561	199.915780	170		
10	8	3	10	7	4	199.93859	199.938512	-78		
11	8	3	11	7	4	200.35937	200.359436	65		

(Table continued)

Table 1. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
12	8	5	12	7	6	200.71264	200.712291	-348		
6	3	4	5	2	3	202.46807			0.46792	
4	4	1	3	3	0	202.68922			0.68895	
6	6	1	7	3	4	202.70138				
4	4	0	3	3	1	202.91489			0.91477	
13	2	11	13	1	12	204.57432	204.574188	-132		
13	3	11	13	2	12	205.69061	205.690352	-258		
5	3	2	4	2	3	208.44982			0.44974	
15	6	9	14	7	8	208.54017				
5	4	1	5	1	4	210.88377	210.883601	-168	0.88372	-119
11	0	11	10	1	10	212.56011	212.560245	135	0.55985	395
11	1	11	10	0	10	212.58537	212.585220	-150	0.58535	-130
10	1	9	9	2	8	212.63279			0.63284	
4	4	0	4	1	3	212.63722				
7	3	5	6	2	4	213.92088			0.9206	
10	2	9	9	1	8	214.55451			0.55449	
6	3	3	6	0	6	214.85240	214.852321	-78	0.85241	-89
6	4	2	6	1	5	214.87447	214.874424	-45	0.87455	-126
3	3	1	2	0	2	215.12859	215.128560	-24	0.12847	90
9	9	0	9	8	1	215.66435	215.664093	-257		
9	9	1	9	8	2	215.66451	215.664093	-417		
12	1	11	12	0	12	216.77187	216.771858	-11	0.77188	-22
12	2	11	12	1	12	216.90345	216.903343	-106	0.90344	-97
10	9	1	10	8	2	216.97076	216.971065	304		
11	9	2	11	8	3	218.15555	218.155749	198		
12	4	8	11	5	7	219.86785	219.867814	-35		
5	2	3	4	1	4	221.67231			0.67228	
10	2	8	9	3	7	221.73722	221.737182	-38	0.73736	-178
14	2	12	14	1	13	222.99856	222.998726	166		
14	3	12	14	2	13	223.56951	223.569547	36		
8	3	6	7	2	5	223.70613			0.70611	
5	4	2	4	3	1	226.27197			0.27204	
7	4	3	7	1	6	227.02313	227.022995	-135	0.02311	115
5	4	1	4	3	2	227.82440			0.82417	
12	0	12	11	1	11	230.72683	230.726703	-127	0.72705	-347
12	1	12	11	0	11	230.73773			0.73776	
11	1	10	10	2	9	231.21387	231.213306	-563	0.21388	-574
11	3	8	10	4	7	231.88732	231.887343	22	0.88752	-177
11	2	10	10	1	9	232.11789	232.117831	-58	0.11793	-99
11	10	1	11	9	2	232.40635	232.408292	1941		
9	3	7	8	2	6	233.31967	233.320052	382	0.31965	402
13	1	12	13	0	13	235.64053	235.640502	-28	0.64063	-128
13	2	12	13	1	13	235.70238	235.702511	130		

(Table continued)

Table 1. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
10	3	8	9	2	7	244.20682	244.206873	53	0.20672	153
11	2	9	10	3	8	244.53613	244.535995	-135	0.53634	-345
6	3	3	5	2	4	245.34021			0.34034	
4	3	2	3	0	3	245.75526			0.75525	
6	4	3	5	3	2	247.91277			0.91272	
13	0	13	12	1	12	248.82236	248.822280	-79	0.82255	-270
13	1	13	12	0	12	248.82715	248.826994	-155		
8	4	4	8	1	7	248.88518	248.885207	27	0.88522	-13
12	1	11	11	2	10	249.48030	249.480223	-77	0.48039	-167
12	2	11	11	1	10	249.90327	249.903090	-180	0.90333	-240
6	4	2	5	3	3	253.81209			0.81209	
5	5	1	4	4	0	253.93887			0.93904	
5	5	0	4	4	1	253.96859			0.96858	
14	1	13	14	0	14	254.36892	254.368703	-216		
14	2	13	14	1	14	254.39856	254.398276	-283		
7	3	4	7	0	7	256.11307	256.113055	-15	0.11321	-155
11	3	9	10	2	8	257.10020	257.100056	-143	0.10029	-234
13	4	9	12	5	8	258.42033	258.420280	-49		
12	3	9	11	4	8	262.83836	262.838200	-160		
4	4	1	4	1	4	263.26942	263.269300	-120	0.26945	-150
12	2	10	11	3	9	265.13848	265.138678	198	0.13892	-242
7	4	4	6	3	3	266.19504			0.19519	
14	0	14	13	1	13	266.84330	266.843933	632	0.84517	-1237
14	1	14	13	0	13	266.84550	266.843933	-1567	0.84517	-1237
13	1	12	12	2	11	267.55944	267.559409	-30	0.55966	-251
13	2	12	12	1	11	267.75766	267.757763	103	0.75806	-297
12	3	10	11	2	9	271.84252	271.842491	-28	0.84267	-179
15	1	14	15	0	15	272.96722	272.967448	227		
15	2	14	15	1	15	272.98275	272.981831	-919		
8	5	3	8	2	6	272.99993	272.999814	-115	0.00022	-406
9	5	4	9	2	7	275.37587	275.375875	4	0.37622	-345
6	2	4	5	1	5	276.14799	276.148070	80	0.14812	-50
7	5	2	7	2	5	277.42567	277.425599	-71	0.42581	-211
6	5	2	5	4	1	278.25755			0.25760	
6	5	1	5	4	2	278.51828			0.51840	
8	4	5	7	3	4	280.35195			0.35220	
9	4	5	9	1	8	281.15585	281.155726	-123	0.15596	-234
5	3	3	4	0	4	281.91544	281.915370	-69	0.91559	-220
7	4	3	6	3	4	282.25849			0.25861	
5	4	2	5	1	5	283.48900	283.488958	-41	0.48931	-352
13	2	11	12	3	10	284.37798	284.377868	-112	0.37813	-262
15	0	15	14	1	14	284.78615	284.786018	-132	0.78627	-252
14	1	13	13	2	12	285.50984	285.509625	-214		
14	2	13	13	1	12	285.60353	285.603384	-145	0.60369	-306

(Table continued)

Table 1. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
6	5	1	6	2	4	285.85929	285.859148	-141		
10	5	5	10	2	8	286.73700	286.736808	-192		
13	3	11	12	2	10	287.85742	287.857071	-348		
7	3	4	6	2	5	289.44525			0.44545	
13	3	10	12	4	9	289.77198	289.771941	-38		
9	4	6	8	3	5	290.72727	290.726562	-707	0.72747	-908
5	5	0	5	2	3	295.56570	295.565598	-101		
10	4	7	9	3	6	298.41700	298.416795	-204	0.41714	-345
7	5	3	6	4	2	301.86651			0.86679	
16	0	16	15	1	15	302.64330	302.644396	1095		
16	1	16	15	0	15	302.64380	302.644396	596		
14	2	12	13	3	11	302.81779	302.817944	154		
6	6	1	5	5	0	302.98169			0.98285	
6	6	0	5	5	1	302.98535			0.98285	
7	5	2	6	4	3	303.11069			0.11093	
15	1	14	14	2	13	303.35481	303.354817	7		
15	2	14	14	1	13	303.40096	303.399695	-1264		
14	3	12	13	2	11	304.59872	304.598655	-65		
11	4	8	10	3	7	304.88014	304.880125	-14	0.88055	-425
8	3	5	8	0	8	306.09403	306.093967	-62		
11	5	6	11	2	9	308.33093	308.330956	25		
6	4	3	6	1	6	309.47252	309.472420	-99		
12	4	9	11	3	8	311.72806	311.727960	-100	0.72853	-570
4	4	1	3	1	2	314.74201	314.741830	-180	0.74240	-570
8	4	4	7	3	5	315.08127			0.08156	
13	4	10	12	3	9	320.32826	320.328605	344		
17	0	17	16	1	16	320.41750	320.413529	-3971		
17	1	17	16	0	16	320.41770	320.413529	-4171		
15	2	13	14	3	12	320.79053	320.790779	248		
16	2	15	15	1	14	321.12514	321.124843	-296		
15	3	13	14	2	12	321.68905	321.689901	851		
10	4	6	10	1	9	323.43488	323.434882	1		
6	3	4	5	0	5	323.63083			0.63147	
8	5	4	7	4	3	323.92961			0.92876	
5	5	1	5	2	4	325.86439	325.864255	-135		
7	6	2	6	5	1	327.55714			0.55790	
7	6	1	6	5	2	327.59581			0.59558	
8	5	3	7	4	4	328.16769	328.167370	-319	0.16808	-710
11	6	5	11	3	8	330.82297	330.822857	-112		
15	3	12	14	4	11	334.15528	334.155200	-80		
5	4	2	4	1	3	334.61745	334.617325	-125	0.61796	-635
7	2	5	6	1	6	335.15754	335.157884	344	0.15772	164
6	5	2	6	2	5	335.68740	335.687340	-60		
10	6	4	10	3	7	337.31228	337.312355	75		

