Microwave Spectra of Molecules of Astrophysical Interest
V. Water Vapor*

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The available data on the microwave spectrum of water vapor are critically reviewed for information applicable to radio astronomy. Molecular data such as rotational constants, centrifugal distortion constants, hyperfine coupling parameters, and dipole moments are tabulated. A detailed centrifugal distortion calculation has been carried out for the most abundant isotopic form of this molecule $H_2{}^{16}O$, as well as for $H_2{}^{18}O$ and $HD^{16}O$. Transitions have been predicted and tabulated for the frequency range 1 MHz to 800 GHz. All predicted trasitions include 95 percent confidence limits; estimated error limits have been reported for all measured transitions. Observed transitions of $H_2{}^{17}O$ are also listed.

Key words: Hyperfine structure; interstellar molecules; microwave spectra; molecular parameters; radio astronomy; rotational transitions; water.

Contents

1. Introduction

The present tables represent the 5th part of a series of critical reviews [1–4][1] which are intended to update and revise the existing tabulated literature on the microwave spectra of molecules already identified in interstellar observations. For $H_2{}^{16}O$ and $H_2{}^{18}O$ all transitions below 800 GHz and between levels with total rotational energy below 1000 cm^{-1} have been observed in the laboratory and are listed in the tables in this review. Since the astrophysical observation of molecules is a relatively new field with poorly defined limitations, $HD^{16}O$ is also included in this review, although the cosmic abundance of deuterium is expected to be low. The spectral information reported for $HD^{16}O$ includes all predicted and observed transitions between 1 MHz and 800 GHz. The predicted transitions are further limited by fixing a maximum value of 1000 cm^{-1} for the total rotational energy of the lower state of the transition. It is felt that these limits are generous enough to allow for the presentation of all transitions which might be observed in the relatively near future. Several lines of the species $H_2{}^{17}O$ have been identified and measured; these lines are also listed in this review.

Rotational transitions of H_2O and HDO in vibrationally excited states have not been included in this review because of the large vibrational energies involved. Several rotational transitions of $H_2{}^{16}O$ and $HD^{16}O$ in the ν_2 excited state have recently been observed in the laboratory [5].

1.1. Molecular Parameter Table

The rotational and centrifugal distortion constants for $H_2{}^{16}O$ and $H_2{}^{18}O$ are shown in table 1. These were obtained from a weighted least-squares analysis of the observed microwave lines and selected infrared transitions [6, 7] using the following Hamiltonian:

$$\mathcal{H} = \mathcal{H}_r + \mathcal{H}_d^{(4)} + \mathcal{H}_d^{(6)} + \mathcal{H}_d^{(8)} + \mathcal{H}_d^{(10)}$$

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[1] Figures in brackets indicate literature references in section 1.4.

where

$$\mathscr{H}_r=\tfrac{1}{2}(B+C)\mathbf{P}^2+[A-\tfrac{1}{2}(B+C)]\mathbf{P}_z^2+\tfrac{1}{2}(B-C)\mathbf{P}_-^2,$$

$$\mathscr{H}_d^{(4)}=-\Delta_J\mathbf{P}^4-\Delta_{JK}\mathbf{P}^2\mathbf{P}_z^2-\Delta_K\mathbf{P}_z^4-2\delta_J\mathbf{P}^2\mathbf{P}_-^2$$

$$-\delta_K(\mathbf{P}_z^2\mathbf{P}_-^2+\mathbf{P}_-^2\mathbf{P}_z^2),$$

$$\mathscr{H}_d^{(6)}=H_J\mathbf{P}^6+H_{JK}\mathbf{P}^4\mathbf{P}_z^2+H_{KJ}\mathbf{P}^2\mathbf{P}_z^4+H_K\mathbf{P}_z^6$$

$$+2h_J\mathbf{P}^4\mathbf{P}_-^2+h_{JK}\mathbf{P}^2(\mathbf{P}_z^2\mathbf{P}_-^2+\mathbf{P}_-^2\mathbf{P}_z^2)$$

$$+h_K(\mathbf{P}_z^4\mathbf{P}_-^2+\mathbf{P}_-^2\mathbf{P}_z^4),$$

$$\mathscr{H}_d^{(8)}=L_J\mathbf{P}^8+L_{JK}\mathbf{P}^4\mathbf{P}_z^4+L_{KKJ}\mathbf{P}^2\mathbf{P}_z^6+L_K\mathbf{P}_z^8$$

$$+l_K(\mathbf{P}_z^6\mathbf{P}_-^2+\mathbf{P}_-^2\mathbf{P}_z^6),$$

$$\mathscr{H}_d^{(10)}=P_K\mathbf{P}_z^{10}+p_K(\mathbf{P}_z^8\mathbf{P}_-^2+\mathbf{P}_-^2\mathbf{P}_z^8),$$

