Linelists of water vapor parameters from 500 to 8000 cm^{-1}

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tables: 8

ABSTRACT

The line parameters of water vapor are given in files that are available to users for the spectral region from 500 to 8000 cm^{-1}. The parameters include computed and observed values of line positions, strengths, self-broadened half-width coefficients, and air-broadened half-width and pressure-induced frequency-shift coefficients. The HITRAN formatted list also includes values of the exponent, η, which relates the air-broadened width coefficient at a temperature, T, to that at 296K. The isotopic species include $H_2{}^{16}O$, $H_2{}^{18}O$, $H_2{}^{17}O$, $HD^{16}O$, $HD^{18}O$, and $HD^{17}O$. This study culminates several years of research by this author.

1. INTRODUCTION

Water vapor is the most important molecule for which an accurate knowledge of the spectroscopic parameters is necessary for the analysis of atmospheric data. Due to the complexity of the quantum theory for H_2O and HDO, results derived from laboratory measurements of these molecules are essential to obtain the line parameters and for application to theory. This study presents measured and computed line parameter values for water vapor transitions located between 500 and 8000 cm^{-1} that are applicable for atmospheric monitoring. The listings are available to users and this report describes the content of the several listings.

Many studies have been reported on this subject and the relevant publications [1-178] are listed, in the references, in chronological order of publication date. References [179,180] are the previous reports in this edition of this journal. To aid the reader, Table 1 displays the reference numbers given in terms of the type of research and spectral coverage of the study. The spectral coverage displayed in the table for the references may be limited in some cases and for those, a study mainly covers the region shown in the table as well as part of one or more other region(s). The region listed in the table as “higher” pertains to studies covering the spectral region above

8000 cm^{-1}. These studies were included in the references because part of their research reported parameters that are related to the lower spectral region. One example is energy levels of upper rotation-vibration states derived from measured transitions originating from the ground state and these upper states levels are the same as those involved in hot band transitions in the 1.4μm region. Reports labeled in the table as line position studies may include experimental and/or theoretical results of energy level values. Other reports given in the table for the region above 8000 cm^{-1} involve pressure-broadening studies. The pressure-broadening parameters obtained in those studies relate to the parameters (self- and air-broadened half-width coefficients) measured in the lower spectral regions since these parameters are slightly influenced by vibration.

2. PARAMETER LISTINGS

Two related formats are used to list the line parameter values. One list is labeled SISAM.H2O which gives computed as well as experimental values of line positions and strengths. The listing includes rotational quantum assignments and the associated band with band notation showing the upper and lower states in the $\nu_1\nu_2\nu_3$ nomenclature. Other entries include broadening parameters: smoothed values of self- and air-broadened half-width coefficients and air-broadened pressure-induced frequency shift coefficients. The other listing is given in the HITRAN [177] format including values of the exponent, η. η is defined in the expression:

$$b^o(T) = b^o(T^o)[T^o/T]^\eta , \quad (1)$$

where $b^o(T)$ and $b^o(T^o)$ are pressure broadened half-width coefficients for a given transition at sample temperature of T and T^o, respectively.

Table 2 outlines the frequency and strength information given in the SISAM.H2O compilation. The table gives the molecule (H_2O or HDO) and oxygen isotopic species, band, number of lines, frequency extent and minimum and maximum strengths and maximum J value for all of the assigned transitions. Line strength values are given in cm^{-2}/atm. at 296K. Several bands given are not included in the present HITRAN compilation, HITRAN2000 [177], and are denoted in the table by an asterisk placed between the molecule and isotopic species entries. Table 3 gives information of the measured H_2O and HDO broadening parameters. The air- and self-broadened half-width measurements above 4300 cm^{-1} are discussed in the previous report [180]. The smoothed values of the broadening parameters given in SISAM.H2O and the HITRAN formatted listings were derived from the measured values as described in the previous report [180].

The computed and measured values given in SISAM.H2O were mainly derived in previous studies by this author [84,90,93,94,95,105,106,107,122,123,135,141,142143,146,179,180] along with co-authors [59,63,134,171]. The early $HD^{16}O$ studies [59,63] were reanalyzed using more recent data including oxygen-enriched-18 spectra covering the 2450 to 4435 cm^{-1} for the (100)-(000), (020)-(000), (001)-(000), (110)-(000) and (030)-(000) bands with inclusions of the (011)-(010) band and the $HD^{18}O$ bands: (100)-(000) and (001)-(000). The line strengths of the $HD^{16}O$ bands were fitted to a quantum model that included perturbation theory for the (100)-(000) and (020) bands and the (110)-(000) and (030)-(000) bands using the technique presented for the hot band pair: (020)-(010), (100)-(010) [141]. The $HD^{18}O$ analysis involved quantum assignments, line position measurements and determination of rotational energy levels. The $HD^{18}O$ study covered more bands than reported in the line parameter listings and the energy level values for these upper states are given in Table 4. The values were derived from the measured transition frequencies and the ground state energy levels given in ref. [141]. The results obtained in this manner were weighted and average for each level. The highest weight was given for an observed, unblended transition of moderate or strong intensity (not saturated). The uncertainties, un, given in the table were determined from the averaging program.

Table 5 shows a small portion of the SISAM.H2O listing. The format is similar in some ways to that of the HITRAN format. One of the differences is the molecule and isotopic species codes for HDO. As shown in the table the molecule code for HDO is 49 with the same codes for the oxygen isotopic species. Another difference is the band notation. The table labels the bands with upper and lower states given in the usual $\nu_1\nu_2\nu_3$ fashion whereas HITRAN gives codes for the upper and lower states. The line strengths are given in cm^{-2}/atm. at 296K whereas HITRAN list the strengths in $mol.cm^{-2}cm^{-1}$ at 296K. The conversion between the two types of units is:

$$S(cm^{-2}/atm.) = S(mol.cm^{-2}cm^{-1}) \times 2.48 \times 10^{19} \quad at\ 296K. \qquad (2)$$

The strength entry given in the table after the lower state quantum assignment is the computed or observed value. The computed strengths were derived from a quantum model and discussed in previous reports. When such analyses were not performed, the observed strength was inserted in that location. For the spectral region above 4300 cm^{-1}, a quantum model was used to fit the strength data of the (030)-(000), (110)-(000), and (011)-(000) bands of $H_2{}^{16}O$ and $H_2{}^{18}O$ ($H_2{}^{17}O$ was derived from the $H_2{}^{16}O$ values for like transitions) and the (021)-(010) bands of $H_2{}^{16}O$ [179]. Therefore the strengths of transitions of other bands of H_2O in this spectral region along with transitions of HDO in the region above 4800 cm^{-1} were not computed and the strength given in that location in the table was the observed value.

Features that SISAM.H2O has that the HITRAN compilation does not include are the following: uncertainties in the computed line positions, un, the difference between the observed and computed position, o-c, from which the observed value can be determined, and the measured line strength with the associated estimated uncertainty given in percent, Δs%. un for a given transition was derived from the expression:

$$un(position) = \{ un(upper\ state\ level)^2 + un(lower\ state\ level)^2 \}^{1/2}, \qquad (3)$$

where the upper and lower state values of un are given in the energy level listings for the various vibrational states of the molecular species. These listings are also available to the users. A study of Table 5 shows that some lines contain a "9" located between the molecule and isotope codes. This means that the line is doubled with the stronger of the two comparable, unresolved, transitions given for the H_2O species and either given for the two equal strength lines of HDO. The listed strength represents the sum of the two strengths. The values of Δs% go from 1 to 15% in the total listing with Δs%=15% meaning that the observed absorption is either weak or blended from which an accurate determination of the measured strength could not be derived and the uncertainty of the strength could be even higher than 15%: to possibly over 50%. This reflects into the values of o-c for these lines in which for many cases, o-c > 100×10^{-5} cm^{-1}. Other factors can cause high values for o-c such as blending with other lines that are not reported or the line is assigned incorrectly. These conditions may occur more frequently in the higher spectral region than in the lower (below 6000 cm^{-1}) region because computed line strengths for the higher region were not derived and if more than one transition was determined to lie within the location of an absorption, only the quantum assignment of the strongest transition was given unless information for the weaker transition(s) was obtained elsewhere, for example $H_2{}^{17}O$, $H_2{}^{18}O$, and HDO line positions and strengths were mainly derived from spectra of enriched samples of those species.

Other situations given in Table 5 shows that a few lines were not measured and this is indicated by the omission of the values of o-c, observed strength, and Δs%. For situations like this, the HITRAN2000 [177] line strength value is inserted in the observed strength location if the transition is included in the HITRAN listing. For the three entries with this condition shown in Table 5, HITRAN2000 did not contain these lines. It should be noted that this condition occurs for lines with computed line strength values. Another condition observed in the table is that four lines do not have quantum assignments. In all about 160 lines (of over 39,000) were not assigned in the listing with all but two located above 6000 cm^{-1}. The four in the table are located at 7478.983, 7480.400, 7639.02, and 7639.489 cm^{-1}. The parameters assumed for these measured absorptions are the following: lower state energy of 1500 cm^{-1}, b^o(air)=.035cm^{-1}/atm. and b^o(self)=.25cm^{-1}/atm. As noted in the previous report [179], impurities due to NH_3, CO, and N_2O were found in the H_2O samples for this spectral region, however their spectral features were accounted for in the data. This does not dismiss the possibility that some of the unknown absorptions were due to other impurities that were not accounted for.

The listing is also given in the HITRAN format and includes values of η derived from unpublished work [180] covering transitions in the 6 μm region and the values may be in error by 15% or a little more. For the purpose of this work, the results were analyzed only in terms of J or more specifically, $|m|$. These values are given in Table 6. A sample of the HITRAN formatted listing is given in Table 7. It is assumed that the reader is familiar with the HITRAN format for H_2O and additional information is not required. However, additional data are included and located in the last rows of the table. These are the measured line strengths (converted to mol cm^{-1} cm^{-2} at 296K) and uncertainties. The last row specifies were the values come from. "meas." means that the strength was measured whereas "HITRAN" denotes that the strength value is the same as given in HITRAN2000 [177]. If no entry is given means that the transition was not measured and not included in the present HITRAN listing.

3. AVAILABLE FILES

A total of 12 files are available from the website (http://www.mark4sun.jpl.nasa.gov) which are listed in Table 8. The table also gives the descriptions of the files.

4. CONCLUSIONS

This study and the previous two studies [179,180] represent the culmination of several years of research by this author on the spectral parameters of water vapor between 500 and 8000 cm^{-1}. The listings resulting from this work of which samples are given in Tables 6 and 7, can be obtained from a website (http://www.mark4sun.jpl.nasa.gov). Additional listings of energy levels, width, and shift coefficients are also available. The listings provide a more accurate representation of the parameters than is presently available from HITRAN [177] however improvements will be forthcoming from the scientific community. For example, the method used in this work to derive computed line strengths has been improved in the theory proposed by Mikhailenko et al. [174]. In addition, the analyses of the measured line strengths for the 6×6 (or higher) bands located above 5800 cm^{-1} were not attempted here but a theory for this is continuing by several scientists. The measurements provided in this study should be of great help for these and other studies.