(Table continued)

Table 1. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
17	1	16	16	2	15	338.75616	338.754812	-1348		
16	3	14	15	2	13	338.93887	338.938371	-498		
8	3	5	7	2	6	340.54953	340.548981	-548	0.55021	-1229
7	4	4	7	1	7	341.26480	341.264722	-77		
9	5	5	8	4	4	343.20536	343.204987	-372	0.20590	-913
4	4	0	3	1	3	345.85580	345.855710	-90		
9	6	3	9	3	6	348.46394	348.463912	-27		
7	7	1	6	6	0	349.75583			0.75583	
7	7	0	6	6	1	349.75629			0.75583	
7	5	3	7	2	6	350.03856	350.038435	-125	0.0374	1035
8	6	3	7	5	2	351.77602	351.775832	-188	0.7772	-1368
8	6	2	7	5	3	351.99526	351.994838	-421	0.9950	-162
9	4	5	8	3	6	354.11948	354.117997	-1483	0.1205	-2503
9	5	4	8	4	5	354.58886	354.588672	-188	0.5897	-1028
6	4	3	5	1	4	357.26737	357.266727	-643	0.2679	-1173
10	5	6	9	4	5	358.48350	358.482901	-598	0.4840	-1099
8	6	2	8	3	5	361.48429	361.484196	-93		
9	3	6	9	0	9	362.75076	362.750706	-54	0.7503	406
11	5	7	10	4	6	369.33194	369.331750	-189	0.3338	-2050
8	5	4	8	2	7	369.56654	369.566500	-39	0.5663	200
7	3	5	6	0	6	369.99781	369.997374	-436	0.9978	-426
7	6	1	7	3	4	373.83796	373.837850	-110	0.8371	750
11	4	7	11	1	10	374.16027	374.160246	-24		
8	7	2	7	6	1	374.49567			0.4982	
8	7	1	7	6	2	374.50095			0.4982	
9	6	4	8	5	3	375.33393	375.333601	-329	0.3353	-1699
9	6	3	8	5	4	376.21634	376.215706	-633	0.2160	-294
12	5	8	11	4	7	376.36470	376.364595	-105	0.3651	-505
8	4	5	8	1	8	378.54590	378.545822	-78	0.5460	-178
13	5	9	12	4	8	380.87703	380.876923	-107		
6	6	0	6	3	3	383.50953	383.509347	-182		
10	5	5	9	4	6	383.82062	383.820385	-235	0.8210	-615
14	5	10	13	4	9	384.45199	384.451750	-240		
7	4	4	6	1	5	384.83819	384.837863	-326	0.8388	-937
5	4	1	4	1	4	385.50292	385.502644	-276	0.5043	-1656
8	8	1	7	7	0	394.22897	394.228144	-826	0.2295	-1356
8	8	0	7	7	1	394.22939	394.228144	-1246	0.2295	-1356
9	5	5	9	2	8	394.59550	394.595327	-173		
6	6	1	6	3	4	396.07932	396.079217	-102		
8	2	6	7	1	7	396.43256	396.432206	-354	0.4356	-3394
9	3	6	8	2	7	397.31894	397.318905	-35	0.3201	-1195
10	6	5	9	5	4	397.67574	397.675165	-575	0.6752	-35
9	7	3	8	6	2	398.94149	398.941192	-297	0.9663	-25108

(Table continued)

Table 1. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
9	7	2	8	6	3	398.97649	398.976069	-421	0.9663	9769
7	6	2	7	3	5	399.49555	399.495512	-37		
10	4	6	9	3	7	400.22174	400.221654	-86	0.2225	-846
10	6	4	9	5	5	400.48094	400.480847	-92	0.4823	-1453
8	6	3	8	3	6	405.49556	405.495494	-66	0.4969	-1406
7	7	1	8	2	6	411.90256	411.903281	720		
9	6	4	9	3	7	415.01419	415.014144	-45		
5	5	0	5	0	5	416.72846	416.728302	-157		
11	5	6	10	4	7	417.65926	417.659204	-56	0.6599	-696
11	6	6	10	5	5	417.89224	417.892201	-39	0.8934	-1199
8	4	5	7	1	6	418.49453	418.493953	-577	0.4949	-947
9	8	1	8	7	2	419.11491	419.114463	-447	0.1137	763
9	8	2	8	7	1	419.11421	419.114463	253	0.1137	763
8	3	6	7	0	7	419.87242	419.872046	-373	0.8737	-1654
9	4	6	9	1	9	420.67487	420.674851	-19	0.6750	-149
10	7	4	9	6	3	422.96227	422.962047	-223	0.9630	-953
10	7	3	9	6	4	423.12331	423.123105	-204	0.1245	-1395
10	3	7	10	0	10	423.61725	423.617288	37		
10	5	6	10	2	9	425.08484	425.084807	-32	0.0867	-1893
11	6	5	10	5	6	425.32752	425.327390	-130	0.3282	-810
5	5	1	4	2	2	426.29358	426.293468	-112	0.2944	-932
10	6	5	10	3	8	428.84479	428.844763	-26		
6	4	2	5	1	5	431.15478	431.154675	-105	0.1552	-525
12	6	7	11	5	6	434.80516	434.805015	-144	0.8044	615
9	9	1	8	8	0	436.42588	436.426225	345	0.4261	125
9	9	0	8	8	1	436.42625	436.426225	-25	0.4261	125
5	5	0	4	2	3	441.71408	441.713984	-96	0.7142	-216
6	5	1	6	0	6	441.93622	441.936062	-157		
6	5	2	5	2	3	442.08816	442.087990	-170	0.0884	-410
10	8	3	9	7	2	443.69596	443.695749	-211	0.6975	-1751
10	8	2	9	7	3	443.70100	443.701063	62	0.6975	3563
11	7	5	10	6	4	446.35129	446.351178	-112	0.3526	-1422
11	7	4	10	6	5	446.93282	446.932613	-206	0.9314	1213
13	6	8	12	5	7	447.41443	447.414537	107	0.4128	1737
9	7	2	9	4	5	450.35257	450.352531	-39		
12	6	6	11	5	7	451.71728	451.716992	-288	0.7177	-708
11	4	7	10	3	8	452.87987	452.879804	-66	0.8800	-196
14	6	9	13	5	8	455.50229	455.501169	-1121		
7	5	3	6	2	4	456.87330	456.873150	-149	0.8739	-750
12	5	7	11	4	8	457.65578	457.655410	-369	0.6574	-1990
9	2	7	8	1	8	457.75889	457.758797	-92	0.7606	-1803
10	3	7	9	2	8	457.76416	457.763553	-607	0.7606	2953
9	4	6	8	1	7	457.99457	457.994434	-135	0.9944	34

(Table continued)

Table 1. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
10	9	2	9	8	1	461.45006	461.449844	-216	0.4496	244
10	9	1	9	8	2	461.45022	461.449844	-376	0.4496	244
7	7	0	7	4	3	463.57712	463.577201	81		
10	4	7	10	1	10	466.78622	466.786037	-182	0.7856	437
11	8	4	10	7	3	467.89249	467.892571	80	0.9134	-20829
11	8	3	10	7	4	467.91997	467.919813	-157	0.9134	6413
8	7	2	8	4	5	467.98168	467.981360	-319		
12	7	6	11	6	5	468.75345	468.753434	-15	0.7539	-466
12	7	5	11	6	6	470.50699	470.506863	-126	0.5071	-237
9	3	7	8	0	8	472.16770	472.167404	-296	0.1671	304
6	5	1	5	2	4	472.42403	472.423838	-192	0.4246	-762
8	5	4	7	2	5	472.75694	472.756733	-206	0.7567	33
10	7	4	10	4	7	473.00921	473.008949	-261		
7	5	2	7	0	7	473.59196	473.591918	-41		
10	10	1	9	9	0	476.41976	476.419232	-527	0.4206	-1368
10	10	0	9	9	1	476.41976	476.419232	-527	0.4206	-1368
13	6	7	12	5	8	481.04249	481.042370	-119	0.0440	-1630
7	4	3	6	1	6	483.98487	483.984582	-288	0.9849	-318
11	3	8	11	0	11	486.11343	486.113349	-80		
11	9	3	10	8	2	486.13635	486.136839	489	0.1368	39
13	7	7	12	6	6	489.57306	489.573261	201		
12	8	5	11	7	4	491.60657	491.606419	-150	0.6079	-1481
12	8	4	11	7	5	491.71115	491.715614	4464	0.7153	314
9	5	5	8	2	6	492.06924	492.068973	-266	0.0696	-627
13	7	6	12	6	7	494.14093	494.140834	-96	0.1422	-1366
11	10	2	10	9	1	501.57204	501.572319	278	0.5736	-1281
10	4	7	9	1	8	502.25658	502.256270	-310	0.2568	-530
13	5	8	12	4	9	504.38305	504.383054	3	0.3847	-1646
7	5	2	6	2	5	506.92414	506.923871	-269	0.9244	-529
14	7	8	13	6	7	507.92245	507.921879	-571	0.8984	23479
12	9	4	11	8	3	510.42479	510.424678	-112	0.4257	-1022
12	9	3	11	8	4	510.42957	510.429872	301	0.4257	4172
12	4	8	11	3	9	510.58411	510.584066	-44	0.5853	-1234
11	11	1	10	10	0	514.30482	514.304527	-292	0.3032	1327
11	11	0	10	10	1	514.30482	514.304527	-292	0.3032	1327
13	8	5	12	7	6	515.06214	515.062189	48	0.0633	-1111
10	5	6	9	2	7	516.79739	516.797109	-280	0.7970	109
10	2	8	9	1	9	517.75849	517.758393	-97	0.7581	293
11	3	8	10	2	9	519.58939	519.589167	-223	0.5893	-133
13	7	6	12	6	7	494.14093	494.140834	-96	0.1422	-1366
11	10	2	10	9	1	501.57204	501.572319	278	0.5736	-1281
10	4	7	9	1	8	502.25658	502.256270	-310	0.2568	-530
13	5	8	12	4	9	504.38305	504.383054	3	0.3847	-1646

