High-resolution far-infrared (20–350-cm^{-1}) spectra of several isotopic species of H_2O

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Far-infrared pure rotational spectra of $H_2{}^{16}O$, $H_2{}^{18}O$, $HD^{16}O$, $HD^{18}O$, $D_2{}^{16}O$, and $D_2{}^{18}O$ have been measured with a high-resolution Fourier-transform spectrometer with an apparatus function of 0.004 cm^{-1} in the region from 20 to 350 cm^{-1}. Altogether about 1200 lines have been assigned and measured with an accuracy that is believed to be ~0.0002 cm^{-1} (~6 MHz), so that many of the frequencies should be of use in the calibration of far-infrared spectrometers.

INTRODUCTION

The past 10 years or so have seen increasing use of infrared spectrometers with resolution capabilities better than 0.01 cm^{-1}. The introduction of these instruments, using both Fourier and laser techniques, has created an urgent need for convenient standards over the whole of the infrared region. In the far infrared, i.e., in the region below 300 cm^{-1}, pure rotation transitions of water vapor are particularly strong, and indeed it is often quite difficult to eliminate them entirely from a spectrum. Water-vapor lines are thus often a natural choice for calibration in the region.

Fourier-transform infrared spectrometers with mirror movements of the order of 1 m have instrument functions with full width at half-maxima of only a few thousandths of a wave-number unit so that, with good signal-to-noise ratio, line measurements can attain a precision of the order of one ten thousandth of a wave-number unit (i.e., of the order of 3 MHz). The best available measurement of the spectrum of H_2O below 300 cm^{-1} has been recorded by Kauppinnen *et al.*[1] with an apparatus function of about 0.01 cm^{-1}; the precision was of the order of 10^{-3} cm^{-1}. At the same time the extensive predictions of Flaud *et al.*,[2] based on mid-infrared data, have about the same precision. It thus seemed of value to undertake new measurements of the pure rotation spectrum of H_2O so that the resulting line frequencies could be used to calibrate infrared spectrometers in the far infrared.

While recording the spectra of some deuterated species it was found that the lines of H_2O were too weak to be used as calibrants. However, lines of HDO were prominent, thus prompting careful measurement of some deuterated samples of water vapor (using the previously measured lines of H_2O as standards). In addition, the spectra of some samples of H_2O enriched in ^{18}O were also recorded. Since the absorption cell was at that time heavily contaminated with deuterium, a number of the rarer isotopic water species were readily identified and measured. Thus, in addition to $H_2{}^{16}O$, the following isotopic species have been included in the present study: $H_2{}^{18}O$, $HD^{16}O$, $HD^{18}O$, $D_2{}^{16}O$, and $D_2{}^{18}O$. Of these, only $H_2{}^{18}O$ appears to have been studied previously at a resolution as high as 0.01 cm^{-1}, by Kauppinen and Kyrö.[3] All the spectra have been fitted to molecular parameters that serve to reproduce the data, for the most part, to within the accuracy of measurement.

EXPERIMENT

The spectra were recorded with a Bomem DA 3.002 Fourier-transform spectrometer. The instrument was operated with the maximum possible optical path difference (MOPD) of 246 cm, which, with the Hamming apodization function [0.53856 + 0.46144 cos π(OPD/MOPD)] gives rise to an instrument function of full width at half-maximum of 0.0036 cm^{-1}. Two bolometers (Infrared Laboratories, Inc., Tucson, Arizona) were used: one had an effective size of 3 mm in diameter and was operated at 1.6 K and the other was 2 mm in diameter and was operated at 4.2 K. Three different cooled filters served to limit the radiation reaching the bolometers: the first was of crystal quartz together with a layer of garnet powder and covered the region below 100 cm^{-1}, the second was of calcium fluoride and crystal quartz for the region below 200 cm^{-1}, and the third was of sapphire together with layers of diamond and garnet powder for the region below 350 cm^{-1}. Because the bolometers are background-limited devices the best signal-to-noise ratios were obtained with the narrowest optical bandwidth, i.e., with the lower-temperature bolometer and the quartz filter. In order to cover the whole region from 15 to 350 cm^{-1}, several Mylar film beam splitters were used, ranging in thickness from 80 to 3 μm. Most spectra were run overnight, maximum observation times being set by the hold times of the two detector Dewars (~12 h at 1.6 K, ~25 h at 4.2 K).

The stainless-steel sample cell was 15 cm long and was fitted with high-density polyethylene windows. For the most part sample pressures were limited to less than 1 Torr (except below 30 cm^{-1} where 2 Torr was used) in order to minimize possible pressure shifts and pressure broadening. No attempt was made to record very weak lines, which would have only limited use as calibrants. Two examples that illustrate the

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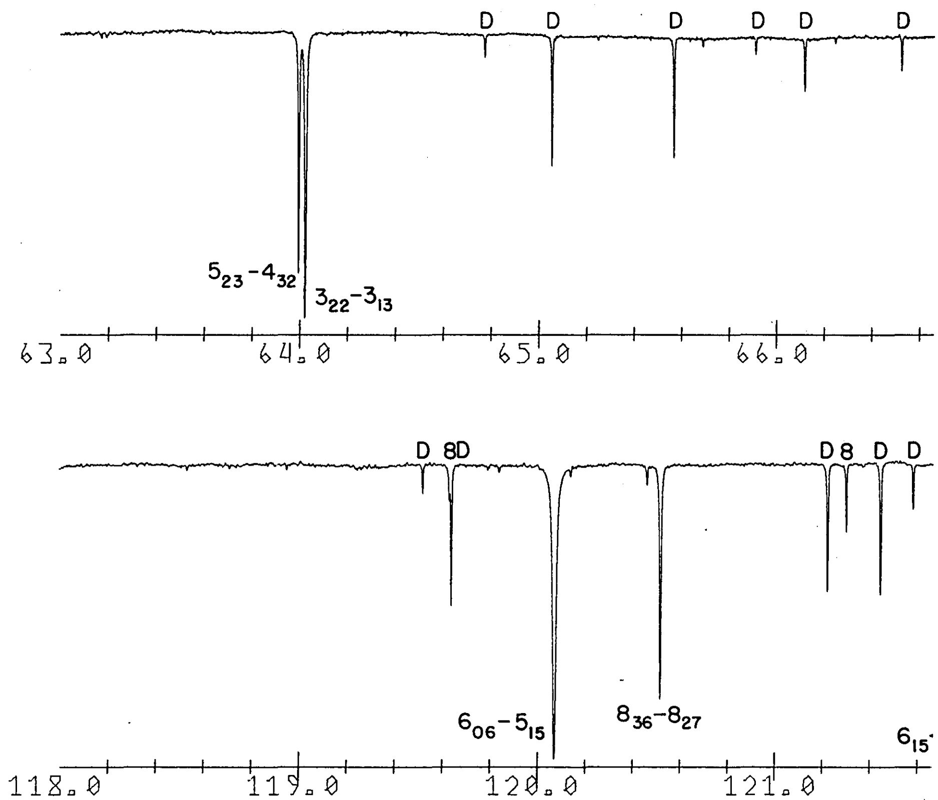

Fig. 1. Two portions of the FIR spectrum of water vapor. The top spectrum (near 65 cm^{-1}) was obtained with the 1.6-K bolometer and the quartz filter, the bottom spectrum (near 120 cm^{-1}) with the 4-K bolometer and the sapphire filter (see text). Assignments to lines of $H_2{}^{16}O$ are given, and isotopic lines have been indicated as follows: D for $HD^{16}O$ and 8 for $H_2{}^{18}O$. HDO was present in much greater than natural abundance because of contamination of the absorption cell by deuterium.

quality of the spectra obtained are shown in Fig. 1. A complete atlas of the spectrum from 25 to 350 cm^{-1} will be published elsewhere.[4]

Some care had to be taken in order to obtain good recordings of the stronger H_2O lines. The problem here is due to residual water vapor in the spectrometer, which causes an attenuation at the H_2O frequencies that increases as the optical path difference increases. This results in what can be described as a self-apodization and consequent broadening of the stronger H_2O lines. Neighboring strong isotopic lines are, of course, not affected since there were never enough of these species in the spectrometer to cause any significant attenuation. To a large degree the problem was overcome by installing a 5-cm diffusion pump and cold trap attached directly to the spectrometer sample chamber to augment the standard spectrometer pumping system. In this way the residual pressure in the instrument was reduced to less than 5 mTorr. At the same time, most of the spectra were recorded during the winter months when the relative humidity in the laboratory was low. Under these conditions the strongest water lines were still detectable but were too weak for accurate measurement.

The spectra were calibrated using HF and HCl lines measured recently by Jennings *et al.*[5] using heterodyne methods together with a few H_2O lines below 33 cm^{-1} measured by Helminger *et al.*[6] and one HCl line measured by De Lucia *et al.*[7] using microwave techniques. For convenience these lines are listed in Table 1. A typical calibration curve covering the region from 75 to 200 cm^{-1} is shown in Fig. 2. Here the differences between the frequencies given in Table 1 and those given by the spectrometer system have been plotted in inverse centimeters against the line frequency. The fact that the

Table 1. Lines Used for Calibration[a]

Molecule	Transition	ν (MHz)	ν (cm^{-1})
$H_2{}^{16}O$	4_{22}–3_{31}	916 171.58[b]	30.56019
	5_{24}–4_{31}	970 315.02[b]	32.36623
	2_{02}–1_{11}	987 926.76[b]	32.95369
	7_{26}–7_{17}	3 691 315.55	123.12903
HF	1–0	1 232 476.28	41.11098
	2–1	2 463 428.77	82.17114
	3–2	3 691 334.63	123.12967
	4–3	4 914 682.59	163.93617
$H^{35}Cl$	1–0	625 915.20[c]	20.87828
	3–2	1 876 226.63	62.58418
	4–3	2 499 864.44	83.38650
	5–4	3 121 986.49	104.13826
	6–5	3 742 216.58	124.82691
	7–6	4 360 179.79	145.43994
	8–7	4 975 504.74	165.96497
$H^{37}Cl$	1–0	624 975.04[c]	20.84692
	2–1	1 249 571.40	41.68122
	7–6	4 353 662.88	145.22256
	8–7	4 968 078.30	165.71725
	9–8	5 579 495.42	186.11193

[a] Lines not otherwise attributed taken from Jennings *et al.*[5]
[b] Taken from Helminger *et al.*[6]
[c] Taken from De Lucia *et al.*[7]

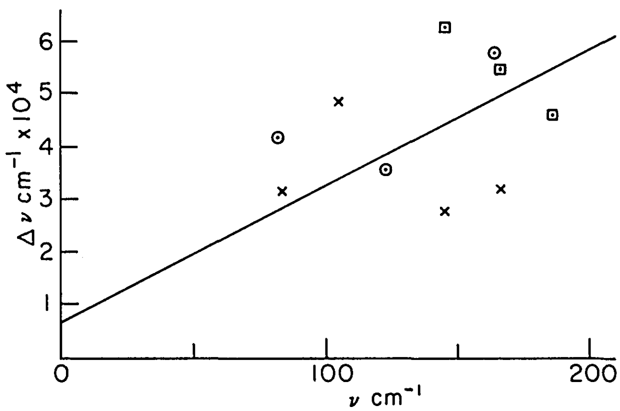

Fig. 2. Calibration curve for the region from 75 to 200 cm^{-1}. Points derived from HF lines are indicated by circles, from $H^{35}Cl$ lines by crosses, and from $H^{37}Cl$ lines by squares.

differences are not zero arises mainly from the difficulty in ensuring that the He–Ne laser beam, used as reference, and the infrared beam are exactly parallel and also from nonparallelism caused by the use of a finite entrance iris aperture. These corrections should be zero at zero frequency, and this has been taken into account by adding one or more dummy points with zero difference at zero wave number. A least-squares fit, including two dummy points at zero, is shown in the line in Fig. 2; the rms deviation of the calibration points from this line is 0.00012 cm^{-1} (3.6 MHz). Allowing for the possibility of small systematic errors it seems reasonable to assume that the measurement accuracy of lines with high signal-to-noise ratio should be of the order of 0.0002 cm^{-1} (6 MHz). Above 186 cm^{-1}, the highest-frequency HCl line measured by Jennings *et al.*, the wave-number scale depends on the assumption that the correction to be applied is proportional to wave number. Thus the estimated accuracy at 350 cm^{-1} can be no better than 0.0004 cm^{-1}. Actually the situation is somewhat worse, since the signal-to-noise ratio of the spectra deteriorates significantly above 280 cm^{-1}. Evidence based on fitting the data to a molecular Hamiltonian, described in the next section, indicates that these error estimates are reasonable.

DATA FITTING AND LINE ASSIGNMENTS

In order to get an independent assessment of the measurement accuracy and also to aid in the assignments of the weaker isotopes the observed lines have been fitted to a molecular Hamiltonian. The Hamiltonian most often used for asymmetric rotor molecules such as H_2O is the A-reduced form that is due to Watson,[8] and it is particularly convenient because it is easy to extend it to arbitrary high order.[9] Here, all terms involving up to the tenth power in the angular momenta have been included together with one term in the twelfth power, i.e., the term involving K^{12}. This is exactly the Hamiltonian used by Messer *et al.*[9] in their recent study of the microwave spectra of $HD^{16}O$ and $D_2{}^{16}O$, thus making it easy to compare their results with the present ones.

Assignment of lines involving hydrogen and the three isotopes of oxygen was simple since all the lines have been calculated and have been given in the tabulation of Flaud *et al.*[2] Too few lines of $H_2{}^{17}O$ were observed to make a fit meaningful, and no species containing ^{17}O has therefore been considered here. For the isotopic species involving deuterium a fit was first made to available microwave data, and the resulting constants used to predict far-infrared (FIR) lines (in all the calculations the velocity of light was taken to be 2.99792458 $\times 10^{10}$ cm/sec). Lines whose assignments became obvious were then added to the fit and new predictions made. As lines were added some new constants had to be added in order to keep the fit as far as possible as good as the data. Initial assignments of many lines involving deuterium and ^{18}O became obvious after the corresponding ^{16}O species had been assigned and fitted. Further assignments were then made as indicated above. In this way assignments to the species $HD^{16}O$, $HD^{18}O$, $D_2{}^{16}O$, and $D_2{}^{18}O$ were completed. The measured line frequencies and quantum-number assignments have been collected in Tables 2–7. In these tables lines from other sources that were included in the fits have also been listed, and references are given in footnotes to each table. In addition to the measured lines, the tables also give calculated line positions, standard errors of the calculated frequencies, and the residuals, observed − calculated. The parameters used to obtain the calculated frequencies are given in Table 8.

DISCUSSION

Some statistics from the fits are given in Table 9. In addition to the overall standard deviations and the number of parameters used, the rms errors of the microwave data and of the Fourier-transform data have been included separately. The number of parameters and the rms errors obtained by Messer *et al.*[9] for the microwave spectra of $HD^{16}O$ and $D_2{}^{16}O$ have also been included in the table. It may be noted that the rms errors of the microwave data for $HD^{16}O$ and $D_2{}^{16}O$ obtained here are slightly lower than those obtained by Messer *et al.* This is perhaps not too surprising since the inclusion of the FIR data has forced the addition of a few more parameters. However, the indication is quite strong that the FIR data do not have significant systematic errors because such errors would presumably have worsened the fit to the microwave data. A further assurance that systematic errors are not serious can be obtained from consideration of the $H_2{}^{16}O$ fit, which also includes the excellent recent measurements of Kauppinen *et al.*[10] in the region from 500 to 700 cm^{-1}. These data were obtained using an instrument of approximately the same resolution capability as the Bomem instrument and were calibrated with heterodyne measurements of carbonyl sulfide that are due to Wells *et al.*[11] The inclusion of these data without degradation of the fit is evidence of the absence of serious systematic error. The addition of the water line at 123 cm^{-1} measured recently by Jennings *et al.*[5] also results in no degradation of the fit. Indeed, a fit excluding this line predicts the frequency to be 3 691 316.327 MHz, only about 800 kHz above the value given in Table 1. The fit with this line included gives a residual of 129 kHz, which is well within the 250-kHz estimate of the measurement accuracy.[5] The rms errors of the FIR lines are similar for all the istopic species, viz., 0.00016 cm^{-1}, in agreement with conclusions based on the calibration data. To be sure, not all the lines were included to obtain these rms values. In particular, lines of $H_2{}^{16}O$ (and of $HD^{16}O$) above 300 cm^{-1} in the present measurements were excluded because of increasing calibration uncertainty and because of decreasing signal-to-noise ratio. Also excluded

Table 2. Pure Rotational Transitions of $H_2{}^{16}O$[a]