$$\mathbf{P}^2=\mathbf{P}_x^2+\mathbf{P}_y^2+\mathbf{P}_z^2,$$

and

$$\mathbf{P}_-^2=\mathbf{P}_x^2-\mathbf{P}_y^2.$$

Also in table 1 are the molecular parameters for $HD^{16}O$ which were obtained from an analysis of 53 microwave transitions [8]. Details of these calculations and the statistical analysis have been discussed by Cook, Helminger, and De Lucia [6–11]. This analysis procedure is similar to ones reported by Kirchhoff [12] and Steenbeckeliers [13, 14]; relations among these formulations are discussed in reference 10. All analyses reported in this review are performed in the semi-rigid rotor basis [10]. As pointed out in an earlier part of this series [1–4], it is necessary to retain more significant figures in the spectral constants than indicated by the statistical error limits if the constants are to reproduce the observed spectra within experimental error. This is particularly true for light molecules such as water where the obtained values of the parameters are extremely sensitive to the choice of which parameters are to be varied.

1.2. Microwave Spectral Tables

Table 2 contains the results of the experimental work on $H_2{}^{16}O$ and $H_2{}^{18}O$. Unlike the previous molecules reviewed in this series, all of the transitions that satisfy the appropriate criteria for inclusion in this table, i.e., which occur between 1 MHz and 800 GHz and whose lower energy state is below 1000 cm^{-1}, have been observed in the laboratory. Table 2, therefore, lists only the upper and lower state quantum numbers in the form J (K_p,K_o), the observed frequency for each isotopic species and an estimate of its uncertainty, the energy of the lower state, the strength of the transition, and the reference. Table 3 contains the results of the statistical analysis of the spectrum of $HD^{16}O$. For each spectral line the first column of table 3 contains the upper state and lower state quantum numbers in the form, J (K_p,K_o) for a rigid asymmetric rotor. The quantum numbers are followed by the observed line frequency and, in parentheses, the estimated experimental uncertainty in MHz. The third column contains the calculated line frequency and estimated uncertainty in MHz. The calculated uncertainties represent 95 percent confidence levels, which are approximately twice (this varies slightly with the amount of data included in the calculation) the standard deviation obtained from the least squares analysis. The line strengths for the rotational transitions are shown in column 4, followed by the total rotational energy of each rotational level. These energies were calculated from the rotation and distortion constants listed in table 1. References to the laboratory measurements are shown in the last column of table 3.

It should be pointed out that the rotation-distortion analysis of asymmetric molecules with large rotational constants is somewhat less straightforward than the analysis of heavier molecules. It is clear that as more transitions at higher J are added to the analysis, more terms must also be added to the Hamiltonian. A corollary of this is that the statistical uncertainty of a transition beyond the range of the observed data set may be unrealistically small because the uncertainties in these additional terms in the Hamiltonian would contribute additional unaccounted error to the calculated uncertainty.

In both tables 2 and 3 the line strengths for the unsplit rotational transitions are listed. These line strengths, denoted by ${}^xS(J'_{K'_p,K'_o};\,J''_{K''_p,K''_o})$, are defined in this review as:

$$ {}^xS(J'_{K'_p,K'_o};\,J''_{K''_p,K''_o})=\frac{(2J+1)|\mu_{J'\leftarrow J''}|^2}{\mu_x^2}$$

where the superscript x refers to one of the principal axes of the molecule ($x=a$, b or c); $|\mu_{J'}\leftarrow{}_{J''}|$ is the dipole moment matrix element connecting the upper, $J'_{K'_p,K'_o}$, and lower, $J''_{K''_p,K''_o}$, rotational levels involved in the transition; and μ_x is the magnitude of the component of μ along the x axis. Thus the line strength as defined is independent of the absolute magnitude of the dipole moment. It should be noted that these line strengths were calculated using wave functions which included the centrifugal distortion constants of table 1 but ignoring the effects of centrifugal distorition on the dipole operator itself [15].

Since in the case of H_2O the two hydrogens are indistinguishable particles, the statistical weight of each rotational state must be considered in any calculation of spectral intensities. States for which the K_p, K_o subscripts are both even (*ee*) or both odd (*oo*) have statistical weight one, while the remaining states have statistical weight three. These factors are not included in the tabulated line strengths.

Table 4 lists observed transitions of $H_2{}^{17}O$. Although it is not possible to analyze this isotopic species in the above manner because of the limited number of laboratory measurements, these transitions would appear to be prime candidates for astrophysical observation.

Because of the nuclear moments of the hydrogen and deuterium nucleus, small splittings of the rotational levels listed in these tables exist. These splittings may be calculated from the hyperfine constants listed in table 5. Calculation of splittings from these constants is somewhat complicated because of the asymmetric nature of the molecule and the fact that there is more than one coupling nucleus in each case. This problem has been discussed by several authors [16–18]. The splittings have not been listed in the tables primarily because their small size makes it unlikely that they will be observed astrophysically, and because of the complexity involved in the calculation of the structure for each transition. If these calculations are required for the positive identification of an astrophysical observation, the authors of this review possess the necessary programs.

