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Emission Spectrum of Hot HDO in the 380–2190 cm^{-1} Region

T. Parekunnel,* P. F. Bernath,*[,1] N. F. Zobov,†[,2] S. V. Shirin,†[,2] Oleg L. Polyansky,†[,2] and Jonathan Tennyson†

*Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada N2L 3G1; and †Department of Physics and Astronomy, University College London, London WC1E 6BT, United Kingdom

E-mail: bernath@uwaterloo.ca, j.tennyson@ucl.ac.uk

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Fourier transform emission spectra were recorded using a mixture of H_2O and D_2O at a temperature of 1500°C. The spectra were recorded in three overlapping sections and cover the wavenumber range 380–2190 cm^{-1}. A total of 22 106 lines were measured, of which 60% are thought to belong to HDO. A total of 6430 HDO transitions are assigned, including the first transitions to the (040) vibrational state, with a term value of 5420.042 cm^{-1}. A total of 1536 new energy levels of HDO belonging to the (000), (010), (020), (030), and (040) states are presented, significantly extending the degree of rotational excitation compared to previous studies. © 2001 Elsevier Science

Key Words: water vapor; infrared spectrum; emission; line assignments; hot bands.

1. INTRODUCTION

In recent years there has been great progress in the experimental and theoretical understanding of the energy level structure of water (*1*). On the experimental side, new overtone spectra of water have been recorded in the visible and near UV regions (*2*–*3*). In the infrared, new spectra of hot water emission have now been measured (*4*–*7*) from 400 to 6000 cm^{-1} in the laboratory. Hot water vapor lines have also been seen in absorption in the spectra of sunspots (*4, 6, 8*) ("Water on the Sun"). On the theoretical side, the availability of high quality *ab initio* potential energy surfaces (*9*) and the direct variational calculation of vibration–rotation energy levels have revolutionized the analysis of water spectra (*10*).

Progress for the HDO isotopomer has been much less satisfactory. In particular, no spectra of hot HDO have been analyzed to date. We report such observations in this paper.

The HDO molecule is of interest for a number of reasons. Because H_2O is so abundant in our atmosphere, HDO can be detected readily in atmospheric absorption spectra using the sun as a source (*11*). Astrophysicists are also interested in HDO because nearly all of the deuterium now in the Universe was formed in the Big Bang (*12*). The D/H ratio is thus an important parameter with cosmological significance. The ratio D/H can be determined for objects such as comets from the relative HDO to H_2O abundances (*13*).

In molecular physics, the HDO energy levels can be used to study the breakdown of the Born–Oppenheimer approximation. At the moment, this breakdown is the largest source of error in the calculation of water vibration–rotation energy levels from an *ab initio* potential energy surface. The potential surface can be corrected empirically (*9*–*10*), but recently Schwenke (*14*) calculated *ab initio* a complete set of corrections for the breakdown of the Born–Oppenheimer approximation in water. The experimental energy levels of both HDO and H_2O are needed for comparison with theory. The HDO molecule is also a popular molecule for mode-selective laser chemistry by dissociation (e.g., *15*).

The infrared spectra of HDO were first measured by Benedict *et al.* (*16*) in 1956, followed by work in France (e.g., *17*). Since then there has been considerable additional work, mainly by Toth and co-workers (*18*–*23*) on the room temperature infrared absorption spectra. Toth has recently published a list of the energy levels for the (000), (010), (100), and (020) vibrational states of HDO. Note that we adopt the traditional labeling convention of v_1 for the OD stretching mode and for the v_3 OH stretching mode, in spite of the Mulliken convention (24). Other infrared measurements include the detection of several transitions near 1 μm by Bykov *et al*. (*25, 26*) and the 300–000 and 111–000 bands by Hu *et al*. (*27*).

The pure rotational lines of HDO were measured in the submillimeter wave region by Messer *et al*. (*28*) and by Baskakov *et al*. (*29*). To higher frequency, the pure rotational transitions in the regions 20–350 cm^{-1} (*30*) and 110–500 cm^{-1} (*31*) were recorded by Fourier transform absorption spectroscopy.

The most highly excited levels of HDO have been recorded by overtone spectroscopy in the visible and near-UV regions.

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[1] Also Department of Chemistry, University of Arizona, Tucson, Arizona 85721.

[2] Permanent address: Institute of Applied Physics, Russian Academy of Science, Uljanov Street 46, Nizhnii Novgorod, Russia 603950.