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Table 1. Reference numbers and type of research that applies for $H_2{}^{16}O$, $H_2{}^{18}O$, $H_2{}^{17}O$, $HD^{16}O$, and $HD^{18}O$

	rotational	1000-2000 cm^{-1}	2000-4000 cm^{-1}	4000-6000 cm^{-1}	6000-8000 cm^{-1}	higher
$H_2{}^{16}O$						
positions	9,48,49,52,53,67,75 83,109,115,117,119,120 130,135,139,148,154	6,15,29,32,53,62,84 89,93,95,103,111,116 128,130,135,142,148,154	8,16,17,19,27 51,53,93,95,125 142,148,154,179	6,16,26,27,31 34,125,154 161,179	23,33,42,47,105 154,159,159,179	44,70,154 159,175 176
strengths	53,135,165	6,22,29,39,53,84,93,95 124,128,135,142,165	18,25,51,53,93 95,142,165,179	6,37,98,167 179	72,105,108,131 155,159,167,179	
widths, foreign	3,60,69,77,92,97 113,140,158,168,170	2,4,6,11,13,20,39,43 45,57,64,76,78,82,85 100,113,146,149,165 168,170,171,180	18,87,163,165 168,170,180	6,98,168,170 180	101,118,153 168,170,180	46,61,79 127,150,151 152,164 166,169
widths, self	69,77,86,97,104,173	11,39,43,56,76,133 134,147,160,165	165,179 180	98,179 180	108,118,131 159,179,180	61,80,102 157,159 162,166
freqency shifts	104,110,173	20,126,132,133,134 137,146,165,171	165			61,127 150,169
theory	3,5,112,121,129 140,168,170	3,5,29,84,89,103,112 121,128,129,133,135 142,168,170	3,5,25,51,112 121,129,142 168,170,179	3,5,26,34,112 121,129,161 168,170,179	3,5,42,112 121,129 168,170	129,150
emission	86,115,117,119 120,130,139	116,124,130	27	27,31	33	
continuum	96,156	60	60	99		
$H_2{}^{18}O$						
positions	9,10,28,30,40,49 52,67,136,174	50,62,90,93	7,24,55,93 107	35,38,41,66	36,71,106	
strengths		90,93	93,107	41,66	106	
width, foreign		147				
theory		90,121	55,121	66,121	121	
emission	174					
$H_2{}^{17}O$						
positions	8,21,28,30,40 49,52,136	50,62,90,93	54,55,93,107	35,179	36,106	
strengths		90,93	54,93,107	179	106	
theory	130	90,121	54,55,121	121	121	
$HD^{16}O$						
positions	65,67,141	1,62,68,73,94,141 145,172	1,59,63,172	74,123	81,122,144	
strengths	12,14,141	68,94,141	58,59,63	74,123	122	
widths, foreign	168	143,168	88,168			
theory	168	68,73,168	58,168	74		
emission		172	172			
$HD^{18}O$						
positions	67	94,114				
strengths	14	94				

Table 2. Frequency and strength extent of transitions given in the SISAM.H2O listing

			all transitions						measured transitions					
M	I	band	no.	min. freq.	max. freq.	min. str.	max. str.	J_{max}	no.	min. freq.	max. freq.	min. str.	max. str.	J_{max}
1	1	000 000	627	500.0350	1743.9773	5.09E-08	4.07E-01	21	307	590.3311	1285.6899	1.67E-07	9.54E-02	19
1	1	010 010	202	502.1937	1029.4600	5.17E-08	2.08E-04	18	49	590.6003	851.2487	4.72E-07	8.10E-05	15
1	1	010 000	1903	701.9643	2819.8482	5.01E-08	7.41E+00	21	1282	783.2109	2582.6184	1.72E-07	7.40E+00	20
1	1	020 010	872	877.3133	2628.5774	5.07E-08	6.88E-03	16	505	995.9774	2276.5521	1.24E-07	6.82E-03	14
1	1	100 010	532	1221.4102	2611.6646	5.01E-08	9.66E-05	14	255	1247.8814	2423.0689	1.51E-07	9.68E-05	12
1	1	001 010	484	1298.1172	2716.1280	5.15E-08	2.33E-04	14	229	1298.1172	2571.9108	1.56E-07	2.35E-04	13
1	1	030 020	215	1223.6274	2017.9823	3.58E-08	5.47E-06	11	33	1293.6548	1841.5484	4.42E-07	5.46E-06	6
1	1	020 000	1135	2565.2831	4402.7739	2.05E-09	7.35E-02	17	660	2622.5755	4402.7739	7.60E-08	7.40E-02	15
1	1	030 010	313	2813.5890	3916.7097	2.69E-07	5.34E-05	12	96	2926.4559	3375.7254	5.59E-07	5.45E-05	10
1	1	100 000	1326	2823.0743	4495.9911	3.43E-08	5.58E-01	17	876	2912.3764	4495.9911	3.59E-08	5.50E-01	17
1	1	110 010	372	3172.3397	4173.8405	1.95E-10	3.41E-04	12	77	3325.6623	4173.8405	1.15E-07	2.30E-04	10
1	1	001 000	1626	2894.6577	4640.3609	2.33E-13	6.06E+00	20	1090	2992.1594	4640.3609	1.00E-07	6.13E+00	19
1	1	011 010	533	3203.9027	4323.1554	2.06E-07	2.99E-03	15	200	3351.2812	4323.1554	1.92E-07	2.82E-03	14
1	1	021 020	49	3570.3183	3868.3919	2.51E-07	1.27E-06	8						
1	1	030 000	655	4331.3505	5931.9594	1.23E-08	4.41E-04	15	500	4359.3120	5924.1403	2.36E-08	4.18E-04	15
1	1	110 000	921	4568.0670	6071.3992	9.01E-08	8.98E-02	17	803	4568.0670	6071.3992	2.14E-08	8.93E-02	17
1	1	011 000	1221	4608.2066	6227.1887	1.16E-07	6.99E-01	19	1095	4608.2066	6227.1887	1.00E-07	6.95E-01	19
1*	1	120 010	146	4884.9663	5524.2168	2.30E-08	6.92E-05	12	134	4884.9663	5524.2168	8.17E-08	6.95E-05	12
1	1	021 010	348	4833.6529	5791.0001	2.01E-07	6.89E-04	13	314	4833.6529	5791.0001	3.40E-08	6.77E-04	13
1*	1	040 010	5	4862.0731	5437.9696	3.00E-07	1.05E-05	9	5	4862.0731	5437.9696	1.71E-07	1.05E-05	9
1*	1	200 010	37	5472.1938	5824.8819	1.70E-07	1.70E-06	8	36	5472.1938	5824.8819	1.70E-07	1.70E-06	8
1*	1	101 010	26	5146.4168	5760.9331	2.21E-07	9.50E-07	9	26	5146.4168	5760.9331	9.87E-08	9.50E-07	9
1*	1	002 010	3	5930.2897	5990.0362	2.00E-07	3.36E-07	5	3	5930.2897	5990.0362	2.00E-07	3.36E-07	5
1	1	040 000	260	5904.1890	7460.3308	1.36E-07	5.90E-04	14	260	5904.1890	7460.3308	1.36E-07	5.90E-04	14
1	1	120 000	496	6301.9499	7761.6665	2.00E-07	4.25E-03	13	496	6301.9499	7761.6665	2.00E-07	4.25E-03	13
1	1	021 000	757	5962.3431	7804.6095	1.20E-07	3.48E-02	15	757	5962.3431	7804.6095	1.20E-07	3.48E-02	15
1	1	200 000	774	6421.3968	7939.5930	3.00E-07	6.60E-02	18	774	6421.3968	7939.5930	3.00E-07	6.60E-02	18
1	1	101 000	901	6441.9552	7971.9153	3.00E-07	4.60E-01	17	901	6441.9552	7971.9153	3.00E-07	4.60E-01	17
1	1	002 000	590	6552.7186	7973.0819	2.22E-07	5.26E-03	14	590	6552.7186	7973.0819	2.22E-07	5.26E-03	14
1*	1	050 000	6	7195.2892	7653.7109	2.00E-06	6.64E-05	5	6	7195.2892	7653.7109	2.00E-06	6.64E-05	5
1	1	111 010	153	6932.3517	7538.9079	3.30E-07	2.07E-04	12	153	6932.3517	7538.9079	3.30E-07	2.07E-04	12
1	1	210 010	68	6537.3321	7360.2854	5.80E-07	9.18E-05	8	68	6537.3321	7360.2854	5.80E-07	9.18E-05	8
1	1	031 010	133	6572.1139	7370.5624	2.99E-07	4.28E-05	11	133	6572.1139	7370.5624	2.99E-07	4.28E-05	11
1*	1	130 010	26	6531.0242	7371.8907	2.93E-07	4.40E-06	10	26	6531.0242	7371.8907	2.93E-07	4.40E-06	10
1*	1	012 010	7	7044.4791	7639.4968	2.91E-07	4.90E-05	6	7	7044.4791	7639.4968	2.91E-07	4.90E-05	6
1	2	000 000	199	500.7524	1107.8835	5.04E-08	7.32E-04	17	76	595.5295	943.9840	3.90E-07	1.20E-04	16
1	2	010 010	20	501.6760	674.0171	5.08E-08	4.45E-07	12						
1	2	010 000	1031	893.5514	2310.5115	5.04E-08	1.50E-02	18	731	1009.5539	2219.1683	2.06E-07	1.52E-02	17
1	2	020 010	303	1203.3157	2014.5525	5.02E-08	1.45E-05	12	167	1284.7791	1934.9395	8.93E-08	1.52E-05	11
1	2	100 010	63	1807.7876	2248.8805	5.12E-08	2.61E-07	8						
1	2	001 010	59	2004.6187	2305.8356	5.14E-08	4.87E-07	8						
1	2	020 000	388	2806.9048	4045.9928	1.92E-07	1.34E-04	13	330	2892.7951	3981.5073	1.81E-07	1.40E-04	13
1	2	100 000	572	3001.8909	4193.4293	4.97E-09	2.24E-03	13	472	3001.8909	4193.4293	8.11E-08	2.44E-03	13
1	2	001 000	721	3160.6760	4290.8130	1.23E-07	1.26E-02	16	594	3160.6760	4290.8130	2.57E-07	1.26E-02	16
1	2	110 010	4	3624.2062	4024.2763	3.00E-07	8.75E-07	8	1	4024.2763	4024.2763	9.27E-07	9.27E-07	8
1	2	011 010	101	3525.8313	3911.0661	2.50E-07	4.79E-06	9						
1*	2	030 000	54	4476.4357	5584.7154	9.41E-08	5.49E-06	10	1	4661.7763	4661.7763	3.07E-07	3.07E-07	2
1	2	110 000	338	4876.8053	5655.4885	9.51E-08	2.04E-04	13	162	4954.3400	5655.4885	1.94E-07	2.11E-04	11
1	2	011 000	582	4839.9607	5910.2198	9.51E-08	1.39E-03	15	402	4927.6856	5869.1798	2.28E-08	1.41E-03	14
1*	2	021 010	89	5082.4704	5465.4576	9.43E-08	1.41E-06	9	8	5232.5519	5420.5897	2.79E-07	1.11E-06	8
1*	2	120 010	3	5140.9614	5375.5935	1.02E-07	1.41E-07	4						
1*	2	040 000	3	6630.6781	6999.4815	2.18E-07	1.08E-06	9	3	6630.6781	6999.4815	2.18E-07	1.08E-06	9
1*	2	120 000	125	6540.4462	7137.1483	8.48E-08	4.81E-05	9	125	6540.4462	7137.1483	8.48E-08	4.81E-05	9
1*	2	021 000	250	6481.3641	7507.8576	8.16E-08	7.35E-05	10	250	6481.3641	7507.8576	8.16E-08	7.35E-05	10
1*	2	200 000	317	6530.1832	7622.8460	8.36E-08	1.63E-04	11	317	6530.1832	7622.8460	8.36E-08	1.63E-04	11
1*	2	101 000	419	6739.6970	7696.8481	8.99E-08	9.04E-04	12	419	6739.6970	7696.8481	8.99E-08	9.04E-04	12
1*	2	002 000	152	6700.0517	7732.0894	9.05E-08	1.23E-05	8	152	6700.0517	7732.0894	9.05E-08	1.23E-05	8
1	3	000 000	129	500.8874	976.2445	5.11E-08	1.53E-04	15	31	598.9986	797.3165	3.00E-07	2.25E-05	14
1	3	010 010	4	502.7523	559.2258	5.04E-08	7.94E-08	10						
1	3	010 000	841	1007.7228	2260.6045	5.04E-08	3.00E-03	17	660	1063.7848	2224.1543	4.48E-08	2.78E-03	17
1	3	020 010	190	1270.3185	1939.9008	5.11E-08	2.61E-06	11	109	1314.1474	1939.9008	5.67E-08	2.40E-06	9
1	3	020 000	292	2887.1297	3993.9411	1.94E-11	1.70E-05	12	264	2927.2546	3944.7876	1.12E-07	1.70E-05	12
1	3	100 000	435	3201.6459	4151.1924	3.29E-11	2.66E-04	12	382	3201.6459	4151.1924	1.23E-07	1.47E-04	12
1	3	001 000	603	3163.3984	4298.2354	6.62E-12	2.24E-03	15	534	3163.3984	4298.2354	1.00E-07	2.28E-03	15
1	3	011 010	34	3591.5801	3857.3357	2.48E-07	9.00E-07	7						