As a convenience to the user, the calculated unsplit transition frequencies of HDO from table 3 have been listed according to increasing frequency in table 6.

1.3. List of Symbols and Conversion Factors

a. Symbols

A, B, C	Rotational constants (MHz). $A \geqslant B \geqslant C$. These correspond to $\mathscr{A}$, $\mathscr{B}$, $\mathscr{C}$ in references 6–11.
Δ, δ	Quartic centrifugal distortion constants (MHz).
H, h	Sextic centrifugal distortion constants (MHz).
L, l	Octic centrifugal distortion constants (MHz).
P, p	Dectic centrifugal distortion constants (MHz).
$\mathbf{P}_x^2 \mathbf{P}_y^2 \mathbf{P}_z^2$	Angular momentum operators.
a, b, c	Principal axes corresponding to A, B, and C, respectively.
$\mu_{a,b,c}$	Components of the dipole moment along the principal axes (Debye).
χ_{ij}	Elements of the quadrupole coupling tensor (kHz).
T_{ij}	Elements of the spin-rotation tensor (Dimensionless).
$I_{a,b,c}$	Monents of inertia of whole molecule with respect to the indicated principal axis.
F	Total angular momentum quantum number which includes the nuclear spin for the ^{17}O coupling.
J	Total rotational angular momentum quantum number.
K_p	Projection of J on the summetry axis in the limiting prolate symmetric top.
K_o	Projection of J on the symmetry axis in the limiting oblate symmetric top.

b. Conversion Factors

The following conversion factors have been used:

$$A, B, C \text{ (MHz)} = \frac{5.05376 \times 10^5}{I_{a,b,c}\,(\text{amu Å}^2)}.$$

Frequency-wave number conversion factor: 29979.25 MHz/cm^{-1}.

In keeping with commonly accepted conventions in molecular spectroscopy, certain energies have been expressed in their wavenumber (cm^{-1}) equivalents. The actual energy can be obtained by multiplying the cm^{-1} equivalent by hc.

In an attempt to increase the usefulness of this series, the format of the earlier contributions to this series by D. R. Johnson, F. J. Lovas, and W. H. Kirchhoff of the National Bureau of Standards has been followed whenever possible. We are also indebted to R. L. Cook for the development of the computer programs used in the analysis, and to Professor Walter Gordy for his support and encouragement during this work.

1.4. References

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2. Water Spectral Tables

TABLE 1. Molecular parameters for water

	$H_2{}^{16}O$	$H_2{}^{18}O$	$HD^{16}O$
Rotational constants (MHz)	Ref. 72A	Ref. 72C	Ref. 71E
A	$835\,840.288 \pm 1.00$	$825\,366.08 \pm 8.7$	$701\,931.502 \pm 0.22$
B	$435\,351.717 \pm 0.90$	$435\,331.59 \pm 8.0$	$272\,912.599 \pm 0.11$
C	$278\,138.700 \pm 0.90$	$276\,950.46 \pm 8.0$	$192\,055.245 \pm 0.10$
Distortion constants (MHz)	Ref. 72A	Ref. 72C	Ref. 71E
Δ_J	$(3.759422 \pm 0.0049) \times 10^{1}$	$(3.72938 \pm 0.030) \times 10^{1}$	$(1.083749 \pm 0.00058) \times 10^{1}$
Δ_{JK}	$(-1.729128 \pm 0.0034) \times 10^{2}$	$(-1.70204 \pm 0.013) \times 10^{2}$	$(3.420729 \pm 0.0037) \times 10^{1}$
Δ_K	$(9.7329052 \pm 0.0019) \times 10^{2}$	$(9.596441 \pm 0.023) \times 10^{2}$	$(3.7707828 \pm 0.00026) \times 10^{2}$
δ_J	$(1.521040 \pm 0.0020) \times 10^{1}$	$(1.52431 \pm 0.012) \times 10^{1}$	$(3.647126 \pm 0.0014) \times 10^{0}$
δ_K	$(4.10502 \pm 0.030) \times 10^{1}$	$(3.1463 \pm 0.12) \times 10^{1}$	$(6.308750 \pm 0.0035) \times 10^{1}$
H_J	$(1.56556 \pm 0.039) \times 10^{-2}$	$(1.412 \pm 0.34) \times 10^{-2}$	$(1.1275 \pm 0.099) \times 10^{-3}$
H_{JK}	$(-4.2081 \pm 1.1) \times 10^{-2}$		$(7.3435 \pm 0.091) \times 10^{-2}$
H_{KJ}	$(-5.09508 \pm 0.21) \times 10^{-1}$	$(-4.5260 \pm 0.71) \times 10^{-1}$	$(-2.740667 \pm 0.022) \times 10^{-1}$
H_K	$(3.733028 \pm 0.015) \times 10^{0}$	$(5.08511 \pm 0.24) \times 10^{0}$	$(1.465159 \pm 0.0027) \times 10^{0}$
h_J	$(7.79579 \pm 0.18) \times 10^{-3}$	$(7.8937 \pm 1.1) \times 10^{-3}$	$(6.5461 \pm 0.15) \times 10^{-4}$
h_{JK}	$(-2.5165 \pm 0.22) \times 10^{-2}$	$(-1.716 \pm 2.8) \times 10^{-2}$	$(3.0963 \pm 0.037) \times 10^{-2}$
h_K	$(1.0971 \pm 0.052) \times 10^{0}$		$(5.54951 \pm 0.055) \times 10^{-1}$
L_J			$(2.1939 \pm 0.40) \times 10^{-6}$
L_{JK}	$(-3.0647 \pm 0.93) \times 10^{-3}$		$(-7.45685 \pm 0.45) \times 10^{-4}$
L_{KKJ}	$(1.02952 \pm 0.24) \times 10^{-2}$		$(2.86575 \pm 0.091) \times 10^{-3}$
L_K	$(-2.340138 \pm 0.15) \times 10^{-2}$	$(-9.59337 \pm 0.83) \times 10^{-2}$	$(-7.557072 \pm 0.10) \times 10^{-3}$
l_K	$(-1.3546 \pm 0.20) \times 10^{-2}$	$(2.351 \pm 0.24) \times 10^{-2}$	$(-5.69461 \pm 0.24) \times 10^{-3}$
P_K	$(5.19841 \pm 0.15) \times 10^{-5}$	$(1.4491 \pm 0.13) \times 10^{-3}$	$(1.90459 \pm 0.10) \times 10^{-5}$
p_K	$(3.7603 \pm 2.1) \times 10^{-5}$		$(1.4074 \pm 0.39) \times 10^{-5}$
Dipole moment (Debye)	Ref. 73A and 73B		Ref. 73A
μ_a			0.6567 ± 0.0004
μ_b	1.8546 ± 0.0004		1.7318 ± 0.0009