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Most notably, Campargue and co-workers (*32–36*) have recently used the ultrasensitive technique of intracavity laser absorption spectroscopy to measure a number of overtone bands. Our contribution in this area has been to record long-path Fourier transform absorption spectra in the region 16 300–22 800 cm^{-1} (*37*). The most highly excited vibrational state known to date is (007) with a band origin at 22 625.50 cm^{-1} (*37*). Other experiments on HDO are the intracavity Fourier transform measurements of the 500–000 transition (*38*), as well as Russian intracavity measurements of the (003) and (005) levels (*39*).

2. EXPERIMENTAL DETAILS

The hot HDO emission spectra were recorded on November 6, 1997 at the University of Waterloo with a Bruker IFS 120HR Fourier transform spectrometer. The spectrometer was operated with a KBr beamsplitter and either a Si : B or a HgCdTe detector. The spectra reported here in the region 350–2200 cm^{-1} were recorded in three pieces. The section 350–750 cm^{-1} used a liquid-He-cooled Si : B detector and a cold longwave pass filter at 750 cm^{-1}. A separate cold bandpass filter was used to cover the region 750–1300 cm^{-1}. The region 1200–2200 cm^{-1} was recorded with a HgCdTe detector and an uncooled 2200 cm^{-1} longwave pass filter. Forty-five scans were co-added with the Si : B detector and forty with the HgCdTe detector at a resolution of 0.01 cm^{-1}.

A KRS-5 window was used on the emission port of the spectrometer. The water vapor was heated in the center of a 1-m-long, 5-cm-diameter alumina tube sealed with cooled KRS-5 windows. The tube was placed inside a furnace and heated to 1500°C. A slow flow of water vapor through the cell was maintained at a pressure of 2.5 Torr. An equimolar mixture of H_2O and D_2O liquids was used to provide the vapor. The thermal emission from the cell was focused into the emission port of the spectrometer with an off-axis parabolic mirror. The lines were measured with the PC-Decomp program of Brault and has an estimated accuracy of ± 0.001 cm^{-1} for strong unblended lines. The spectrum, however, was very dense with H_2O, D_2O and HDO lines present.

The three spectra analyzed for this paper have lines in the regions 380–746, 750–1249, and 1250–2180 cm^{-1}. There were enough strong common lines in the two higher wavenumber spectra to put them on a common wavenumber scale and then calibrate them with the water lines reported in Polyansky *et al.* (*40*). Because of a lack of strong common lines between the two lower wavenumber regions, the lines in the region 380–746 cm^{-1} were just calibrated with our previous measurements (*40*) in this region. This means that in the region 750–2190 cm^{-1} our lines have a wavenumber scale that is in excellent agreement with that of Toth (*41, 42*), but the region 380–746 cm^{-1} is on a scale slightly different from that of Toth. Fortunately, this difference is less than 0.001 cm^{-1}, our estimated absolute accuracy.

3. LINE ASSIGNMENTS

A total of 22 106 lines were measured in the emission spectrum. Of course not all of these transitions correspond to HDO and before starting detailed analysis of these lines it was necessary to eliminate those due to H_2O and D_2O. The H_2O lines were identified by comparison with previously published (*5, 6*) hot emission spectra. For D_2O similar comparisons were made with a "pure" D_2O emission spectrum recorded in Waterloo which is yet to be fully analyzed; in practice this D_2O spectrum contained approximately 10% HDO. As the intensities differ in the three regions of the HDO spectrum, these regions were analysed separately. Lines were identified as H_2O or D_2O by matching both frequency and intensity. This is because the line density of the spectra is such that inevitably some HDO lines coincide with lines from the other isotopomers. We identified 4155 H_2O lines (322 also belonging to HDO) and 5423 D_2O (447 also HDO). H_2O and D_2O lines are marked in the full linelist which is given in the supplementary data for this article.

Energy levels for the ground, (010), (020), (030), (100), (001), and (110) vibrational states of HDO with low J and K_a values have been given by Toth (*18, 19, 21, 22*). These were used to conduct an initial analysis of the spectrum to identify "trivial" assignments were both upper and lower energy levels were already known.