(Table continued)

Table 1. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
7	5	2	6	2	5	506.92414	506.923871	-269	0.9244	-529
14	7	8	13	6	7	507.92245	507.921879	-571	0.8984	23479
12	9	4	11	8	3	510.42479	510.424678	-112	0.4257	-1022
12	9	3	11	8	4	510.42957	510.429872	301	0.4257	4172
12	4	8	11	3	9	510.58411	510.584066	-44	0.5853	-1234
11	11	1	10	10	0	514.30482	514.304527	-292	0.3032	1327
11	11	0	10	10	1	514.30482	514.304527	-292	0.3032	1327
13	8	5	12	7	6	515.06214	515.062189	48	0.0633	-1111
10	5	6	9	2	7	516.79739	516.797109	-280	0.7970	109
10	2	8	9	1	9	517.75849	517.758393	-97	0.7581	293
11	3	8	10	2	9	519.58939	519.589167	-223	0.5893	-133

[a] The first six columns give the assignment of the transition. Calc is the value of the transition (in reciprocal centimeters) calculated from the energy levels given by Toth.[7–9] Obs. stands for the observed peak position. The observed value is missing if the line was too strong in the spectrum. O − C represents the difference (observed − calculated) $\times 10^6$ cm. Lit stands for the decimal part of the observed values obtained by Johns[3] and those above 350 cm^{-1} obtained by Kauppinen *et al.*[2] The last column, O − L, gives the difference (observed − literature[3] values) $\times 10^6$ cm.

Table 2. Absorption Peaks (in Reciprocal Centimeters) Assigned to the Pure Rotational Transitions[a] of HDO Between 170 and 520 cm^{-1}

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
11	6	6	10	6	5	170.61147	170.611371	-99		
11	6	5	10	6	4	170.63544	170.635285	-154		
12	1	11	11	2	10	170.90460	170.904568	-31		
14	1	13	14	0	14	171.15902	171.159006	-13		
14	2	13	14	1	14	171.60530	171.605134	-166		
11	5	7	10	5	6	171.77234	171.772249	-91		
11	4	8	10	4	7	172.17403	172.173801	-228		
13	0	13	12	1	12	172.20187	172.201855	-15		
13	1	13	12	1	12	172.22580	172.225641	-158		
11	5	6	10	5	5	172.23081	172.230733	-77		
13	0	13	12	0	12	172.24960	172.249546	-53		
13	1	13	12	0	12	172.27353	172.273382	-147	0.2735*	-118
12	2	11	11	2	10	172.41288	172.412867	-12		
7	3	5	6	2	4	173.35572			0.35573	
12	1	11	11	1	10	173.55471	173.554692	-18		
3	3	1	2	1	2	174.89684	174.896816	-21		
12	2	11	11	1	10	175.06299	175.062957	-33		
6	3	3	5	2	4	176.02710			0.02707	
11	4	7	10	4	6	176.47909	176.478897	-193		
11	2	9	10	2	8	176.84111	176.841007	-102		
6	2	4	5	1	5	177.68416			0.68412	
14	3	11	13	4	10	178.30603	178.306256	225		
7	3	4	7	0	7	178.80060	178.800540	-59		
8	3	6	7	2	5	181.49692			0.49704	
6	2	4	5	0	5	181.60292	181.602891	-29		
11	3	8	10	3	7	182.18618	182.185942	-237		

(Table continued)

Table 2. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
12	3	10	11	3	9	182.61029	182.610258	-32		
13	1	12	12	2	11	184.28104	184.280985	-55		
15	1	14	15	0	15	184.29663	184.294765	-1864		
13	7	6	13	6	7	184.45760	184.457124	-476		
15	2	14	15	1	15	184.53804	184.535721	-2318		
5	4	2	4	3	1	184.56517			0.56522	
13	7	7	13	6	8	184.70408	184.704186	105		
14	0	14	13	1	13	184.75837	184.758403	32		
14	1	14	13	1	13	184.77013				
5	4	1	4	3	2	184.77162			0.77164	
14	0	14	13	0	13	184.78230	184.782121	-179		
14	1	14	13	0	13	184.79406	184.794079	19		
12	7	5	11	7	4	185.03362	185.033926	305		
13	2	12	12	2	11	185.11944	185.119445	5		
13	2	11	12	3	10	185.61195	185.611838	-112		
13	1	12	12	1	11	185.78932	185.789326	5		
12	7	5	12	6	6	185.99095	185.991027	77		
12	7	6	12	6	7	186.08685	186.086828	-22		
12	6	7	11	6	6	186.22395	186.223683	-267		
12	6	6	11	6	5	186.28873	186.288666	-63		
13	2	12	12	1	11	186.62772	186.627736	15		
3	3	1	2	0	2	186.85061	186.850576	-33		
11	7	4	11	6	5	187.24606	187.245874	-186		
11	7	5	11	6	6	187.27929	187.279179	-111		
12	4	9	11	4	8	187.39134	187.391259	-81		
12	5	8	11	5	7	187.50165	187.501286	-364		
9	3	7	8	2	6	188.27888			0.27887	
10	7	3	10	6	4	188.27973				
10	7	4	10	6	5	188.28992	188.289756	-163		
12	5	7	11	5	6	188.48017	188.479855	-315		
9	7	2	9	6	3	189.13283	189.132318	-512	0.13337	-1052
9	7	3	9	6	4	189.13535	189.134826	-524	0.13337	1456
12	2	10	11	2	9	189.52522	189.525313	93		
8	7	1	8	6	2	189.83250	189.832894	394	0.83304	-146
8	7	2	8	6	3	189.83302	189.832894	-126	0.83304	-146
7	7	0	7	6	1	190.40358	190.403542	-38	0.40376	-218
7	7	1	7	6	2	190.40362	190.403542	-78	0.40376	-218
5	3	2	4	1	3	191.42645	191.426308	-146		
10	3	8	9	2	7	194.14937	194.149067	-303	0.1478*	1267
12	4	8	11	4	7	194.20495	194.204960	10		
4	3	2	3	1	3	195.09638	195.096246	-128		
13	2	11	12	3	10	196.12387	196.123735	-135		
7	3	4	6	2	5	197.08652	197.086608	88	0.08669	-82
14	1	13	13	2	12	197.24882	197.248824	4		

(Table continued)