TABLE 2. Microwave spectra of $H_2{}^{16}O$ and $H_2{}^{18}O$ [a]

Transition		$H_2{}^{16}O$				$H_2{}^{18}O$			
Upper state	Lower state	Observed frequency (MHz) (Est. uncertainty)	Lower state energy level (cm^{-1})	Line strength	Ref.	Observed frequency (MHz) (Est. uncertainty)	Lower state energy level (cm^{-1})	Line strength	Ref.
1(1, 0)–	1(0, 1)	556 936.002(0.089)	23.794	1.500	72A	547 676.44(0.06)	23.754	1.500	72C
2(1, 1)–	2(0, 2)	752 033.227(0.489)	70.091	2.073	72A	745 320.20(0.48)	69.925	2.061	72C
3(1, 3)–	2(2, 0)	183 310.0906(0.0015)	136.164	0.102	71A	203 407.52(0.02)	134.780	0.100	72C
4(1, 4)–	3(2, 1)	380 197.372(0.025)	212.157	0.123	72A	390 607.76(0.04)	210.795	0.119	72C
4(2, 3)–	3(3, 0)	448 001.075(0.022)	285.419	0.132	72A	489 054.26(0.08)	282.302	0.132	72C
5(1, 5)–	4(2, 2)	325 152.919(0.027)	315.780	0.091	72A	322 465.17(0.05)	314.455	0.086	72C
5(3, 3)–	4(4, 0)	474 689.127(0.072)	488.135	0.118	72A	537 337.57(0.47)	482.671	0.119	72C
5(3, 2)–	4(4, 1)	620 700.807(0.387)	488.108	0.122	72A	692 079.14(0.60)	482.642	0.123	72C
6(1, 6)–	5(2, 3)	22 235.07985(0.00005)	446.511	0.057	69G	5 625.147(0.015)	445.155	0.053	70B
6(4, 3)–	5(5, 0)	439 150.812(0.053)	742.078	0.101	72A	520 137.32(0.47)	733.696	0.103	72C
6(4, 2)–	5(5, 1)	470 888.947(0.192)	742.074	0.102	72A	554 859.87(0.49)	733.692	0.103	72C
6(2, 4)–	7(1, 7)	488 491.133(0.375)	586.480	0.036	72A	517 181.96(0.21)	583.987	0.033	72C
7(5, 3)–	6(6, 0)	437 346.667(0.201)	1 045.063	0.088	72A				
7(5, 2)–	6(6, 1)	443 018.295(0.210)	1 045.062	0.088	72A				
10(2, 9)–	9(3, 6)	321 225.644(0.244)	1 282.924	0.089	72A				

[a] For $H_2{}^{16}O$ and $H_2{}^{18}O$ all transitions below 800 GHz and between levels with total rotational energy below 1000 cm^{-1} have been observed in the laboratory and are listed in this table.