Table 2 continued

M I	band	all transitions no.	min. freq.	max. freq.	min. str.	max. str.	J_{max}	measured transitions no.	min. freq.	max. freq.	min. str.	max. str.	J_{max}
1*3	110 000	213	4940.9761	5664.1062	4.79E-08	6.11E-05	11	180	4940.9761	5664.1062	7.00E-08	6.11E-05	11
1 3	011 000	440	4909.0652	5838.2591	2.36E-08	2.60E-04	15	390	4909.0652	5818.9367	7.34E-08	2.60E-04	15
1*3	021 010	26	5142.8754	5412.8427	9.00E-08	2.56E-07	7						
1*3	120 000	53	6616.7594	7056.0842	6.68E-08	3.20E-06	6	53	6616.7594	7056.0842	6.68E-08	3.20E-06	6
1*3	021 000	191	6502.2778	7380.5257	9.00E-08	1.24E-05	12	191	6502.2778	7380.5257	9.00E-08	1.24E-05	12
1*3	200 000	261	6826.4499	7781.9979	7.50E-08	2.70E-05	11	261	6826.4499	7781.9979	7.50E-08	2.70E-05	11
1*3	101 000	335	6686.3614	7604.9751	4.63E-08	1.72E-04	11	335	6686.3614	7604.9751	4.63E-08	1.72E-04	11
1*3	002 000	58	7033.1997	7639.2273	9.00E-08	1.32E-06	6	58	7033.1997	7639.2273	9.00E-08	1.32E-06	6
49 1	000 000	123	504.5735	834.7326	5.01E-08	7.74E-06	17	56	651.0778	834.7326	4.74E-08	1.74E-06	16
49 1	010 000	1710	917.3648	1921.2779	5.01E-08	6.21E-04	20	1413	917.3648	1921.2779	3.66E-08	6.24E-04	19
49 1	020 010	435	1145.2243	1695.0543	5.01E-08	1.61E-06	13	325	1155.8371	1695.0543	4.80E-08	1.66E-06	13
49 1	100 010	33	1230.7725	1574.1042	5.01E-08	9.72E-08	7	24	1230.7725	1574.1042	4.65E-08	9.45E-08	6
49 1	020 000	610	2575.2579	3262.6872	4.78E-09	2.87E-05	15	420	2591.8247	3262.6872	1.11E-07	2.91E-05	15
49 1	100 000	812	2450.3977	3059.2576	2.40E-09	2.34E-04	16	494	2453.0028	3059.2576	1.13E-07	2.35E-04	16
49 1	001 000	1257	3289.0747	4103.0239	7.02E-08	4.34E-04	17	1019	3304.2474	4103.0239	7.02E-08	4.42E-04	17
49*1	011 010	174	3530.7092	3816.2754	7.07E-08	5.34E-07	10						
49 1	110 000	585	3825.6065	4426.4111	2.12E-08	2.10E-05	16	555	3825.6065	4426.4111	4.28E-08	2.21E-05	16
49 1	030 000	376	3950.3362	4435.0167	5.98E-08	1.99E-05	14	357	3950.3362	4435.0167	7.99E-09	2.00E-05	14
49 1	200 000	252	5118.8720	5595.5566	6.90E-08	1.85E-05	14	225	5118.8720	5595.5566	6.90E-08	1.85E-05	14
49*1	120 000	28	5400.6167	5607.6961	1.93E-07	7.92E-07	6	27	5400.6167	5607.6961	1.70E-07	4.10E-07	6
49 1	011 000	526	4814.1532	5366.4719	1.33E-07	9.06E-05	14	498	4814.1532	5366.4719	1.29E-07	3.66E-05	14
49*1	101 000	337	6151.2972	6687.4862	6.71E-08	2.43E-06	11	317	6151.2972	6640.3680	5.28E-08	2.43E-06	11
49*1	021 000	144	6266.6580	6634.3342	9.77E-08	1.92E-06	11	140	6266.6580	6634.3342	6.93E-09	1.57E-06	11
49*1	210 000	138	6586.7469	6912.2570	5.61E-08	1.59E-06	11	135	6601.9203	6912.2570	8.88E-09	9.90E-07	11
49*1	002 000	629	6895.8667	7571.5864	9.58E-08	2.50E-05	15	614	6895.8667	7513.7914	4.20E-08	2.50E-05	15
49 2	010 000	438	1173.7720	1684.2263	5.04E-08	1.26E-06	13	410	1173.7720	1684.2263	4.83E-08	1.28E-06	13
49*2	100 000	73	2586.9104	2812.0584	1.50E-07	4.93E-07	8	62	2586.9104	2812.0584	1.59E-07	4.75E-07	8
49*2	001 000	148	3568.3434	3824.7175	1.51E-07	8.84E-07	10	131	3568.3434	3824.7175	1.53E-07	8.68E-07	9
49 3	010 000	175	1234.2347	1598.7655	5.04E-08	2.31E-07	10	137	1234.2347	1598.7655	4.50E-08	2.28E-07	10

M= molecule, 1=H_2O, 49=HDO
I=oxygen isotopic species, 1=16, 2=18, 3=17
no.=number of vibration-rotation transitions
freq. is the frequency in cm^{-1}
str. is the strength in cm^{-2}/atm. at 296K
J_{max} is the maximum upper state J value
an asterisk, *, between molecule and isotopic species codes denotes that transitions of the band are not contained in HITRAN2000.

Table 3. Frequency extent of H_2O and HDO broadening measurements

			air-broadening				self-broadening			
M	I	band	no.	min. frq.	max. frq.	Jmax	no.	min. frq.	max. frq.	Jmax
1	1	000-000	149	604.4482	1153.1903	18	106	600.6621	1153.1903	17
1	1	010-010	1	676.5496		12	2	609.7160	676.5496	12
1	1	010-000	792	896.5048	2271.7235	18	800	897.6940	2281.7859	17
1	1	020-010	113	1207.2742	2026.1207	11	204	1207.2742	2026.1207	11
1	1	100-010	13	1956.8087	2227.4019	4	31	1933.5548	2251.8697	8
1	1	001-010	27	1981.0268	2289.8940	6	0			
1	1	020-000	367	2864.3511	4260.4087	15	0			
1	1	030-010	5	2981.3638	3174.6872	5	0			
1	1	100-000	368	2912.3764	4304.4911	16	0			
1	1	001-000	494	3013.2146	4339.9831	18	10	4356.2226	4448.2253	13
1	1	011-010	9	3572.2124	3912.3372	10	0			
1	1	030-000	61	4405.9842	5562.6989	14	167	4428.4819	5643.5839	12
1	1	110-000	171	4900.7207	5753.4196	13	423	4761.5976	5840.4648	13
1	1	011-000	458	4901.3357	6018.0629	18	624	4787.8768	5992.4248	16
1	1	120-010	0				5	5137.8365	5405.7198	5
1	1	021-010	25	5045.8239	5437.0643	10	118	5067.7914	5499.8687	11
1	1	040-000	5	6011.4863	7031.4738	9	118	5904.1890	7031.4738	12
1	1	120-000	139	6505.4849	7438.2301	11	324	6301.9499	7640.5650	12
1	1	021-000	239	6443.0852	7541.9944	13	530	6271.0338	7804.6095	13
1	1	200-000	219	6641.2667	7620.8435	13	563	6516.2772	7939.5930	13
1	1	101-000	326	6660.7548	7728.8588	15	600	6441.9553	7859.1041	17
1	1	002-000	125	7003.1045	7758.5553	11	390	6710.4781	7919.8769	12
1	1	111-010	5	7091.4263	7301.4349	7	57	7007.6054	7489.3979	12
1	1	210-010	0				20	6900.7387	7288.7380	7
1	1	031-010	0				45	6645.8556	6942.6383	8
1	2	000-000	3	639.4312	742.2072	14	4	617.3500	702.5895	12
1	2	010-000	174	1170.0349	2078.1670	15	261	1242.2439	2078.1670	13
1	2	020-000	4	2982.6360	3165.1023	7	0			
1	2	100-000	5	3350.0442	3541.6190	6	0			
1	2	001-000	23	3376.2887	3961.1484	13	0			
1	2	110-000	0				24	5081.0632	5517.6333	8
1	2	011-000	0				162	5061.9475	5580.5284	11
1	2	120-000	0				2	6670.5677	6852.4753	4
1	2	021-000	0				7	6481.3641	6986.6457	8
1	2	200-000	0				15	7158.7137	7474.2564	8
1	2	101-000	12	7060.3074	7372.2612	9	60	7060.3074	7398.2435	11
1	3	010-000	69	1359.0129	2058.5764	12	142	1315.6066	2010.9119	12
1	3	001-000	15	3581.5092	3939.4868	11	0			
1	3	011-000	4	5214.5816	5482.7397	6	82	5131.2366	5540.7963	9
1	3	200-000	1	7099.3683		1	0			
1	3	101-000	2	7060.8160	7154.7658	7	20	7153.4683	7370.2193	8
49	1	000-000	15	709.8113	825.9693	15	0			
49	1	010-000	549	931.5905	1936.0780	19	0			
49	1	020-010	4	1186.7011	1403.7577	4	0			
49	2	010-000	41	1173.7720	1713.3820	12	0			

M=molecule, 1=H_2O, 49=HDO frq.=frequency in cm^{-1} Jmax is the maximum upper state J

I=oxygen isotopic species, 1=16, 2=18, 3=17 no.=number of transitions.

Table 4. Experimental vibration-rotation energy level values (cm^{-1}) of the (100), (020), (001), (110) and (030) states of $HD^{18}O$