To identify transitions involving previously unobserved energy levels in the system it was necessary to use variational predictions to aid the assignment process. There is no linelist available to us for hot HDO, but Partridge and Schwenke (*9*) have computed a room temperature linelist with states extending to energies about 8000 cm^{-1} above the ground state. This linelist was transformed to a temperature of 1800 K using Boltzmann statistics. The spectral region 380–2190 cm^{-1} covers both pure rotational transitions of HDO, particularly with high J or K_a, and the first bending fundamental, with a band origin at 1403.48 cm^{-1}, as well as associated hot bands.

Trivial assignments and other isotopomers having been eliminated from our list of transitions, the unassigned lines were analyzed using a computer program. Candidate transitions were identified using the variational linelist and then confirmed, or otherwise, by the presence, or not, of the appropriate combination difference transitions. In this way we were able to identify numerous new transitions involving known vibrational states and also to identify 190 transitions involving the (040) bending state.

The Partridge and Schwenke linelist (*9*) proved to be too restricted for the analysis of hot rotational levels. However, they also provided (*43*) energy levels for higher states of HDO. These were used to provide estimates of frequencies for pure rotational transitions which were then used to seed a further search.

TABLE 1
Summary of Assigned HDO Emission Lines

Transition	Number
Pure rotations	
000-000	516
010-010	372
020-020	170
030-030	77
Bending modes	
010-000	1723
020-010	1676
030-020	1011
040-030	74
110-010	362
011-001	123
Difference bands	
100-010	65
110-020	132

We have assigned 1146 pure HDO rotational transitions spanning all HDO states up to (110). A total of 5085 transitions were assigned to bending transitions which involve a change of one quantum in the ν_2 mode. In addition 199 transitions were assigned to assorted difference bands. It has already been found that these difference bands are common in the emission spectrum of hot H_2O (*5*, *44*). Table 1 gives a summary of all bands for which more than 10 transitions were assigned.

Experimental energy levels, which can be calculated by linking known energy levels and newly assigned transitions, are an important product of our analysis. This work has more than tripled the number of known energy levels for the states (000), (010), (020), (030) and (040). Tables 2 and 3 present energy levels for the first four of these states. The lowest *J* levels have been omitted from these tabulations as they have been well-determined previously (*18*, *19*). Our results for the previously unobserved (040) state are given in Table 4.

Altogether we have assigned 6430 HDO transitions in the emission spectrum. This number represents approximately half the transitions which we identify as belonging to HDO. There is no doubt that many of the unassigned lines in the lower wavenumber portion of the spectrum belong to pure rotational transitions of vibrational states with excited stretching modes. Analysis of these states is best conducted in conjunction with analysis of associated vibrational transitions involving these stretching modes. Such transitions lie to somewhat higher frequency than the spectra reported here. An emission spectrum covering this region has been recorded in Waterloo and will be analyzed together with the unassigned transitions remaining from the present study.

TABLE 2
Experimental Term Values in cm^{-1} for the Ground and (010) Vibrational States of HDO

J	K_a	K_c	(000)		(010))	
11	0	11	916.029	a	2316.312	a
11	1	11	916.124	a	2316.446	a
11	1	10	1046.474	a	2459.361	a
11	2	10	1049.124	a	2462.887	a
11	2	9	1141.691	a	2561.580	a
11	3	9	1164.510	a	2589.750	a
11	3	8	1206.754	a	2632.660	a
11	4	8	1278.438	a	2716.170	a
11	4	7	1287.239	a	2724.463	a
11	5	7	1410.566	a	2863.369	a
11	5	6	1411.319	a	2864.036	a
11	6	6	1570.061	a	3040.100	a
11	6	5	1570.095	a	3040.129	a
11	7	5	1757.340	a	3246.058	a
11	7	4	1757.341	a	3246.059	a
11	8	4	1971.030	a	3479.363	a
11	8	3	1971.030	a	3479.363	a
11	9	3	2209.906	a	3738.413	a
11	9	2	2209.906	a	3738.413	a
11	10	2	2472.974	a	4021.937	d
11	10	1	2472.974	a	4021.937	d
11	11	1	2759.426	d	4328.919	d
11	11	0	2759.426	d	4328.919	d
12	0	12	1075.715	a	2474.835	a
12	1	12	1075.762	a	2474.904	a
12	1	11	1220.028	a	2633.352	a
12	2	11	1221.536	a	2635.417	a
12	2	10	1331.217	a	2752.926	a
12	3	10	1347.119	a	2773.107	a
12	3	9	1405.125	a	2832.490	a
12	4	9	1465.831	a	2904.291	a
12	4	8	1481.443	a	2919.136	a
12	5	8	1598.066	a	3051.433	a
12	5	7	1599.798	a	3052.969	a
12	6	7	1756.284	a	3226.829	a
12	6	6	1756.384	a	3226.912	a
12	7	6	1942.372	a	3431.571	a
12	7	5	1942.375	a	3431.573	a
12	8	5	2155.016	a	3663.801	a
12	8	4	2155.016	a	3663.801	a
12	9	4	2392.886	a	3921.804	a
12	9	3	2392.886	a	3921.804	a
12	10	3	2654.916	d	4204.229	d
12	10	2	2654.916	d	4204.229	d
12	11	2	2940.256	d	4510.028	d
12	11	1	2940.256	d	4510.028	d
12	12	1	3248.227	d	4838.388	d
12	12	0	3248.227	d	4838.388	d
13	0	13	1247.964	a	2645.775	a
13	1	13	1247.988	a	2645.811	a
13	1	12	1405.818	a	2819.396	a
13	2	12	1406.656	a	2820.577	a
13	2	11	1532.728	a	2956.268	a
13	3	11	1543.243	a	2970.013	a
13	3	10	1618.698	a	3047.832	a