TABLE 3. Microwave spectrum of HD^{16}O. Frequencies are in MHz units

Transition		Observed frequency (Est. uncertainty)[a]	Calculated frequency (Est. uncertainty)[b]	Line strength	Energy levels in cm^{-1}		
Upper state	Lower state				Upper state	Lower state	Ref.
1(1, 0)–	1(1, 1)	80 578.150	80 578.283(0.052)	1.500	32.496	29.809	56B
1(0, 1)–	0(0, 0)	464 924.520(0.032)	464 924.503(0.154)	1.000	15.508	0.0	71E
1(1, 0)–	1(0, 1)	509 292.420(0.045)	509 292.435(0.150)	1.500	32.496	15.508	71E
2(1, 1)–	2(1, 2)	241 561.550(0.037)	241 561.524(0.113)	0.833	66.185	58.127	71E
2(2, 0)–	2(2, 1)	10 278.2455(0.0010)	10 278.280(0.013)	3.315	109.269	108.926	64A
2(1, 1)–	2(0, 2)	599 926.710(0.122)	599 926.747(0.129)	2.279	66.185	46.173	71E
2(0, 2)–	1(1, 1)	490 596.640(0.058)	490 596.693(0.153)	0.633	46.173	29.809	71E
3(1, 2)–	3(1, 3)	481 779.500(0.282)	481 779.345(0.137)	0.587	116.461	100.391	71E
3(2, 1)–	3(2, 2)	50 236.300	50 236.435(0.047)	2.274	157.065	155.389	56B
3(3, 0)–	3(3, 1)	824.6706(0.0020)	824.672(0.003)	5.238	233.051	233.024	62A
2(2, 0)–	3(0, 3)		537 792.770(0.239)	0.006	109.269	91.330	
3(1, 2)–	3(0, 3)	753 411.150(0.376)	753 411.151(0.208)	2.752	116.461	91.330	71E
2(2, 0)–	3(1, 3)	266 161.070(0.025)	266 160.964(0.140)	0.132	109.269	100.391	71E
3(1, 2)–	2(2, 1)	225 896.720(0.038)	225 896.661(0.157)	0.228	116.461	108.926	71E
4(1, 3)–	4(1, 4)		797 486.719(0.253)	0.463	182.984	156.382	
4(2, 2)–	4(2, 3)	143 727.210(0.037)	143 727.393(0.087)	1.684	221.836	217.042	71E
4(3, 1)–	4(3, 2)	5 702.780	5 702.841(0.015)	4.010	295.677	295.487	53E
4(4, 0)–	4(4, 1)		54.618(0.001)	7.190	402.331	402.329	
3(2, 1)–	4(0, 4)	207 110.65(0.1)[c]	207 111.227(0.276)	0.018	157.065	150.156	73C
3(2, 1)–	4(1, 4)	20 460.010	20 460.065(0.130)	0.223	157.065	156.382	70G
3(3, 0)–	4(2, 3)	479 947.370(0.104)	479 947.467(0.158)	0.131	233.051	217.042	71E
3(3, 1)–	4(2, 2)	335 395.500(0.026)	335 395.402(0.159)	0.138	233.024	221.836	71E
5(2, 3)–	5(2, 4)	310 533.290(0.051)	310 533.472(0.116)	1.296	303.995	293.637	71E
5(3, 2)–	5(3, 3)	22 307.670(0.050)	22 307.495(0.044)	3.218	374.410	373.666	48B
5(4, 1)–	5(4, 2)	486.528(0.002)	486.521(0.004)	5.835	480.259	480.243	62A
5(5, 0)–	5(5, 1)		3.259(0.000)	9.157	615.970	615.970	
5(0, 5)–	4(2, 2)		3 296.488(0.243)	0.026	221.946	221.836	
5(1, 5)–	4(2, 2)	120 778.190(0.014)	120 778.173(0.153)	0.238	225.865	221.836	71E
4(3, 1)–	5(2, 4)	61 185.950	61 186.057(0.133)	0.298	295.677	293.637	70D
5(2, 3)–	4(3, 2)	255 050.260(0.059)	255 050.256(0.149)	0.338	303.995	295.487	71E
6(2, 4)–	6(2, 5)	559 816.740(0.285)	559 816.651(0.218)	1.029	403.549	384.876	71E
6(3, 3)–	6(3, 4)	64 427.340	64 427.239(0.088)	2.643	469.664	467.515	70D
6(4, 2)–	6(4, 3)	2 394.560(0.050)	2 394.534(0.015)	4.890	573.972	573.892	55A
6(5, 1)–	6(5, 2)		35.484(0.001)	7.710	709.172	709.170	
6(0, 6)–	5(2, 3)	69 550.580	69 550.561(0.233)	0.027	306.315	303.995	70G
5(3, 2)–	6(1, 5)		356 839.620(1.793)	0.017	374.410	362.507	
6(1, 6)–	5(2, 3)	138 530.570(0.057)	138 530.586(0.150)	0.200	308.616	303.995	71E
6(2, 5)–	5(3, 2)	313 750.620(0.031)	313 750.749(0.208)	0.450	384.876	374.410	71E
5(4, 1)–	6(3, 4)	382 065.100(0.090)	382 065.035(0.171)	0.267	480.259	467.515	71E
5(4, 2)–	6(3, 3)	317 151.250(0.048)	317 151.275(0.172)	0.270	480.243	469.664	71E
7(3, 4)–	7(3, 5)	151 616.190(0.026)	151 616.055(0.122)	2.188	581.964	576.906	71E
7(4, 3)–	7(4, 4)	8 577.812	8 577.761(0.040)	4.183	683.614	683.328	68A
7(5, 2)–	7(5, 3)		209.887(0.005)	6.643	818.022	818.015	
7(6, 1)–	7(6, 2)		2.340(0.000)	9.617	981.144	981.144	
6(2, 4)–	7(0, 7)	11 618.2(0.1)[c]	11 618.083(0.351)	0.022	403.549	403.162	73D
7(1, 6)–	6(3, 3)		127 527.533(3.002)	0.033	473.918	469.664	
7(1, 7)–	6(2, 4)	26 880.380(0.050)	26 880.371(0.206)	0.148	404.446	403.549	53E
7(2, 6)–	6(3, 3)		622 483.456(0.613)	0.548	490.428	469.664	
7(3, 5)–	6(4, 2)	87 962.810(0.014)	87 962.882(0.178)	0.448	576.906	573.972	71E
7(3, 4)–	6(4, 3)	241 973.570(0.039)	241 973.471(0.178)	0.460	581.964	573.892	71E
6(5, 1)–	7(4, 4)		774 776.302(2.124)	0.231	709.172	683.328	
6(5, 2)–	7(4, 3)		766 163.057(2.144)	0.231	709.170	683.614	
8(3, 5)–	8(3, 6)	305 038.550(0.112)	305 038.652(0.225)	1.812	711.799	701.624	71E
8(4, 4)–	8(4, 5)	24 884.770(0.050)	24 884.785(0.081)	3.620	809.402	808.572	53E
8(5, 3)–	8(5, 4)		892.229(0.017)	5.818	942.579	942.549	
7(2, 5)–	8(0, 8)		228 072.253(0.511)	0.016	520.124	512.516	
8(1, 7)–	7(3, 4)		497 675.668(4.533)	0.049	598.564	581.964	
7(2, 5)–	8(1, 8)	207 345.710(0.072)	207 345.707(0.235)	0.105	520.124	513.208	71E
8(3, 6)–	7(4, 3)	539 935.900(0.336)	539 935.881(0.237)	0.629	701.624	683.614	71E
7(5, 2)–	8(4, 5)	283 318.590(0.023)	283 318.515(0.173)	0.401	818.022	808.572	71E
7(5, 3)–	8(4, 4)	258 223.760(0.104)	258 223.843(0.172)	0.402	818.015	809.402	71E
9(3, 6)–	9(3, 7)		540 375.466(0.943)	1.503	859.401	841.376	