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
1	6	1	6	5	2	3	22235.080	22235.080(	0)	0
2	3	1	3	2	2	0	183310.117	183310.117(	1)	0
3	10	2	9	9	3	6	321225.644	321225.645(	41)	0
4	5	1	5	4	2	2	325152.919	325152.899(	16)	19
5	4	1	4	3	2	1	380197.372	380197.416(	14)	-43
6	10	3	7	11	2	10	390134.508	390134.503(	180)	5
7	7	5	3	6	6	0	437346.667	437346.619(	106)	48
8	6	4	3	5	5	0	439150.812	439150.819(	38)	-7
9	7	5	2	6	6	1	443018.295	443018.356(	109)	-60
10	4	2	3	3	3	0	448001.075	448001.087(	16)	-12
11	6	4	2	5	5	1	470888.947	470888.829(	97)	118
12	5	3	3	4	4	0	474689.127	474689.121(	52)	6
13	6	2	4	7	1	7	488491.133	488490.862(	96)	271
14	8	6	3	7	7	0	503568.532	503568.536(	97)	-3
15	8	6	2	7	7	1	504482.692	504482.688(	101)	3
16	1	1	0	1	0	1	556936.002	556935.838(	58)	164
17	1	1	0	1	0	1	18.57799	18.57738(	0)	61
18	5	3	2	4	4	1	620700.807	620700.451(	114)	356
19	2	1	1	2	0	2	752033.227	752032.854(	56)	372
20	2	1	1	2	0	2	25.08516	25.08512(	0)	4
21	4	2	2	3	3	1	916171.582	916171.607(	71)	-25
22	4	2	2	3	3	1	30.55987	30.56020(	0)	-33
23	5	2	4	4	3	1	32.36608	32.36622(	0)	-14
24	5	2	4	4	3	1	970315.022	970314.837(	68)	185
25	2	0	2	1	1	1	32.95371	32.95369(	0)	2
26	2	0	2	1	1	1	987926.764	987926.770(	18)	-5
27	3	1	2	3	0	3	36.60403	36.60414(	0)	-11
28	1	1	1	0	0	0	37.13709	37.13712(	0)	-3
29	3	1	2	2	2	1	38.46408	38.46417(	0)	-9
30	6	3	4	5	4	1	38.63735	38.63756(	1)	-21
31	3	2	1	3	1	2	38.79061	38.79055(	0)	6
32	4	2	2	4	1	3	40.28243	40.28249(	0)	-6
33	2	2	0	2	1	1	40.98795	40.98797(	0)	-2
34	7	4	3	6	5	2	42.63838	42.63849(	3)	-11
35	8	2	7	7	3	4	43.24340	43.24360(	1)	-20
36	6	2	5	5	3	2	44.09924	44.09932(	0)	-8
37	5	2	3	5	1	4	47.05316	47.05316(	0)	0
38	7	2	6	6	3	3	48.05927	48.05929(	1)	-2
39	6	3	3	5	4	2	51.43437	51.43448(	1)	-11
40	4	1	3	4	0	4	53.44416	53.44428(	0)	-12
41	2	2	1	2	1	2	55.40533	55.40525(	0)	8
42	2	1	2	1	0	1	55.70200	55.70202(	0)	-2
43	4	3	2	5	0	5	57.16912	57.16899(	0)	13
44	3	0	3	2	1	2	57.26528	57.26528(	0)	0
45	6	3	3	6	2	4	58.77541	58.77545(	1)	-4
46	7	3	5	6	4	2	58.91410	58.91410(	1)	0
47	6	2	4	6	1	5	59.86800	59.86775(	1)	25
48	7	3	4	7	2	5	59.94692	59.94679(	1)	13
49	5	3	2	5	2	3	62.30138	62.30141(	0)	-3
50	8	4	5	7	5	2	62.87289	62.87323(	4)	-34
51	5	2	3	4	3	2	63.99404	63.99378(	0)	26
52	3	2	2	3	1	3	64.02304	64.02293(	0)	11
53	8	3	5	8	2	6	67.24602	67.24596(	2)	6
54	4	3	1	4	2	2	68.06300	68.06300(	0)	0
55	4	1	3	3	2	2	69.19583	69.19563(	0)	20
56	3	1	3	2	0	2	72.18770	72.18765(	0)	5
57	3	3	0	3	2	1	73.26240	73.26221(	0)	19
58	5	1	4	5	0	5	74.10959	74.10961(	0)	-2
59	8	3	6	7	4	3	74.87896	74.87890(	2)	6
60	8	3	6	7	4	3	74.87880	74.87890(	2)	-10
61	4	2	3	4	1	4	75.52391	75.52390(	0)	1
62	9	4	5	9	3	6	77.31608	77.31630(	3)	-22
63	9	4	5	9	3	6	77.31617	77.31630(	3)	-13
64	7	2	5	7	1	6	78.19588	78.19585(	1)	3
65	10	4	6	10	3	7	78.30365	78.30360(	4)	5
66	3	3	1	3	2	2	78.91798	78.91792(	0)	6
67	4	0	4	3	1	3	79.77428	79.77428(	0)	0
68	9	3	6	9	2	7	80.99764	80.99761(	2)	3
69	8	4	4	8	3	5	81.61791	81.61798(	2)	-7
70	4	3	2	4	2	3	82.15452	82.15463(	0)	-11
71	12	4	9	13	1	12	82.63893	82.64031(	12)	-138*
72	9	3	7	8	4	4	84.45568	84.45575(	3)	-7
73	7	3	4	6	4	3	85.63185	85.63180(	2)	5
74	11	4	7	11	3	8	85.78477	85.78458(	7)	19
75	10	3	8	9	4	5	85.89278	85.89297(	4)	-19
76	5	3	3	5	2	4	87.75941	87.75942(	0)	-1
77	4	1	4	3	0	3	88.07670	88.07671(	0)	-1
78	7	4	3	7	3	4	88.88060	88.88058(	2)	2
79	5	2	4	5	1	5	89.58323	89.58328(	0)	-5
80	2	2	1	1	1	0	92.52981	92.52988(	0)	-7
81	6	3	4	6	2	5	96.06730	96.06740(	1)	-10
82	6	1	5	6	0	6	96.20908	96.20919(	1)	-11
83	6	4	2	6	3	3	96.23115	96.23133(	1)	-18
84	6	2	4	5	3	3	98.80528	98.80539(	1)	-11
85	2	2	0	1	1	1	99.02676	99.02678(	0)	-2
86	5	1	4	4	2	3	99.09500	99.09525(	1)	-25
87	11	5	6	11	4	7	99.98711	99.98684(	7)	26
88	8	2	6	8	1	7	100.02144	100.02150(	1)	-6
89	10	3	7	10	2	8	100.18074	100.18089(	3)	-15
90	5	0	5	4	1	4	100.50941	100.50953(	0)	-12
91	5	4	1	5	3	2	101.52912	101.52916(	1)	-4
92	10	4	7	9	5	4	104.03833	104.03834(	5)	-1
93	4	4	0	4	3	1	104.29175	104.29171(	0)	4
94	5	1	5	4	0	4	104.57251	104.57270(	0)	-19
95	9	4	5	8	5	4	105.06834	105.06868(	5)	-34
96	4	4	1	4	3	2	105.59066	105.59086(	0)	-20
97	6	2	5	6	1	6	105.65890	105.65905(	0)	-15
98	5	4	2	5	3	3	106.14626	106.14636(	1)	-10
99	7	3	5	7	2	6	107.08607	107.08615(	1)	-8
100	6	4	3	6	3	4	107.74609	107.74611(	1)	-2
101	10	5	5	10	4	6	108.25210	108.25249(	4)	-39
102	7	4	4	7	3	5	111.04966	111.04967(	1)	-1
103	3	2	2	2	1	1	111.12548	111.12547(	1)	1
104	8	4	5	8	3	6	116.59263	116.59257(	2)	6
105	9	5	4	9	4	5	117.06200	117.06213(	3)	-13
106	7	1	6	7	0	7	117.97053	117.97048(	1)	5
107	6	0	6	5	1	5	120.07107	120.07115(	1)	-8
108	8	3	6	8	2	7	120.51567	120.51588(	2)	-21
109	6	1	6	5	0	5	121.90449	121.90446(	1)	3
110	8	3	5	7	4	4	122.41384	122.41376(	3)	8
111	11	3	8	11	2	9	122.55884	122.55911(	5)	-26
112	9	2	7	9	1	8	122.84186	122.84206(	2)	-20
113	7	2	6	7	1	7	3691315.550	3691315.680(	169)	-129
114	7	2	6	7	1	7	123.12899	123.12904(	0)	-5
115	8	5	3	8	4	4	124.13592	124.13594(	3)	-2
116	9	4	6	9	3	7	124.65360	124.65351(	2)	9
117	6	1	5	5	2	4	126.69700	126.69705(	1)	-5
118	4	2	3	3	1	2	126.99655	126.99647(	1)	8
119	7	5	2	7	4	3	128.59828	128.59824(	3)	4
120	6	5	1	6	4	2	130.85244	130.85240(	2)	4
121	5	5	0	5	4	1	131.73519	131.73517(	1)	2
122	6	5	2	6	4	3	131.87394	131.87389(	2)	5
123	7	5	3	7	4	4	131.90270	131.90266(	3)	4
124	5	5	1	5	4	2	131.95858	131.95865(	1)	-7
125	8	5	4	8	4	5	132.45823	132.45820(	3)	3
126	3	2	1	2	1	2	132.65990	132.65996(	0)	-6
127	7	2	5	6	3	4	133.43107	133.43112(	2)	-5
128	9	5	5	9	4	6	134.09587	134.09611(	3)	-24
129	10	4	7	10	3	8	135.20783	135.20749(	3)	34
130	9	3	7	9	2	8	135.84573	135.84597(	2)	-24
131	10	5	6	10	4	7	137.38294	137.38331(	4)	-37
132	8	1	7	8	0	8	138.82664	138.82661(	1)	3
133	7	0	7	6	1	6	138.99126	138.99124(	1)	2
134	7	1	7	6	0	6	139.78256	139.78264(	1)	-8
135	5	2	4	4	1	3	140.71165	140.71170(	1)	-5
136	8	2	7	8	1	8	141.43745	141.43754(	1)	-9
137	10	2	8	10	1	9	144.95034	144.95061(	2)	-26
138	11	6	5	11	5	6	145.05084	145.05080(	10)	4
139	11	4	8	11	3	9	147.96106	147.96059(	5)	47*
140	3	3	0	3	0	3	148.65694	148.65690(	1)	4
141	3	3	1	2	2	0	149.05524	149.05542(	1)	-18
142	3	3	0	2	2	1	150.51704	150.51693(	1)	11
143	10	6	4	10	5	5	150.75623	150.75642(	5)	-19
144	7	1	6	6	2	5	151.30281	151.30267(	2)	14
145	10	3	8	10	2	9	152.49411	152.49434(	3)	-23
146	6	2	5	5	1	4	153.45387	153.45390(	1)	-3
147	9	6	3	9	5	4	154.08567	154.08561(	4)	6
148	8	6	2	8	5	3	155.73035	155.73035(	4)	0
149	10	6	5	10	5	6	156.25424	156.25413(	5)	11
150	9	6	4	9	5	5	156.26472	156.26467(	4)	5
151	7	6	1	7	5	2	156.35901	156.35913(	4)	-12
152	6	6	0	6	5	1	156.42571	156.42572(	1)	-1
153	8	6	3	8	5	4	156.44481	156.44470(	4)	11
154	6	6	1	6	5	2	156.45916	156.45923(	1)	-7
155	7	6	2	7	5	3	156.54319	156.54319(	4)	0
156	14	6	9	13	7	6	156.89833	156.93207(	196)	-3374*
157	8	0	8	7	1	7	157.58450	157.58455(	2)	-5
158	8	1	8	7	0	7	157.91910	157.91919(	1)	-9
159	9	1	8	9	0	9	158.91125	158.91114(	2)	11
160	9	2	8	9	1	9	160.17543	160.17540(	2)	3
161	9	3	6	8	4	5	160.21050	160.21058(	4)	-8
162	4	3	1	4	0	4	161.78980	161.78976(	1)	4
163	12	4	9	12	3	10	162.44330	162.44408(	7)	-78*
164	11	2	9	11	1	10	165.81653	165.81665(	4)	-12
165	8	2	6	7	3	5	166.21750	166.21747(	3)	3
166	7	2	6	6	1	5	166.70245	166.70249(	1)	-4
167	11	3	9	11	2	10	169.93268	169.93278(	4)	-10
168	4	3	2	3	2	1	170.36056	170.36055(	1)	1
169	8	1	7	7	2	6	173.28212	173.28212(	2)	0
170	4	2	2	3	1	3	173.50106	173.50105(	1)	1
171	9	0	9	8	1	8	176.00575	176.00576(	2)	-1

(continued overleaf)