			--------(100)-------		------- (020)-------		-------(001)-------		-------(110)-------		-------(030)-------	
J	K_a	K_c	*Energy*	*un*	*Energy*	*un*	*Energy*	*un*	*Energy*	*un*	*Energy*	*un*
0	0	0	2709.28466	40.	2767.20936	40.	3696.33049	4.	4080.54526	40.	4121.75456	40.
1	0	1	2724.42956	6.	2782.72628	50.	3711.66184	4.	4095.86026	8.	4137.19681	8.
1	1	1	2738.54080	50.	2801.01750	25.	3724.69134	7.	4114.30766	15.	4156.43778	25.
1	1	0	2741.17653	5.	2804.09643	30.	3727.44905	9.	4117.34448	10.	4159.52537	45.
2	0	2	2754.37682	10.	2813.38861	45.	3741.92433	3.	4126.12810	15.	4167.73382	15.
2	1	2	2766.18129	5.	2828.95916	30.	3752.58655	6.	4141.83600	15.	4184.28050	30.
2	1	1	2774.08105	10.	2838.19123	20.	3760.85276	3.	4150.92500	10.	4193.54715	25.
2	2	1	2816.10393	6.	2892.72819	15.	3799.80272	5.	4203.09923	10.	4253.19923	8.
2	2	0	2816.43948	15.	2893.08313	25.	3800.19420	6.	4203.44890	15.	4253.53739	50.
3	0	3	2798.47684	15.	2858.50440	10.	3786.37088	6.	4170.65598	8.	4212.70429	8.
3	1	3	2807.43429	15.	2870.65076	25.	3794.18867	7.	4182.91180	40.	4225.83152	20.
3	1	2	2823.18791	10.	2889.06828	55.	3810.66844	4.	4201.00765	30.	4244.34915	40.
3	2	2	2861.45764	7.	2939.22185	10.	3845.73541	9.	4248.71522	15.	4299.73042	50.
3	2	1	2863.09516	7.	2940.96040	40.	3847.63933	9.	4250.43224	25.	4301.38245	45.
3	3	1	2937.50519	7.	3036.75254	40.	3917.31654	17.	4337.47450	70.	4409.27524	50.
3	3	0	2937.53189	5.	3036.77790	90.	3917.35172	15.	4337.50151	50.	4409.29980	50.
4	0	4	2855.92420	30.	2917.18864	29.	3844.11270	9.	4228.56094	50.	4271.26004	40.
4	1	4	2862.08745	5.	2925.86260	95.	3849.25643	18.	4237.31185	20.	4280.86844	40.
4	1	3	2888.16142	40.	2956.37590	60.	3876.50001	5.	4267.21324	15.	4311.62465	30.
4	2	3	2921.64157	10.	3000.56900	60.	3906.64378	5.	4309.23017	35.	4361.48095	20.
4	2	2	2926.32033	10.	3005.91195	40.	3912.04139	15.	4314.15865	20.	4366.27031	40.
4	3	2	2998.45480	20.	3099.28198	60.	3979.15175	15.	4398.67419	40.		
4	3	1	2998.63978	10.	3099.46020	90.	3979.39384	23.	4398.85800	40.		
4	4	1	3102.92955	25.	3232.28424	50.	4077.54344	20.	4516.98690	90.		
4	4	0	3102.93122	15.	3232.28930	50.	4077.54610	35.	4516.98910	90.		
5	0	5	2926.02612	6.	2988.63070	40.	3914.45433	5.	4299.03024	10.	4342.61443	20.
5	1	5	2929.91065	15.	2994.34153	15.	3917.53632	6.	4304.78979	40.	4349.14559	25.
5	1	4	2968.49892	5.	3039.58875	15.	3957.74955	5.	4348.99174	15.	4394.90524	25.
5	2	4	2996.41482	15.	3077.32160	80.	3982.24865	10.	4384.38995	30.	4438.21027	85.
5	2	3	3006.52018	15.	3088.44506	50.	3993.76684	7.	4395.08498	8.	4448.73286	40.
5	3	3	3074.74305	20.	3177.55645	40.	4056.54777	15.	4475.28337	25.		
5	3	2	3075.46559	15.	3178.25301	15.	4057.48908	5.	4476.00410	15.		
5	4	2	3178.92835	20.	3310.46841	50.	4154.68262	5.	4593.23783	40.		
5	4	1	3178.94235	35.	3310.48200	300.	4154.70569	15.	4593.25180	30.		
5	5	1	3311.59960	50.			4279.73500	40.	4741.24870	40.		
5	5	0	3311.59960	50.			4279.73560	40.	4741.24870	40.		
6	0	6	3008.40320	30.	3072.32380	50.	3997.07714	8.	4381.56044	35.	4426.24435	40.
6	1	6	3010.68643	15.	3075.84434	40.	3998.79680	7.	4385.10952	25.	4430.42034	40.
6	1	5	3063.50552	10.	3137.98790	50.	4053.59311	10.	4445.59176	50.	4493.54863	30.
6	2	5	3085.48942	6.	3168.76595	25.	4072.21917	10.	4473.88815	25.	4529.62502	50.
6	2	4	3103.70948	18.	3188.68600	300.	4092.70893	30.	4493.27272	70.	4548.96906	20.
6	3	4	3166.32869	20.	3271.55325	50.	4149.43832	6.	4567.26348	33.		
6	3	3	3168.41497	45.	3273.56557	130.	4152.13394	10.	4569.35332	20.		
6	4	3	3270.27580	30.			4247.42960	16.	4684.89635	40.		
6	4	2	3270.35282	15.			4247.54263	10.	4684.96983	50.		
6	5	2	3402.45990	100.			4372.00213	25.	4832.39017	300.		
6	5	1	3402.46220	40.			4372.00440	35.	4832.39350	200.		
6	6	1	3562.49320	20.			4522.87150	60.	5009.23476	50.		
6	6	0	3562.49320	20.			4522.87150	60.	5009.23476	50.		
7	0	7	3102.95394	15.	3168.09267	60.	4091.93777	10.	4475.98410	50.	4521.92950	50.
7	1	7	3104.22930	15.	3170.15800	40.	4092.84985	15.	4478.06794	30.	4524.48144	50.
7	1	6	3172.32250	8.	3250.66850	50.	4163.05044	5.	4556.08808	50.	4606.73420	50.
7	2	6	3188.54295	10.	3274.28302	40.	4176.19152	21.	4577.38282	40.	4635.39332	50.
7	2	5	3217.52514	5.	3306.28002	50.	4208.36444	15.	4608.37502	40.	4666.76642	50.
7	3	5	3273.08923	15.	3381.13442	40.	4257.65862	10.	4674.50032	60.		
7	3	4	3278.01088	15.	3385.92378	40.	4263.91537	25.	4679.43792	50.		
7	4	4	3377.03160	30.			4355.83857	6.	4792.02457	50.		
7	4	3	3377.30815	15.			4356.24188	15.	4792.28851	15.		
7	5	3	3508.59320	45.			4479.78634	18.	4938.83800	300.		
7	5	2	3508.59959	50.			4479.79737	12.	4938.84200	300.		
7	6	2	3668.07266	50.			4630.12080	50.	5114.50576	300.		
7	6	1	3668.07266	50.			4630.12080	50.	5114.50576	300.		
7	7	1	3854.27382	50.			4805.81902	25.				
7	7	0	3854.27382	50.			4805.81902	25.				

Table 4 continued

			(100)		(020)		(001)		(110)		(030)	
J	K_a	K_c	*Energy*	*un*	*Energy*	*un*	*Energy*	*un*	*Energy*	*un*	*Energy*	*un*
8	0	8	3209.70825	10.	3275.94150	50.	4199.08880	6.	4582.31910	50.	4629.63940	40.
8	1	8	3210.39562	10.	3277.11191	40.	4199.55602	9.	4583.50038	30.	4631.14676	50.
8	1	7	3294.06360	30.	3376.64425	25.	4285.19844	14.	4679.49155	40.	4733.52986	50.
8	2	7	3305.23755	30.	3393.71895	20.	4293.79586	8.	4694.51772	40.	4755.16822	50.
8	2	6	3347.35378	15.	3440.57208	300.	4339.98275	8.	4739.75318	50.		
8	3	6	3394.81815	30.			4380.94633	29.	4796.77546	50.		
8	3	5	3404.72586	30.			4393.29536	40.	4806.77882	20.		
8	4	5	3499.21686	15.			4479.92172	28.	4914.64641	50.		
8	4	4	3500.02095	30.			4481.08400	12.	4915.41657	50.		
8	5	4	3630.02750	55.			4603.14226	30.				
8	5	3	3630.05360	60.			4603.18928	29.				
8	6	3	3788.80987	50.			4752.78200	40.				
8	6	2	3788.80987	50.			4752.78200	40.				
8	7	2					4927.87870	15.				
8	7	1					4927.87870	15.				
8	8	1					5127.39110	300.				
8	8	0					5127.39110	300.				
9	0	9	3328.71667	15.	3395.93143	50.	4318.58237	30.	4700.63012	50.	4749.41272	50.
9	1	9	3329.07682	20.	3396.58122	50.	4318.81500	20.	4701.28593	50.	4750.28143	50.
9	1	8	3428.03283	40.	3515.06208	300.	4419.42460	30.	4814.97978	50.	4873.07388	60.
9	2	8	3435.25113	30.	3526.78411	300.	4424.68308	20.	4824.94391	50.		
9	2	7	3492.41512	30.			4486.63268	20.	4886.58398	50.		
9	3	7	3531.23097	25.			4518.95842	15.	4933.85200	300.		
9	3	6	3548.79307	25.			4540.34850	35.	4951.66378	300.		
9	4	6	3636.80708	15.			4619.62323	50.				
9	4	5	3638.80487	50.			4622.47576	60.				
9	5	5	3766.80403	70.			4742.12222	300.				
9	5	4	3766.90309	50.			4742.28248	15.				
9	6	4					4890.88400	200.				
9	6	3					4890.88700	200.				
9	7	3					5065.24626	80.				
9	7	2					5065.24626	80.				
9	8	2					5264.06863	300.				
9	8	1					5264.06863	300.				
10	0	10	3460.01012	5.	3528.11600	300.	4450.44258	15.	4830.98671	50.	4881.29261	50.
10	1	10	3460.19593	15.	3528.46811	50.	4450.55715	15.	4831.34456	50.	4881.78796	50.
10	1	9	3574.24940	15.			4565.50415	10.	4962.07728	50.		
10	2	9	3578.28154	40.			4568.55209	15.				
10	2	8	3651.79004	15.			4647.24589	15.				
10	3	8	3681.98546	40.			4671.28800	60.				
10	3	7	3710.03650	30.			4704.66655	35.				
10	4	7	3791.06063	50.			4774.79803	40.				
10	4	6	3794.07406	50.			4780.92896	50.				
10	5	6					4896.76088	50.				
10	5	5					4897.21906	50.				
11	0	11	3603.59612	10.			4594.67237	25.	4973.41452	50.		
11	1	11	3603.69115	20.			4594.72784	45.	4973.60665	50.		
11	1	10	3731.49273	50.			4723.46099	15.				
11	2	10	3734.07725	40.			4725.15720	50.				
11	2	9					4820.73799	50.				
11	3	9					4837.52855	50.				
11	3	8					4885.47486	50.				
12	0	12	3759.46655	50.			4751.25688	50.				
12	1	12	3759.51460	50.			4751.28350	50.				
12	1	11					4893.43740	50.				
12	2	11					4894.31414	50.				
13	0	13	3927.45855	300.			4920.16705	50.				
13	1	13	3927.45855	300.			4920.18796	50.				
13	1	12					5075.54074	300.				
13	2	12					5075.88863	50.				
14	0	14					5101.38118	50.				
14	1	14					5101.38753	300.				
15	0	15					5294.88155	300.				
15	1	15					5294.88155	300.				

un is the estimated uncertainty of the energy level value in $cm^{-1} \times 10^5$