Table 2. Continued

J'	$K_a{}'$	$K_c{}'$	J''	$K_a{}''$	$K_c{}''$	Calc	Obs	O − C	Lit	O − L
15	0	15	14	1	14	197.26436	197.265043	682		
15	1	15	14	1	14	197.26960	197.271840	2240		
15	0	15	14	0	14	197.27612	197.277822	1701		
15	1	15	14	0	14	197.28136	197.283684	2323		
16	1	15	16	0	16	197.30243	197.301972	-457		
16	2	15	16	1	16	197.43134	197.430792	-548		
14	2	13	13	2	12	197.70686	197.706772	-88		
14	1	13	13	1	12	198.08722	198.087273	53		
12	3	9	11	3	8	198.37088	198.370955	75		
14	2	13	13	1	12	198.54526	198.545201	-59		
8	3	5	8	0	8	199.27960	199.279472	-127		
6	4	3	5	3	2	199.48077			0.48090	
11	3	9	10	2	8	199.65929	199.659217	-72	0.6600*	-783
6	4	2	5	3	3	200.30471			0.30477	
13	2	11	12	2	10	201.51520	201.515018	-181		
13	6	8	12	6	7	201.83926	201.839305	45		
13	6	7	12	6	6	201.99814	201.998283	142		
13	4	10	12	4	9	202.26657	202.266553	-17		
15	3	12	14	4	11	202.29521	202.296240	1030		
14	2	12	13	2	11	202.65265	202.653008	358		
13	5	9	12	5	8	203.13929	203.139258	-31		
4	3	2	3	0	3	204.15704	204.156918	-117		
6	3	3	5	1	4	204.42741	204.427283	-127		
13	5	8	12	5	7	205.04004	205.039933	-107		
12	3	10	11	2	9	205.42847	205.428472	1		
14	3	12	13	2	11	209.29378	209.293693	-87		
7	4	3	7	1	6	209.69243	209.692278	-152		
16	0	16	15	1	15	209.72595	209.726025	74		
16	1	16	15	1	15	209.72885	209.726025	-2825		
16	1	16	15	0	15	209.73409	209.734803	712		
15	1	14	14	2	13	209.95569	209.955552	-137		
15	2	14	14	2	13	210.20234	210.202444	104		
15	1	14	14	1	13	210.41373	210.413479	-250		
15	2	14	14	1	13	210.66038	210.660358	-22		
8	4	4	8	1	7	210.83014	210.829990	-149		
6	4	2	6	1	5	211.46346	211.463319	-140		
7	2	5	6	1	6	211.50782	211.507808	-11	0.50801	-202
13	4	9	12	4	8	211.99948	211.999376	-103		
13	2	11	12	2	10	212.02712	212.026895	-225		
12	8	4	12	7	5	212.64169	212.640681	-1009		
12	8	4	12	7	5	212.64169	212.644262	2571		
14	2	12	13	2	11	213.16457	213.164679	109		
13	3	10	12	3	9	213.57512	213.574871	-248		

(Table continued)

Table 2. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
5	5	1	4	4	0	213.63778			0.63868	
5	5	0	4	4	1	213.63964			0.6453*	
7	4	4	6	3	3	213.66035			0.66032	
11	8	3	11	7	4	213.68752	213.688788	1267		
7	2	5	6	0	6	213.80875	213.808676	-74		
10	8	2	10	7	3	214.59453	214.594982	451		
5	4	1	5	1	4	215.02267	215.022538	-132		
9	8	1	9	7	2	215.37468	215.375269	588	0.37591	-641
9	8	2	9	7	3	215.37478	215.375269	489	0.37591	-641
9	4	5	9	1	8	215.90050	215.900424	-76		
8	8	0	8	7	1	216.04189	216.042032	142	0.04261	-578
8	8	1	8	7	2	216.04189	216.042032	142	0.04261	-578
7	4	3	6	3	4	216.09553	216.095733	202	0.09563	103
14	4	11	13	4	10	216.74673	216.746282	-448		
5	3	3	4	1	4	217.28367	217.283535	-132		
15	2	13	14	3	12	218.12308	218.123173	93		
14	5	10	13	5	9	218.61526	218.614801	-459		
4	4	0	4	1	3	219.34744	219.347300	-144		
7	3	4	6	1	5	219.45493	219.454819	-111		
14	3	12	13	2	11	219.80570	219.805627	-73		
8	3	5	7	2	6	221.36804	221.368099	58	0.36783	269
14	5	9	13	5	8	221.99024	221.991721	1481		
17	0	17	16	1	16	222.13994	222.138004	-1936		
17	0	17	16	1	16	222.13994	222.142224	2284		
17	1	17	16	1	16	222.14144	222.142224	784		
15	3	13	14	3	12	222.17008	222.170276	195		
16	1	15	15	2	14	222.49034	222.492284	1944		
16	2	15	15	2	14	222.62215	222.624067	1916		
16	1	15	15	1	14	222.73699	222.739146	2156		
16	2	15	15	1	14	222.86880	222.870954	2154		
5	3	3	4	0	4	223.50966	223.509523	-139		
15	2	13	14	2	12	224.76421	224.764160	-49		
9	3	6	9	0	9	224.96434	224.964317	-22		
10	4	6	10	1	9	225.69524	225.695061	-179		
8	4	5	7	3	4	226.60109			0.60087	
14	3	11	13	3	10	227.70159	227.701824	233		
15	3	13	14	2	12	228.81121	228.811269	59		
6	5	2	5	4	1	228.90773			0.90790	
6	5	1	5	4	2	228.92514			0.92512	
14	4	10	13	4	9	229.44516	229.444973	-186		
8	5	4	8	3	5	230.73702				
15	4	12	14	4	11	230.80113	230.801903	773		
8	4	4	7	3	5	232.48852			0.48874	

(Table continued)

Table 2. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
9	4	6	8	3	5	237.78203	237.782478	448	0.78200	478
8	3	5	7	1	6	237.87775	237.877638	-112		
11	9	2	11	8	3	238.87620	238.875305	-895		
10	9	1	10	8	2	239.77020	239.769995	-204		
9	9	0	9	8	1	240.56027	240.560028	-242		
11	4	7	11	1	10	240.76451	240.764356	-154		
6	3	4	5	1	5	241.64972	241.649617	-101		
7	5	3	6	4	2	244.03606	244.035731	-328	0.03612	-389
7	5	2	6	4	3	244.12289	244.122870	-20	0.12299	-120
4	4	0	3	2	1	245.26628	245.266080	-195		
6	3	4	5	0	5	245.56848	245.568276	-203		
4	4	1	4	1	4	245.94692	245.946834	-83		
15	4	11	14	4	10	246.17047	246.171004	534		
11	5	6	11	3	9	246.81014	246.810520	380		
10	4	7	9	3	6	246.87184	246.871499	-340		
4	4	1	3	2	2	246.94015	246.939954	-200		
8	2	6	7	1	7	248.64311	248.642992	-118	0.64309	-98
9	3	6	8	2	7	249.44599	249.445804	-185	0.44595	-146
8	2	6	7	0	7	249.92727	249.927171	-99		
9	4	5	8	3	6	250.01521			0.01519	
11	4	8	10	3	7	253.86983	253.869500	-330		
5	4	2	5	1	5	254.37782	254.377666	-151		
10	3	7	10	0	10	255.63855	255.638533	-17		
6	6	1	5	5	0	256.82173			0.82174	
6	6	0	5	5	1	256.82176			0.82174	
5	4	1	4	2	2	258.42277	258.422501	-264		
8	5	4	7	4	3	258.92234			0.92238	
12	4	9	11	3	8	259.07499	259.074809	-180		
8	5	3	7	4	4	259.23820			0.23829	
9	3	6	8	1	7	260.82944	260.829417	-22		
12	4	8	12	1	11	261.41475	261.414655	-95		
13	4	10	12	3	9	262.97068	262.970378	-302		
5	4	2	4	2	3	263.20077	263.200618	-150		
6	4	3	6	1	6	265.27506	265.274923	-136		
14	4	11	13	3	10	266.14229	266.141794	-495		
7	3	5	6	1	6	268.28903	268.288899	-131		
12	5	7	12	2	10	268.58327	268.582825	-445		
15	4	12	14	3	11	269.24183	269.241989	158		
10	4	6	9	3	7	269.39220	269.391820	-380	0.3887*	3120
11	5	6	11	2	9	269.62832	269.628311	-8		
6	4	2	5	2	3	269.97578	269.975585	-194		
7	3	5	6	0	6	270.58996	270.589762	-198		
7	6	2	6	5	1	271.96020			0.96089	
7	6	1	6	5	2	271.96143			0.96089	

(Table continued)