Table 2. Continued

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
172	9	1	9	8	0	8	176.14627	176.14643(	2)	-16
173	4	3	1	3	2	2	177.54103	177.54111(	1)	-8
174	10	1	9	10	0	10	178.48587	178.48580(	3)	7
175	7	7	0	7	6	1	178.61983	178.61976(	3)	7
176	8	7	1	8	6	2	179.04874	179.05094(	45)	-220*
177	8	7	2	8	6	3	179.07982	179.08074(	45)	-92*
178	10	2	9	10	1	10	179.08424	179.08411(	3)	13
179	9	7	2	9	6	3	179.20474	179.20577(	78)	-103*
180	10	7	4	10	6	5	179.37238	179.36878(	104)	360*
181	11	4	7	10	5	6	180.28915	180.28902(	7)	13
182	8	2	7	7	1	6	181.38626	181.38624(	1)	2
183	5	3	2	5	0	5	183.46411	183.46419(	1)	-8
184	12	3	10	12	2	11	187.75593	187.75584(	6)	9
185	5	3	3	4	2	2	188.18867	188.18863(	1)	4
186	9	1	8	8	2	7	193.47937	193.47936(	2)	1
187	10	0	10	9	1	9	194.32229	194.32228(	2)	1
188	10	1	10	9	0	9	194.38154	194.38164(	2)	-10
189	9	2	7	8	3	6	195.80563	195.80555(	3)	8
190	10	3	7	9	4	6	197.26473	197.26470(	5)	3
191	9	2	8	8	1	7	197.49514	197.49522(	2)	-8
192	11	1	10	11	0	11	197.73804	197.73787(	4)	17
193	11	2	10	11	1	11	198.01830	198.01844(	4)	-14
194	8	8	1	8	7	2	198.35279	198.33224(	97)	2055*
195	9	8	1	9	7	2	199.21706	199.20833(	295)	873*
196	6	3	4	5	2	3	202.46792	202.46813(	1)	-21
197	4	4	1	3	3	0	202.68895	202.68920(	1)	-25
198	4	4	0	3	3	1	202.91477	202.91490(	1)	-13
199	5	3	2	4	2	3	208.44974	208.44983(	1)	-9
200	5	4	1	5	1	4	210.88372	210.88374(	2)	-2
201	11	0	11	10	1	10	212.55985	212.56005(	3)	-20
202	11	1	11	10	0	10	212.58535	212.58537(	3)	-2
203	10	1	9	9	2	8	212.63284	212.63268(	2)	16
204	7	3	5	6	2	4	213.92060	213.92088(	1)	-28
205	10	2	9	9	1	8	214.55449	214.55461(	2)	-12
206	6	3	3	6	0	6	214.85241	214.85239(	1)	2
207	6	4	2	6	1	5	214.87455	214.87453(	2)	2
208	3	3	1	2	0	2	215.12847	215.12851(	1)	-4
209	12	1	11	12	0	12	216.77188	216.77193(	6)	-5
210	12	2	11	12	1	12	216.90344	216.90351(	6)	-7
211	5	2	3	4	1	4	221.67228	221.67231(	1)	-3
212	10	2	8	9	3	7	221.73736	221.73732(	4)	4
213	8	3	6	7	2	5	223.70611	223.70627(	2)	-16
214	5	4	2	4	3	1	226.27204	226.27200(	1)	4
215	7	4	3	7	1	6	227.02311	227.02322(	2)	-11
216	5	4	1	4	3	2	227.82417	227.82436(	1)	-19
217	12	0	12	11	1	11	230.72705	230.72679(	5)	26
218	12	1	12	11	0	11	230.73776	230.73776(	5)	0
219	11	1	10	10	2	9	231.21388	231.21382(	2)	6
220	11	3	8	10	4	7	231.88752	231.88775(	6)	-23
221	11	2	10	10	1	9	232.11793	232.11801(	2)	-8
222	9	3	7	8	2	6	233.31965	233.31969(	2)	-4
223	13	1	12	13	0	13	235.64063	235.64043(	10)	20
224	10	3	8	9	2	7	244.20672	244.20688(	3)	-16
225	11	2	9	10	3	8	244.53634	244.53613(	5)	21
226	6	3	3	5	2	4	245.34034	245.34026(	1)	8
227	4	3	2	3	0	3	245.75525	245.75524(	2)	1
228	6	4	3	5	3	2	247.91272	247.91283(	1)	-11
229	13	0	13	12	1	12	248.82255	248.82269(	7)	-14
230	13	1	13	12	0	12		248.82754(	7)	
231	8	4	4	8	1	7	248.88522	248.88544(	3)	-22
232	12	1	11	11	2	10	249.48039	249.48029(	3)	10
233	12	2	11	11	1	10	249.90333	249.90340(	3)	-7
234	6	4	2	5	3	3	253.81209	253.81217(	1)	-8
235	5	5	1	4	4	0	253.93904	253.93893(	1)	11
236	5	5	0	4	4	1	253.96858	253.96867(	1)	-9
237	7	3	4	7	0	7	256.11321	256.11312(	1)	9
238	11	3	9	10	2	8	257.10029	257.10018(	4)	11
239	4	4	1	4	1	4	263.26945	263.26939(	2)	6
240	12	2	10	11	3	9	265.13892	265.13873(	7)	19
241	7	4	4	6	3	3	266.19519	266.19510(	2)	9
242	14	0	14	13	1	13	266.84517	266.84512(	14)	5
243	14	1	14	13	0	13	266.84517	266.84731(	14)	-214*
244	13	1	12	12	2	11	267.55966	267.55961(	8)	5
245	13	2	12	12	1	11	267.75806	267.75814(	8)	-8
246	12	3	10	11	2	9	271.84267	271.84260(	5)	7
247	8	5	3	8	2	6	273.00022	272.99988(	4)	34
248	9	5	4	9	2	7	275.37622	275.37604(	4)	18
249	6	2	4	5	1	5	276.14812	276.14809(	2)	3
250	7	5	2	7	2	5	277.42581	277.42561(	3)	20
251	6	5	2	5	4	1	278.25760	278.25756(	2)	4
252	6	5	1	5	4	2	278.51840	278.51820(	2)	20
253	8	4	5	7	3	4	280.35220	280.35205(	3)	15
254	9	4	5	9	1	8	281.15596	281.15598(	3)	-2
255	5	3	3	4	0	4	281.91559	281.91540(	2)	19
256	7	4	3	6	3	4	282.25861	282.25849(	2)	12
257	5	4	2	5	1	5	283.48931	283.48906(	2)	25
258	13	2	11	12	3	10	284.37813	284.37778(	14)	35
259	15	0	15	14	1	14	284.78627	284.79080(	51)	-453*
260	15	1	15	14	0	14	284.78627	284.79181(	51)	-554*
261	14	2	13	13	1	12	285.60369	285.60421(	23)	-52
262	7	3	4	6	2	5	289.44545	289.44531(	2)	14
263	9	4	6	8	3	5	290.72747	290.72724(	3)	23
264	10	4	7	9	3	6	298.41714	298.41677(	4)	37
265	7	5	3	6	4	2	301.86679	301.86643(	2)	36*
266	6	6	1	5	5	0	302.98285	302.98162(	2)	123*
267	6	6	0	5	5	1	302.98285	302.98528(	2)	-243*
268	7	5	2	6	4	3	303.11093	303.11063(	2)	30*
269	11	4	8	10	3	7	304.88055	304.87988(	6)	67*
270	12	4	9	11	3	8	311.72853	311.72757(	7)	96*
271	4	4	1	3	1	2	314.74240	314.74195(	2)	45*
272	8	4	4	7	3	5	315.08156	315.08142(	3)	14*
273	6	3	4	5	0	5	323.63147	323.63091(	2)	56*
274	8	5	4	7	4	3	323.92876	323.92967(	3)	-91*
275	7	6	2	6	5	1	327.55790	327.55722(	3)	68*
276	7	6	1	6	5	2	327.59558	327.59587(	3)	-29*
277	8	5	3	7	4	4	328.16808	328.16768(	3)	40*
278	5	4	2	4	1	3	334.61796	334.61748(	2)	48*
279	7	2	5	6	1	6	335.15772	335.15757(	2)	15*
280	8	3	5	7	2	6	340.55021	340.54958(	3)	63*
281	9	5	5	8	4	4	343.20590	343.20537(	3)	53*
282	7	7	1	6	6	0	349.75583	349.75596(	4)	-13*
283	7	7	0	6	6	1	349.75583	349.75640(	4)	-56*
284	8	6	3	7	5	2		351.77613(	4)	
285	8	6	2	7	5	3		351.99537(	4)	
286	9	4	5	8	3	6		354.11946(	4)	
287	9	5	4	8	4	5		354.58902(	4)	
288	6	4	3	5	1	4		357.26740(	2)	
289	10	5	6	9	4	5		358.48377(	5)	
290	7	3	5	6	0	6		369.99782(	2)	
291	8	7	2	7	6	1		374.49774(	46)	
292	8	7	1	7	6	2		374.50313(	46)	
293	9	6	4	8	5	3		375.33411(	5)	
294	9	6	3	8	5	4		376.21643(	5)	
295	10	5	5	9	4	6		383.82078(	6)	
296	7	4	4	6	1	5		384.83831(	3)	
297	5	4	1	4	1	4		385.50288(	3)	
298	8	8	1	7	7	0		394.21022(	127)	
299	8	8	0	7	7	1		394.21027(	127)	
300	8	2	6	7	1	7		396.43265(	3)	
301	9	3	6	8	2	7		397.31903(	3)	
302	10	6	5	9	5	4		397.67578(	6)	
303	9	7	3	8	6	2		398.94241(	79)	
304	9	7	2	8	6	3		398.97750(	79)	
305	10	4	6	9	3	7		400.22180(	5)	
306	10	6	4	9	5	5		400.48109(	6)	
307	11	5	6	10	4	7		417.65917(	11)	
308	8	4	5	7	1	6		418.49469(	3)	
309	9	8	1	8	7	2		419.10509(	330)	
310	8	3	6	7	0	7		419.87260(	2)	
311	10	7	4	9	6	3		422.95894(	104)	
312	11	6	5	10	5	6		425.32666(	12)	
313	9	9	0	8	8	1		436.19728(	1052)	
314	6	5	2	5	2	3		442.08813(	3)	
315	10	8	3	9	7	2		443.67341(	515)	
316	9	2	7	8	1	8		457.75896(	3)	
317	9	4	6	8	1	7		457.99470(	4)	
318	9	3	7	8	0	8		472.16780(	3)	
319	8	5	4	7	2	5		472.75704(	4)	
320	7	4	3	6	1	6		483.98494(	3)	
321	11	10	2	10	9	1		500.16772(	7056)	
322	11	10	1	10	9	2		500.16773(	7056)	
323	10	4	7	9	1	8		502.25644(	5)	
324	10	4	7	9	1	8	502.25802	502.25644(	5)	158*
325	13	5	8	12	4	9	504.38306	504.37695(	67)	611*
326	7	5	2	6	2	5		506.92413(	3)	
327	12	9	4	11	8	3		509.99319(	3023)	
328	12	9	3	11	8	4		509.99761(	3023)	
329	12	4	8	11	3	9	510.58403	510.58396(	12)	7
330	13	8	5	12	7	6		514.86284(	1084)	
331	10	5	6	9	2	7	516.79775	516.79769(	5)	6
332	10	2	8	9	1	9	517.75917	517.75869(	4)	48
333	11	3	8	10	2	9	519.58952	519.58958(	5)	-6
334	12	10	3	11	9	2		524.65304(	8975)	
335	12	10	2	11	9	3		524.65316(	8975)	
336	10	3	8	9	0	9	525.96024	525.96008(	4)	16
337	13	9	5	12	8	4		533.55701(	3767)	
338	13	9	4	12	8	5		533.57627(	3766)	
339	6	6	1	5	3	2	536.24615	536.24595(	3)	20
340	6	6	0	5	3	3	541.09037	541.09028(	3)	9
341	8	4	4	7	1	7	545.29660	545.29660(	3)	0
342	8	5	3	7	2	6	546.30359	546.30350(	4)	9

Table 2. Continued

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
343	11	5	7	10	2	8	547.81661	547.81675(	7)	-14
344	11	4	8	10	1	9	550.01159	550.01138(	6)	21
345	7	6	2	6	3	3	554.64087	554.64094(	5)	-7
346	6	5	2	5	0	5	563.25099	563.25091(	3)	8
347	7	6	1	6	3	4	567.21597	567.21587(	5)	10
348	8	6	3	7	3	4	569.25512	569.25495(	4)	17
349	13	4	9	12	3	10	571.28643	571.28689(	39)	-46*
350	11	2	9	10	1	10	576.11444	576.11458(	5)	-14
351	11	3	9	10	0	10	580.53641	580.53659(	5)	-18
352	12	3	9	11	2	10	580.73189	580.73247(	15)	-58*
353	9	6	4	8	3	5	581.08810	581.08803(	5)	7
354	12	5	8	11	2	9	584.70877	584.70905(	12)	-28
355	9	5	4	8	2	7	591.69728	591.69747(	4)	-19
356	10	6	5	9	3	6	592.05415	592.05421(	6)	-6
357	8	6	2	7	3	5	594.94735	594.94770(	4)	-35
358	12	4	9	11	1	10	600.10368	600.10333(	8)	35
359	11	6	6	10	3	7	604.44853	604.44827(	10)	26
360	7	5	3	6	0	6	612.95023	612.95015(	3)	8
361	9	4	5	8	1	8	616.07278	616.07287(	4)	-9
362	12	6	7	11	3	8	620.57733	620.57564(	35)	169*
363	9	6	3	8	3	6	625.26726	625.26720(	5)	6
364	13	5	9	12	2	10		626.32356(	38)	
365	12	2	10	11	1	11	633.08992	633.08995(	7)	-3
366	12	3	10	11	0	11	635.39701	635.39712(	6)	-11
367	7	7	1	6	4	2	637.03392	637.03408(	4)	-16
368	7	7	0	6	4	3	638.08957	638.08952(	4)	5
369	13	3	10	12	2	11	639.97230	639.97362(	37)	-132*
370	10	5	5	9	2	8	644.32015	644.32026(	5)	-11
371	13	4	10	12	1	11	651.58024	651.58025(	13)	-1
372	10	6	4	9	3	7	659.23058	659.23071(	6)	-13
373	8	7	2	7	4	3		659.45512(	46)	
374	8	7	1	7	4	4		662.94897(	45)	
375	8	5	4	7	0	7	668.92369	668.92338(	4)	31
376	14	5	10	13	2	11		671.36359(	104)	
377	9	7	3	8	4	4		678.80870(	78)	
378	9	7	2	8	4	5		687.88040(	78)	
379	13	2	11	12	1	12		689.03713(	14)	
380	13	3	11	12	0	12	690.22009	690.22022(	12)	-13
381	10	7	4	9	4	5		694.10669(	104)	
382	10	4	6	9	1	9	696.24299	696.24317(	5)	-18
383	14	3	11	13	2	12		697.05686(	86)	
384	11	6	5	10	3	8		697.91747(	11)	
385	14	4	11	13	1	12		703.71343(	56)	
386	11	7	5	10	4	6		705.34908(	128)	
387	11	5	6	10	2	9	705.35115	705.36101(	10)	-985*
388	8	6	3	7	1	6	707.39737	707.39759(	4)	-22
389	10	7	3	9	4	6		713.48068(	103)	
390	12	7	6	11	4	7		713.76767(	175)	

[a] In the columns headed OBS and CALC those frequencies given to three decimal places are in units of megahertz; those given to five places are in inverse centimeters. SDC is the standard error (1σ) of the calculation and O-C is the residual, observed − calculated, both given in units of the last figure quoted. Lines given in megahertz have been taken from Refs. 5, 6, and 12–14; lines given in inverse centimeters above 500 cm^{-1} are from Ref. 10.

Table 3. Pure Rotational Transitions of $H_2{}^{18}O$[a]

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
1	6	1	6	5	2	3	5625.147	5625.149(	9)	-2
2	3	1	3	2	2	0	203407.520	203407.520(	13)	0
3	5	1	5	4	2	2	322465.170	322465.132(	28)	38
4	4	1	4	3	2	1	390607.760	390607.774(	25)	-14
5	4	2	3	3	3	0	489054.260	489054.244(	54)	15
6	6	2	4	7	1	7	517181.960	517182.068(	128)	-108
7	6	4	3	5	5	0	520137.320	520137.245(	271)	75
8	5	3	3	4	4	0	537337.570	537337.682(	283)	-111
9	1	1	0	1	0	1	547676.440	547676.455(	40)	-14
10	6	4	2	5	5	1	554859.870	554860.010(	277)	-140
11	5	3	2	4	4	1	692079.140	692079.224(	341)	-84
12	2	1	1	2	0	2	745320.200	745320.018(	140)	182
13	2	0	2	1	1	1	33.17852	33.17877(	1)	-25
14	3	1	2	3	0	3	36.54629	36.54624(	1)	5
15	1	1	1	0	0	0	36.74851	36.74866(	0)	-15
16	3	2	1	3	1	2	37.91637	37.91635(	1)	2
17	3	1	2	2	2	1	39.40702	39.40712(	2)	-10
18	4	2	2	4	1	3	39.65607	39.65628(	1)	-21
19	2	2	0	2	1	1	39.99423	39.99448(	1)	-25
20	6	2	5	5	3	2	44.72184	44.72205(	2)	-21
21	5	2	3	5	1	4	46.79803	46.79809(	2)	-6
22	4	1	3	4	0	4	53.56904	53.56917(	1)	-13
23	2	2	1	2	1	2	54.48708	54.48712(	1)	-4
24	2	1	2	1	0	1	55.23377	55.23375(	0)	2
25	3	0	3	2	1	2	57.34810	57.34801(	2)	9
26	6	3	3	6	2	4	57.37222	57.37237(	3)	-15
27	7	3	4	7	2	5	59.09673	59.09675(	4)	-2
28	6	2	4	6	1	5	60.05781	60.05768(	3)	13
29	5	3	2	5	2	3	60.57031	60.57028(	2)	3
30	3	2	2	3	1	3	63.18781	63.18782(	1)	-1
31	5	2	3	4	3	2	65.86717	65.86696(	3)	21
32	4	3	1	4	2	2	66.24314	66.24306(	2)	8
33	4	1	3	3	2	2	70.04731	70.04730(	3)	1
34	3	3	0	3	2	1	71.50798	71.50781(	1)	17
35	3	1	3	2	0	2	71.64075	71.64063(	1)	12
36	5	1	4	5	0	5	74.31376	74.31375(	2)	1
37	4	2	3	4	1	4	74.79170	74.79163(	1)	7
38	3	3	1	3	2	2	77.33878	77.33865(	1)	13
39	7	2	5	7	1	6	78.75872	78.75859(	3)	13
40	4	0	4	3	1	3	79.66599	79.66596(	2)	3
41	4	3	2	4	2	3	80.67156	80.67149(	1)	7
42	9	3	6	9	2	7	81.59820	81.59837(	9)	-17
43	7	4	3	7	3	4	86.15040	86.15037(	4)	3
44	5	3	3	5	2	4	86.42814	86.42813(	1)	1
45	4	1	4	3	0	3	87.49194	87.49186(	1)	8
46	7	3	4	6	4	3	88.51661	88.51654(	5)	7
47	5	2	4	5	1	5	88.95240	88.95247(	2)	-7
48	2	2	1	1	1	0	91.45249	91.45236(	1)	13
49	6	4	2	6	3	3	93.57733	93.57745(	3)	-12
50	6	3	4	6	2	5	94.93189	94.93182(	2)	7
51	6	1	5	6	0	6	96.33380	96.33396(	2)	-16
52	2	2	0	1	1	1	98.03443	98.03445(	1)	-2
53	5	4	1	5	3	2	99.06428	99.06414(	3)	14
54	5	1	4	4	2	3	99.74028	99.74036(	3)	-8
55	5	0	5	4	1	4	100.21815	100.21823(	2)	-8
56	6	2	4	5	3	3	100.64136	100.64151(	3)	-15
57	8	2	6	8	1	7	100.72748	100.72752(	4)	-4
58	4	4	0	4	3	1	101.96996	101.97016(	1)	-20
59	4	4	1	4	3	2	103.35240	103.35196(	2)	44*
60	5	4	2	5	3	3	103.94774	103.94798(	3)	-24
61	5	1	5	4	0	4	103.98182	103.98173(	1)	9
62	6	2	5	6	1	6	105.10447	105.10470(	2)	-23
63	6	4	3	6	3	4	105.65051	105.65039(	3)	12
64	7	3	5	7	2	6	106.16386	106.16391(	3)	-5
65	7	4	4	7	3	5	109.13414	109.13416(	4)	-2
66	3	2	2	2	1	1	109.96722	109.96725(	2)	-3
67	9	5	4	9	4	5	113.41263	113.41267(	12)	-4
68	8	4	5	8	3	6	114.93054	114.93033(	5)	21
69	7	1	6	7	0	7	117.91647	117.91649(	3)	-2
70	6	0	6	5	1	5	119.63065	119.63047(	2)	18
71	8	3	6	8	2	7	119.79182	119.79163(	5)	19
72	8	5	3	8	4	4	120.76696	120.76696(	8)	0
73	6	1	6	5	0	5	121.29947	121.29948(	2)	-1
74	7	2	6	7	1	7	122.61143	122.61148(	3)	-5
75	9	4	6	9	3	7	123.29339	123.29342(	7)	-3
76	9	2	7	9	1	8	123.43658	123.43666(	7)	-8
77	8	3	5	7	4	4	125.43259	125.43294(	6)	-35
78	7	5	2	7	4	3	125.50328	125.50335(	6)	-7
79	4	2	3	3	1	2	125.73729	125.73725(	2)	4
80	6	1	5	5	2	4	127.01201	127.01197(	3)	4
81	5	5	0	5	4	1	128.89017	128.89022(	2)	-5
82	6	5	2	6	4	3	129.04319	129.04325(	5)	-6
83	7	5	3	7	4	4	129.09425	129.09444(	5)	-19
84	5	5	1	5	4	2	129.13517	129.13522(	2)	-5
85	8	5	4	8	4	5	129.73232	129.73252(	7)	-20
86	3	2	1	2	1	2	131.81073	131.81059(	2)	14
87	10	4	7	10	3	8	134.16146	134.16139(	12)	7
88	7	2	5	6	3	4	135.07036	135.07019(	4)	17
89	9	3	7	9	2	8	135.27611	135.27610(	7)	1
90	7	0	7	6	1	6	138.43168	138.43163(	2)	5
91	8	1	7	8	0	8	138.58268	138.58262(	4)	6
92	7	1	7	6	0	6	139.14030	139.14031(	2)	-1
93	5	2	4	4	1	3	139.36503	139.36502(	3)	1
94	8	2	7	8	1	8	140.91545	140.91570(	4)	-25
95	3	3	0	3	0	3	145.97027	145.97039(	2)	-12