TABLE 3. Microwave spectrum of $HD^{16}O$. Frequencies are in MHz units—Continued

Transition		Observed frequency (Est. uncertainty)[a]	Calculated frequency (Est. uncertainty)[b]	Line strength	Energy levels in cm^{-1}		
Upper state	Lower state				Upper state	Lower state	Ref.
9(4, 5)–	9(4, 6)	61 704.590	61 704.801(0.118)	3.148	951.653	949.594	70D
9(5, 4)–	9(5, 5)	3 044.710(0.100)	3 044.641(0.049)	5.152	1 082.918	1 082.816	55A
8(2, 6)–	9(0, 9)		559 427.696(1.958)	0.011	653.091	634.430	
9(1, 8)–	8(3, 5)		717 684.049(6.106)	0.058	735.739	711.799	
8(4, 4)–	9(2, 7)		232 421.557(21.849)	0.024	809.402	801.649	
8(2, 6)–	9(1, 9)		548 552.311(1.772)	0.075	653.091	634.793	
9(4, 6)–	8(5, 3)	210 310.650(0.021)	210 310.585(0.178)	0.587	949.594	942.579	71E
9(4, 5)–	8(5, 4)	272 907.540(0.026)	272 907.615(0.180)	0.590	951.653	942.549	71E
10(4, 6)–	10(4, 7)	134 770.220(0.039)	134 770.134(0.225)	2.734	1 110.791	1 106.296	71E
10(5, 5)–	10(5, 6)	8 837.210	8 837.102(0.110)	4.597	1 239.144	1 238.850	71B
10(1, 9)–	9(3, 6)		769 625.323(9.026)	0.055	885.073	859.401	
10(2, 8)–	9(4, 5)		395 998.169(30.834)	0.041	964.862	951.653	
9(6, 3)–	10(5, 6)	169 246.050	169 245.965(0.178)	0.532	1 244.495	1 238.850	71E
9(6, 4)–	10(5, 5)	160 329.460	160 329.545(0.178)	0.533	1 244.492	1 239.144	71E
11(5, 6)–	11(5, 7)	22 581.570	22 581.668(0.166)	4.117	1 411.413	1 410.660	71B
12(5, 7)–	12(5, 8)	51 917.870	51 917.861(0.233)	3.690	1 599.950	1 598.219	71B
11(7, 4)–	12(6, 7)	31 670.430		0.662	1 757.574	1 756.516	71B
11(7, 5)–	12(6, 6)	28 668.340		0.662	1 757.574	1 756.615	71B
13(2,12)–	12(3, 9)	45 902.540		0.175	1 406.716	1 405.184	71B