Table 2. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
13	5	8	13	2	11	272.10811	272.107835	-274		
16	4	13	15	3	12	272.96573	272.967448	1717		
9	5	5	8	4	4	273.39185	273.391107	-742	0.39181	-703
10	5	5	10	2	8	274.23862	274.238581	-39		
9	5	4	8	4	5	274.32346	274.323871	410	0.32344	431
7	4	4	7	1	7	278.87834	278.878131	-208		
7	4	3	6	2	4	280.06109	280.060901	-188		
6	4	3	5	2	4	280.25423	280.254020	-209		
9	5	4	9	2	7	281.24256	281.242395	-165		
10	3	7	9	2	8	281.47120	281.471096	-104		
4	4	1	3	1	2	285.86782	285.867582	-233		
8	6	3	7	5	2	286.98974			0.98991	
8	6	2	7	5	3	286.99724			0.99693	
10	5	6	9	4	5	287.15881	287.158387	-423	0.1563*	2087
13	4	9	13	1	12	287.62491	287.624809	-100		
9	2	7	8	1	8	288.43688	288.436699	-180		
10	3	7	9	1	8	288.83344	288.833284	-156		
9	2	7	8	0	8	289.12825	289.127915	-335		
8	4	4	7	2	5	289.26973	289.269539	-190		
8	5	3	8	2	6	289.47343	289.473166	-264		
10	5	5	9	4	6	289.51180	289.511682	-117		
11	3	8	11	0	11	290.72571	290.726562	852		
11	4	7	10	3	8	291.44548	291.445163	-316	0.4426*	2563
8	4	5	8	1	8	295.35598	295.355783	-197		
8	3	6	7	1	7	297.17480	297.174622	-178		
5	4	2	4	1	3	297.25913	297.258906	-227		
7	5	2	7	2	5	297.89013	297.889967	-162		
7	4	4	6	2	5	298.44842	298.448224	-196		
8	3	6	7	0	7	298.45896	298.458702	-257		
9	4	5	8	2	6	298.54690	298.546662	-237		
7	7	1	6	6	0	298.74111	298.741420	310	0.74111	310
7	7	0	6	6	1	298.74111	298.741420	310	0.74111	310
11	5	7	10	4	6	299.80697	299.806833	-136		
9	6	4	8	5	3	301.87507				
9	6	3	8	5	4	301.90743	301.907146	-283		
4	4	0	3	1	3	301.94009	301.939984	-101		
11	5	6	10	4	7	305.05567	305.055550	-120	0.0566*	-1050
6	5	1	6	2	4	305.61880	305.618602	-198		
6	4	3	5	1	4	308.65454	308.654356	-183		
10	4	6	9	2	7	309.11576	309.115596	-164		
12	5	8	11	4	7	310.82953	310.829344	-185		
8	7	2	7	6	1	313.70836	313.708334	-26	0.70838	-46
8	7	1	7	6	2	313.70840	313.708334	-66	0.70838	-46

(Table continued)

Table 2. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
9	4	6	9	1	9	314.78644	314.786295	-145		
10	6	5	9	5	4	316.56378	316.563652	-128	0.5637*	-48
10	6	4	9	5	5	316.67564	316.675579	-60	0.6749*	679
12	4	8	11	3	9	316.93395	316.933826	-123		
11	3	8	10	2	9	317.17889	317.178700	-190		
8	4	5	7	2	6	318.13579	318.135618	-171		
13	5	9	12	4	8	319.76387	319.763671	-199		
7	4	4	6	1	5	320.81683	320.816623	-206		
12	5	7	11	4	8	321.36181	321.361652	-157		
11	3	8	10	1	9	321.69018	321.689901	-278		
5	5	1	5	2	4	322.33223	322.331988	-241		
11	4	7	10	2	8	322.38829	322.388040	-249		
5	4	1	4	1	4	323.87666	323.876493	-164		
6	5	2	6	2	5	324.29106	324.290909	-151		
14	5	10	13	4	9	326.37965	326.379128	-522		
7	5	3	7	2	6	327.57929	327.579294	3		
9	7	3	8	6	2	328.56869	328.568211	-478	0.56837	-159
9	7	2	8	6	3	328.56931	328.568211	-1099	0.56837	-159
9	3	7	8	0	8	328.85181	328.851614	-196		
12	3	9	12	0	12	329.41091	329.410688	-222		
10	2	8	9	1	9	330.05962	330.059432	-187		
10	2	8	9	0	9	330.42242	330.422042	-378		
15	5	11	14	4	10	330.78649	330.783635	-2855		
11	6	6	10	5	5	330.97263	330.972527	-102	0.9728*	-273
11	6	5	10	5	6	331.30172	331.301397	-322		
8	5	4	8	2	7	332.58588	332.585716	-163		
8	4	5	7	1	6	334.64550	334.645336	-164		
6	5	1	5	3	2	334.75782	334.757809	-10		
6	5	2	5	3	3	335.50072	335.500551	-169		
10	4	7	10	1	10	337.14750	337.147420	-79		
13	5	8	12	4	9	339.01051	339.010303	-206		
8	8	1	7	7	0	339.34667	339.346892	222	0.34734	-448
8	8	0	7	7	1	339.34667	339.346892	222	0.34734	-448
9	4	6	8	2	7	339.63089	339.630735	-155		
13	6	7	13	3	10	339.68228	339.682606	326		
9	5	5	9	2	8	339.68771	339.687557	-152		
12	4	8	11	2	9	339.75213	339.752043	-87		
10	7	4	9	6	3	343.30046	343.300770	310		
12	6	7	11	5	6	344.96577	344.965563	-207		
12	6	6	11	5	7	345.81811	345.818005	-104		
13	4	9	12	3	10	346.32314	346.322975	-165		
6	4	2	5	1	5	348.10576	348.105602	-156		
7	5	2	6	3	3	348.35002	348.350071	51		

(Table continued)

Table 2. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
10	5	6	10	2	9	349.21858	349.218550	-29		
7	5	3	6	3	4	350.49210	350.492025	-74		
9	4	6	8	1	7	351.01434	351.014169	-171		
9	8	2	8	7	1	354.11097	354.110890	-80		
12	3	9	11	2	10	356.00113	356.001190	60		
11	7	5	10	6	4	357.88043	357.880287	-142		
11	7	4	10	6	5	357.89183	357.891528	-302		
13	6	8	12	5	7	358.32486	358.325003	142		
12	3	9	11	1	10	358.65124	358.651263	22		
14	5	9	13	4	10	358.73418	358.735592	1412		
13	6	7	12	5	8	360.31460	360.314988	388		
8	5	3	7	3	4	360.60010	360.600007	-92		
10	3	8	9	1	9	361.00243	361.002300	-130		
10	3	8	9	0	9	361.36523	361.365059	-171		
11	5	7	11	2	10	361.44228	361.442277	-2		
10	4	7	9	2	8	363.16700	363.166842	-157		
8	5	4	7	3	5	365.62771	365.627588	-121		
10	8	3	9	7	2	368.76230	368.763073	773		
10	4	7	9	1	8	370.52924	370.529027	-213		
14	6	9	13	5	8	370.72343	370.724220	789		
9	5	4	8	3	5	371.09121	371.091050	-159		
12	7	6	11	6	5	372.27650	372.276312	-187		
12	7	5	11	6	6	372.31398	372.313983	2		
11	2	9	10	1	10	372.57485	372.574649	-201		
10	6	4	10	3	7	374.89215	374.892128	-22		
14	6	8	13	5	9	374.96926	374.970134	873		
7	4	3	6	1	6	374.99440	374.994181	-218		
12	5	8	12	2	11	376.53105	376.530734	-315		
9	9	1	8	8	0	378.62935	378.628703	-647		
14	4	10	13	2	11	379.64443	379.644199	-230		
10	5	5	9	3	6	379.69670	379.696661	-39		
9	5	5	8	3	6	381.16466	381.164406	-254		
15	5	10	14	4	11	381.33194	381.332830	890		
11	8	4	10	7	3	383.28929	383.289919	629		
9	6	3	9	3	6	385.04732	385.047298	-22		
13	7	7	12	6	6	386.44426	386.444276	16		
13	7	6	12	6	7	386.55482	386.554611	-208		
12	4	9	12	1	12	390.06729	390.066800	-490		
10	9	2	9	8	1	393.15782	393.157874	53		
8	6	2	8	3	5	393.20849	393.208529	39		
11	4	8	10	1	9	393.37383	393.373424	-405		
5	5	1	4	2	2	394.13264	394.132440	-195		

(Table continued)

Table 2. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
11	3	9	10	0	10	395.57988	395.579721	-158		
13	3	10	12	2	11	397.16337	397.163183	-186		
12	8	5	11	7	4	397.67531	397.675165	-145		
5	5	0	4	2	3	398.92689	398.926871	-18		
14	7	8	13	6	7	400.30495	400.318005	13055		
14	7	7	13	6	8	400.59591	400.608395	12485		
9	6	4	9	3	7	403.06962	403.069495	-124		
8	6	3	8	3	6	403.38295	403.382923	-26		
10	6	5	10	3	8	403.65697	403.656959	-11		
8	4	4	7	1	7	404.94761	404.947384	-225		
6	5	2	5	2	3	405.17179	405.171657	-133		
11	6	6	11	3	9	405.55196	405.551906	-54		
11	9	3	10	8	2	407.57096	407.570291	-669		
13	8	6	12	7	5	411.89854	411.899669	1128		
13	8	5	12	7	6	411.90180	411.903281	1481		
7	5	3	6	2	4	414.45766	414.457441	-218		
12	2	10	11	1	11	415.09295	415.093031	81		
6	5	1	5	2	4	415.53128	415.531138	-141		
15	4	11	14	3	12	416.52112	416.521595	474		
12	4	9	11	1	10	419.35535	419.355196	-154	0.3579*	-2704
8	5	4	7	2	5	422.40892	422.408758	-162		
9	5	5	8	2	6	429.69635	429.696105	-245		
12	3	10	11	0	11	431.09115	431.091106	-44		
7	5	2	6	2	5	433.13809	433.137928	-161		
10	5	6	9	2	7	437.15039	437.150251	-138		
9	4	5	8	1	8	438.42846	438.428280	-180		
14	3	11	13	2	12	439.74552	439.745573	52		
11	5	7	10	2	8	445.71617	445.716131	-38		
13	4	10	12	1	11	448.06721	448.067019	-190		
8	5	3	7	2	6	452.13480	452.134661	-138		
12	5	8	11	2	9	456.37671	456.376454	-255		
13	2	11	12	1	12	456.96969	456.969504	-186		
13	2	11	12	0	12	467.52934	467.529151	-188		
13	5	9	12	2	10	469.99078	469.990371	-408		
9	5	4	8	2	7	472.94007	472.939870	-200		
10	4	6	9	1	9	475.96882	475.968671	-149		
14	4	11	13	1	12	479.02462	479.023971	-649		
15	3	12	14	2	13	482.77457	482.775098	528		
14	5	10	13	2	11	487.09084	487.090308	-532		
10	5	5	9	2	8	495.99186	495.991708	-151		
14	2	12	13	1	13	497.90846	497.908570	110		
14	3	12	13	0	13	504.57352	504.573368	-151		