(continued overleaf)

Table 3. Continued

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
96	3	3	1	2	2	0	147.31162	147.31142(	2)	20
97	3	3	0	2	2	1	148.83129	148.83127(	2)	2
98	9	6	3	9	5	4	150.44370	150.44374(	51)	-4*
99	7	1	6	6	2	5	151.24364	151.24342(	4)	22
100	10	3	8	10	2	9	152.02086	152.02095(	12)	-9
101	6	2	5	5	1	4	152.09037	152.09043(	3)	-6
102	8	6	2	8	5	3	152.25496	152.25720(	14)	-224*
103	7	6	1	7	5	2	152.97172	152.97154(	9)	18
104	8	6	3	8	5	4	153.05951	153.05935(	12)	16
105	6	6	0	6	5	1	153.08002	153.08003(	9)	-1
106	6	6	1	6	5	2	153.11770	153.11787(	9)	-17
107	7	6	2	7	5	3	153.17886	153.17893(	9)	-7
108	8	0	8	7	1	7	156.92574	156.92586(	3)	-12
109	8	1	8	7	0	7	157.22077	157.22087(	2)	-10
110	9	1	8	9	0	9	158.50525	158.50536(	6)	-11
111	4	3	1	4	0	4	159.46864	159.46851(	3)	13
112	9	2	8	9	1	9	159.61636	159.61623(	5)	13
113	9	3	6	8	4	5	163.15988	163.16187(	8)	-199*
114	7	2	6	6	1	5	165.41784	165.41782(	4)	2
115	8	2	6	7	3	5	167.46077	167.46061(	7)	16*
116	4	3	2	3	2	1	168.49238	168.49239(	2)	-1
117	4	2	2	3	1	3	172.89171	172.89140(	3)	31
118	8	1	7	7	2	6	172.89679	172.89699(	5)	-20
119	7	7	0	7	6	1	174.81163	174.81158(	14)	5
120	8	7	2	8	6	3	175.25044	175.25050(	13)	-6
121	9	0	9	8	1	8	175.25926	175.25914(	4)	12
122	9	1	9	8	0	8	175.38136	175.38134(	4)	2
123	4	3	1	3	2	2	175.94663	175.94664(	2)	-1
124	10	1	9	10	0	10	177.94763	177.94755(	7)	8
125	10	2	9	10	1	10	178.46530	178.46518(	7)	12
126	8	2	7	7	1	6	180.22008	180.22008(	4)	0
127	5	3	2	5	0	5	181.68219	181.68213(	3)	6
128	5	3	3	4	2	2	186.13636	186.13688(	3)	-52*
129	9	1	8	8	2	7	192.84905	192.84880(	6)	25*
130	10	0	10	9	1	9	193.49348	193.49361(	5)	-13
131	10	1	10	9	0	9	193.54435	193.54447(	4)	-12
132	9	2	8	8	1	7	196.41503	196.41495(	5)	8
133	9	2	7	8	3	6	196.49225	196.49383(	10)	-158*
134	11	1	10	11	0	11	197.08665	197.08672(	13)	-7
135	10	3	7	9	4	6	199.89026	199.89011(	13)	15
136	6	3	4	5	2	3	200.22409	200.22415(	3)	-6
137	4	4	1	3	3	0	200.33654	200.33655(	2)	-1
138	4	4	0	3	3	1	200.57806	200.57815(	2)	-9
139	5	4	1	5	1	4	206.43244	206.43251(	4)	-7
140	5	3	2	4	2	3	207.10883	207.10873(	2)	10
141	6	4	2	6	1	5	211.00709	211.00750(	5)	-41*
142	7	3	5	6	2	4	211.52420	211.52405(	4)	15
143	11	0	11	10	1	10	211.65246	211.65237(	9)	9
144	11	1	11	10	0	10	211.67378	211.67380(	9)	-2
145	10	1	9	9	2	8	211.82549	211.82493(	8)	56*
146	3	3	1	2	0	2	212.16725	212.16710(	3)	15
147	10	2	9	9	1	8	213.50424	213.50429(	8)	-5
148	12	1	11	12	0	12	216.01257	216.01803(	58)	-546*
149	12	2	11	12	1	12	216.12921	216.12882(	59)	39*
150	5	2	3	4	1	4	221.32979	221.33008(	3)	-29
151	5	4	2	4	3	1	223.84172	223.84180(	3)	-8
152	5	4	1	4	3	2	225.50127	225.50137(	3)	-10
153	6	4	3	5	3	2	245.30435	245.30426(	3)	9
154	5	5	1	4	4	0	251.00686	251.00685(	3)	1
155	5	5	0	4	4	1	251.03954	251.03963(	3)	-9
156	6	5	2	5	4	1	275.28342	275.28338(	5)	4
157	7	4	3	6	3	4	280.31769	280.31730(	5)	39

[a] See footnote to Table 2 for explanation of column headings. Lines given in megahertz have been taken from Ref. 15.

Table 4. Pure Rotational Transitions of $HD^{16}O$[a]

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
1	5	4	1	5	4	2	486.528	486.528(	0)	0
2	3	3	0	3	3	1	824.671	824.670(	0)	0
3	6	4	2	6	4	3	2394.560	2394.559(	1)	1
4	9	5	4	9	5	5	3044.710	3044.714(	9)	-3
5	4	3	1	4	3	2	5702.780	5702.842(	2)	-62
6	7	4	3	7	4	4	8577.812	8577.808(	4)	4
7	10	5	5	10	5	6	8837.210	8837.139(	19)	70
8	2	2	0	2	2	1	10278.246	10278.245(	0)	0
9	6	2	4	7	0	7	11618.200	11617.961(	40)	238*
10	3	2	1	4	1	4	20460.010	20460.007(	14)	2
11	5	3	2	5	3	3	22307.670	22307.535(	6)	135
12	11	5	6	11	5	7	22581.570	22581.511(	29)	59
13	8	4	4	8	4	5	24884.770	24884.780(	8)	-10
14	7	1	7	6	2	4	26880.380	26880.446(	35)	-66
15	11	7	5	12	6	6	28668.340	28668.227(	146)	112
16	11	7	4	12	6	7	31670.430	31670.540(	138)	-110
17	13	2	12	12	3	9	45902.540	45902.539(	54)	0
18	3	2	1	3	2	2	50236.300	50236.343(	3)	-42
19	12	5	7	12	5	8	51917.870	51917.833(	53)	36
20	4	3	1	5	2	4	61185.950	61186.047(	20)	-96
21	9	4	5	9	4	6	61704.590	61704.631(	15)	-40
22	6	3	3	6	3	4	64427.340	64427.367(	11)	-27
23	6	0	6	5	2	3	69550.580	69550.595(	26)	-15
24	1	1	0	1	1	1	80578.150	80578.246(	5)	-95
25	7	3	5	6	4	2	87962.810	87962.820(	13)	-9
26	5	1	5	4	2	2	120778.190	120778.177(	13)	13
27	10	4	6	10	4	7	134770.220	134770.352(	33)	-131
28	6	1	6	5	2	3	138530.570	138530.519(	20)	50
29	4	2	2	4	2	3	143727.210	143727.303(	9)	-93
30	7	3	4	7	3	5	151616.190	151616.225(	17)	-34
31	9	6	4	10	5	5	160329.460	160329.408(	48)	52
32	9	6	3	10	5	6	169246.050	169245.904(	31)	146
33	3	2	1	4	0	4	207110.650	207110.879(	31)	-229*
34	7	2	5	8	1	8	207345.710	207345.687(	40)	23
35	9	4	6	8	5	3	210310.650	210310.598(	19)	51
36	3	1	2	2	2	1	225896.720	225896.701(	22)	19
37	2	1	1	2	1	2	241561.550	241561.494(	13)	56
38	7	3	4	6	4	3	241973.570	241973.603(	19)	-33
39	5	2	3	4	3	2	255050.260	255050.203(	20)	56
40	7	5	3	8	4	4	258223.760	258223.877(	23)	-116
41	2	2	0	3	1	3	266161.070	266160.994(	18)	75
42	9	4	5	8	5	4	272907.540	272907.497(	18)	42
43	7	5	2	8	4	5	283318.590	283318.556(	22)	33
44	8	3	5	8	3	6	305038.550	305038.552(	26)	-2
45	5	2	3	5	2	4	310533.290	310533.408(	20)	-118
46	6	2	5	5	3	2	313750.620	313750.631(	23)	-11
47	5	4	2	6	3	3	317151.250	317151.208(	20)	42
48	11	5	7	10	6	4	332949.590	332949.523(	33)	67
49	3	3	1	4	2	2	335395.500	335395.543(	22)	-43
50	11	5	6	10	6	5	355841.380	355841.388(	64)	-8
51	5	3	2	6	1	5	356835.850	356835.939(	90)	-88
52	5	4	1	6	3	4	382065.100	382065.103(	18)	-2
53	1	0	1	0	0	0	464924.520	464924.482(	13)	38
54	3	3	0	4	2	3	479947.370	479947.516(	24)	-146
55	3	1	2	3	1	3	481779.500	481779.451(	20)	49
56	2	0	2	1	1	1	490596.640	490596.682(	18)	-41
57	1	1	0	1	0	1	509292.420	509292.372(	18)	48
58	10	7	4	11	6	5	528958.354	528958.340(	79)	14
59	10	7	3	11	6	6	529990.765	529990.793(	69)	-28
60	8	3	6	7	4	3	539935.900	539936.058(	30)	-157
61	9	3	6	9	3	7	540374.264	540374.140(	49)	124
62	8	2	6	9	1	9	548555.008	548555.019(	53)	-10
63	6	2	4	6	2	5	559816.740	559816.187(	43)	553*
64	2	1	1	2	0	2	599926.710	599926.588(	17)	122
65	2	1	1	2	0	2	20.01090	20.01140(	0)	-50
66	7	2	6	6	3	3	622482.571	622482.691(	28)	-119
67	8	6	3	9	5	4	663044.564	663044.732(	44)	-167
68	8	6	2	9	5	5	666105.694	666105.604(	30)	89
69	10	4	7	9	5	4	700845.589	700845.744(	39)	-155
70	3	1	2	3	0	3	753411.150	753411.010(	22)	140
71	3	1	2	3	0	3	25.13126	25.13109(	0)	17
72	6	5	2	7	4	3	766165.655	766165.686(	33)	-31
73	6	5	1	7	4	4	774779.016	774778.980(	34)	36
74	4	1	3	4	1	4	797487.016	797487.008(	25)	7
75	4	1	3	3	2	2	27.59439	27.59453(	0)	-14
76	4	1	3	3	2	2	827263.389	827263.344(	25)	45
77	4	4	1	5	3	2	836994.625	836994.618(	36)	7
78	10	4	6	9	5	5	838660.821	838660.809(	41)	11
79	8	2	7	7	3	4	838953.288	838953.207(	51)	80
80	2	1	2	1	1	1	848961.843	848961.776(	22)	67
81	2	1	2	1	1	1	28.31819	28.31832(	0)	-13
82	8	3	5	7	4	4	853552.362	853552.417(	35)	-55
83	1	1	1	0	0	0	893638.666	893638.608(	28)	57
84	1	1	1	0	0	0	29.80834	29.80858(	0)	-24