[a] From Toth (18).
[d] Levels treated as degenerate.

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
13	4	10	1668.095	a	3107.381	a
13	4	9	1693.446	a	3131.745	a
13	5	9	1801.207	a	3255.187	a
13	5	8	1804.840	a	3258.418	a
13	6	8	1958.125	a	3429.192	a
13	6	7	1958.383	a	3429.410	a
13	7	7	2142.829	a	3632.524	a
13	7	6	2142.841	a	3632.533	a
13	8	6	2354.274	a	3863.529	a
13	8	5	2354.274	a	3863.529	a
13	9	5	2591.018	a	4120.363	d
13	9	4	2591.018	a	4120.363	d
13	10	4	2851.907	a	4401.589	d
13	10	3	2851.907	a	4401.589	d
13	11	3	3136.039	d	4706.101	d
13	11	2	3136.039	d	4706.101	d
13	12	2	3442.703	d	5033.060	d
13	12	1	3442.703	d	5033.060	d
13	13	1	3771.349	d	5381.836	d
13	13	0	3771.349	d	5381.836	d
14	0	14	1432.747	a	2829.106	a
14	1	14	1432.758	a	2829.125	a
14	1	13	1603.905	a	3017.575	a
14	2	13	1604.362	a	3018.240	a
14	2	12	1745.896	a	3171.148	a
14	3	12	1752.537	a	3180.106	a
14	3	11	1846.401	a	3277.601	a
14	4	11	1884.843	a	3325.047	a
14	4	10	1922.888	a	3362.052	a
14	5	10	2019.821	a	3474.478	a
14	5	9	2026.831	a	3480.745	a
14	6	9	2175.564	a	3647.170	a
14	6	8	2176.177	a	3647.687	a
14	7	8	2358.688	a	3848.900	a
14	7	7	2358.721	a	3848.926	a
14	8	7	2568.783	a	4078.518	d
14	8	6	2568.783	a	4078.518	d
14	9	6	2804.271	a	4334.055	d
14	9	5	2804.271	a	4334.055	d
14	10	5	3063.912	a	4613.975	d
14	10	4	3063.912	a	4613.975	d
14	11	4	3346.714	d	4917.099	d
14	11	3	3346.714	d	4917.099	d
14	12	3	3652.000	d	5242.558	d
14	12	2	3652.000	d	5242.558	d
14	13	2	3979.121	d	5589.694	d
14	13	1	3979.121	d	5589.694	d
14	14	1	4327.677	d	5958.044	d
14	14	0	4327.677	d	5958.044	d
15	0	15	1630.024	a	3024.796	a
15	1	15	1630.029	a	3024.805	a
15	1	14	1814.319	a	3227.938	a
15	2	14	1814.565	a	3228.307	a
15	2	13	1970.655	a	3397.438	a
15	3	13	1974.708	a	3403.071	a
15	3	12	2087.137	a	3520.662	a
15	4	12	2115.644	a	3556.859	a
15	4	11	2169.061	a	3609.422	a
15	5	11	2253.675	a	3709.077	a
15	5	10	2266.175	a	3720.348	a