(Table continued)

Table 2. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
10	7	4	9	5	5	504.95523	504.953380	-1849		
7	6	2	6	3	3	511.46438	511.464384	3		
15	4	12	14	1	13	511.73853	511.738539	8		
7	6	1	6	3	4	513.61348	513.613470	-9		
11	4	7	10	1	10	518.12203	518.121625	-405		

[a] See the footnote of Table 1 for the definitions of the columns. The literature values marked with an asterisk (*) are taken from Ref. 1.

Table 3. Absorption Peaks (in Reciprocal Centimeters) Assigned to Pure Rotational Transitions[a] of $D_2{}^{16}O$ Between 110 and 420 cm^{-1}

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
10	2	8	9	3	7	110.58680	110.586802	2	0.58676	42
10	1	9	9	2	8	110.60346	110.603195	-264	0.60339	-195
5	3	2	4	2	3	110.89925	110.899068	-181	0.89917	-102
11	0	11	10	1	10	111.26224	111.262050	-190	0.26199	60
11	1	11	10	0	10	111.29759	111.297637	46	0.29755	87
6	3	4	5	2	3	111.39692	111.396611	-309	0.39682	-209
12	1	11	12	0	12	111.39580	111.396611	810		
10	7	3	10	6	4	112.01743	112.017291	-139	0.01726	31
9	7	2	9	6	3	112.24910	112.249126	26		
9	7	3	9	6	4	112.26857	112.268268	-301		
7	7	0	7	6	1	112.31984	112.320058	218	0.31998	78
7	7	1	7	6	2	112.32051	112.320058	-452	0.31998	78
8	7	1	8	6	2	112.33393	112.333849	-80	0.33390	-51
8	7	2	8	6	3	112.33804	112.338114	73		
5	2	3	4	1	4	112.67997	112.679903	-66	0.67989	13
4	4	1	3	3	0	112.71256	112.712388	-171	0.71221	178
4	4	0	3	3	1	112.77577	112.775759	-9	0.77573	29
6	3	3	6	0	6	112.92511	112.925104	-5		
10	2	9	9	1	8	112.96321	112.963150	-60	0.96324	-90
7	3	5	6	2	4	117.93372	117.933508	-211	0.93369	-182
11	1	10	10	2	9	120.71554	120.715355	-185	0.71526	95
12	0	12	11	1	11	120.85260	120.852297	-303	0.85248	-183
12	1	12	11	0	11	120.86830	120.868175	-125	0.86825	-75
13	1	12	13	0	13	121.36956	121.369419	-141		
13	2	12	13	1	13	121.46154	121.461231	-309		
11	2	10	10	1	9	121.90906				
8	3	6	7	2	5	123.34648	123.346414	-66	0.34633	84
11	2	9	10	3	8	124.50533	124.505035	-294	0.50502	15
5	4	2	4	3	1	124.79544	124.795281	-158	0.79534	-59
5	4	1	4	3	2	125.23748	125.237541	60	0.23765	-109
6	4	2	6	1	5	125.96711	125.967457	346		
12	3	9	11	4	8	126.64486	126.644485	-374		
8	8	0	8	7	1	126.90713	126.907119	-11		
9	8	1	9	7	2	127.03911	127.039259	149		

(Table continued)

Table 3. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
10	8	2	10	7	3	127.10818	127.107735	-444		
6	3	3	5	2	4	127.86137	127.861262	-107	0.86139	-128
9	3	7	8	2	6	128.16769	128.167704	13	0.16759	114
7	4	3	7	1	6	128.83369	128.833512	-177		
13	0	13	12	1	12	130.41942	130.419255	-165		
13	1	13	12	0	12	130.42643	130.426269	-161		
12	1	11	11	2	10	130.54014	130.539979	-161	0.54016	-181
12	2	11	11	1	10	131.13039	131.130353	-36	0.13050	-147
10	3	8	9	2	7	133.04900	133.049013	12	0.04907	-57
4	3	2	3	0	3	135.43884	135.438809	-26		
8	4	4	8	1	7	135.76385	135.763810	-39		
6	4	3	5	3	2	136.27327	136.273181	-89	0.27313	51
12	2	10	11	3	9	136.87129	136.871071	-218	0.87107	1
6	4	2	5	3	3	138.00129	138.001261	-29	0.00127	9
11	3	9	10	2	8	138.60825	138.608148	-101	0.60808	68
6	2	4	5	1	5	139.02225	139.022101	-145	0.02206	41
14	0	14	13	1	13	139.96432	139.963989	-330		
14	1	14	13	0	13	139.96715	139.967075	-75		
13	1	12	12	2	11	140.20411	140.203990	-119		
13	2	12	12	1	11	140.49217	140.492074	-95		
5	5	1	4	4	0	142.16061	142.160315	-294	0.16052	-205
5	5	0	4	4	1	142.16691	142.166820	-90	0.16676	60
13	3	10	12	4	9	143.83857	143.838442	-128		
12	3	10	11	2	9	145.18210	145.182139	39	0.18205	89
7	4	4	6	3	3	146.57490	146.574848	-52	0.57492	-72
7	3	4	6	2	5	147.96643	147.966401	-29	0.96643	-29
13	2	11	12	3	10	148.07194	148.071782	-157		
15	0	15	14	1	14	149.48664	149.487334	694		
14	1	13	13	2	12	149.77668	149.776448	-232		
14	2	13	13	1	12	149.91625	149.915982	-267		
7	4	3	6	3	4	151.49175	151.491586	-163	0.49213	-544
5	3	3	4	0	4	152.54413	152.543959	-170		
13	3	11	12	2	10	152.74031	152.740217	-92		
6	5	2	5	4	1	154.47031	154.470298	-11	0.47058	-282
6	5	1	5	4	2	154.52803	154.527971	-58	0.52814	-169
8	4	5	7	3	4	155.15833	155.158147	-182	0.15820	-53
14	2	12	13	3	11	158.50115	158.501053	-96		
16	0	16	15	1	15	158.98600	158.985763	-236		
14	3	11	13	4	10	159.10463	159.104286	-343		
15	1	14	14	2	13	159.29233	159.292243	-86		
15	2	14	14	1	13	159.35980	159.359697	-102		
13	3	12	13	2	11	161.03734	161.037344	3		
9	4	6	8	3	5	161.82053	161.820501	-28	0.82073	-229

(Table continued)