Table 4. Continued

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
85	6	2	4	5	3	3	29.88270	29.88315(	0)	-45
86	6	2	4	5	3	3	895874.360	895874.353(	37)	7
87	2	0	2	1	0	1	919310.885	919310.808(	21)	76
88	2	0	2	1	0	1	30.66468	30.66491(	0)	-23
89	4	1	3	4	0	4	984137.828	984137.881(	31)	-52
90	4	1	3	4	0	4	32.82737	32.82731(	0)	6
91	3	0	3	2	1	2	33.20341	33.20335(	0)	6
92	3	0	3	2	1	2	995411.501	995411.487(	22)	13
93	2	1	1	1	1	0	33.68813	33.68814(	0)	-1
94	2	1	1	1	1	0	1009944.697	1009945.024(	22)	-326
95	5	2	3	5	1	4	38.75849	38.75857(	0)	-8
96	6	2	4	6	1	5	41.04189	41.04182(	0)	7
97	3	1	3	2	1	2	42.26418	42.26401(	0)	17
98	5	1	4	5	0	5	43.29004	43.29012(	0)	-8
99	3	0	3	2	0	2	45.15700	45.15713(	0)	-13
100	7	2	5	7	1	6	46.20579	46.20582(	0)	-3
101	3	2	2	2	2	1	46.46269	46.46277(	0)	-8
102	3	2	1	2	2	0	47.79547	47.79563(	0)	-16
103	5	1	4	4	2	3	48.19430	48.19431(	0)	-1
104	4	0	4	3	1	3	49.76524	49.76533(	0)	-9
105	3	1	2	2	1	1	50.27686	50.27681(	0)	5
106	9	3	6	8	4	5	50.82934	50.82944(	0)	-10
107	7	2	5	6	3	4	52.60898	52.60897(	0)	1
108	8	2	6	8	1	7	54.52575	54.52568(	0)	7
109	4	1	4	3	1	3	55.99135	55.99133(	0)	2
110	6	1	5	6	0	6	56.19242	56.19240(	0)	2
111	9	3	6	9	2	7	57.74837	57.74844(	1)	-7
112	8	3	5	8	2	6	58.70670	58.70653(	1)	17
113	4	0	4	3	0	3	58.82597	58.82598(	0)	-1
114	4	2	3	3	2	2	61.65279	61.65285(	0)	-6
115	7	3	4	7	2	5	61.83852	61.83851(	0)	1
116	4	3	2	3	3	1	62.46344	62.46350(	0)	-6
117	4	3	1	3	3	0	62.62619	62.62622(	0)	-3
118	4	2	2	3	2	1	64.77141	64.77138(	0)	3
119	4	1	4	3	0	3	65.05205	65.05198(	0)	7
120	5	0	5	4	1	4	65.56390	65.56382(	0)	8
121	9	2	7	9	1	8	65.90897	65.90894(	0)	3
122	6	3	3	6	2	4	66.11468	66.11452(	0)	16
123	4	1	3	3	1	2	66.52223	66.52220(	0)	3
124	5	2	4	5	1	5	67.77176	67.77164(	0)	12
125	6	1	5	5	2	4	68.87067	68.87064(	0)	3
126	5	3	2	5	2	3	70.41514	70.41512(	0)	2
127	7	1	6	7	0	7	70.75634	70.75614(	0)	20
128	5	0	5	4	0	4	71.78980	71.78982(	0)	-2
129	5	1	5	4	0	4	75.70859	75.70858(	0)	1
130	8	2	6	7	3	5	76.18416	76.18408(	0)	8
131	6	2	5	6	1	6	76.25980	76.25984(	0)	-4
132	5	2	4	4	2	3	76.59457	76.59460(	0)	-3
133	5	4	2	4	4	1	77.91340	77.91347(	0)	-7
134	5	4	1	4	4	0	77.92793	77.92787(	0)	6
135	5	3	3	4	3	2	78.17858	78.17858(	0)	0
136	5	3	2	4	3	1	78.73246	78.73245(	0)	1
137	5	3	3	5	2	4	80.02934	80.02930(	0)	4
138	6	0	6	5	1	5	80.44988	80.44988(	0)	0
139	5	1	4	4	1	3	82.25220	82.25263(	0)	-43*
140	6	3	4	6	2	5	82.63919	82.63892(	0)	26
141	6	1	6	5	1	5	82.75102	82.75080(	0)	22
142	6	0	6	5	0	5	84.36878	84.36864(	0)	14
143	7	2	6	7	1	7	85.98181	85.98168(	0)	13
144	8	1	7	8	0	8	86.04735	86.04720(	0)	15
145	7	3	5	7	2	6	86.47736	86.47725(	0)	11
146	6	1	6	5	0	5	86.66962	86.66956(	0)	6
147	7	1	6	6	2	5	89.04224	89.04207(	0)	17
148	6	2	5	5	2	4	91.23897	91.23900(	0)	-3
149	8	3	6	8	2	7	91.67380	91.67378(	1)	2
150	9	4	5	9	3	6	92.24298	92.24310(	3)	-12
151	6	5	2	5	5	1	93.19840	93.19785(	1)	55*
152	6	5	1	5	5	0	93.19840	93.19892(	1)	-52*
153	6	4	3	5	4	2	93.64795	93.64802(	0)	-7
154	6	4	2	5	4	1	93.71163	93.71166(	0)	-3
155	6	3	4	5	3	3	93.84846	93.84861(	0)	-15
156	6	3	3	5	3	2	95.25352	95.25358(	0)	-6
157	7	1	7	6	1	6	95.82984	95.82993(	0)	-9
158	8	2	7	8	1	8	96.73914	96.73928(	0)	-14
159	7	0	7	6	0	6	96.84672	96.84668(	0)	4
160	6	1	5	5	1	4	97.27089	97.27092(	0)	-3
161	8	4	4	8	3	5	97.59775	97.59779(	2)	-4
162	7	1	7	6	0	6	98.13084	98.13085(	0)	-1
163	9	3	7	9	2	8	98.27014	98.27024(	1)	-10
164	6	2	4	5	2	3	99.55428	99.55417(	0)	11
165	9	2	7	8	3	6		100.02371(	1)	
166	4	2	3	3	1	2	100.58039	100.58052(	0)	-13
167	9	1	8	9	0	9	101.30672	101.30688(	1)	-16
168	7	4	3	7	3	4	101.64811	101.64791(	1)	20
169	6	4	2	6	3	3	104.30696	104.30692(	0)	4
170	7	2	6	6	2	5	105.55182	105.55177(	0)	5
171	5	4	1	5	3	2	105.84903	105.84883(	0)	20
172	6	4	3	6	3	4	106.37615	106.37611(	0)	4
173	7	4	4	7	3	5	106.41909	106.41916(	1)	-7
174	5	4	2	5	3	3	106.57670	106.57670(	0)	0
175	8	4	5	8	3	6	106.94262	106.94271(	2)	-9
176	8	0	8	7	1	7	108.07007	108.07013(	0)	-6
177	8	1	7	7	2	6	108.13573	108.13565(	0)	8
178	9	4	6	9	3	7	108.20929	108.20979(	3)	-50
179	9	2	8	9	1	9	108.30623	108.30634(	1)	-11
180	7	6	2	6	6	1	108.33742	108.33765(	3)	-23*
181	7	6	1	6	6	0	108.33742	108.33772(	3)	-30*
182	8	1	8	7	1	7	108.76179	108.76149(	0)	30
183	7	5	3	6	5	2	108.83992	108.83999(	2)	-7
184	7	5	2	6	5	1	108.84546	108.84581(	2)	-35
185	8	0	8	7	0	7	109.35438	109.35430(	0)	8
186	7	3	5	6	3	4	109.39012	109.39011(	0)	1
187	7	4	4	6	4	3	109.43319	109.43316(	1)	3
188	7	4	3	6	4	2	109.63953	109.63941(	1)	12
189	8	1	8	7	0	7	110.04566	110.04566(	0)	0
190	5	2	4	4	1	3	110.65307	110.65291(	0)	16
191	7	1	6	6	1	5	111.41053	111.41043(	0)	10
192	7	3	4	6	3	3	112.29845	112.29841(	0)	4
193	7	2	5	6	2	4	116.57448	116.57443(	0)	5
194	8	2	7	7	2	6	119.51907	119.51909(	0)	-2
195	6	2	5	5	1	4	119.63927	119.63928(	0)	-1
196	9	0	9	8	1	8	121.22089	121.22094(	1)	-5
197	4	2	2	3	1	3	121.44515	121.44518(	0)	-3
198	9	1	9	8	1	8	121.58372	121.58370(	1)	2
199	9	1	9	8	0	8	122.27520	122.27506(	1)	14
200	8	6	3	7	6	2	123.87537	123.87552(	4)	-15*
201	8	6	2	7	6	1	123.87537	123.87598(	4)	-61*
202	8	5	4	7	5	3	124.52587	124.52584(	2)	3
203	8	5	3	7	5	2	124.54857	124.54860(	2)	-3
204	8	1	7	7	1	6	124.64528	124.64536(	0)	-8
205	8	3	6	7	3	5	124.71561	124.71561(	1)	0
206	8	4	5	7	4	4	125.23765	125.23916(	1)	-151*
207	8	4	4	7	4	3	125.78409	125.78310(	1)	99*
208	9	1	8	8	2	7	125.78851	125.78854(	1)	-3
209	7	2	6	6	1	5	127.92027	127.92013(	0)	14
210	8	3	5	7	3	4	129.83345	129.83323(	1)	22
211	9	5	4	9	4	5	131.25091	131.25117(	4)	-26
212	8	2	6	7	2	5	132.96510	132.96521(	1)	-11
213	9	2	8	8	2	7	133.15101	133.15075(	1)	26
214	8	5	3	8	4	4	133.16907	133.16902(	2)	5
215	8	5	4	8	4	5	133.96966	133.96932(	2)	34
216	10	1	10	9	1	9	134.32604	134.32576(	1)	28
217	7	5	2	7	4	3	134.40351	134.40353(	1)	-2
218	10	0	10	9	0	9	134.50174	134.50169(	1)	5
219	7	5	3	7	4	4	134.68280	134.68265(	1)	15
220	6	5	1	6	4	2	135.19742	135.19713(	1)	29
221	6	5	2	6	4	3	135.27611	135.27582(	1)	29
222	5	5	0	5	4	1	135.70999	135.70987(	0)	12
223	5	5	1	5	4	2	135.72598	135.72599(	0)	-1
224	8	2	7	7	1	6	136.02884	136.02880(	1)	4
225	9	1	8	8	1	7	137.17202	137.17198(	1)	4
226	4	3	2	3	2	1	138.42277	138.42247(	0)	30
227	9	3	7	8	3	6	139.74745	139.74721(	2)	24
228	9	5	5	8	5	4	140.25252	140.25282(	4)	-30
229	4	3	1	3	2	2	140.28857	140.28840(	0)	17
230	9	5	4	8	5	3	140.32439	140.32462(	4)	-23
231	9	4	6	8	4	5	141.01409	141.01429(	2)	-20
232	9	4	5	8	4	4	142.24260	142.24247(	2)	13
233	9	2	8	8	1	7	144.53417	144.53419(	1)	-2
234	10	2	9	9	2	8	146.47849	146.47839(	2)	10
235	9	3	6	8	3	5	147.59733	147.59716(	2)	17
236	5	2	3	4	1	4	147.61273	147.61250(	0)	23
237	9	2	7	8	2	6	148.55539	148.55524(	1)	15
238	10	1	9	9	1	8	149.32940	149.32947(	2)	-7
239	5	3	3	4	2	2	151.82986	151.82967(	0)	19
240	10	3	8	9	3	7	154.42578	154.42590(	3)	-12
241	10	4	7	9	4	6	156.68692	156.68711(	4)	-19
242	5	3	2	4	2	3	157.36803	157.36800(	0)	3
243	10	4	6	9	4	5	159.12425	159.12432(	4)	-7
244	9	6	3	9	5	4	161.55333	161.55371(	6)	-38
245	9	6	4	9	5	5	161.65214	161.65262(	6)	-48
246	8	6	2	8	5	3	162.44191	162.44195(	4)	-4
247	8	6	3	8	5	4	162.47092	162.47117(	4)	-25
248	7	6	1	7	5	2	163.11465	163.11456(	2)	9
249	7	6	2	7	5	3	163.12164	163.12148(	2)	16
250	10	2	8	9	2	7	163.20650	163.20661(	3)	-11
251	6	3	4	5	2	3	163.51974	163.51963(	1)	11
252	6	6	0	6	5	1	163.62346	163.62265(	2)	81*
253	6	6	1	6	5	2	163.62346	163.62383(	2)	-37*
254	10	3	7	9	3	6	165.17601	165.17612(	3)	-11
255	4	4	1	3	3	0	169.27789	169.27781(	0)	8
256	4	4	0	3	3	1	169.30719	169.30714(	0)	5

(*continued overleaf*)

Table 4. Continued

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
257	7	3	5	6	2	4	173.35573	173.35557(	1)	16
258	6	3	3	5	2	4	176.02707	176.02698(	1)	9
259	6	2	4	5	1	5	177.68412	177.68410(	0)	2
260	8	3	6	7	2	5	181.49704	181.49675(	2)	29
261	5	4	2	4	3	1	184.56522	184.56506(	1)	16
262	5	4	1	4	3	2	184.77164	184.77151(	1)	13
263	9	3	7	8	2	6	188.27887	188.27874(	3)	13
264	9	7	2	9	6	3	189.13337	189.13325(	11)	12*
265	9	7	3	9	6	4	189.13337	189.13586(	11)	-249*
266	8	7	1	8	6	2	189.83304	189.83335(	7)	-31*
267	8	7	2	8	6	3	189.83304	189.83388(	7)	-84*
268	7	7	0	7	6	1	190.40376	190.40389(	10)	-13
269	7	7	1	7	6	2	190.40376	190.40397(	10)	-21
270	7	3	4	6	2	5	197.08669	197.08640(	1)	29
271	6	4	3	5	3	2	199.48090	199.48062(	1)	28
272	6	4	2	5	3	3	200.30477	200.30459(	1)	18
273	7	2	5	6	1	6	211.50801	211.50773(	1)	28
274	5	5	1	4	4	0	213.63868	213.63764(	1)	104*
275	5	5	0	4	4	1	213.63868	213.63957(	1)	-89*
276	7	4	4	6	3	3	213.66032	213.66020(	2)	12
277	9	8	1	9	7	2	215.37591	215.37590(	3)	1
278	9	8	2	9	7	3	215.37591	215.37594(	3)	-3
279	8	8	0	8	7	1	216.04261	216.04231(	27)	30
280	8	8	1	8	7	2	216.04261	216.04232(	27)	29
281	7	4	3	6	3	4	216.09563	216.09539(	2)	24
282	8	3	5	7	2	6	221.36783	221.36786(	2)	-3
283	8	4	5	7	3	4	226.60087	226.60095(	3)	-8
284	6	5	2	5	4	1	228.90790	228.90761(	2)	29
285	6	5	1	5	4	2	228.92512	228.92502(	2)	10
286	8	4	4	7	3	5	232.48874	232.48839(	3)	35
287	9	4	6	8	3	5	237.78200	237.78201(	4)	-1
288	7	5	3	6	4	2	244.03612	244.03594(	3)	18
289	7	5	2	6	4	3	244.12299	244.12281(	3)	18
290	8	2	6	7	1	7	248.64309	248.64301(	1)	8
291	9	3	6	8	2	7	249.44595	249.44593(	3)	2
292	9	4	5	8	3	6	250.01519	250.01525(	4)	-6
293	6	6	1	5	5	0	256.82174	256.82157(	3)	17
294	6	6	0	5	5	1	256.82174	256.82168(	3)	6
295	8	5	4	7	4	3	258.92238	258.92236(	4)	2
296	8	5	3	7	4	4	259.23829	259.23825(	4)	4
297	7	6	2	6	5	1	271.96089	271.96029(	4)	60*
298	7	6	1	6	5	2	271.96089	271.96155(	4)	-66*
299	9	5	5	8	4	4	273.39181	273.39208(	7)	-26
300	9	5	4	8	4	5	274.32344	274.32370(	7)	-26
301	8	6	3	7	5	2	286.98991	286.99000(	7)	-9*
302	8	6	2	7	5	3	286.99693	286.99754(	7)	-61*
303	7	7	1	6	6	0	298.74111	298.74161(	10)	-50*
304	7	7	0	6	6	1	298.74111	298.74162(	10)	-51*
305	9	6	3	8	5	4		301.90809(	10)	
306	8	7	2	7	6	1	313.70838	313.70933(	10)	-95*
307	8	7	1	7	6	2	313.70838	313.70941(	10)	-103*
308	9	7	3	8	6	2	328.56837	328.56960(	17)	-123*
309	9	7	2	8	6	3	328.56837	328.57017(	17)	-180*
310	8	8	0	7	7	1	339.34734	339.34775(	21)	-41*
311	8	8	1	7	7	0	339.34734	339.34775(	21)	-41*

[a] See footnote to Table 2 for explanation of column headings. Lines given in megahertz have been taken from Ref. 9.

Table 5. Pure Rotational Transitions of $HD^{18}O$[a]

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
1	7	4	3	7	4	4	9032.200	9032.257(	23)	-56
2	10	5	5	10	5	6	9477.100	9476.720(	137)	380
3	3	2	1	4	1	4	9526.600	9526.895(	67)	-294
4	2	2	0	2	2	1	10458.600	10458.481(	6)	118
5	7	1	7	6	2	4	22733.200	22733.365(	93)	-164
6	5	3	2	5	3	3	23080.250	23080.275(	22)	-25
7	11	5	6	11	5	7	24218.400	24217.978(	418)	422
8	8	4	4	8	4	5	26196.850	26196.811(	30)	39
9	4	3	1	5	2	4	37889.850	37889.863(	46)	-13
10	3	2	1	3	2	2	51087.680	51087.625(	20)	55
11	9	4	5	9	4	6	64908.690	64908.794(	41)	-104
12	6	3	3	6	3	4	66601.940	66602.139(	32)	-198
13	1	1	0	1	1	1	80616.300	80616.289(	17)	11
14	7	3	5	6	4	2	121185.070	121185.082(	46)	-12
15	5	1	5	4	2	2	127224.800	127224.791(	44)	8
16	6	1	6	5	2	3	139788.680	139788.689(	44)	-9
17	10	4	6	10	4	7	141550.340	141550.325(	46)	15
18	4	2	2	4	2	3	145984.850	145984.828(	40)	22
19	7	3	4	7	3	5	156479.350	156479.244(	44)	105
20	7	5	3	8	4	4	212375.510	212375.598(	40)	-87
21	7	2	5	8	1	8	216553.110	216553.116(	46)	-5
22	7	5	2	8	4	5	238797.230	238797.146(	34)	84
23	3	1	2	2	2	1	240872.000	240872.012(	46)	-11
24	2	1	1	2	1	2	241680.380	241680.385(	42)	-4
25	3	1	2	3	0	3	24.89980	24.89975(	0)	5
26	4	1	3	3	2	2	27.99580	27.99602(	0)	-22
27	1	1	1	0	0	0	29.45970	29.46004(	1)	-34
28	4	1	3	4	0	4	32.63009	32.63011(	0)	-2
29	3	0	3	2	1	2	33.16789	33.16787(	1)	2
30	5	2	3	5	1	4	38.15183	38.15172(	2)	11
31	6	2	4	6	1	5	40.55151	40.55151(	2)	0
32	3	1	3	2	1	2	41.98972	41.98975(	1)	-3
33	5	1	4	5	0	5	43.12906	43.12914(	1)	-8
34	3	0	3	2	0	2	44.86689	44.86681(	2)	8
35	7	2	5	7	1	6	45.86075	45.86093(	2)	-18
36	3	2	2	2	2	1	46.19154	46.19161(	2)	-7
37	3	2	1	2	2	0	47.54693	47.54685(	2)	8
38	5	1	4	4	2	3	48.48328	48.48339(	1)	-11
39	4	0	4	3	1	3	49.60076	49.60077(	1)	-1
40	3	1	2	2	1	1	50.00607	50.00603(	1)	4
41	7	2	5	6	3	4	53.43775	53.43758(	3)	17
42	8	2	6	8	1	7	54.34277	54.34288(	3)	-11
43	4	1	4	3	1	3	55.62124	55.62118(	2)	6
44	6	1	5	6	0	6	56.04464	56.04464(	2)	0
45	9	3	6	9	2	7	56.79660	56.79670(	6)	-10
46	8	3	5	8	2	6	57.54878	57.54883(	4)	-5
47	4	0	4	3	0	3	58.42245	58.42265(	2)	-20
48	7	3	4	7	2	5	60.54873	60.54867(	3)	6
49	4	2	3	3	2	2	61.28777	61.28774(	2)	3
50	4	3	2	3	3	1	62.10717	62.10703(	2)	14
51	4	1	4	3	0	3	64.44310	64.44305(	2)	5
52	4	2	2	3	2	1	64.45316	64.45317(	2)	-1
53	6	3	3	6	2	4	64.76792	64.76756(	2)	36
54	5	0	5	4	1	4	65.25577	65.25568(	1)	9
55	9	2	7	9	1	8	65.87374	65.87402(	7)	-28
56	4	1	3	3	1	2	66.15297	66.15300(	2)	-3
57	5	2	4	5	1	5	67.01918	67.01921(	1)	-3
58	6	1	5	5	2	4	69.02194	69.02187(	2)	7
59	5	3	2	5	2	3	69.06964	69.06959(	2)	5
60	7	1	6	7	0	7	70.57483	70.57477(	3)	6
61	5	0	5	4	0	4	71.27616	71.27608(	2)	8
62	5	1	5	4	0	4	75.03513	75.03512(	2)	1
63	6	2	5	6	1	6	75.51141	75.51097(	1)	44
64	5	2	4	4	2	3	76.13260	76.13250(	1)	10
65	8	2	6	7	3	5	76.92178	76.92177(	4)	1
66	5	4	2	4	4	1	77.46168	77.46143(	4)	25
67	5	3	3	4	3	2	77.73529	77.73533(	2)	-4
68	5	3	2	4	3	1	78.30844	78.30833(	2)	11
69	5	3	3	5	2	4	78.80250	78.80232(	2)	18
70	6	0	6	5	1	5	79.99630	79.99644(	1)	-14
71	6	3	4	6	2	5	81.44306	81.44290(	2)	16
72	5	1	4	4	1	3	81.77520	81.77511(	2)	9
73	6	1	6	5	1	5	82.18483	82.18467(	1)	16
74	6	0	6	5	0	5	83.75559	83.75548(	2)	11
75	7	2	6	7	1	7	85.23012	85.23006(	2)	6
76	7	3	5	7	2	6	85.32432	85.32425(	3)	7
77	8	1	7	8	0	8	85.77731	85.77717(	3)	14
78	6	1	6	5	0	5	85.94367	85.94371(	2)	-4
79	7	1	6	6	2	5	89.01941	89.01955(	3)	-14
80	9	4	5	9	3	6	90.21304	90.21292(	5)	12
81	8	3	6	8	2	7	90.57353	90.57356(	4)	-3
82	6	2	5	5	2	4	90.67627	90.67643(	1)	-16
83	6	5	2	5	5	1	92.64373	92.64317(	7)	56*
84	6	5	1	5	5	0	92.64373	92.64432(	7)	-59*
85	6	4	3	5	4	2	93.11216	93.11229(	2)	-13
86	6	4	2	5	4	1	93.17917	93.17931(	2)	-14
87	6	3	4	5	3	3	93.31687	93.31701(	1)	-14
88	6	3	3	5	3	2	94.76882	94.76874(	1)	8
89	7	1	7	6	1	6	95.16624	95.16622(	1)	2
90	8	4	4	8	3	5	95.63444	95.63440(	3)	4
91	8	2	7	8	1	8	95.97460	95.97433(	3)	26