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
15	6	10	2408.557	a	3880.715	a
15	6	9	2409.903	a	3881.850	a
15	7	9	2589.973	a	4080.660	
15	7	8	2590.057	a	4080.742	
15	8	8	2798.509	a	4308.719	
15	8	7	2798.513	a	4308.722	
15	9	7	3032.606	a	4562.833	d
15	9	6	3032.606	a	4562.833	d
15	10	6	3290.888	d	4841.335	d
15	10	5	3290.888	d	4841.335	d
15	11	5	3572.309	d	5142.978	d
15	11	4	3572.309	d	5142.978	d
15	12	4	3876.050	d	5466.838	d
15	12	3	3876.050	d	5466.838	d
15	13	3	4201.580	d	5812.270	d
15	13	2	4201.580	d	5812.270	d
15	14	2	4548.373	d	6178.683	d
15	14	1	4548.373	d	6178.683	d
15	15	1	4916.149	d	6565.872	d
15	15	0	4916.149	d	6565.872	d
16	0	16	1839.754	a	3232.804	a
16	1	16	1839.757	a	3232.809	a
16	1	15	2037.056	a	3450.501	a
16	2	15	2037.188	a	3450.705	a
16	2	14	2207.117	a	3635.201	a
16	3	14	2209.513		3638.648	a
16	3	13	2339.944		3776.003	
16	4	13	2360.075		3802.374	
16	4	12	2430.992	a	3872.934	
16	5	12	2502.437	a	3958.678	a
16	5	11	2523.127		3977.541	
16	6	11	2657.013	a	4129.736	
16	6	10	2659.764		4132.058	
16	7	10	2836.617		4327.808	
16	7	9	2836.823	a	4327.975	
16	8	9	3043.420	a	4554.094	
16	8	8	3043.431	a	4554.090	
16	9	8	3275.978	a	4806.638	d
16	9	7	3275.978	a	4806.638	d
16	10	7	3532.781	d	5083.618	d
16	10	6	3532.781	d	5083.618	d
16	11	6	3812.705	d	5383.681	d
16	11	5	3812.705	d	5383.681	d
16	12	5	4114.878	d	5705.846	d
16	12	4	4114.878	d	5705.846	d
16	13	4	4438.651	d	6049.390	d
16	13	3	4438.651	d	6049.390	d
16	14	3	4783.618	d	6413.860	d
16	14	2	4783.618	d	6413.860	d
16	15	2	5149.378	d	6798.868	d
16	15	1	5149.378	d	6798.868	d
16	16	1	5535.745	d	7204.241	d
16	16	0	5535.745	d	7204.241	d
17	0	17	2061.897	a	3453.092	a
17	1	17	2061.898	a	3453.094	a
17	1	16	2272.103	a	3685.259	a
17	2	16	2272.172	a	3685.371	a
17	2	15	2455.379	a	3884.565	a
17	3	15	2456.767		3886.630	a
17	3	14	2604.144		4042.765	

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
17	4	14	2617.726		4061.184	
17	4	13	2707.595	a	4151.511	
17	5	13	2765.744		4222.914	
17	5	12	2797.620		4252.371	
17	6	12	2920.783	a	4394.100	
17	6	11	2926.032		4398.558	
17	7	11	3098.595		4590.252	
17	7	10	3099.058	a	4590.627	
17	8	10	3303.477		4814.593	
17	8	9	3303.503		4814.593	
17	9	9	3534.342	d	5065.396	d
17	9	8	3534.342	d	5065.396	d
17	10	8	3789.538	d	5340.750	d
17	10	7	3789.538	d	5340.750	d
17	11	7	4067.863	d	5639.141	d
17	11	6	4067.863	d	5639.141	d
17	12	6	4368.360	d	5959.524	d
17	12	5	4368.360	d	5959.524	d
17	13	5	4690.352	d	6301.143	d
17	13	4	4690.352	d	6301.143	d
17	14	4	5033.327	d	6663.518	d
17	14	3	5033.327	d	6663.518	d
17	15	3	5397.011	d	7046.250	d
17	15	2	5397.011	d	7046.250	d
17	16	2	5781.098	d	7449.132	d
17	16	1	5781.098	d	7449.132	d
17	17	1	6185.485	d	7872.136	d
17	17	0	6185.485	d	7872.136	d
18	0	18	2296.384	a	3685.619	a
18	1	18	2296.384	a	3685.619	a
18	1	17	2519.416	a	3932.188	a
18	2	17	2519.452	a	3932.250	a
18	2	16	2715.533		4145.632	
18	3	16	2716.330		4146.842	
18	3	15	2879.423		4320.513	
18	4	15	2888.238		4332.875	
18	4	14	2997.706		4443.997	
18	5	14	3043.157		4501.367	
18	5	13	3089.176		4544.524	
18	6	13	3199.653		4673.591	
18	6	12	3209.060		4681.624	
18	7	12	3375.825		4867.944	
18	7	11	3376.824		4868.733	
18	8	11	3578.631		5090.161	
18	8	10	3578.700		5090.218	
18	9	10	3807.626		5339.075	
18	9	9	3807.623		5339.124	
18	10	9	4061.120	d	5612.657	
18	10	8	4061.120	d	5612.668	
18	11	8	4337.716		5909.282	d
18	11	7	4337.732		5909.282	d
18	12	7	4636.448	d	6227.795	d
18	12	6	4636.448	d	6227.795	d
18	13	6	4956.561	d	6567.408	d
18	13	5	4956.561	d	6567.408	d
18	14	5	5297.521	d	6927.609	d
18	14	4	5297.521	d	6927.609	d
18	15	4	5658.963	d	7307.960	d
18	15	3	5658.963	d	7307.960	d
18	16	3	6040.706	d	7708.295	d