Table 5. Extract from SISAM.H2O compilation

M	I	computed position	upper J	upper K_a	upper K_c	lower J	lower K_a	lower K_c	strength	lower energy	linewidth air	linewidth self	shift air	band	un	o-c	measured strength	Δs%
1	3	5476.94385	7	2	6	6	2	5	5.45E-05	551.60934	.0652	.377	-.01820	011 000	4.	-3.	5.41E-05	3.
1	2	5477.33424	6	4	3	5	4	2	3.91E-05	604.54412	.0638	.358	-.01050	011 000	6.	7.	3.96E-05	2.
1	2	5477.49300	11	2	9	11	2	10	1.38E-07	1518.78785	.0430	.272	-.01800	011 000	40.			
4991		5477.76551	10	6	5	9	6	4	1.99E-07	1244.43726	.0530	.283	.00000	200 000	15.	199.	1.99E-07	3.
1	1	5477.76824	8	0	8	7	3	5	9.90E-07	2439.95442	.0758	.354	.00000	200 010	8.	100.	9.90E-07	10.*
1	2	5477.79945	5	4	1	4	3	2	9.26E-07	379.29154	.0724	.365	-.00840	110 000	26.	-13.	1.07E-06	10.
1	1	5477.86421	4	3	1	4	1	4	1.68E-06	1821.59680	.0845	.434	.00210	021 010	9.	46.	1.50E-06	10.
1	1	5477.93537	5	4	1	5	1	4	3.68E-04	399.45752	.0870	.415	-.00100	110 000	1.	1.	3.66E-04	2.
1	1	5478.03172	11	2	9	10	3	8	4.66E-05	1446.12824	.0465	.280	-.02200	110 000	17.	10.	4.77E-05	1.
1	2	5478.19009	6	4	2	5	4	1	1.17E-04	604.79280	.0654	.370	-.00910	011 000	17.	7.	1.16E-04	1.
1	1	5478.47116	10	2	8	10	2	9	5.68E-04	1293.63404	.0540	.312	-.01860	011 000	9.	7.	5.65E-04	2.
1	3	5478.55731	9	1	9	8	1	8	2.91E-05	742.49066	.0395	.310	-.01030	011 000	27.	-28.	2.98E-05	3.
1	3	5478.59575	9	0	9	8	0	8	9.73E-06	742.39854	.0373	.300	-.01020	011 000	31.	-25.	1.00E-05	3.
1	2	5478.69012	6	3	3	5	2	4	1.24E-06	414.16812	.0860	.430	-.00300	110 000	33.	38.	1.24E-06	10.
1	1	5479.03183	13	2	12	12	1	11	7.95E-06	1774.61629	.0160	.173	-.00600	110 000	50.	0.	7.86E-06	5.
1	1	5479.16758	7	4	4	7	2	5	9.94E-07	2392.59252	.0764	.392	-.00260	021 010	34.	-18.	1.05E-06	10.
1	1	5479.24580	8	3	6	7	3	5	1.12E-05	2439.95442	.0637	.340	-.01200	021 010	8.	-10.	1.05E-05	4.*
1	1	5479.33740	11	5	7	10	2	8	2.76E-06	1437.96860	.0660	.325	.00000	030 000	60.	62.	2.77E-06	7.
1	3	5479.58664	7	4	3	7	1	6	1.12E-07	702.88581	.0830	.391	-.00100	110 000	60.			
1	1	5479.61062	3	2	1	2	0	2	7.26E-03	70.09081	.0987	.434	.00150	011 000	2.	-2.	7.43E-03	1.
1	2	5479.83532	4	3	1	4	1	4	4.45E-06	223.82849	.0890	.434	.00210	011 000	17.	48.	3.90E-06	10.
1	1	5479.85016	4	3	2	3	0	3	3.60E-06	1731.89669	.0960	.456	-.00100	120 010	9.	600.	3.60E-06	15.
1	1	5479.87866	6	4	2	6	1	5	1.55E-04	542.90577	.0830	.404	-.00100	110 000	3.	4.	1.55E-04	1.
192		5480.13460	7	7	0	7	6	1	1.02E-07	1204.17475	.0440	.210	-.01590	110 000	33.			
49	1	5480.31811	10	2	9	9	2	8	1.90E-06	743.09739	.0676	.285	.00000	200 000	10.	-11.	1.90E-06	4.
49	1	5480.33751	11	1	11	10	1	10	1.82E-06	769.11689	.0509	.250	.00000	200 000	20.	-11.	1.82E-06	5.
1	3	7007.11385	4	0	4	5	2	3	8.95E-07	445.79341	.0950	.488	-.01000	101 000	25.	15.	8.95E-07	10.
1	2	7007.14179	7	1	7	8	0	8	6.85E-06	740.91225	.0512	.370	-.01780	200 000	28.	1.	6.85E-06	3.
1	2	7007.27629	7	3	5	8	3	6	2.42E-05	1001.70568	.0680	.363	-.00880	101 000	36.	-9.	2.42E-05	3.
1	1	7007.31986	8	5	4	9	6	3	2.36E-05	1631.38300	.0565	.300	-.01200	002 000	7.	4.	2.36E-05	3.
1	1	7007.39738	6	2	4	7	2	5	2.70E-06	2392.59252	.0779	.425	-.00730	111 010	31.	-38.	2.70E-06	15.*
1	2	7007.43529	3	1	3	4	2	2	5.20E-06	314.45943	.0995	.445	-.00580	200 000	37.	-9.	5.20E-06	4.
1	1	7007.48606	9	3	6	9	5	5	3.66E-05	1474.98078	.0758	.332	.00000	101 000	10.	-16.	3.66E-05	3.
1	1	7007.60543	7	1	6	8	1	7	3.12E-06	2490.35404	.0613	.367	-.01370	111 010	10.	7.	3.12E-06	4.
1	2	7007.79207	7	2	5	8	2	6	8.56E-06	980.22225	.0807	.439	-.00880	101 000	20.	3.	8.56E-06	4.
1	1	7008.04530	6	1	6	7	2	5	2.02E-06	2392.59252	.0893	.428	-.00700	060 010	100.	0.	2.02E-06	10.*
1	1	7008.07888	7	2	6	8	2	7	9.00E-06	2495.16582	.0579	.343	-.01350	111 010	60.	12.	9.00E-06	5.
1	2	7008.12241	6	5	1	7	5	2	9.18E-06	1051.20304	.0567	.290	-.01160	101 000	23.	4.	9.18E-06	3.
1	3	7008.24681	6	1	5	7	2	6	8.13E-07	708.01628	.0750	.415	-.01300	200 000	61.	74.	8.13E-07	7.
1	2	7008.30762	6	5	2	7	5	3	3.10E-06	1050.99014	.0567	.290	-.01090	101 000	11.	18.	3.10E-06	7.
1	1	7008.31540	9	0	9	9	1	8	3.85E-04	1079.07958	.0498	.290	-.01180	200 000	6.	-10.	3.85E-04	3.
1	1	7008.36418	7	1	7	6	4	2	1.32E-05	757.78018	.0700	.360	.00000	200 000	10.	82.	1.32E-05	15.
1	1	7008.40020	4	1	3	5	3	2	2.06E-03	508.81205	.0916	.460	-.01100	101 000	6.	-3.	2.06E-03	3.
1	1	7008.44079	5	3	2	5	0	5	9.50E-05	325.34790	.0915	.442	-.00300	120 000	12.	41.	9.50E-05	5.
1	1	7008.68391	8	5	3	9	6	4	7.20E-06	1631.24548	.0540	.296	-.01200	002 000	20.	-11.	7.20E-06	3.
1	1	7008.73749	10	1	9	10	2	8	4.02E-05	1437.96860	.0560	.328	-.00400	200 000	20.	35.	4.02E-05	2.
1	2	7008.83621	3	2	1	4	3	2	3.40E-05	379.29154	.0894	.469	-.00400	200 000	25.	-31.	3.40E-05	4.
1	1	7008.87102	4	1	3	5	2	4	2.18E-06	2024.15264	.0874	.469	-.00900	210 010	202.	-202.	2.18E-06	10.
1	3	7008.95708	5	2	3	4	2	2	1.33E-06	315.07850	.0862	.452	-.01000	021 000	7.	7.	1.33E-06	6.
1	1	7008.98648	11	6	6	11	6	5	4.80E-06	2144.04627	.0424	.249	-.01100	021 000	97.	252.	4.80E-06	15.
1	2	7009.06050	5	3	3	4	3	2	1.94E-05	379.29154	.0761	.382	-.01230	021 000	10.	0.	1.94E-05	3.
1	1	7009.50720	9	4	6	10	5	5	2.16E-06	1724.70541	.0680	.364	.00000	002 000	31.	-190.	2.16E-06	5.
1	1	7194.57595	7	1	6	7	4	3	1.00E-03	931.23710	.0840	.399	.00000	002 000	9.	13.	1.00E-03	3.
1	1	7194.68594	3	2	2	3	2	1	7.90E-05	1819.33510	.0903	.456	-.01050	111 010	21.	16.	7.90E-05	5.
1	1	7194.80522	1	1	0	2	1	1	7.60E-02	95.17593	.1001	.460	-.00400	101 000	3.	3.	7.60E-02	2.
1	1	7194.96209	4	3	2	5	4	1	2.80E-04	610.34116	.0768	.395	-.00900	002 000	30.	26.	2.80E-04	2.*
1	2	7195.06226	5	4	2	5	4	1	1.34E-04	604.79280	.0675	.365	-.01030	101 000	59.	64.	1.34E-04	5.
1	1	7195.28917	4	1	4	5	4	1	2.00E-06	610.34116	.0905	.407	-.01200	050 000	48.	-66.	2.00E-06	10.*
1	1	7195.45621	3	0	3	4	3	2	2.00E-05	382.51688	.0945	.456	-.01600	002 000	14.	-41.	2.00E-05	5.
49	1	7195.51216	10	5	6	10	5	5	1.02E-07	1239.08924	.0507	.343	.00000	002 000	15.	-16.	1.02E-07	10.
49	1	7195.56658	7	1	6	7	2	5	2.29E-06	520.12352	.0902	.442	.00000	002 000	12.	12.	2.29E-06	3.
49	1	7195.67424	2	0	2	3	1	3	7.76E-06	100.39090	.0995	.439	.00000	002 000	16.	9.	7.77E-06	2.
49	1	7195.71562	2	2	1	3	2	2	7.70E-06	155.38900	.0902	.500	.00000	002 000	15.	-2.	7.71E-06	3.
1	2	7195.83976	5	4	1	5	4	2	4.62E-05	604.54412	.0718	.365	-.00790	101 000	29.	-30.	4.62E-05	3.
1	3	7196.37970	4	2	3	3	3	0	1.47E-07	283.76774	.0888	.428	-.01000	200 000	47.	-270.	1.47E-07	15.
49	1	7196.40721	10	5	5	10	5	6	1.07E-07	1238.79446	.0507	.343	.00000	002 000	20.	-1.	1.07E-07	10.
1	1	7196.63208	9	5	5	8	5	4	3.04E-04	1255.16675	.0527	.308	-.01200	021 000	20.	-3.	3.04E-04	2.
1	1	7196.66664	10	0	10	11	1	11	3.88E-05	1327.11762	.0252	.265	-.01900	002 000	11.	-14.	3.88E-05	2.
1	1	7196.68339	10	1	10	11	0	11	1.16E-04	1327.10996	.0266	.266	-.02000	002 000	30.	211.	1.16E-04	2.
1	1	7196.69531	13	3	11	12	3	10	4.00E-06	1962.50690	.0290	.217	-.01700	021 000	141.	169.	4.00E-06	15.
49	1	7196.69790	9	5	5	9	5	4	2.90E-06	1082.88663	.0552	.310	.00000	002 000	20.	-60.	2.90E-06	3.
1	1	7196.82650	13	2	11	12	2	10	6.80E-06	1960.20733	.0288	.228	-.01000	021 000	150.	0.	6.80E-06	10.
1	1	7196.84967	9	5	4	8	5	3	1.10E-04	1255.91153	.0565	.321	-.01200	021 000	13.	-7.	1.10E-04	2.