Table 5. Continued

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
92	7	0	7	6	0	6	96.14400	96.14399(	1)	1
93	6	1	5	5	1	4	96.67077	96.67099(	2)	-22
94	9	3	7	9	2	8	97.22781	97.22802(	6)	-21
95	7	1	7	6	0	6	97.35449	97.35445(	2)	4
96	6	2	4	5	2	3	99.07075	99.07077(	1)	-2
97	4	2	3	3	1	2	99.44463	99.44473(	4)	-10
98	7	4	3	7	3	4	99.77124	99.77130(	2)	-6
99	9	2	7	8	3	6	100.62616	100.62643(	7)	-26
100	9	1	8	9	0	9	100.90643	100.90602(	5)	41
101	6	4	2	6	3	3	102.50272	102.50276(	1)	-4
102	5	4	1	5	3	2	104.09223	104.09219(	2)	4
103	6	4	3	6	3	4	104.64005	104.64026(	1)	-21
104	7	4	4	7	3	5	104.68934	104.68960(	2)	-26
105	5	4	2	5	3	3	104.84470	104.84498(	2)	-28
106	7	2	6	6	2	5	104.88537	104.88530(	2)	7
107	8	4	5	8	3	6	105.23540	105.23579(	3)	-39
108	9	4	6	9	3	7	106.54641	106.54647(	5)	-6
109	8	0	8	7	1	7	107.35592	107.35603(	2)	-11
110	9	2	8	9	1	9	107.51466	107.51440(	6)	26
111	7	6	2	6	6	1	107.67403	107.67427(	8)	-24
112	7	6	1	6	6	0	107.67403	107.67435(	8)	-32
113	8	1	7	7	2	6	107.90291	107.90314(	4)	-23
114	8	1	8	7	1	7	108.00169	108.00179(	2)	-10
115	7	5	3	6	5	2	108.20135	108.20119(	4)	16
116	7	5	2	6	5	1	108.20929	108.20742(	4)	187*
117	8	0	8	7	0	7	108.56633	108.56650(	2)	-17
118	7	4	4	6	4	3	108.81580	108.81600(	2)	-20
119	7	4	3	6	4	2	109.03315	109.03319(	2)	-4
120	8	1	8	7	0	7	109.21233	109.21226(	2)	7
121	5	2	4	4	1	3	109.42411	109.42423(	3)	-12
122	7	1	6	6	1	5	110.67427	110.67411(	2)	16
123	7	3	4	6	3	3	111.76472	111.76464(	1)	8
124	7	2	5	6	2	4	115.98350	115.98353(	2)	-3
125	6	2	5	5	1	4	118.32564	118.32555(	3)	9
126	8	2	7	7	2	6	118.74615	118.74607(	2)	8
127	4	2	2	3	1	3	120.39299	120.39213(	3)	86*
128	9	0	9	8	1	8	120.39299	120.39427(	3)	-128*
129	9	1	9	8	1	8	120.72983	120.72994(	3)	-11
130	9	1	9	8	0	8	121.37573	121.37570(	3)	3
131	8	6	3	7	6	2	123.12899	123.12672(	9)	227*
132	8	6	2	7	6	1	123.12899	123.12722(	9)	177*
133	8	1	7	7	1	6	123.76899	123.76889(	2)	10
134	8	5	4	7	5	3	123.80648	123.80639(	4)	9
135	8	5	3	7	5	2	123.83072	123.83078(	4)	-6
136	8	3	6	7	3	5	123.99530	123.99537(	3)	-7
137	8	4	5	7	4	4	124.54165	124.54156(	2)	9
138	8	4	4	7	4	3	125.11421	125.11410(	2)	11
139	9	1	8	8	2	7	125.32590	125.32596(	6)	-6
140	7	2	6	6	1	5	126.53991	126.53987(	2)	4
141	9	5	4	9	4	5	128.92879	128.92915(	8)	-36
142	8	3	5	7	3	4	129.25108	129.25101(	2)	7
143	8	5	3	8	4	4	130.92227	130.92237(	4)	-10
144	8	5	4	8	4	5	131.76418	131.76431(	4)	-13
145	7	5	2	7	4	3	132.20576	132.20569(	2)	7
146	8	2	6	7	2	5	132.25068	132.25085(	2)	-17
147	9	2	8	8	2	7	132.27006	132.27000(	3)	6
148	7	5	3	7	4	4	132.49945	132.49947(	2)	-2
149	6	5	1	6	4	2	133.03150	133.03146(	3)	4
150	6	5	2	6	4	3	133.11423	133.11429(	3)	-6
151	10	1	10	9	1	9	133.37966	133.37980(	5)	-14
152	10	0	10	9	0	9	133.54418	133.54426(	5)	-8
153	5	5	0	5	4	1	133.56643	133.56644(	7)	-1
154	5	5	1	5	4	2	133.58318	133.58341(	7)	-23
155	8	2	7	7	1	6	134.61201	134.61182(	3)	19
156	9	1	8	8	1	7	136.16889	136.16889(	4)	0
157	4	3	2	3	2	1	136.78300	136.78314(	3)	-14
158	9	6	4	8	6	3	138.60808	138.60311(	14)	497*
159	9	6	3	8	6	2	138.60808	138.60540(	14)	268*
160	4	3	1	3	2	2	138.68410	138.68412(	3)	-2
161	9	3	7	8	3	6	138.92459	138.92446(	4)	13
162	9	5	5	8	5	4	139.45636	139.45623(	7)	13
163	9	5	4	8	5	3	139.53322	139.53322(	7)	0
164	9	4	6	8	4	5	140.23532	140.23514(	4)	18
165	9	4	5	8	4	4	141.52655	141.52643(	4)	12
166	9	2	8	8	1	7	143.11311	143.11293(	5)	18
167	10	2	9	9	2	8	145.49055	145.49063(	8)	-8
168	5	2	3	4	1	4	146.53666	146.53654(	3)	12
169	9	3	6	8	3	5	146.94795	146.94791(	4)	4
170	9	2	7	8	2	6	147.70000	147.70004(	4)	-4
171	10	1	9	9	1	8	148.22332	148.22325(	9)	7
172	5	3	3	4	2	2	150.06525	150.06530(	3)	-5
173	10	3	8	9	3	7	153.49498	153.49504(	7)	-6
174	5	3	2	4	2	3	155.70479	155.70470(	3)	9
175	10	4	7	9	4	6	155.82263	155.82279(	10)	-16
176	10	4	6	9	4	5	158.37939	158.37928(	10)	11
177	9	6	3	9	5	4	158.94494	158.94480(	12)	14
178	9	6	4	9	5	5	159.05082	159.05078(	12)	4
179	8	6	2	8	5	3	159.87268	159.87261(	5)	7
180	8	6	3	8	5	4	159.90404	159.90391(	5)	13
181	7	6	1	7	5	2	160.57638	160.57617(	6)	21
182	7	6	2	7	5	3	160.58359	160.58358(	6)	1
183	6	6	0	6	5	1	161.11000	161.10924(	9)	76
184	6	6	1	6	5	2	161.11000	161.11050(	9)	-50
185	6	3	4	5	2	3	161.61666	161.61672(	3)	-6
186	10	2	8	9	2	7	162.19132	162.19146(	10)	-14
187	10	3	7	9	3	6	164.42831	164.42846(	7)	-15
188	4	4	1	3	3	0	167.19729	167.19744(	5)	-15
189	4	4	0	3	3	1	167.22772	167.22782(	5)	-10
190	7	3	5	6	2	4	171.31278	171.31261(	3)	17
191	6	3	3	5	2	4	174.34094	174.34094(	3)	0
192	6	2	4	5	1	5	176.59256	176.59259(	3)	-3
193	8	3	6	7	2	5	179.32474	179.32445(	4)	29
194	5	4	2	4	3	1	182.38331	182.38343(	3)	-12
195	5	4	1	4	3	2	182.59746	182.59740(	3)	6
196	9	3	7	8	2	6	185.99811	185.99807(	6)	4
197	9	7	2	9	6	3	186.23470	186.23467(	23)	3*
198	9	7	3	9	6	4	186.23470	186.23751(	23)	-281*
199	8	7	1	8	6	2	186.97030	186.96977(	11)	53
200	8	7	2	8	6	3	186.97030	186.97035(	11)	-5
201	7	7	0	7	6	1	187.56955	187.56983(	10)	-28
202	7	7	1	7	6	2	187.56955	187.56992(	10)	-37
203	7	3	4	6	2	5	195.42933	195.42914(	3)	19
204	6	4	3	5	3	2	197.18732	197.18740(	3)	-8
205	6	4	2	5	3	3	198.04128	198.04137(	3)	-9
206	7	2	5	6	1	6	210.39134	210.39145(	3)	-11
207	5	5	1	4	4	0	211.04392	211.04293(	5)	99*
208	5	5	0	4	4	1	211.04392	211.04496(	5)	-104*
209	7	4	4	6	3	3	211.23482	211.23466(	3)	16
210	9	8	1	9	7	2	212.23682	212.23687(	12)	-5
211	9	8	2	9	7	3	212.23682	212.23691(	13)	-9
212	8	8	0	8	7	1	212.93735	212.93727(	13)	8
213	8	8	1	8	7	2	212.93735	212.93728(	12)	7
214	7	4	3	6	3	4	213.75764	213.75755(	3)	9
215	8	3	5	7	2	6	219.79475	219.79485(	4)	-10

[a] See footnote to Table 2 for explanation of column headings. Lines given in megahertz have been taken from Ref. 14.

Table 6. Pure Rotational Transitions of $D_2{}^{16}O$[a]

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
1	3	1	3	2	2	0	10919.410	10919.358(	38)	52
2	4	4	1	5	3	2	10947.180	10947.115(	40)	64
3	8	7	2	9	6	3	30182.490	30182.466(	47)	24
4	8	7	1	9	6	4	30778.500	30778.458(	44)	42
5	4	2	3	3	3	0	43414.560	43414.503(	37)	57
6	4	4	0	5	3	3	55482.320	55482.359(	39)	-39
7	8	5	4	7	6	1	70240.630	70240.514(	39)	115
8	8	5	3	7	6	2	74471.690	74471.567(	41)	123
9	6	1	6	5	2	3	93350.060	93350.120(	50)	-59
10	9	8	2	10	7	3	103076.400	103076.330(	61)	69
11	9	8	1	10	7	4	103152.890	103152.817(	34)	73
12	6	2	4	7	1	7	104875.710	104875.824(	54)	-113
13	11	2	10	10	3	7	120183.280	120183.292(	75)	-11
14	10	9	2	11	8	3	145134.800	145134.723(	76)	76
15	10	9	1	11	8	4	145143.820	145143.959(	25)	-138
16	4	1	4	3	2	1	151710.400	151710.375(	37)	24
17	5	5	1	6	4	2	180171.220	180170.994(	35)	225
18	5	1	5	4	2	2	181833.020	181833.171(	39)	-151
19	5	5	0	6	4	3	187633.100	187633.084(	35)	15
20	7	4	4	6	5	1	192519.440	192519.487(	33)	-47

(continued overleaf)

Table 6. Continued

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
21	12	8	5	11	9	2	215689.010	215689.046(	84)	-35
22	12	8	4	11	9	3	215731.730	215731.757(	107)	-26
23	7	4	3	6	5	2	218442.500	218442.449(	38)	50
24	4	2	2	3	3	1	227010.500	227010.506(	37)	-6
25	11	3	8	12	2	11	254484.270	254484.273(	79)	-3
26	11	7	5	10	8	2	265060.070	265059.910(	59)	159
27	11	7	4	10	8	3	265381.300	265381.224(	28)	76
28	6	6	1	7	5	2	307107.530	307107.585(	41)	-54
29	6	3	4	5	4	1	307743.140	307743.143(	37)	-3
30	6	6	0	7	5	3	308133.650	308133.468(	41)	181
31	1	1	0	1	0	1	316799.810	316799.862(	19)	-51
32	5	2	4	4	3	1	339035.260	339035.166(	41)	93
33	10	6	5	9	7	2	345039.170	345039.290(	49)	-119
34	10	6	4	9	7	3	347278.230	347278.350(	55)	-119
35	7	2	5	8	1	8	393332.820	393332.795(	75)	24
36	7	7	1	8	6	2	403251.620	403251.778(	45)	-158
37	7	7	0	8	6	3	403377.360	403377.484(	47)	-124
38	2	1	1	2	0	2	403561.820	403561.993(	23)	-172
39	10	2	9	9	3	6	428706.470	428706.433(	61)	37
40	6	3	3	5	4	2	430949.260	430949.206(	47)	54
41	9	5	5	8	6	2	452326.480	452326.547(	55)	-66
42	3	1	2	2	2	1	458531.450	458531.329(	38)	121
43	9	5	4	8	6	3	466238.740	466238.727(	56)	13
44	2	0	2	1	1	1	468246.570	468246.526(	29)	43
45	8	8	1	9	7	2	469619.170	469619.135(	42)	34
46	8	8	0	9	7	3	469633.530	469633 477(	54)	52
47	3	1	2	3	0	3	555330.360	555330.291(	30)	68
48	8	4	5	7	5	2	571220.050	571219.997(	52)	53
49	6	2	5	5	3	2	572114.910	572114.947(	43)	-36
50	1	1	1	0	0	0	607349.600	607349.442(	33)	157
51	9	2	8	8	3	5	642615.950	642615.987(	54)	-36
52	8	4	4	7	5	3	643247.420	643247.336(	64)	84
53	7	3	5	6	4	2	649560.460	649560.336(	53)	123
54	4	2	2	4	1	3	692243.600	692243.529(	37)	70
55	3	2	1	3	1	2	697922.720	697922.772(	31)	-52
56	7	2	6	6	3	3	714087.250	714087.359(	47)	-108
57	5	2	3	4	3	2	722669.850	722669.943(	48)	-93
58	8	2	7	7	3	4	740648.840	740648.829(	52)	11
59	2	2	0	2	1	1	24.80270	24.80261(	0)	9
60	2	2	0	2	1	1	743563.430	743563.563(	34)	-133
61	5	2	3	5	1	4	25.05420	25.05435(	0)	-15
62	5	2	3	5	1	4	751110.670	751110.519(	42)	151
63	4	1	3	4	0	4	26.10042	26.10042(	0)	0
64	4	1	3	4	0	4	782470.880	782471.027(	37)	-146
65	3	0	3	2	1	2	28.37790	28.37822(	0)	-32
66	3	0	3	2	1	2	850757.720	850757.629(	33)	90
67	6	2	4	6	1	5	29.70054	29.70042(	0)	12
68	6	2	4	6	1	5	890396.080	890396.238(	53)	-157
69	2	1	2	1	0	1	29.95218	29.95229(	0)	-11
70	2	1	2	1	0	1	897947.110	897947.160(	44)	-49
71	4	1	3	3	2	2	31.05305	31.05290(	0)	15
72	4	1	3	3	2	2	930942.470	930942.628(	41)	-157
73	2	2	1	2	1	2	947556.570	947556.592(	34)	-21
74	2	2	1	2	1	2	31.60719	31.60709(	0)	10
75	7	3	4	7	2	5	34.79779	34.79783(	0)	-4
76	3	2	2	3	1	3	35.52770	35.52781(	0)	-11
77	3	2	2	3	1	3	1065097.240	1065097.070(	37)	170
78	8	3	5	8	2	6	35.83265	35.83280(	0)	-15
79	5	1	4	5	0	5	35.89911	35.89906(	0)	5
80	6	3	3	6	2	4	36.18162	36.18163(	0)	-1
81	7	2	5	7	1	6	37.21541	37.21557(	0)	-16
82	3	1	3	2	0	2	38.62819	38.62822(	0)	-3
83	5	3	2	5	2	3	39.01826	39.01817(	0)	9
84	9	3	6	9	2	7	39.85558	39.85568(	1)	-10
85	4	0	4	3	1	3	40.48027	40.48029(	0)	-2
86	3	3	0	3	2	1	44.41111	44.41131(	0)	-20
87	11	4	7	11	3	8	46.20579	46.20536(	3)	43*
88	10	4	6	10	3	7	46.23044	46.23061(	2)	-17
89	3	3	1	3	2	2	46.57127	46.57141(	0)	-14
90	5	1	4	4	2	3	46.82643	46.82659(	0)	-16
91	4	1	4	3	0	3	46.86455	46.86454(	0)	1
92	10	3	7	10	2	8	47.01726	47.01718(	1)	8
93	6	1	5	6	0	6	47.04303	47.04295(	0)	8
94	8	2	6	8	1	7	47.22563	47.22581(	0)	-18
95	5	2	4	5	1	5	47.34227	47.34251(	0)	-24
96	9	4	5	9	3	6	48.75267	48.75287(	2)	-20
97	12	4	8	12	3	9	49.31784	49.31783(	8)	1
98	5	3	3	5	2	4	49.94491	49.94497(	0)	-6
99	2	2	1	1	1	0	50.99198	50.99207(	0)	-9
100	5	0	5	4	1	4	51.72650	51.72648(	0)	2
101	8	4	4	8	3	5	52.70508	52.70518(	1)	-10
102	6	3	4	6	2	5	53.29501	53.29497(	0)	4
103	2	2	0	1	1	1	53.88298	53.88301(	0)	-3
104	10	4	6	9	5	5	54.24217	54.24225(	2)	-8
105	6	2	5	6	1	6	54.98818	54.98804(	0)	14
106	5	1	5	4	0	4	55.25639	55.25648(	0)	-9
107	7	4	3	7	3	4	56.82022	56.82020(	0)	2
108	11	3	8	11	2	9	56.93608	56.93608(	3)	0
109	7	3	5	7	2	6	57.93250	57.93257(	0)	-7
110	7	1	6	7	0	7	58.55179	58.55181(	0)	-2
111	9	2	7	9	1	8	58.80755	58.80742(	1)	13
112	7	2	5	6	3	4	59.87374	59.87361(	0)	13
113	6	4	2	6	3	3	60.08505	60.08496(	0)	9
114	3	2	2	2	1	1	60.69473	60.69465(	0)	8
115	12	5	7	12	4	8	61.37760	61.37776(	6)	-16
116	6	1	5	5	2	4	61.97916	61.97921(	0)	-5
117	5	4	1	5	3	2	62.11344	62.11346(	0)	-2
118	6	0	6	5	1	5	62.27884	62.27877(	0)	7
119	4	4	0	4	3	1	63.10466	63.10466(	0)	0
120	4	4	1	4	3	2	63.48922	63.48900(	0)	22
121	7	2	6	7	1	7	63.49946	63.49930(	0)	16
122	5	4	2	5	3	3	63.54141	63.54137(	0)	4
123	8	3	6	8	2	7	63.84338	63.84324(	0)	14
124	6	4	3	6	3	4	63.89473	63.89460(	0)	13
125	6	1	6	5	0	5	64.06730	64.06724(	0)	6
126	7	4	4	7	3	5	64.82295	64.82292(	0)	3
127	11	5	6	11	4	7	66.27280	66.27267(	3)	13
128	8	4	5	8	3	6	66.60955	66.60960(	1)	-5
129	9	3	6	8	4	5	68.19907	68.19904(	2)	3
130	12	3	9	12	2	10	68.70044	68.70033(	6)	11
131	4	2	3	3	1	2	69.13968	69.13966(	0)	2
132	8	1	7	8	0	8	69.80436	69.80431(	0)	5
133	3	2	1	2	1	2	70.18238	70.18224(	0)	14
134	10	2	8	10	1	9	70.88322	70.88312(	2)	10
135	9	3	7	9	2	8	70.89948	70.89956(	1)	-8
136	10	5	5	10	4	6	71.16029	71.16023(	2)	6
137	8	2	7	8	1	8	72.62360	72.62339(	0)	21
138	7	1	7	6	0	6	73.24515	73.24509(	0)	6
139	10	4	7	10	3	8	73.58553	73.58561(	2)	-8
140	9	5	4	9	4	5	75.09850	75.09851(	1)	-1
141	7	1	6	6	2	5	75.95302	75.95301(	0)	1
142	5	2	4	4	1	3	76.49858	76.49857(	0)	1
143	8	5	3	8	4	4	77.74887	77.74888(	1)	-1
144	8	2	6	7	3	5	77.85007	77.85014(	1)	-7
145	10	3	8	10	2	9	78.89351	78.89333(	1)	18
146	11	4	8	11	3	9	78.92712	78.92699(	2)	13
147	7	5	2	7	4	3	79.28408	79.28418(	1)	-10
148	8	5	4	8	4	5	79.97684	79.97677(	1)	7
149	6	5	1	6	4	2	80.06836	80.06817(	0)	19
150	7	5	3	7	4	4	80.10796	80.10877(	1)	-81*
151	6	5	2	6	4	3	80.31062	80.31059(	0)	3
152	5	5	0	5	4	1	80.41857	80.41858(	0)	-1
153	5	5	1	5	4	2	80.46990	80.46974(	0)	16
154	9	1	8	9	0	9	80.62930	80.62926(	1)	4
155	10	5	6	10	4	7	80.74849	80.74859(	2)	-10
156	9	2	8	9	1	9	82.13688	82.13662(	1)	26
157	11	5	7	11	4	8	82.16589	82.16596(	3)	-7
158	8	0	8	7	1	7	82.25220	82.25189(	0)	31*
159	3	3	1	2	2	0	82.46362	82.46345(	0)	17
160	8	1	8	7	0	7	82.64725	82.64721(	0)	4
161	11	2	9	11	1	10	82.68325	82.68306(	3)	19
162	3	3	0	2	2	1	82.98656	82.98647(	0)	9
163	6	2	5	5	1	4	83.15638	83.15622(	0)	16
164	12	5	8	12	4	9	84.58365	84.58366(	6)	-1
165	12	4	9	12	3	10	85.41655	85.41636(	4)	19
166	11	3	9	11	2	10	87.58214	87.58216(	3)	-2
167	10	3	7	9	4	6	88.11822	88.11831(	4)	-9
168	8	1	7	7	2	6	88.55682	88.55690(	0)	-8
169	4	2	2	3	1	3	89.67162	89.67148(	0)	14
170	7	2	6	6	1	5	89.70151	89.70144(	0)	7
171	12	6	6	12	5	7	89.73313	89.73284(	10)	29
172	10	1	9	10	0	10	91.09680	91.09668(	3)	12
173	10	2	9	10	1	10	91.86934	91.86936(	3)	-2
174	9	0	9	8	1	8	91.98281	91.98291(	1)	-10
175	9	1	9	8	0	8	92.16165	92.16166(	1)	-1
176	11	6	5	11	5	6	92.76328	92.76355(	5)	-26
177	4	3	2	3	2	1	93.63486	93.63473(	0)	13
178	12	4	8	11	5	7	93.79642	93.79630(	11)	12
179	12	2	10	12	1	11	93.91315	93.91320(	7)	-5
180	10	6	4	10	5	5	94.66951	94.66935(	2)	16
181	9	2	7	8	3	6	94.95292	94.95296(	2)	-4
182	9	6	4	9	5	5	96.21955	96.21931(	1)	24
183	4	3	1	3	2	2	96.24255	96.24248(	0)	7
184	8	6	2	8	5	3	96.38502	96.38527(	1)	-25
185	8	6	3	8	5	4	96.52169	96.52159(	1)	10
186	7	6	1	7	5	2	96.68746	96.68765(	1)	-19