Table 3. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
10	4	6	10	1	9	164.13064	164.130871	231		
8	4	4	7	3	5	166.38814	166.388043	-96	0.38822	-177
7	5	3	6	4	2	166.59873	166.598586	-143	0.59880	-214
10	4	7	9	3	6	166.77911	166.778893	-216	0.77913	-237
7	5	2	6	4	3	166.88124	166.881124	-115	0.88129	-166
7	2	5	6	1	6	168.15676	168.156552	-207	0.15713	-578
17	0	17	16	1	16	168.45945	168.460320	869		
16	1	15	15	2	14	168.76850	168.768244	-255		
16	2	15	15	1	14	168.80078	168.800676	-103		
15	3	13	14	2	12	169.80569	169.805269	-420		
11	4	8	10	3	7	170.51803	170.517822	-208	0.51823	-408
6	6	1	5	5	0	170.86648	170.866654	174	0.86696	-306
6	6	0	5	5	1	170.86695	170.866654	-296	0.86696	-306
8	3	5	7	2	6	171.61551	171.615366	-144	0.61544	-74
6	3	4	5	0	5	172.35036	172.350274	-85		
12	4	9	11	3	8	173.66277	173.662421	-348		
13	4	10	12	3	9	176.91571	176.915722	11		
18	0	18	17	1	17	177.90945	177.908863	-586		
16	2	14	15	3	13	178.13511	178.134980	-129		
17	1	16	16	2	15	178.21176	178.211518	-241		
17	2	16	16	1	15	178.22753	178.227464	-66		
8	5	4	7	4	3	178.31481	178.314645	-164	0.31491	-265
16	3	14	15	2	13	178.84155	178.841573	22		
8	5	3	7	4	4	179.31415	179.313932	-218	0.31418	-248
14	4	11	13	3	10	180.93748	180.937550	69		
7	6	2	6	5	1	183.25176	183.251564	-195	0.25198	-416
7	6	1	6	5	2	183.25836	183.258127	-233	0.25849	-363
9	4	5	8	3	6	183.56157	183.561430	-139	0.56156	-130
15	4	12	14	3	11	186.13871	186.136703	-2006		
19	0	19	18	1	18	187.32961	187.330194	584		
18	1	17	17	2	16	187.62515	187.625009	-141		
17	3	15	16	2	14	188.01568	188.015828	148		
9	5	5	8	4	4	189.22216	189.221947	-213	0.22209	-143
5	4	2	4	1	3	189.98510	189.984834	-270		
9	5	4	8	4	5	192.05037	192.050222	-148	0.05058	-358
7	3	5	6	0	6	194.67712	194.676934	-186		
8	6	3	7	5	2	195.55234	195.552031	-309	0.55216	-129
8	6	2	7	5	3	195.59063	195.590371	-259	0.59066	-289
9	3	6	8	2	7	198.65182	198.651788	-32	0.65173	58
7	7	1	6	6	0	198.76348	198.763202	-278	0.76334	-138
7	7	0	6	6	1	198.76353	198.763202	-328	0.76334	-138
10	5	6	9	4	5	198.77475	198.774588	-162	0.77471	-122
8	2	6	7	1	7	199.28213	199.281668	-461	0.28122	448

(Table continued)

Table 3. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
6	4	3	5	1	4	200.34594	200.345802	-138		
10	4	6	9	3	7	203.83456	203.834495	-65	0.83453	-35
10	5	5	9	4	6	205.50932	205.508966	-354	0.50915	-184
11	5	7	10	4	6	206.45346	206.453176	-283		
9	6	4	8	5	3	207.69253	207.692370	-159	0.69270	-330
9	6	3	8	5	4	207.85294	207.852693	-247	0.85281	-117
8	7	2	7	6	1	211.20268	211.202917	237		
8	7	1	7	6	2	211.20340	211.202917	-483	0.20327	-353
12	5	8	11	4	7	212.04080	212.040686	-113		
7	4	4	6	1	5	212.45702	212.456924	-96		
13	5	9	12	4	8	215.74413	215.743829	-301		
8	3	6	7	0	7	219.11378	219.113782	1		
10	6	5	9	5	4	219.53772	219.537559	-161	0.53758	-21
10	6	4	9	5	5	220.07169	220.071651	-38	0.07166	-9
11	5	6	10	4	7	220.33377	220.333584	-185		
9	7	3	8	6	2	223.57580	223.575675	-124		
9	7	2	8	6	3	223.58040	223.580362	-37		
8	8	1	7	7	0	225.79002	225.789958	-61		
8	4	5	7	1	6	227.17171	227.171570	-139		
11	4	7	10	3	8	227.64671	227.646524	-186		
10	3	7	9	2	8	228.50349	228.503382	-108		
11	6	6	10	5	5	230.84887	230.848899	28		
9	2	7	8	1	8	231.41977	231.419432	-337		
11	6	5	10	5	6	232.34865	232.348567	-82		
10	7	4	9	6	3	235.84737	235.847360	-10		
10	7	3	9	6	4	235.86985	235.869697	-153		
12	5	7	11	4	8	237.34011	237.340015	-95		
9	8	2	8	7	1	238.28142	238.281333	-87		
12	6	7	11	5	6	241.24346	241.243449	-11		
9	4	6	8	1	7	244.87914	244.879135	-5		
12	6	6	11	5	7	244.90707	244.907028	-42		
9	3	7	8	0	8	245.19790	245.197734	-166		
11	7	5	10	6	4	247.96707	247.966762	-308		
11	7	4	10	6	5	248.05184	248.051671	-168		
13	6	8	12	5	7	250.20843	250.208341	-89		
10	8	3	9	7	2	250.70896	250.709108	147		
9	9	1	8	8	0	251.90791	251.907651	-258		
12	4	8	11	3	9	254.88922	254.889254	33		
13	5	8	12	4	9	257.32537	257.324971	-399		
13	6	7	12	5	8	258.13939	258.139383	-6		
12	7	6	11	6	5	259.85333	259.853204	-126		
12	7	5	11	6	6	260.12405	260.123914	-135		
11	3	8	10	2	9	260.33453	260.334391	-138		

(Table continued)

Table 3. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
7	5	3	6	2	4	262.86543	262.865206	-224		
11	8	4	10	7	3	263.04857	263.047948	-622		
11	8	3	10	7	4	263.05147	263.050774	-696		
10	2	8	9	1	9	263.62302	263.622837	-183		
10	9	2	9	8	1	264.45179	264.451153	-637		
10	4	7	9	1	8	265.44213	265.441946	-184		
8	5	4	7	2	5	269.93292	269.932601	-319		
13	7	7	12	6	6	271.36981	271.369819	9		
13	7	6	12	6	7	272.12166	272.121452	-208		
10	3	8	9	0	9	272.48573	272.485661	-68		
14	6	8	13	5	9	272.63189	272.631536	-354		
12	8	5	11	7	4	275.27035	275.270282	-67		
12	8	4	11	7	5	275.28236	275.283102	742		
11	9	3	10	8	2	276.92782	276.927806	-14		
10	10	1	9	9	0	277.09812	277.097923	-197		
9	5	5	8	2	6	277.76017	277.759973	-197		
14	5	9	13	4	10	280.77382	280.773707	-112		
14	7	8	13	6	7	282.28833	282.288449	119		
14	7	7	13	6	8	284.14688	284.146770	-110		
13	4	9	12	3	10	285.00675	285.006513	-237		
13	8	6	12	7	5	287.33965	287.339731	80		
13	8	5	12	7	6	287.38223	287.382807	577		
8	4	4	7	1	7	287.82014	287.819876	-263		
11	4	8	10	1	9	288.41806	288.418085	24		
12	9	4	11	8	3	289.31754	289.317977	436		
11	10	2	10	9	1	289.69256	289.692977	416		
15	7	9	14	6	8	292.25747	292.257689	219		
12	3	9	11	2	10	293.15386	293.153550	-310		
11	2	9	10	1	10	295.26809	295.267704	-385		
14	8	7	13	7	6	299.20542	299.205413	-6		
14	8	6	13	7	7	299.33684	299.337275	434		
11	5	7	10	2	8	299.70122	299.700894	-325		
11	3	9	10	0	10	300.58792	300.587763	-157		
11	11	1	10	10	0	301.35867	301.358691	21		
13	9	5	12	8	4	301.60026	301.600043	-216		
12	10	3	11	9	2	302.21747	302.215620	-1849		
12	4	9	11	1	10	313.28176	313.281463	-297		
12	11	2	11	10	1	314.00374	314.004029	289		
13	10	4	12	9	3	314.64918	314.648702	-477		
12	5	8	11	2	9	315.18218	315.182064	-115		
13	3	10	12	2	11	325.98994	325.989402	-538		
12	2	10	11	1	11	326.16162	326.161326	-294		
13	11	3	12	10	2	326.56833	326.569492	1162		

(Table continued)

Table 3. Continued

J'	K_a'	K_c'	J''	K_a''	K_c''	Calc	Obs	O − C	Lit	O − L
14	10	5	13	9	4	326.97251	326.974611	2100		
12	3	10	11	0	11	329.18795	329.187663	-287		
13	5	9	12	2	10	333.76206	333.762057	-2		
13	4	10	12	1	11	339.52943	339.529330	-99		
10	5	5	9	2	8	345.89447	345.894209	-261		
11	6	6	10	3	7	348.23985	348.239728	-121		
13	3	11	12	0	12	358.04933	358.049112	-218		
14	3	11	13	2	12	358.14189	358.141520	-369		
14	2	12	13	1	13	386.12405	386.123937	-112		
11	7	5	10	4	6	413.79668	413.794939	-1740		

[a] See the footnote of Table 1 for the definitions of the columns.

increase when the wave number increases. At 500 cm^{-1} the average value is approximately-0.000017 cm^{-1}. The result that the averageO − C value is negative and not 0 is statistically significant because the standard error was ~0.00017 cm^{-1}. The uncertainties of the energy levels given by Toth[7] increase when J and especially K_a increase. The corresponding increase in the O − C values could be observed, but it seemed not to be so remarkable that it could exclusively explain the large scattering of the O − C values in Fig. 2.