Table 5 continued

M	I	computed position	upper J	upper K_a	upper K_c	lower J	lower K_a	lower K_c	strength	lower energy	linewidth air	linewidth self	shift air	band	un	o-c	measured strength	Δs%
1	1	7196.96042	4	3	1	5	4	2	1.02E-04	610.11442	.0784	.415	-.00800	002 000	19.	-22.	1.02E-04	2.
1	3	7197.01149	6	3	4	6	3	3	2.11E-06	659.98667	.0839	.436	-.00670	101 000	46.	1.	2.11E-06	5.
1	1	7228.79668	6	3	3	5	4	2	8.83E-06	610.11442	.0850	.417	-.00600	200 000	6.	-28.	8.83E-06	3.
1	1	7228.85376	4	4	1	3	2	2	9.00E-06	206.30142	.0845	.416	-.00600	021 000	22.	54.	9.00E-06	6.
1	1	7229.13305	5	2	3	6	3	4	3.22E-04	648.97869	.0885	.459	-.00590	002 000	8.	-5.	3.22E-04	2.*
1	3	7229.34758	2	2	1	2	2	0	5.18E-05	135.43118	.0924	.480	-.00850	101 000	2.	2.	5.18E-05	3.
49	1	7229.42179	5	2	4	5	2	3	3.16E-06	303.99483	.0916	.475	.00000	002 000	10.	21.	3.15E-06	3.
1	1	7229.57071	5	0	5	6	3	4	2.13E-05	648.97869	.0828	.422	-.01400	050 000	44.	28.	2.13E-05	3.*
1	3	7229.66403	2	2	0	3	0	3	4.18E-07	136.53762	.1000	.490	-.00930	101 000	44.	-603.	4.18E-07	15.
1	1	7229.78276	11	5	6	11	4	7	4.10E-05	1899.00816	.0700	.390	-.00800	200 000	45.	74.	4.10E-05	7.
1	1	7229.82028	3	2	1	4	0	4	1.47E-04	222.05276	.0970	.473	-.00930	101 000	5.	18.	1.47E-04	3.
49	1	7229.88062	2	0	2	2	1	1	9.17E-06	66.18451	.1032	.460	.00000	002 000	16.	21.	9.18E-06	2.
1	1	7229.89946	7	5	3	7	6	2	3.65E-05	1216.18976	.0540	.240	-.00800	002 000	4.	4.	3.65E-05	3.
1	1	7230.05217	2	1	2	2	1	1	2.91E-02	95.17593	.0986	.503	-.00940	101 000	3.	3.	2.91E-02	1.
1	1	7230.21638	7	5	2	7	6	1	1.13E-04	1216.19450	.0540	.290	-.00800	002 000	15.	52.	1.13E-04	3.
1	2	7230.23920	4	1	3	4	0	4	1.20E-05	221.23399	.0930	.490	-.00400	200 000	58.	20.	1.20E-05	8.
1	1	7230.31561	4	2	2	4	1	3	1.23E-02	275.49704	.0961	.479	-.00330	200 000	3.	-2.	1.23E-02	1.
1	1	7230.56289	5	2	3	6	0	6	3.10E-05	446.69659	.0881	.437	-.00930	101 000	14.	211.	3.10E-05	7.
1	1	7230.62720	9	4	5	9	3	6	6.00E-04	1282.91910	.0800	.402	-.00500	200 000	21.	20.	6.00E-04	7.
1	1	7230.91394	4	3	1	4	3	2	1.34E-01	382.51688	.0816	.441	-.00850	101 000	2.	-2.	1.34E-01	1.
49	1	7230.96010	3	1	3	3	1	2	3.74E-06	116.46133	.0956	.499	.00000	002 000	8.	30.	3.75E-06	10.
1	3	7231.26142	1	1	1	1	1	0	1.10E-04	42.18695	.1021	.495	-.00900	101 000	3.	-2.	1.10E-04	2.
49	1	7231.29699	4	3	2	4	3	1	9.25E-06	295.67750	.0830	.441	.00000	002 000	5.	4.	9.24E-06	2.
1	1	7231.35875	5	3	2	5	3	3	1.77E-02	503.96809	.0825	.437	-.00850	101 000	10.	-9.	1.77E-02	1.
49	1	7231.77478	4	3	1	4	3	2	9.48E-06	295.48727	.0830	.441	.00000	002 000	9.	7.	9.48E-06	7.
1	1	7231.79368	4	1	3	3	3	0	8.10E-04	285.41857	.0910	.438	-.01000	101 000	6.	16.	8.10E-04	5.
1	1	7231.87230	3	2	1	3	1	2	4.90E-02	173.36580	.0944	.470	-.00300	200 000	6.	10.	4.90E-02	1.
1	1	7478.22400	17	3	15	16	3	14	8.00E-07	3211.21261	.0140	.164	-.02000	101 000	300.	0.	8.00E-07	15.
1	1	7478.30108	9	4	6	8	5	3	1.67E-05	1255.91153	.0610	.317	.00000	002 000	31.	-8.	1.67E-05	2.
1	1	7478.52193	3	1	2	2	2	1	1.61E-05	134.90164	.0981	.486	-.00900	002 000	6.	-53.	1.61E-05	2.
1	1	7478.65423	5	2	3	5	1	4	1.02E-03	399.45752	.0890	.473	-.00570	002 000	8.	11.	1.02E-03	3.*
1	1	7478.71763	7	3	4	7	2	5	2.75E-04	782.40982	.0910	.439	-.00300	002 000	19.	-3.	2.75E-04	2.
1	1	7478.86493	14	3	11	13	3	10	1.90E-05	2414.72341	.0398	.276	-.01000	101 000	7.	-3.	1.90E-05	2.
9	9	7478.98338	9	9	9	9	9	9	5.40E-06	1500.00000	.0300	.250	.25000	999 999	0.	0.	5.40E-06	5.
1	1	7479.09189	5	0	5	5	1	4	6.64E-05	399.45752	.0970	.453	-.00879	050 000	44.	-58.	6.64E-05	2.*
1	1	7479.47380	11	4	7	11	3	8	4.20E-06	1813.22339	.0800	.415	.00000	002 000	52.	-80.	4.20E-06	5.
1	1	7479.54433	6	3	3	6	2	4	1.64E-04	602.77349	.0860	.429	-.00500	002 000	32.	15.	1.64E-04	2.
1	1	7479.63554	1	1	1	0	0	0	3.42E-04	.00000	.1030	.498	-.00220	002 000	9.	6.	3.42E-04	3.
1	1	7479.74214	6	4	3	6	1	6	4.35E-05	447.25235	.0820	.374	-.00400	200 000	11.	36.	4.35E-05	3.
49	91	7479.80506	9	8	2	8	7	1	1.01E-07	1294.83641	.0347	.229	.00000	002 000	11.	14.	1.01E-07	3.
1	1	7479.81008	10	3	8	9	4	5	3.20E-05	1360.23533	.0720	.384	.00000	002 000	25.	22.	3.20E-05	2.
1	1	7479.95535	4	3	2	5	0	5	8.44E-07	325.34790	.0890	.426	.00000	002 000	30.	-211.	8.44E-07	15.*
9	9	7480.40080	9	9	9	9	9	9	2.49E-06	1500.00000	.0300	.250	.25000	999 999	0.	0.	2.49E-06	2.
1	2	7480.61582	4	2	3	4	1	4	2.26E-06	223.82849	.0910	.465	-.00470	002 000	29.	-32.	2.26E-06	10.
49	1	7480.80267	9	3	6	8	2	7	1.69E-07	609.94656	.0880	.389	.00000	002 000	9.	3.	1.68E-07	2.
49	91	7481.07581	9	7	2	8	6	3	2.10E-07	1105.00339	.0480	.245	.00000	002 000	40.	-51.	2.10E-07	2.
1	2	7481.20321	5	3	3	5	2	4	4.69E-07	414.16812	.0824	.411	-.00330	002 000	30.	30.	4.69E-07	15.
1	2	7481.23554	5	4	1	5	3	2	6.71E-07	505.72873	.0805	.417	-.00880	002 000	28.	27.	6.71E-07	15.
1	1	7481.53120	15	5	11	14	5	10	1.66E-06	2918.24498	.0272	.244	-.02000	101 000	150.	0.	1.66E-06	7.
1	2	7481.86155	5	3	3	4	1	4	5.00E-06	223.82849	.0891	.439	-.00200	101 000	47.	-55.	5.00E-06	15.
1	2	7481.88638	5	1	4	5	0	5	1.45E-06	324.04672	.0895	.457	-.00890	002 000	80.	-98.	1.45E-06	10.
1	1	7482.09050	15	3	12	14	3	11	1.46E-06	2739.42833	.0300	.247	-.01000	101 000	150.	0.	1.46E-06	6.
1	1	7504.71476	5	3	3	4	1	4	2.42E-03	224.83838	.0891	.439	-.00200	101 000	10.	20.	2.42E-03	2.
49	1	7504.75570	8	4	4	7	2	5	9.87E-08	520.12352	.0840	.396	.00000	002 000	10.	-30.	9.90E-08	5.
1	1	7504.94097	4	3	2	4	2	3	8.40E-04	300.36228	.0850	.440	-.00580	002 000	30.	3.	8.40E-04	3.*
1	91	7504.94262	8	7	2	7	6	1	5.00E-05	1216.19450	.0418	.235	-.01800	200 000	20.	788.	5.00E-05	5.
1	1	7505.09225	12	5	8	11	4	7	6.54E-05	1899.00816	.0690	.370	.00000	200 000	13.	-5.	6.54E-05	2.
1	1	7505.26805	4	1	4	4	2	3	8.40E-06	300.36228	.0840	.444	-.00580	050 000	48.	-35.	8.40E-06	2.*
1	1	7505.71657	7	5	3	7	2	6	1.70E-06	709.60821	.0685	.317	-.00700	200 000	12.	763.	1.70E-06	10.
1	3	7506.55923	7	3	4	6	1	5	3.68E-07	541.99675	.0915	.466	-.00460	101 000	44.	-123.	3.68E-07	15.
1	1	7506.77997	4	1	3	3	2	2	2.33E-05	206.30142	.0956	.485	-.00900	002 000	20.	-27.	2.33E-05	3.
1	1	7506.90298	13	4	9	12	4	8	1.24E-05	2205.65288	.0736	.378	-.02300	101 000	396.	485.	1.24E-05	5.
1	1	7507.10906	7	4	4	7	1	7	5.17E-06	586.47918	.0780	.362	.00000	200 000	5.	24.	5.17E-06	3.
1	2	7507.31301	5	1	4	4	2	3	2.90E-07	298.62009	.0885	.468	-.00860	002 000	80.	47.	2.90E-07	15.
1	1	7507.46553	4	2	3	4	1	4	1.06E-03	224.83838	.0910	.465	-.00470	002 000	9.	4.	1.06E-03	3.
1	2	7507.72222	2	2	0	1	1	1	1.00E-06	36.74866	.1000	.509	-.00160	002 000	18.	-22.	1.00E-06	15.
1	2	7507.85753	6	5	2	5	1	5	4.65E-07	325.21571	.0840	.460	-.00250	021 000	26.	86.	4.65E-07	15.
1	1	7508.04764	5	1	4	5	0	5	8.51E-04	325.34790	.0895	.457	-.00890	002 000	22.	31.	8.51E-04	3.
1	1	7508.15382	8	5	3	8	4	4	1.00E-05	1131.77556	.0740	.359	-.01500	002 000	20.	-22.	1.00E-05	2.
1	1	7508.30131	9	7	2	9	6	3	1.74E-06	1631.38300	.0470	.239	.00000	002 000	11.	19.	1.74E-06	6.
1	1	7508.38912	5	3	3	5	2	4	2.30E-04	416.20873	.0824	.411	-.00330	002 000	14.	18.	2.30E-04	3.
1	2	7508.72492	5	0	5	4	1	4	1.34E-06	223.82849	.0807	.471	-.01170	002 000	31.	308.	1.34E-06	10.
1	1	7508.78631	5	4	2	4	1	3	9.45E-05	275.49704	.0920	.437	-.00500	200 000	6.	29.	9.45E-05	2.