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
18	16	2	6040.706	d	7708.295	d
18	17	2	6442.540	d	8128.485	d
18	17	1	6442.540	d	8128.485	d
18	18	1	6864.423	d	8568.592	d
18	18	0	6864.423	d	8568.592	d
19	0	19	2543.209	a	3930.315	a
19	1	19	2543.209	a	3930.315	a
19	1	18	2778.949	a	4191.256	a
19	2	18	2778.969	a	4191.291	a
19	2	17	2987.607		4418.476	
19	3	17	2988.058		4419.190	
19	3	16	3165.744		4609.095	
19	4	16	3171.279		4617.121	
19	4	15	3300.211		4749.217	
19	5	15	3334.237		4793.553	
19	5	14	3396.998		4853.290	
19	6	14	3493.330		4967.941	
19	6	13	3509.153		4981.591	
19	7	13	3668.238		5160.756	
19	7	12	3670.218		5162.347	
19	8	12	3868.826		5380.715	
19	8	11	3868.969		5380.851	
19	9	11	4095.786		5627.594	
19	9	10	4095.789		5627.622	
19	10	10	4347.409	d	5899.252	
19	10	9	4347.409	d	5899.260	
19	11	9	4622.221		6194.051	
19	11	8	4622.256		6194.016	
19	12	8	4919.073	d	6510.577	d
19	12	7	4919.073	d	6510.577	d
19	13	7	5237.223	d	6848.113	d
19	13	6	5237.223	d	6848.113	d
19	14	6	5576.072	d	7206.073	d
19	14	5	5576.072	d	7206.073	d
19	15	5	5935.256	d	7583.951	d
19	15	4	5935.256	d	7583.951	d
19	16	4	6314.483	d	7981.602	d
19	16	3	6314.483	d	7981.602	d
19	17	3	6713.698	d	8398.940	d
19	17	2	6713.698	d	8398.940	d
19	18	2	7132.751	d	8835.273	d
19	18	1	7132.751	d	8835.273	d
19	19	1	7571.635	d	9292.624	d
19	19	0	7571.635	d	9292.624	d
20	0	20	2802.260	d	4187.166	d
20	1	20	2802.260	d	4187.166	d
20	1	19	3050.657	d	4462.397	
20	2	19	3050.657	d	4462.420	
20	2	18	3271.646		4703.124	
20	3	18	3271.881		4703.542	
20	3	17	3463.200		4908.538	
20	4	17	3466.595		4913.621	
20	4	16	3614.113		5066.114	
20	5	16	3638.520		5099.072	
20	5	15	3720.010		5177.710	
20	6	15	3801.480		5276.814	
20	6	14	3826.480		5298.647	
20	7	14	3975.666		5468.553	
20	7	13	3979.411		5471.580	
20	8	13	4173.984		5686.167	