[a] For reference 71E, the estimated experimental uncertainties are the rms deviations of 5 or more measurements of each line frequency and include no correction for possible systematic effects. These may be particularly useful in identifying lines which are difficult to meas because of low signal-to-noise ratio. For all other references, the values are those quoted by the author.

[b] See text.

[c] Recently reported measurements and not included in the least square fit.

TABLE 4. Observed microwave spectrum of $H_2{}^{17}O$.[a] Ref. 71C.

Transition	F–F′	Observed frequency (MHz)
3(1, 3)– 2(2, 0)[b]	7/2–9/2	193 999.94
	7/2–7/2	193 999.94
	5/2–7/2	193 999.94
	5/2–5/2	194 001.70
	9/2–9/2	194 001.70
	3/2–5/2	194 002.98
	9/2–11/2	194 004.13
	3/2–3/2	194 004.13
6(1, 6)– 5(2, 3)[c]	11/2–13/2	13 533.79
	13/2–15/2	13 534.41
	9/2–11/2	13 534.41
	7/2–9/2	13 536.02
	15/2–17/2	13 537.06
	5/2–7/2	13 537.97

[a] The transitions of $H_2{}^{17}O$ are split by a quadrupole interaction of the ^{17}O nucleus (spin 5/2). The quadrupole coupling constants of $H_2{}^{17}O$ are listed in Ref. 71C.

[b] Calculated unsplit frequency: $f_0 = 194\,002.29$ MHz.

[c] Calculated unsplit frequency: $f_0 = 13\,535.51$ MHz.

TABLE 5. Hyperfine constants of water

Elements of the deuterium quadrupole coupling tensor[a]. Ref. 67C.	
χ_{xx}	307.91 ± 0.14 kHz
χ_{yy}	− 133.13 ± 0.14 kHz
χ_{zz}	− 174.78 ± 0.20 kHz
α	−1°16′ ± 3′ (73E)
Elements of the hydrogen spin-rotation tensor[b]. Ref. 67D.	
T_{aa}	$(-4225 \pm 21) \times 10^{-11}$
T_{bb}	$(-7068 \pm 83) \times 10^{-11}$
T_{cc}	$(-11885 \pm 56) \times 10^{-11}$
T_{ab}	$(5344 \pm 9) \times 10^{-11}$

[a] The axis system (*x*, *y*, *z*) is the principal axis system of the deuterium quadrupole coupling tensor in either HDO or D_2O and is related to a set of molecule-fixed axes, centered at either deuterium atom, in the following way. Let *X* be a molecule-fixed axis along the OD bond with the positive sense in the O to D direction. Let *Y* be the other axis in the plane of the molecule with the positive direction pointing away from the bisector of the DOD (or HOD) angle. The *Z* axis is perpendicular to the plane of the molecule and the positive direction is determined by letting *X*, *Y*, *Z* be a right-handed coordinate system. The deuterium fixed coordinates, *x*, *y*, *z*, also form a right-handed coordinate system with the *z* axis being identical to the

Z axis. The x, y axes are obtained by rotation of the X, Y axes about the Z axis by an angle of α. The negative sign of α implies that the x axis is rotated from the X axis toward the bisector of the DOD angle.

[b]The axis system (a, b, c) is the principal inertial axis system of the H_2O molecule.