Table 5 continued

M I	computed position	upper J	upper K_a	upper K_c	lower J	lower K_a	lower K_c	strength	lower energy	linewidth air	linewidth self	shift air	band	un	o-c	measured strength	Δs%
1 1	7509.15754	5	4	1	5	3	2	3.29E-04	508.81205	.0805	.417	-.00880	002 000	14.	16.	3.29E-04	2.
1 3	7510.19553	6	4	2	5	2	3	7.50E-07	445.79341	.0890	.433	-.00660	101 000	30.	25.	7.50E-07	4.
1 1	7510.41650	7	2	5	6	1	6	1.50E-05	447.25235	.0893	.445	-.00400	200 000	9.	-60.	1.50E-05	5.
1 1	7510.52505	5	4	1	4	2	2	5.90E-04	315.77953	.0885	.446	-.00660	101 000	10.	10.	5.90E-04	2.
1 1	7591.17111	11	1	10	11	0	11	1.50E-05	1327.10996	.0320	.240	.00000	002 000	6.	9.	1.50E-05	4.
1 1	7591.18543	5	5	1	4	2	2	1.68E-06	315.77953	.0860	.375	-.00600	200 000	4.	737.	1.68E-06	10.*
1 1	7591.32573	9	0	9	8	1	8	9.80E-06	744.16266	.0436	.320	-.01500	002 000	12.	-3.	9.80E-06	3.
1 2	7591.35234	8	4	5	7	2	6	4.45E-07	706.59776	.0730	.399	-.00150	101 000	58.	105.	4.45E-07	15.
1 1	7591.39460	11	2	10	11	1	11	5.43E-06	1327.11762	.0310	.214	.00000	002 000	150.	25.	5.43E-06	5.
1 1	7591.47633	9	1	9	8	0	8	2.90E-06	744.06366	.0440	.344	-.01400	002 000	30.	-122.	2.90E-06	10.
1 2	7592.18006	6	3	4	5	2	3	9.80E-07	445.15854	.0885	.459	-.01040	002 000	34.	-6.	9.80E-07	15.
1 1	7592.43037	7	5	3	6	1	6	3.82E-05	447.25235	.0750	.360	-.00200	021 000	8.	63.	3.82E-05	2.
1 1	7592.55887	7	5	2	6	3	3	1.49E-04	661.54890	.0825	.402	-.01050	101 000	9.	9.	1.49E-04	2.
1 1	7593.14689	4	3	2	3	2	1	1.26E-03	212.15636	.0894	.469	-.00740	002 000	30.	-1.	1.26E-03	3.*
1 1	7593.47397	4	1	4	3	2	1	1.26E-05	212.15636	.0892	.453	-.00740	050 000	48.	53.	1.26E-05	2.*
1 3	7594.01561	5	3	3	4	2	2	1.28E-07	315.07850	.0902	.448	-.00730	002 000	150.	-1.	1.28E-07	15.
1 2	7594.40859	10	5	5	9	3	6	3.45E-07	1279.79752	.0797	.437	-.00670	101 000	13.	90.	3.45E-07	15.
1 2	7594.91875	8	2	6	7	0	7	1.08E-06	583.77780	.0800	.439	-.00880	101 000	30.	-5.	1.08E-06	10.
1 3	7597.30220	4	4	1	3	3	0	6.15E-07	283.76774	.0725	.405	-.01240	002 000	80.	0.	6.15E-07	10.
1 1	7597.53423	8	2	7	7	1	6	8.69E-05	704.21404	.0690	.376	-.00570	002 000	2.	-3.	8.69E-05	2.
1 1	7598.42859	8	7	2	8	4	5	1.25E-06	1122.70853	.0758	.260	.00000	200 000	20.	441.	1.25E-06	10.
1 2	7599.35981	9	4	6	8	1	7	1.88E-07	879.49476	.0730	.357	-.00410	200 000	70.	88.	1.88E-07	15.
1 1	7599.57652	9	3	6	8	1	7	1.03E-04	882.89032	.0820	.414	-.00240	101 000	10.	8.	1.03E-04	2.
1 1	7599.70751	10	3	7	9	4	6	7.70E-07	1340.88487	.0733	.404	.00000	002 000	10.	-891.	7.70E-07	10.
1 2	7600.03827	7	3	5	6	2	4	1.79E-07	601.23777	.0877	.462	-.01300	002 000	33.	12.	1.79E-07	15.
1 1	7600.77342	4	3	1	3	2	2	4.45E-04	206.30142	.0844	.425	-.00530	002 000	19.	23.	4.45E-04	3.
1 1	7601.29475	6	4	2	5	1	5	2.29E-05	326.62546	.0865	.399	-.00120	200 000	10.	15.	2.29E-05	2.
1 1	7602.14676	12	1	11	12	0	12	1.60E-06	1557.84446	.0260	.192	.00000	002 000	42.	24.	1.60E-06	5.
1 1	7602.21545	12	2	11	12	1	12	5.20E-06	1557.84778	.0260	.186	.00000	002 000	100.	55.	5.20E-06	3.
1 1	7638.12392	10	3	8	9	2	7	4.60E-06	1201.92150	.0630	.360	-.00300	002 000	25.	108.	4.60E-06	10.
1 1	7638.16116	7	6	1	6	4	2	1.71E-05	757.78018	.0692	.324	-.02000	101 000	7.	-6.	1.71E-05	2.*
1 1	7638.60903	11	3	9	10	2	8	1.35E-05	1437.96860	.0570	.330	-.00300	002 000	35.	-33.	1.35E-05	2.
1 2	7638.99660	6	5	2	5	4	1	1.50E-06	604.79280	.0650	.364	-.01520	002 000	100.	0.	1.50E-06	15.
9 9	7639.01999	9	9	9	9	9	9	2.82E-07	1500.00000	.0300	.250	.25000	999 999	0.	0.	2.82E-07	15.
1 1	7639.22173	7	6	2	6	4	3	5.07E-05	756.72478	.0658	.318	-.01600	101 000	17.	7.	5.07E-05	3.*
1 3	7639.22742	5	2	3	4	1	4	1.28E-07	224.30423	.0980	.477	-.00420	002 000	312.	-312.	1.28E-07	15.
1 2	7639.31221	6	5	1	5	4	2	7.00E-07	604.54412	.0615	.339	-.01720	002 000	200.	-1.	7.00E-07	15.
	7639.48900							4.00E-07	1500.00000	.0300	.250	.25000	999 999			4.00E-07	15.
1 1	7639.49814	6	5	1	5	4	2	2.91E-07	2251.69528	.0579	.306	-.01720	012 010	300.	0.	2.91E-07	15.
1 1	7639.50960	7	7	1	6	4	2	2.77E-06	757.78018	.0726	.328	.00000	120 000	22.	180.	2.77E-06	3.*
1 1	7639.57588	3	3	1	2	0	2	7.40E-06	70.09081	.0970	.447	-.00200	002 000	19.	-28.	7.40E-06	3.
1 1	7640.56500	7	7	0	6	4	3	9.97E-06	756.72478	.0715	.298	.00000	120 000	22.	-20.	9.97E-06	2.*
1 1	7640.76422	10	4	7	9	1	8	4.33E-05	1079.07958	.0630	.326	.00100	200 000	32.	48.	4.33E-05	2.
1 1	7641.93813	9	3	7	8	2	6	1.71E-05	982.91171	.0760	.383	-.00800	002 000	19.	-13.	1.71E-05	2.
1 2	7643.82400	6	6	1	5	5	0	1.40E-06	733.68293	.0463	.290	-.01780	002 000	150.	0.	1.40E-06	15.
1 1	7644.32669	6	4	2	5	0	5	2.91E-05	325.34790	.0868	.399	-.00010	101 000	12.	21.	2.91E-05	2.
1 1	7644.56369	5	5	1	4	4	0	3.14E-04	488.13416	.0595	.332	-.01650	002 000	43.	43.	3.14E-04	2.
1 1	7644.59644	5	5	0	4	4	1	8.70E-04	488.10769	.0595	.328	-.01650	002 000	13.	-14.	8.70E-04	3.
1 2	7644.68808	10	3	7	9	1	8	2.94E-07	1074.76293	.0720	.367	-.00940	101 000	41.	84.	2.94E-07	15.
191	7645.72160	14	1	14	13	0	13	1.20E-06	1806.67004	.0110	.204	-.02500	002 000	200.	0.	1.20E-06	15.
1 2	7646.85532	9	2	7	8	0	8	1.69E-07	740.91225	.0725	.404	-.01300	101 000	44.	136.	1.69E-07	15.
1 1	7647.25135	8	5	4	7	1	7	1.23E-06	586.47918	.0700	.300	.00000	021 000	20.	7.	1.23E-06	10.
1 1	7648.47886	11	4	7	10	2	8	1.27E-05	1437.96860	.0785	.376	-.00020	101 000	67.	-26.	1.27E-05	2.
1 1	7648.66442	12	3	10	11	2	9	1.04E-06	1690.66441	.0445	.266	.00000	002 000	38.	-42.	1.04E-06	10.
1 1	7649.34179	7	4	3	6	1	6	3.43E-05	447.25235	.0845	.391	-.00200	200 000	9.	-37.	3.43E-05	2.
1 1	7650.12754	9	4	6	8	2	7	2.97E-04	885.60021	.0665	.354	-.00120	101 000	27.	31.	2.97E-04	3.
1 1	7650.88093	11	7	5	10	5	6	1.42E-06	1718.71880	.0530	.352	-.02000	021 000	64.	-43.	1.42E-06	10.
1 1	7651.37974	12	5	7	11	3	8	2.17E-05	1813.22339	.0800	.429	-.00150	101 000	5.	-4.	2.17E-05	2.
1 1	7651.79444	9	5	5	8	3	6	1.76E-04	1006.11593	.0630	.331	-.00580	101 000	13.	6.	1.76E-04	2.
1 1	7653.07562	6	4	3	5	3	2	5.90E-04	508.81205	.0819	.430	-.01130	002 000	16.	3.	5.90E-04	4.
1 1	7653.27336	5	2	3	4	1	4	2.72E-04	224.83838	.0980	.477	-.00420	002 000	8.	-6.	2.72E-04	3.*
1 1	7653.71102	5	0	5	4	1	4	1.44E-05	224.83838	.0990	.456	-.00428	050 000	44.	38.	1.44E-05	2.*
1 1	7654.15554	8	6	2	7	4	3	6.30E-05	931.23710	.0735	.337	-.01420	101 000	11.	2.	6.30E-05	2.

M=molecule, 1=H_2O 49=HDO. I=oxygen isotopic species, 1=16, 2=18, 3=17. 9 between M and I means the line is doubled and the strength pertains to the sum of the strengths of the two comparable transitions and the computed position represents the transition given.
position and lower energy in cm^{-1}
strength in cm^{-2}/atm. at 296K. If measured strength given but Δs% not given means that strength not measured and value taken from the HITRAN compilation.
un is the estimated uncertainty in the computed line position in $cm^{-1} \times 10^5$. o-c is the observed minus computed line position in $cm^{-1} \times 10^5$.
linewidth and shift in cm^{-1}/atm. at 296K
Δs% is the estimated uncertainty in the measured strength value in percent.
an asterisk, *, in the last column denotes a perturbed transition

Table 6. Values of η for air-broadening used in the HITRAN listing

•m•	η	•m•	η	•m•	η	•m•	η
1	0.78	6	0.64	11	0.41	16	0.38
2	0.78	7	0.59	12	0.39	17	0.41
3	0.77	8	0.53	13	0.37	18	0.41
4	0.73	9	0.49	14	0.36	19	0.41
5	0.69	10	0.45	15	0.36	20	0.41

$m = -J''$ for P-branch transitions, $m = J'$ for R- branch transitions and $m=J$ for Q-branch transitions. Prime and double prime denote upper and lower states, respectively.

η is used in the expression:

$$b^o(T) = b^o(T_o)\,[T_o/T]^\eta$$

where b^o is the half-width coefficient

Table 7. Extract of water vapor listing given in HITRAN format

M	computed freq. (cm^{-1})	strength	$\lvert R \rvert$	b° air	b° self	E″	η	d° air	band	upper J K_a K_c	lower J K_a K_c	observed strength	Δs%
13	3503.473130	1.638E-26	7.013E-06	.1000	.4950	283.7677	.77	-.009000	4	1 3 0 3	3 3 0	1.81E-26	10. meas.
12	3503.579610	7.020E-27	7.499E-03	.0240	.1730	2238.0319	.37	-.005000	5	113 212	13 211	2.98E-25	4. meas.
11	3503.580790	7.060E-24	1.901E-03	.0580	.3450	1813.2234	.41	-.002000	4	111 2 9	11 3 8	6.90E-24	2. meas.
12	3503.615750	3.837E-26	1.521E-03	.0580	.3400	1334.4792	.49	-.014000	4	1 9 3 7	9 4 6	3.72E-26	10. meas.
14	3503.669530	1.501E-26	1.074E-02	.0460	.2620	1587.7405	.45	.000000	5	1 9 7 2	10 7 3	1.53E-26	HITRAN
14	3503.669760	1.501E-26	1.074E-02	.0435	.2620	1587.7402	.45	.000000	5	1 9 7 3	10 7 4	1.53E-26	10. meas.
11	3503.773100	7.947E-26	2.988E-04	.0731	.3430	2129.6186	.73	-.002000	8	2 4 2 3	4 4 0		
13	3503.775670	2.183E-25	4.703E-02	.0610	.3400	1337.4894	.49	-.002800	5	1 8 4 5	9 4 6	2.21E-25	3. meas.
11	3503.959720	4.962E-26	6.335E-05	.0912	.4590	1907.4514	.77	-.007000	8	2 2 1 2	3 3 1	5.16E-26	HITRAN
11	3504.165280	1.146E-21	8.910E-02	.0200	.2400	1557.8478	.39	-.013100	5	111 111	12 112	1.15E-21	3. meas.
11	3504.166140	3.599E-22	8.396E-02	.0225	.2200	1557.8445	.39	-.013100	5	111 011	12 012	3.25E-22	HITRAN
14	3504.261910	6.293E-25	3.389E-03	.0861	.4550	581.9621	.59	.000000	5	1 6 2 5	7 3 4	6.41E-25	2. meas.
12	3504.340000	4.006E-25	2.177E-02	.0460	.2440	1399.4632	.53	-.010800	5	1 7 6 1	8 6 2	4.01E-25	5. meas.
11	3504.343020	5.365E-23	1.111E-03	.0643	.3130	1059.6467	.59	-.003000	4	1 7 4 4	7 5 3	5.37E-23	4. meas.
12	3504.366980	1.202E-24	2.178E-02	.0460	.2530	1399.4278	.53	-.010800	5	1 7 6 2	8 6 3	1.20E-24	2. meas.
11	3504.466880	7.302E-23	6.402E-04	.0580	.3670	882.8903	.53	-.001000	4	1 8 0 8	8 1 7	6.78E-23	3. meas.
11	3504.674480	9.884E-24	1.967E-03	.0590	.2500	1525.1360	.41	.000000	3	110 5 5	11 210	1.37E-23	10. meas.
11	3504.750060	2.606E-21	1.250E-03	.0841	.4690	285.2193	.77	-.005600	4	1 2 2 0	3 3 1	2.54E-21	5. meas.
12	3504.866840	8.956E-26	8.786E-04	.0700	.3600	1047.3285	.53	.000000	3	1 7 6 2	8 3 5	9.92E-26	3. meas.
14	3504.888360	1.811E-26	9.920E-03	.0650	.2310	1532.7322	.37	.000000	5	112 310	13 211	1.83E-26	10. meas.
11	3504.972900	4.196E-26	7.129E-04	.0654	.3500	2439.9544	.59	-.011000	7	2 7 2 6	7 3 5	6.21E-26	HITRAN
13	3505.270220	6.172E-25	3.430E-03	.0602	.3800	585.1619	.59	-.011900	4	1 6 0 6	7 1 7	5.85E-25	4. meas.
11	3505.414850	2.320E-25	2.906E-04	.0756	.3550	2129.5992	.73	-.003900	7	2 4 3 2	4 4 1	2.49E-25	HITRAN
11	3505.554890	3.909E-23	1.070E-02	.0382	.2650	1590.6908	.53	-.012700	5	1 7 7 0	8 7 1	3.89E-23	HITRAN
11	3505.555230	1.174E-22	1.071E-02	.0382	.2650	1590.6901	.53	-.012700	5	1 7 7 1	8 7 2	1.18E-22	2. meas.
12	3505.603760	3.272E-24	1.478E-03	.0907	.4690	414.1681	.69	-.007100	4	1 4 1 3	5 2 4	3.26E-24	2. meas.
13	3505.736870	6.253E-26	3.006E-04	.0838	.4380	781.3773	.59	-.001300	4	1 6 3 4	7 2 5	5.93E-26	2. meas.
11	3505.865600	2.695E-22	8.094E-04	.0700	.3230	888.5987	.64	-.002800	4	1 6 4 3	6 5 2	2.54E-22	5. meas.
13	3505.951420	1.832E-24	3.388E-03	.0595	.3910	584.9409	.59	-.009800	4	1 6 1 6	7 0 7	1.88E-24	3. meas.
11	3505.953510	4.196E-23	6.713E-06	.1000	.4950	285.4186	.77	-.009000	4	1 3 0 3	3 3 0	4.16E-23	5. meas.
11	3506.079440	7.746E-23	3.423E-04	.0760	.3880	742.0730	.69	-.003700	5	1 5 3 2	5 5 1	7.95E-23	3. meas.
12	3506.101980	1.852E-25	1.260E-03	.0655	.3600	1198.1995	.49	-.001200	4	1 9 1 8	9 2 7	1.86E-25	2. meas.
11	3506.178220	4.680E-26	3.106E-05	.0690	.3370	1998.9953	.41	.000000	3	111 6 5	11 5 6	6.29E-26	HITRAN
14	3506.185430	5.325E-26	1.579E-02	.0490	.1730	1406.6568	.37	.000000	5	112 111	13 212	5.28E-26	4. meas.
11	3506.225300	1.037E-26	2.473E-03	.0435	.3230	2983.3963	.36	.000000	4	114 410	14 5 9	1.40E-26	HITRAN
13	3506.408220	8.028E-27	1.729E-03	.0580	.3400	1337.4894	.49	-.014000	4	1 9 3 7	9 4 6	1.17E-26	10. meas.
11	3506.585340	2.170E-26	5.521E-05	.0515	.3310	2275.3729	.37	.000000	3	113 4 9	12 5 8	3.11E-26	HITRAN
11	3506.702950	2.154E-22	1.021E-04	.0804	.3720	508.8121	.64	-.002500	3	1 6 4 3	5 3 2	2.20E-22	3. meas.
14	3506.775480	1.549E-25	6.233E-03	.0825	.3600	995.7934	.45	.000000	5	1 9 2 7	10 3 8	1.56E-25	2. meas.
13	3506.819690	2.380E-25	1.632E-04	.0940	.4500	380.8059	.73	-.007900	5	1 3 1 3	4 3 2	2.48E-25	2. meas.
12	3507.012220	4.478E-24	1.052E-03	.0916	.4600	505.7287	.69	-.007800	5	1 4 1 3	5 3 2	4.56E-24	2. meas.
14	3507.023780	1.049E-25	3.097E-02	.0465	.1980	1405.8184	.37	.000000	5	112 111	13 112	1.10E-25	3. meas.
14	3507.196390	1.041E-25	3.086E-02	.0454	.1850	1406.6568	.37	.000000	5	112 211	13 212	1.04E-25	HITRAN
14	3507.207110	6.818E-26	2.295E-02	.0310	.2040	1432.7584	.36	.000000	5	113 013	14 114	6.82E-26	HITRAN
14	3507.218870	9.964E-26	3.354E-02	.0277	.2000	1432.7466	.36	.000000	5	113 013	14 014	1.07E-25	6. meas.
14	3507.220070	9.924E-26	3.341E-02	.0260	.1900	1432.7584	.36	.000000	5	113 113	14 114	1.07E-25	6. meas.
14	3507.231830	6.777E-26	2.281E-02	.0305	.2070	1432.7466	.36	.000000	5	113 113	14 014	6.78E-26	HITRAN
14	3507.245200	1.481E-26	1.306E-04	.0740	.3820	683.6101	.59	.000000	5	1 7 2 6	7 4 3	1.48E-26	HITRAN
11	3507.247320	1.799E-26	2.886E-03	.0160	.2180	3127.8619	.37	.000000	4	112 9 4	13 8 5	1.86E-26	HITRAN
12	3507.288330	5.446E-26	9.536E-06	.0850	.4300	445.3462	.59	.004200	3	1 7 2 5	6 1 6	4.76E-26	3. meas.
13	3507.329820	7.383E-27	4.355E-03	.0253	.2110	1770.8349	.39	-.012500	5	112 012	12 211	7.42E-27	10. meas.
11	3507.447190	1.323E-26	7.163E-04	.0586	.2600	2904.4283	.45	.000000	6	2 9 5 4	10 2 9	3.03E-26	HITRAN
14	3507.636580	6.979E-26	2.116E-02	.0649	.3480	1411.3201	.41	.000000	5	110 5 5	11 5 6	6.66E-26	4. meas.
12	3507.666370	1.295E-25	4.312E-04	.0720	.3530	1051.2030	.59	-.002700	4	1 7 4 3	7 5 2	1.27E-25	3. meas.
14	3507.699790	1.412E-25	2.901E-02	.0745	.2580	1331.2170	.39	.000000	5	111 2 9	12 210	1.49E-25	2. meas.
12	3507.796360	6.334E-26	2.754E-04	.0674	.3410	880.1145	.64	-.002000	4	1 6 4 2	6 5 1	6.17E-26	2. meas.
11	3507.826150	4.478E-25	7.688E-02	.0228	.2500	2915.8943	.41	-.011000	8	210 110	11 111	4.88E-25	5. meas.
11	3507.835090	1.339E-24	7.665E-02	.0228	.2400	2915.8743	.41	-.013000	8	210 010	11 011	1.42E-24	5. meas.
12	3507.874130	6.616E-26	9.799E-05	.0820	.3840	658.6100	.59	-.001000	3	1 7 4 4	6 3 3	6.33E-26	5. meas.
11	3507.921620	5.083E-26	3.860E-03	.0450	.3650	2748.0995	.37	.000000	5	113 4 9	13 6 8	5.16E-26	HITRAN
14	3507.961130	6.979E-26	2.109E-02	.0643	.3050	1410.5667	.41	.000000	5	110 5 6	11 5 7	7.34E-26	3. meas.
14	3508.034740	5.285E-26	1.560E-02	.0469	.1610	1405.8184	.37	.000000	5	112 211	13 112	5.93E-26	3. meas.
13	3508.249910	3.635E-26	1.921E-03	.0817	.4180	1048.6569	.53	-.004800	4	1 7 4 4	8 3 5	3.69E-26	4. meas.
11	3508.378980	9.480E-24	8.838E-03	.0588	.3280	1843.0297	.41	-.010000	4	110 5 5	11 4 8	9.44E-24	2. meas.
13	3508.414000	5.890E-25	1.431E-03	.0907	.4690	415.1280	.69	-.007100	4	1 4 1 3	5 2 4	5.93E-25	2. meas.
12	3508.604580	2.344E-25	1.667E-04	.0707	.3200	733.6829	.69	-.002000	4	1 5 4 1	5 5 0	2.30E-25	4. meas.

M represents the molecule and isotopic codes. Strengths in $molecules^{-1}\ cm^{-2}\ cm^{-1}$ at 296K. b° and d° are the half-width and pressure-induced frequency-shift coefficients, respectively, in cm^{-1}/atm.

Values given in the last two columns are the observed strength and estimated uncertainties, Δs%. If no value is given for Δs%, then the value for the strength was taken from the HITRAN2000 [177] listing and if no value is given for the observed strength, then the vibration-rotation transition for the molecular species is not given in the HITRAN2000 listing.

Table 8. File names and descriptions available on website (http://mark4sun.jpl.nasa.gov)

File name	Description
SISAM.H2O	Listing of $H_2{}^{16}O$, $H_2{}^{17}O$, $H_2{}^{18}O$, $HD^{16}O$, $HD^{17}O$, and $HD^{18}O$ parameters in a format similar to HITRAN, 500-8000 cm^{-1}
HITTOTH.H2O	Listing of $H_2{}^{16}O$, $H_2{}^{17}O$, $H_2{}^{18}O$, $HD^{16}O$, $HD^{17}O$, and $HD^{18}O$ parameters in HITRAN format, 500-8000, 500-8000 cm^{-1}
LEVELS.H2O	$H_2{}^{16}O$, $H_2{}^{17}O$, and $H_2{}^{18}O$ rotational energy levels with uncertainties for vibrational states that are involved in bands in the 500-8000 cm^{-1} region
LEVELS.HDO	$HD^{16}O$, $HD^{17}O$, and $HD^{18}O$ rotational energy levels with uncertainties for vibrational states that are involved in bands in the 500-8000 cm^{-1} region
WIDTOTH.TRA	Air-and self-broadened width coefficients and air-broadened pressure-induced frequency shifts for A-type transitions of H_2O. Measured and smoothed values
WIDTOTH.TRB	Air-and self-broadened width coefficients and air-broadened pressure-induced frequency shifts for B-type transitions of H_2O. Measured and smoothed values
WIDV20.TRA	Air-and self-broadened width coefficients for A-type transitions of H_2O. fitted values for bands with upper state $\nu_2 = 0$
WIDV21.TRA	Air-and self-broadened width coefficients for A-type transitions of H_2O. fitted values for bands with upper state $\nu_2 > 0$
WIDV20.TRB	Air-and self-broadened width coefficients for B-type transitions of H_2O. fitted values for bands with upper state $\nu_2 = 0$
WIDV21.TRB	Air-and self-broadened width coefficients for B-type transitions of H_2O. fitted values for bands with upper state $\nu_2 > 0$
HDOWID.AIR	Air-broadened width coefficients for transitions of HDO in then ν_2 band. Smoothed and measured values with measured uncertainties
HDOSHFT.AIR	Air-broadened pressure-induced frequency shift coefficients for transitions of HDO in the ν_2 band