In Fig. 3, line positions of this paper (O) are compared with the values obtained in the literature (L) by Johns.[3] The scattering of the O − L values is of the same order as that in Fig. 2. The average value of 62 observations was -0.00020 cm^{-1}, and the rms value was 0.00034 cm^{-1}. At higher wave numbers the differences between our line positions and those of Johns became greater. With a linear least-squares fit, a value -0.00046 cm^{-1} was obtained at 330 cm^{-1}.

Between 350 and 500 cm^{-1} there are, in the literature, the line positions given by Kauppinen *et al.*[2] only. When comparing the line positions of the present work with those of Kauppinen *et al.*[2] we observe that the scattering of the O − L values is much greater. This is due to the lower resolution in Ref. (2). The rms value was found to be ~0.0019 cm^{-1}, but the average deviation was not greater than that in Fig. 3.

The accuracy of the calibration procedure was studied by Horneman *et al.*,[12] who used the ν_1 and $2\nu_2$ bands of OCS as examples. According to their results (see Fig. 1 of Ref. 12) the internal consistency of the lines within a single absorption band of a linear molecule is much better than 0.0001 cm^{-1}. The maximum deviations in Fig. 1 of Ref. 12 were approximately 100×10^{-6} cm^{-1}, and in Figs. 2 and 3 of this paper they are approximately 1000×10^{-6} cm^{-1}. A pure calibration factor is not adequate to explain the scattering of the points in Figs. 2 and 3. Dispersion effects mentioned in Section 1 may produce part of the variation in the case of H_2O because the error depends on the absorption strength of the line. However, if plots similar to those of Fig. 2 are made for D_2O and HDO, similar figures are obtained, and so it seems that the dispersion effect is not the main problem with H_2O. This can also be estimated in another way. During the measurements the total pressure in the spectrometer tank is ~0.02 Torr and the tank is continuously pumped. If we assume that the gas leaking to the tank contains the component gases of air in a normal ratio, then no more than 10% of the leak is water, and the ratio between the absorption in the cell and in the moving mirror arm is ~1000. This is much greater than the signal-to-noise ratio in our measurements, so we believe that the absorption in the moving mirror arm is not a serious problem.

The average difference between our line positions and those of Johns[3] is smaller in lower wave numbers, where the calibration lines used by Johns were made, and increases to higher wave numbers, where the calibration of our measurements were made. This can be partially explained with line-shape differences between the water and the OCS lines, as we show below in this section. But this also indicates that the extrapolation in calibration in Johns' work has caused some errors to line positions.

To estimate accuracy of the wave numbers in the OCS $2\nu_2$ work,[12] the Bruker method for calculating peak positions was compared with the center-of-gravity method,[6]

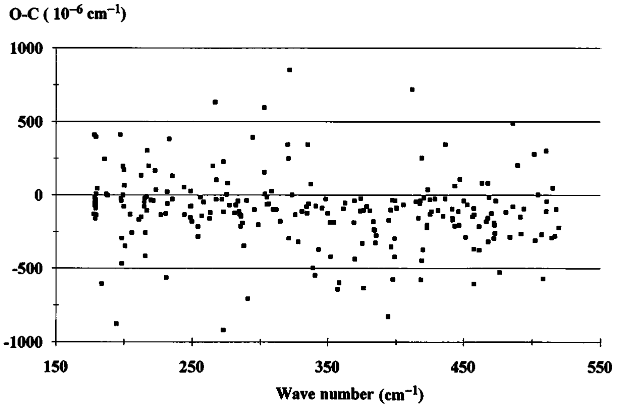

Fig. 2. Differences between the observed (O) and the calculated (C) wave numbers of the absorption peaks of $H_2{}^{16}O$ as functions of wave number. The observed line positions are from this work, and the calculated line positions were derived from the energy levels given by Toth.[7]

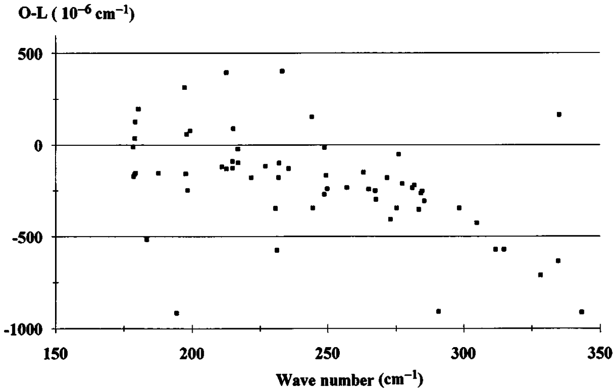

Fig. 3. Differences between the observed line positions of this work (O) and the observed literature values (L) taken from Ref. 3 of $H_2{}^{16}O$ as functions of wave number.

which has been used previously in our accurate measurements for standard purposes, for example, in those produced for the *Handbook of Infrared Standards*.[4] The Bruker method was found to be at least as accurate as the other one. That is why we can also use the standard Bruker method safely in this work. We can also use the estimate $|\Delta\nu| = \delta\nu/q$ (signal to noise) of the center-of-gravity method[6] as the error limit in calculating peak positions. In the formula, $\delta\nu$ = FWHH (full width at half-height) of the line and q is a factor that depends on the line shape [2.8 for the Lor-Sinc (sinc convoluted by a Lorenzian) line shape], which is in this connection a sufficiently good estimate for the line shape in the high-resolution spectrum). For well-separated single lines with an absorption of ~50%, the signal-to-noise ratio is 50, $\delta\nu = 0.0025$ cm^{-1}, and the error limit is $|\Delta\nu| < 18 \times 10^{-6}$ cm^{-1}.

In this work, the phase error in the spectrum was estimated by the calculation of symmetries of the measured line shapes. The symmetries of ~340 lines were analyzed. An interesting effect, which we have also noticed in our earlier H_2O measurements, was found with these calculations. The symmetry of H_2O lines in the same wave-number region is a little bit different from the symmetry of the OCS lines. Having no other explanation of this, we used to think that this is caused by the dispersion effect that is due to H_2O vapor, which is always present in the spectrometer tank. But in one measurement, D_2O, HDO, and H_2O lines had the same symmetry but differed from the OCS lines in the same wave-number region and for equally strong peaks. At this time we have no explanation for this difference. This would be worth another investigation. Nevertheless we can take this difference in line symmetries as a phase error and estimate the corresponding error in line positions with the method described in the dissertation of Horneman.[6] By simulation we could find the error in line positions caused by the different phases in the OCS and the water (H_2O, D_2O, HDO) lines, which increased in wave numbers as $\Delta\nu = \nu \times 0.188 \times 10^{-6}$ cm^{-1}. So we can say that this error is smaller than 47×10^{-6} cm^{-1} in the region below 250 cm^{-1} and smaller than 94×10^{-6} cm^{-1} in the region below 500 cm^{-1}.

We have not found any detailed broadband investigations of the pressure shifts of the pure rotational lines of water vapor. Recently Markov[13] made a study of a single line in the far infrared. According to his results, the pressure self-shift is ~0.000012 cm^{-1}/Torr. The results obtained from the vibration–rotation spectra in the infrared are of the same order in magnitude.[14–17] According to the results of these papers, it seems that the pressure shifts in this paper is smaller than 4×10^{-6} cm^{-1}, which is clearly below the accuracy limit caused by the signal-to-noise ratio and the resolution in this measurement.

The calibration of the OCS ν_2 band has been checked[18] with the help of the accurate $2\nu_2$ band,[12] so the absolute accuracy of the calibration OCS band is believed to be better than 11×10^{-6}. Taken all together, the most important errors in this case are those caused by the different line-shape symmetries between the calibration source and the water lines, the error in calculating peak positions, the error in the calibration source, and the possible error caused by the pressure shift. By adding all these effective errors in the way described by Horneman,[6] we can say that the absolute accuracy of the well-separated single lines is better than 134×10^{-6} cm^{-1} in the wave-number region below 500 cm^{-1}. In the lower region below 250 cm^{-1}, accuracy is better than 78×10^{-6} cm^{-1}. Of course one must remember that in a water spectrum there are many too strong and overlapped lines for which the accuracy is not so good. Its is worth noting that the error is biggest unexpectedly in the region of the calibration spectrum. The reason for this is the different symmetry of line shapes between the calibration and the water spectrum.

As a conclusion, we believe that the peak positions of Tables 1–3 of this paper are more accurate than the previous values given in the literature, especially those between 300 and 500 cm^{-1}, because the calibration conditions, signal-to-noise ratios, and the resolutions were better in our work. With the line-shape analysis described above, we have been able to estimate the absolute accuracy of the measured lines rather reliably. On the other hand, when water is used for calibration, the calibration should not be based on one or two lines. A sufficiently large amount of lines should be taken in order to average out the random variation.

ACKNOWLEDGMENTS

The authors thank S. Alanko for useful comments and R. Anttila for critically reading the manuscript.

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