TABLE 6. Microwave transitions of $HD^{16}O$ in order of frequency

Frequency (MHz)	Transition	Estimated uncertainty (MHz)
2.340	7(6, 1)— 7(6, 2)	(0.000)
3.259	5(5, 0)— 5(5, 1)	(0.000)
35.484	6(5, 1)— 6(5, 2)	(0.001)
54.618	4(4, 0)— 4(4, 1)	(0.001)
209.887	7(5, 2)— 7(5, 3)	(0.005)
486.521	5(4, 1)— 5(4, 2)	(0.004)
824.672	3(3, 0)— 3(3, 1)	(0.003)
892.229	8(5, 3)— 8(5, 4)	(0.017)
2 394.534	6(4, 2)— 6(4, 3)	(0.015)
3 044.641	9(5, 4)— 9(5, 5)	(0.049)
3 296.488	5(0, 5)— 4(2, 2)	(0.243)
5 702.841	4(3, 1)— 4(3, 2)	(0.015)
8 577.761	7(4, 3)— 7(4, 4)	(0.040)
8 837.102	10(5, 5)—10(5, 6)	(0.110)
10 278.280	2(2, 0)— 2(2, 1)	(0.013)
11 618.083	6(2, 4)— 7(0, 7)	(0.351)
20 460.065	3(2, 1)— 4(1, 4)	(0.130)
22 307.495	5(3, 2)— 5(3, 3)	(0.044)
22 581.668	11(5, 6)—11(5, 7)	(0.166)
24 884.785	8(4, 4)— 8(4, 5)	(0.081)
26 880.371	7(1, 7)— 6(2, 4)	(0.206)
50 236.435	3(2, 1)— 3(2, 2)	(0.047)
51 917.861	12(5, 7)—12(5, 8)	(0.233)
61 186.057	4(3, 1)— 5(2, 4)	(0.133)
61 704.801	9(4, 5)— 9(4, 6)	(0.118)
64 427.239	6(3, 3)— 6(3, 4)	(0.088)
69 550.561	6(0, 6)— 5(2, 3)	(0.233)
80 578.283	1(1, 0)— 1(1, 1)	(0.052)
87 962.882	7(3, 5)— 6(4, 2)	(0.178)
120 778.173	5(1, 5)— 4(2, 2)	(0.153)
127 527.533	7(1, 6)— 6(3, 3)	(3.002)
134 770.134	10(4, 6)—10(4, 7)	(0.225)
138 530.586	6(1, 6)— 5(2, 3)	(0.150)
143 727.393	4(2, 2)— 4(2, 3)	(0.087)
151 616.055	7(3, 4)— 7(3, 5)	(0.122)
160 329.545	9(6, 4)—10(5, 5)	(0.178)
169 245.965	9(6, 3)—10(5, 6)	(0.178)
207 111.227	3(2, 1)— 4(0, 4)	(0.276)
207 345.707	7(2, 5)— 8(1, 8)	(0.235)
210 310.585	9(4, 6)— 8(5, 3)	(0.178)
225 896.661	3(1, 2)— 2(2, 1)	(0.157)
228 072.253	7(2, 5)— 8(0, 8)	(0.511)
232 421.557	8(4, 4)— 9(2, 7)	(21.849)
241 561.524	2(1, 1)— 2(1, 2)	(0.113)
241 973.471	7(3, 4)— 6(4, 3)	(0.178)
255 050.256	5(2, 3)— 4(3, 2)	(0.149)
258 223.843	7(5, 3)— 8(4, 4)	(0.172)
266 160.964	2(2, 0)— 3(1, 3)	(0.140)
272 907.615	9(4, 5)— 8(5, 4)	(0.180)
283 318.515	7(5, 2)— 8(4, 5)	(0.173)
305 038.652	8(3, 5)— 8(3, 6)	(0.225)
310 533.472	5(2, 3)— 5(2, 4)	(0.116)
313 750.749	6(2, 5)— 5(3, 2)	(0.208)
317 151.275	5(4, 2)— 6(3, 3)	(0.172)
335 395.402	3(3, 1)— 4(2, 2)	(0.159)
356 839.620	5(3, 2)— 6(1, 5)	(1.793)
382 065.035	5(4, 1)— 6(3, 4)	(0.171)
395 998.169	10(2, 8)— 9(4, 5)	(30.834)
464 924.503	1(0, 1)— 0(0, 0)	(0.154)
479 947.467	3(3, 0)— 4(2, 3)	(0.158)
481 779.345	3(1, 2)— 3(1, 3)	(0.137)
490 596.693	2(0, 2)— 1(1, 1)	(0.153)
497 675.668	8(1, 7)— 7(3, 4)	(4.533)
509 292.435	1(1, 0)— 1(0, 1)	(0.150)
537 792.770	2(2, 0)— 3(0, 3)	(0.239)
539 935.881	8(3, 6)— 7(4, 3)	(0.237)
540 375.466	9(3, 6)— 9(3, 7)	(0.943)
548 552.311	8(2, 6)— 9(1, 9)	(1.772)
559 427.696	8(2, 6)— 9(0, 9)	(1.958)
559 816.651	6(2, 4)— 6(2, 5)	(0.218)
599 926.747	2(1, 1)— 2(0, 2)	(0.129)
622 483.456	7(2, 6)— 6(3, 3)	(0.613)
717 684.049	9(1, 8)— 8(3, 5)	(6.106)
753 411.151	3(1, 2)— 3(0, 3)	(0.208)
766 163.057	6(5, 2)— 7(4, 3)	(2.144)
769 625.323	10(1, 9)— 9(3, 6)	(9.026)
774 776.302	6(5, 1)— 7(4, 4)	(2.124)
797 486.719	4(1, 3)— 4(1, 4)	(0.253)

2.1. Water References

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