Table 6. Continued

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
187	8	2	7	7	1	6	96.71923	96.71879(	0)	44
188	6	6	0	6	5	1	96.80883	96.80876(	1)	7
189	9	1	8	8	2	7	99.98859	99.98878(	1)	-19
190	10	0	10	9	1	9	101.64313	101.64324(	2)	-11
191	11	2	10	11	1	11	101.70819	101.70825(	7)	-6
192	5	3	3	4	2	2	103.35240	103.35278(	0)	-38
193	9	2	8	8	1	7	104.49393	104.49398(	1)	-5
194	10	2	8	9	3	7	110.58676	110.58686(	3)	-10
195	10	1	9	9	2	8	110.60339	110.60329(	2)	10
196	5	3	2	4	2	3	110.89917	110.89910(	0)	7
197	11	0	11	10	1	10	111.26199	111.26213(	4)	-14
198	11	1	11	10	0	10	111.29755	111.29761(	4)	-6
199	6	3	4	5	2	3	111.39682	111.39683(	0)	-1
200	10	7	3	10	6	4	112.01726	112.01733(	5)	-7
201	7	7	0	7	6	1	112.31998	112.31979(	1)	19*
202	7	7	1	7	6	2	112.31998	112.32041(	1)	-43*
203	8	7	1	8	6	2	112.33390	112.33396(	1)	-6
204	5	2	3	4	1	4	112.67989	112.67989(	0)	0
205	4	4	1	3	3	0	112.71221	112.71241(	0)	-20
206	4	4	0	3	3	1	112.77573	112.77573(	0)	0
207	10	2	9	9	1	8	112.96324	112.96320(	1)	4
208	7	3	5	6	2	4	117.93369	117.93359(	1)	10
209	11	1	10	10	2	9	120.71526	120.71551(	2)	-25
210	12	0	12	11	1	11	120.85248	120.85245(	9)	3
211	12	1	12	11	0	11	120.86825	120.86820(	9)	5
212	8	3	6	7	2	5	123.34633	123.34646(	1)	-13
213	11	2	9	10	3	8	124.50502	124.50524(	4)	-22
214	5	4	2	4	3	1	124.79534	124.79534(	0)	0
215	5	4	1	4	3	2	125.23765	125.23730(	0)	35*
216	6	3	3	5	2	4	127.86139	127.86126(	0)	13
217	9	3	7	8	2	6	128.16759	128.16772(	1)	-13
218	12	1	11	11	2	10	130.54016	130.54005(	3)	11
219	12	2	11	11	1	10	131.13050	131.13045(	3)	5
220	10	3	8	9	2	7	133.04907	133.04912(	2)	-5
221	6	4	3	5	3	2	136.27313	136.27327(	1)	-14
222	12	2	10	11	3	9	136.87107	136.87109(	7)	-2
223	6	4	2	5	3	3	138.00127	138.00125(	0)	2
224	11	3	9	10	2	8	138.60808	138.60823(	3)	-15
225	6	2	4	5	1	5	139.02206	139.02214(	0)	-8
226	5	5	1	4	4	0	142.16052	142.16042(	0)	10
227	5	5	0	4	4	1	142.16676	142.16688(	0)	-12
228	12	3	10	11	2	9	145.18205	145.18218(	6)	-13
229	7	4	4	6	3	3	146.57492	146.57489(	1)	3
230	7	3	4	6	2	5	147.96643	147.96642(	0)	1
231	7	4	3	6	3	4	151.49213	151.49165(	1)	48*
232	6	5	2	5	4	1	154.47058	154.47040(	1)	18
233	6	5	1	5	4	2	154.52814	154.52805(	1)	9
234	8	4	5	7	3	4	155.15820	155.15822(	1)	-2
235	9	4	6	8	3	5	161.82073	161.82065(	2)	8
236	8	4	4	7	3	5	166.38822	166.38812(	1)	10
237	7	5	3	6	4	2	166.59880	166.59870(	1)	10
238	10	4	7	9	3	6	166.77913	166.77905(	3)	8
239	7	5	2	6	4	3	166.88129	166.88122(	1)	7
240	7	2	5	6	1	6	168.15713	168.15662(	1)	51
241	11	4	8	10	3	7	170.51823	170.51803(	4)	20
242	6	6	1	5	5	0	170.86696	170.86646(	1)	50*
243	6	6	0	5	5	1	170.86696	170.86707(	1)	-11*
244	8	3	5	7	2	6	171.61544	171.61551(	1)	-7
245	8	5	4	7	4	3	178.31491	178.31480(	2)	11
246	8	5	3	7	4	4	179.31418	179.31407(	2)	11
247	7	6	2	6	5	1	183.25198	183.25173(	2)	25
248	7	6	1	6	5	2	183.25849	183.25828(	2)	21
249	9	4	5	8	3	6	183.56156	183.56151(	2)	5
250	9	5	5	8	4	4	189.22209	189.22214(	2)	-5
251	9	5	4	8	4	5	192.05058	192.05041(	2)	17
252	8	6	3	7	5	2	195.55216	195.55221(	2)	-5
253	8	6	2	7	5	3	195.59066	195.59057(	2)	9
254	9	3	6	8	2	7	198.65173	198.65187(	2)	-14
255	7	7	1	6	6	0	198.76334	198.76338(	2)	-4*
256	7	7	0	6	6	1	198.76334	198.76343(	2)	-9*
257	10	5	6	9	4	5	198.77471	198.77477(	3)	-6
258	8	2	6	7	1	7	199.28122	199.28201(	1)	-79*
259	10	4	6	9	3	7	203.83453	203.83465(	3)	-12
260	10	5	5	9	4	6	205.50915	205.50915(	3)	0
261	9	6	4	8	5	3	207.69270	207.69258(	3)	12
262	9	6	3	8	5	4	207.85281	207.85290(	3)	-9
263	8	7	1	7	6	2	211.20327	211.20334(	3)	-7
264	10	6	5	9	5	4	219.53758	219.53775(	4)	-17
265	10	6	4	9	5	5	220.07166	220.07183(	4)	-17

[a] See footnote to Table 2 for explanation of column headings. Lines given in megahertz have been taken from Ref. 9.

Table 7. Pure Rotational Transitions of $D_2{}^{18}O$[a]

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
1	5	3	3	4	4	0	8898.450	8898.462(	39)	-11
2	10	7	4	9	8	1	26281.930	26281.940(	52)	-9
3	10	7	3	9	8	2	26386.880	26386.870(	55)	9
4	3	1	3	2	2	0	32581.330	32581.323(	40)	6
5	11	2	10	10	3	7	50052.170	50052.170(	45)	0
6	5	3	2	4	4	1	58514.580	58514.565(	39)	15
7	5	5	1	6	4	2	95762.680	95762.595(	33)	84
8	5	5	0	6	4	3	104538.600	104538.681(	32)	-81
9	6	2	4	7	1	7	127557.380	127557.379(	44)	1
10	4	1	4	3	2	1	165718.230	165718.237(	34)	-6
11	8	5	3	7	6	2	175676.750	175676.752(	45)	-1
12	5	1	5	4	2	2	184774.740	184774.733(	40)	6
13	6	6	1	7	5	2	207185.020	207184.996(	32)	23
14	6	6	0	7	5	3	208456.350	208456.376(	28)	-26
15	7	4	4	6	5	1	275475.390	275475.412(	43)	-22
16	4	2	2	3	3	1	279987.590	279987.589(	43)	0
17	7	7	1	8	6	2	288294.200	288294.196(	26)	3
18	7	7	0	8	6	3	288458.260	288458.263(	38)	-3
19	7	4	3	6	5	2	305827.110	305827.085(	42)	24
20	1	1	0	1	0	1	307480.600	307480.595(	43)	5
21	5	2	4	4	3	1	376411.110	376411.119(	43)	-8
22	6	3	3	6	2	4	34.51781	34.51801(	2)	-20
23	3	2	2	3	1	3	34.66893	34.66895(	0)	-2
24	8	3	5	8	2	6	35.09321	35.09351(	3)	-30
25	5	1	4	5	0	5	36.10902	36.10897(	0)	5
26	5	3	2	5	2	3	37.19149	37.19173(	1)	-24
27	3	1	3	2	0	2	38.10143	38.10165(	0)	-22
28	4	0	4	3	1	3	40.46399	40.46405(	0)	-6
29	3	3	0	3	2	1	42.67775	42.67766(	1)	9
30	3	3	1	3	2	2	44.96647	44.96646(	1)	1
31	4	1	4	3	0	3	46.29193	46.29210(	1)	-17
32	5	2	4	5	1	5	46.67326	46.67323(	1)	3
33	6	1	5	6	0	6	47.27506	47.27521(	1)	-15
34	5	1	4	4	2	3	47.61691	47.61696(	0)	-5
35	8	2	6	8	1	7	47.88793	47.88811(	2)	-18
36	5	3	3	5	2	4	48.52262	48.52257(	1)	5
37	2	2	1	1	1	0	49.92209	49.92260(	0)	-51
38	5	0	5	4	1	4	51.53860	51.53851(	1)	9
39	6	3	4	6	2	5	52.03150	52.03151(	1)	-1
40	2	2	0	1	1	1	52.87984	52.87972(	0)	12
41	7	4	3	7	3	4	54.06711	54.06727(	2)	-16
42	6	2	5	6	1	6	54.40902	54.40901(	1)	1
43	5	1	5	4	0	4	54.67418	54.67417(	1)	1
44	7	3	5	7	2	6	56.85982	56.85987(	1)	-5
45	6	4	2	6	3	3	57.50130	57.50142(	1)	-12
46	7	1	6	7	0	7	58.68009	58.68019(	1)	-10
47	3	2	2	2	1	1	59.55396	59.55403(	1)	-7
48	5	4	1	5	3	2	59.69390	59.69377(	1)	13
49	4	4	0	4	3	1	60.78159	60.78147(	1)	12
50	4	4	1	4	3	2	61.21133	61.21132(	1)	1
51	5	4	2	5	3	3	61.28077	61.28083(	1)	-6
52	6	4	3	6	3	4	61.69055	61.69073(	1)	-18
53	6	0	6	5	1	5	61.93876	61.93861(	1)	15
54	6	1	5	5	2	4	62.54061	62.54059(	1)	2
55	7	4	4	7	3	5	62.73380	62.73403(	2)	-23
56	8	3	6	8	2	7	62.97156	62.97149(	2)	7
57	7	2	6	7	1	7	62.98549	62.98540(	2)	9
58	6	1	6	5	0	5	63.48342	63.48323(	1)	19
59	8	4	5	8	3	6	64.70280	64.70289(	2)	-9
60	4	2	3	3	1	2	67.90888	67.90899(	1)	-11
61	3	2	1	2	1	2	69.28402	69.28404(	1)	-2
62	8	1	7	8	0	8	69.76390	69.76384(	3)	6
63	9	3	7	9	2	8	70.21351	70.21366(	3)	-15
64	8	2	7	8	1	8	72.14102	72.14075(	3)	26
65	7	1	7	6	0	6	72.64386	72.64385(	1)	1
66	8	5	3	8	4	4	74.51330	74.51335(	3)	-5

(continued overleaf)

Table 7. Continued

#	J	KA	KC	J	KA	KC	OBS	CALC	SDC	O-C
67	5	2	4	4	1	3	75.17768	75.17768(	2)	0
68	7	1	6	6	2	5	76.19608	76.19604(	2)	4
69	7	5	2	7	4	3	76.23246	76.23247(	1)	-1
70	6	5	1	6	4	2	77.11605	77.11613(	1)	-8
71	6	5	2	6	4	3	77.40075	77.40081(	1)	-6
72	5	5	1	5	4	2	77.57454	77.57442(	1)	12
73	8	2	6	7	3	5	79.49264	79.49264(	6)	0
74	9	1	8	9	0	9	80.41853	80.41816(	5)	37
75	3	3	1	2	2	0	80.72230	80.72221(	2)	9
76	3	3	0	2	2	1	81.28306	81.28285(	2)	21
77	9	2	8	9	1	9	81.65149	81.65147(	5)	2
78	8	0	8	7	1	7	81.68605	81.68595(	2)	10
79	6	2	5	5	1	4	81.78336	81.78327(	2)	9
80	8	1	8	7	0	7	82.00934	82.00924(	2)	10
81	7	2	6	6	1	5	88.35408	88.35404(	2)	4
82	8	1	7	7	2	6	88.46434	88.46439(	3)	-5
83	4	2	2	3	1	3	88.97487	88.97479(	2)	8
84	10	1	9	10	0	10	90.73936	90.73960(	9)	-24*
85	10	6	4	10	5	5	90.86143	90.86134(	9)	9
86	9	0	9	8	1	8	91.33007	91.33027(	3)	-20
87	9	1	9	8	0	8	91.47269	91.47266(	3)	3
88	4	3	2	3	2	1	91.79678	91.79672(	2)	6
89	9	6	4	9	5	5	92.67677	92.67668(	5)	9
90	8	6	2	8	5	3	92.83478	92.83505(	2)	-26
91	7	6	1	7	5	2	93.18809	93.18795(	2)	14
92	6	6	0	6	5	1	93.33745	93.33741(	1)	4
93	12	2	10	12	1	11	94.10674	94.10676(	14)	-2
94	4	3	1	3	2	2	94.58676	94.58677(	2)	-1
95	8	2	7	7	1	6	95.46985	95.46980(	2)	5
96	9	1	8	8	2	7	99.60840	99.60767(	4)	73
97	10	0	10	9	1	9	100.91250	100.91258(	5)	-8
98	11	2	10	11	1	11	101.14339	101.14364(	13)	-25
99	5	3	3	4	2	2	101.35918	101.35922(	3)	-4
100	9	2	8	8	1	7	103.36007	103.36030(	3)	-23
101	6	3	4	5	2	3	109.22159	109.22187(	3)	-28
102	5	3	2	4	2	3	109.40162	109.40160(	3)	2
103	10	1	9	9	2	8	110.00048	110.00071(	4)	-23
104	4	4	1	3	3	0	110.33050	110.33039(	3)	11
105	4	4	0	3	3	1	110.40175	110.40178(	3)	-3
106	11	0	11	10	1	10	110.45822	110.45821(	5)	1
107	11	1	11	10	0	10	110.48504	110.48509(	6)	-5
108	10	2	8	9	3	7	111.34388	111.34413(	8)	-25
109	10	2	9	9	1	8	111.91050	111.91058(	4)	-8
110	5	2	3	4	1	4	112.24026	112.24038(	2)	-12
111	7	3	5	6	2	4	115.59049	115.59041(	3)	8
112	11	1	10	10	2	9	119.94922	119.94926(	4)	-4
113	12	0	12	11	1	11	119.97784	119.97783(	11)	1
114	12	1	12	11	0	11	119.98945	119.98948(	11)	-3
115	5	4	2	4	3	1	122.35920	122.35912(	3)	8
116	5	4	1	4	3	2	122.85701	122.85693(	3)	8
117	9	3	7	8	2	6	125.68573	125.68584(	5)	-11
118	6	3	3	5	2	4	126.68208	126.68210(	3)	-2
119	12	1	11	11	2	10	129.65056	129.65054(	8)	2
120	12	2	11	11	1	10	130.10329	130.10335(	8)	-6
121	10	3	8	9	2	7	130.68327	130.68282(	6)	45
122	6	4	3	5	3	2	133.72066	133.72087(	3)	-21
123	6	4	2	5	3	3	135.66094	135.66096(	3)	-2
124	11	3	9	10	2	8	136.47713	136.47700(	8)	13
125	12	2	10	11	3	9	136.61249	136.61236(	13)	13
126	6	2	4	5	1	5	138.83723	138.83732(	3)	-9
127	5	5	1	4	4	0	139.15208	139.15207(	3)	1
128	5	5	0	4	4	1	139.15971	139.15974(	3)	-3
129	12	3	10	11	2	9	143.31797	143.32259(	13)	-461*
130	7	4	4	6	3	3	143.80646	143.80642(	3)	4
131	7	3	4	6	2	5	147.25708	147.25708(	3)	0
132	7	4	3	6	3	4	149.29291	149.29284(	3)	7
133	6	5	2	5	4	1	151.42792	151.42791(	3)	1
134	6	5	1	5	4	2	151.49595	151.49626(	3)	-31
135	8	4	5	7	3	4	152.08383	152.08314(	3)	69
136	9	4	6	8	3	5	158.41552	158.41560(	4)	-8
137	10	4	7	9	3	6	163.09614	163.09621(	6)	-7
138	7	5	3	6	4	2	163.50012	163.50019(	3)	-7
139	7	5	2	6	4	3	163.83448	163.83458(	3)	-10
140	8	4	4	7	3	5	164.50524	164.50528(	2)	-4
141	11	4	8	10	3	7	166.66803	166.66818(	12)	-15
142	6	6	1	5	5	0	167.25896	167.25849(	3)	47
143	6	6	0	5	5	1	167.25896	167.25925(	3)	-29
144	8	3	5	7	2	6	171.44593	171.44601(	4)	-8
145	8	5	4	7	4	3	175.10601	175.10595(	3)	6
146	8	5	3	7	4	4	176.28459	176.28461(	3)	-2
147	7	6	2	6	5	1	179.61371	179.61353(	3)	18
148	7	6	1	6	5	2	179.62186	179.62171(	3)	15
149	9	4	5	8	3	6	182.22508	182.22507(	4)	1
150	9	5	5	8	4	4	185.79848	185.79847(	5)	1
151	9	5	4	8	4	5	189.11462	189.11446(	4)	16
152	8	6	3	7	5	2	191.87655	191.87667(	4)	-12
153	8	6	2	7	5	3	191.92461	191.92447(	4)	14
154	7	7	1	6	6	0	194.58754	194.58758(	4)	-4
155	7	7	0	6	6	1	194.58754	194.58765(	4)	-11
156	10	5	6	9	4	5	194.99061	194.99053(	8)	8
157	9	3	6	8	2	7	198.98874	198.98895(	6)	-21
158	8	2	6	7	1	7	199.33793	199.33790(	5)	3
159	10	5	5	9	4	6	202.81327	202.81326(	7)	1
160	10	4	6	9	3	7	203.25367	203.25356(	9)	11
161	9	6	4	8	5	3	203.96195	203.96180(	5)	15
162	9	6	3	8	5	4	204.16085	204.16120(	5)	-35
163	8	7	1	7	6	2	206.99739	206.99755(	5)	-16
164	10	6	5	9	5	4	215.71035	215.71058(	10)	-23
165	10	6	4	9	5	5	216.37288	216.37258(	10)	30

[a] See footnote to Table 2 for explanation of column headings. Lines given in megahertz have been taken from Ref. 16.

were lines with high J and K quantum-number assignments and which the limited Hamiltonian was unable to fit, together with a small number of lines that were discarded for reasons such as overlapping. Each excluded line has been indicated with an asterisk after the residual in the tables.

Both observed and calculated frequencies have been given in Tables 2–7. The reason for this is that for some lines the calculated wave number is better than the observation, while for others the reverse is true. Two examples should make this clear. Line 47 in Table 2 is observed at 59.86800 cm^{-1} and calculated at 59.86775, and the difference is 0.00025 cm^{-1}. The standard error on the calculation is low (0.00001 cm^{-1}) because both the J and the K quantum numbers are low and also because the transition falls close to the region where many transitions have been observed by microwave techniques. The calculated frequency is therefore probably the better one to use. Line 325, on the other hand, has been measured by Kauppinen *et al.*[10] at 504.38306 cm^{-1}, whereas the present calculation gives 504.37695 cm^{-1} and the difference is 0.00611 cm^{-1}. The high J and K values of this transition together with the high (but also optimistic) standard error of 0.00067 is clear indication that the observed wave number is the better one in this instance.

Calculated frequencies of some of the stronger $H_2{}^{16}O$ lines in the region from 350 to 500 cm^{-1} have been included in Table 2 despite the lack of observed lines in the region. For those transitions with low values of J and K the calculations can be regarded as interpolations and should therefore be quite reliable and may be of some use until better measurements become available.

The constants presented in Table 8 should not be used to calculate levels outside the range of J or K values observed here. For example, Table 6 shows that in D_2O J values up to 12 and K_a values up to 7 have been observed, and the transitions are reproduced by the constants with an rms error of about 0.00013 cm^{-1}. Papineau *et al.*[17] have observed a more extensive set of data and were able to fit levels with J as high as 19 and K_a as high as 9 with rms errors of about 0.001 cm^{-1}.

Table 8. Molecular Constants (in MHz) for the Ground States of Several Isotopic Species of H_2O[a]

	$H_2{}^{16}O$[b]	$H_2{}^{18}O$[b]	$HD^{16}O$		$HD^{18}O$[b]	$D_2{}^{16}O$		$D_2{}^{18}O$[b]
			b	c		b	c	
A	835839.672(96)	825367.320(82)	701931.489(28)	701931.633(69)	692830.94(43)	462278.840(30)	462279.013(59)	451891.829(78)
B	435346.828(34)	435353.81(22)	272912.857(19)	272912.747(35)	271588.36(13)	218038.256(17)	218038.411(34)	218045.261(48)
C	278140.312(50)	276950.50(10)	192054.973(16)	192055.118(31)	190693.03(16)	145257.985(17)	145257.995(24)	144201.762(35)
Δ_K	974.444(13)	950.799(54)	377.0599(39)	377.0759(100)	356.047(36)	277.4275(25)	277.4489(42)	265.4772(53)
Δ_{JK}	−173.3183(86)	−171.449(30)	34.2412(29)	34.2616(81)	38.291(18)	−45.7213(27)	−45.6957(54)	−44.752(13)
Δ_J	37.5917(15)	37.5559(37)	10.83940(34)	10.84139(120)	10.5898(23)	9.29153(47)	9.3038(12)	9.2696(17)
δ_K	39.603(20)	37.894(63)	63.2532(91)	63.1729(150)	63.294(35)	10.4282(57)	10.4649(62)	9.637(13)
δ_J	15.22164(50)	15.2298(24)	3.64877(12)	3.64967(30)	3.55108(67)	3.68980(29)	3.69396(45)	3.69578(50)
H_K	3.8620(16)	3.7057(71)	1.46574(36)	1.46785(90)	1.3890(54)	0.55446(23)	0.55778(30)	0.51832(54)
$H_{KJ} \times 10$	−5.203(16)	−5.016(54)	−2.7371(18)	−2.7376(50)	−2.635(22)	−0.7555(30)	−0.7481(28)	−0.702(10)
$H_{JK} \times 10^2$	−5.720(46)	−5.73(14)	7.615(13)	7.694(29)	7.500(38)	−0.738(12)	−0.477(19)	−0.838(40)
$H_J \times 10^2$	1.6515(27)	1.6536(37)	0.12204(29)	0.12600(140)	0.1118(16)	0.19803(83)	0.2434(21)	0.1999(29)
h_K	0.9305(29)	0.926(12)	0.5757(16)	0.5564(26)	0.5668(52)	0.11744(71)	0.11169(50)	0.1081(25)
$h_{JK} \times 10^2$	−2.623(28)	−2.75(10)	3.5109(93)	3.6256(150)	3.715(35)	−0.159(14)	0.265(17)	−0.208(12)
$h_J \times 10^3$	8.1761(85)	8.235(31)	0.6231(13)	0.6259(30)	0.5746(80)	0.9675(64)	1.0488(60)	0.9659(65)
$L_K \times 10^2$	−2.650(10)	−2.523(43)	−0.7947(24)	−0.7796(52)	−0.779(21)	−0.1886(13)	−0.15875(50)	−0.1860(49)
$L_{KKJ} \times 10^3$	7.73(12)	8.15(39)	3.177(29)	2.822(59)	3.07(10)	0.572(19)	–	0.646(73)
$L_{JK} \times 10^3$	−2.070(47)	−2.38(15)	−0.987(11)	−0.840(21)	−0.886(52)	−0.1297(72)	–	−0.140(24)
$L_{JJK} \times 10^5$	13.15(63)	15.2(26)	−5.36(17)	−6.80(37)	−5.36*	0.542(97)	−5.02(20)	0.86(24)
$L_J \times 10^6$	−11.07(21)	−11.07*	–	–	–	0.704(42)	−5.26(14)	−0.87(17)
$\ell_K \times 10^3$	−10.35(13)	−11.55(75)	−6.465(98)	−5.035(94)	−6.65(19)	−0.701(23)	−0.1511(34)	−0.702(92)
$\ell_{KJ} \times 10^4$	5.77(22)	6.3(13)	−3.85(17)	−5.05(26)	−5.13(41)	0.134(46)	−1.566(46)	0.266(90)
$\ell_{JK} \times 10^5$	1.60(31)	1.60*	−2.330(43)	−2.393(55)	−2.54(26)	−0.38(17)	−4.10(13)	−0.38*
$\ell_J \times 10^6$	−4.751(40)	−5.17(13)	–	–	–	−0.205(65)	−1.035(41)	−0.205*
$P_K \times 10^5$	17.92(20)	19.9(17)	4.060(95)	2.77(98)	4.38(34)	0.5228(35)	0.4724(51)	0.609(34)
$P_{KKJ} \times 10^6$	−65.2(21)	122.(24)	−14.8(15)	6.86(90)	−14.8*	−0.581(16)	–	−1.45(43)
$P_{KJ} \times 10^6$	26.3(11)	49.2(95)	0.99(70)	−7.49(73)	0.99*	–	–	–
$P_{JK} \times 10^5$	−0.134(28)	−0.134*	0.223(98)	0.254(24)	0.178(21)	–	–	–
$P_{JJK} \times 10^7$	−2.94(25)	−5.18(99)	−0.118(47)	–	0.35(26)	–	–	–
$P_J \times 10^8$	0.329(57)	0.329*	–	–	–	–	–	–
$p_K \times 10^5$	5.90(14)	8.7(14)	2.55(20)	–	2.723(93)	0.1102(44)	–	0.137(62)
$p_{KKJ} \times 10^5$	−0.960(68)	−1.14(21)	0.938(48)	1.105(86)	1.259(96)	–	–	
p_{KJ}	–	–	–	–	–	–	–	
$p_{KJJ} \times 10^7$	−1.50(16)	−1.50*	–	–	–	0.110(57)	–	0.110*
$p_J \times 10^9$	–	–	–	–	–	−0.37(23)	–	−0.47(29)
$T_K \times 10^8$	−56.70(86)	−49.1(48)	−9.40(23)	∓10.64(66)	−11.9(21)	−0.965(14)	−0.937(22)	−0.965*

[a] Estimated errors (1σ) are given in parentheses in units of the last figure quoted.
[b] Present measurements.
[c] Taken from Messer *et al.*[9]
* These constants without error estimates have been fixed at the value found for the corresponding constant of the ^{16}O species.

Table 9. Statistics from the Fits

	$H_2{}^{16}O$[a]	$H_2{}^{18}O$[a]	$HD^{16}O$ *a*	$HD^{16}O$ *b*	$HD^{18}O$[a]	$D_2{}^{16}O$ *a*	$D_2{}^{16}O$ *b*	$D_2{}^{18}O$[a]
No. of Parameters	34	29	30	28	27	30	24	26
J/K (max)	14/7	11/7	13/7	13/7	11/7	12/8	12/8	12/7
Rms MW (MHz)	0.142	0.088	0.080	0.112	0.150	0.096	0.128	0.028
Rms FIR (cm^{-1})	0.00015	0.00013	0.00016	–	0.00016	0.00013	–	0.00017
σ (MHz)	4.6	4.1	4.2	–	4.9	3.6	–	5.2

[a] Present work.
[b] Messer *et al.*[8]

When the present constants are used to predict high J, K lines observed by Papineau *et al.*, errors of up to a few hundredths of a wave-number unit are observed: thus $19_{2,18}$ observed at 2106.6300 is calculated at 2106.6084, and $14_{9,5}$ observed at 2000.2804 is calculated at 2000.2662.

CONCLUSION

Some 300 lines of $H_2{}^{16}O$ have been measured in the region from 20 to 350 cm^{-1} with an accuracy that for the most part is of the order of 0.0002 cm^{-1} (6 MHz). These lines should be of use in the calibration of high-resolution spectrometers working in the FIR region of the spectrum. In addition, about 900 lines of the less abundant species $H_2{}^{18}O$, $HD^{16}O$, $HD^{18}O$, $D_2{}^{16}O$, and $D_2{}^{18}O$ have also been measured with about the same accuracy, and many of these lines may also be useful for calibration purposes, particularly if spectra of deuterated samples are being studied.

Molecular rotation distortion constants for the ground vibrational states of all the species studied have been obtained. Despite the rather restricted range of J and K values included in the calculations, the results, particularly for the less abundant species, are probably the most precise that have been obtained so far.

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