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
20	8	12	4174.310		5686.451	
20	9	12	4398.724		5930.817	
20	9	11	4398.751		5930.876	
20	10	11	4648.370	d	6200.454	
20	10	10	4648.370	d	6200.486	
20	11	10	4921.249		6492.761	
20	11	9	4921.298		6493.259	
20	12	9	5216.184		6807.780	d
20	12	8	5216.183		6807.780	d
20	13	8	5532.262	d	7143.146	d
20	13	7	5532.262	d	7143.146	d
20	14	7	5868.922	d	7498.846	d
20	14	6	5868.922	d	7498.846	d
20	15	6	6225.765	d	7874.153	d
20	15	5	6225.765	d	7874.153	d
20	16	5	6602.449	d	8269.020	d
20	16	4	6602.449	d	8269.020	d
20	17	4	6998.872	d	8683.378	d
20	17	3	6998.872	d	8683.378	d
20	18	3	7415.020	d	9117.080	d
20	18	2	7415.020	d	9117.080	d
20	19	2	7850.792	d		
20	19	1	7850.792	d		
20	20	1	8306.233	d		
20	20	0	8306.233	d		
21	0	21	3073.522	d	4456.096	d
21	1	21	3073.522	d	4456.096	d
21	1	20	3334.489	d	4745.621	
21	2	20	3334.489	d	4745.655	
21	2	19	3567.588		4999.574	
21	3	19	3567.717		4999.845	
21	3	18	3771.939		5219.015	
21	4	18	3773.988		5222.179	
21	4	17	3938.799		5393.863	
21	5	17	3955.624		5417.441	
21	5	16	4057.068		5516.611	
21	6	16	4123.665		5599.847	
21	6	15	4160.851		5632.839	
21	7	15	4297.931		5791.130	
21	7	14	4304.654		5796.611	
21	8	14	4494.019		6006.537	
21	8	13	4494.722		6007.002	
21	9	13	4716.394		6248.737	
21	9	12	4716.430		6248.812	
21	10	12	4963.892		6516.115	
21	10	11	4963.865		6516.170	
21	11	11	5234.753		6806.751	
21	11	10	5234.811		6806.916	
21	12	10	5527.668		7119.314	
21	12	9	5527.638		7119.294	
21	13	9	5841.622	d	7452.436	d
21	13	8	5841.622	d	7452.436	d
21	14	8	6175.990	d	7805.845	d
21	14	7	6175.990	d	7805.845	d
21	15	7	6530.456	d	8178.497	d
21	15	6	6530.456	d	8178.497	d
21	16	6	6904.470	d	8570.474	d
21	16	5	6904.470	d	8570.474	d
21	17	5	7298.083	d	8981.761	d
21	17	4	7298.083	d	8981.761	d

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
21	18	4	7711.152	d	9412.196	d
21	18	3	7711.152	d	9412.196	d
21	19	3	8143.730	d	9862.164	d
21	19	2	8143.730	d	9862.164	d
21	20	2	8595.807	d		
21	20	1	8595.807	d		
22	0	22	3356.925	d	4737.062	d
22	1	22	3356.925	d	4737.062	d
22	1	21	3630.374	d	5040.850	
22	2	21	3630.374	d	5040.747	
22	2	20	3875.405		5307.810	
22	3	20	3875.470		5308.036	
22	3	19	4092.042		5540.636	
22	4	19	4093.277		5542.561	
22	4	18	4273.922		5731.948	
22	5	18	4285.128		5748.263	
22	5	17	4406.977		5868.944	
22	6	17	4459.463		5936.508	
22	6	16	4511.727		5983.725	
22	7	16	4634.736		6128.461	
22	7	15	4646.194		6137.661	
22	8	15	4828.835		6341.365	
22	8	14	4830.210		6342.450	
22	9	14	5048.678		6581.137	
22	9	13	5048.896		6581.252	
22	10	13	5293.884		6845.751	
22	10	12	5293.801		6845.827	
22	11	12	5562.592		7134.677	
22	11	11	5562.690		7134.862	
22	12	11	5853.317		7445.060	
22	12	10	5853.387		7445.120	
22	13	10	6165.160	d	7775.878	d
22	13	9	6165.161	d	7775.878	d
22	14	9	6497.213	d	8127.124	
22	14	8	6497.213	d	8127.271	
22	15	8	6849.654	d	8496.873	d
22	15	7	6849.654	d	8496.873	d
22	16	7	7220.487	d	8885.837	d
22	16	6	7220.487	d	8885.837	d
22	17	6	7611.189	d	9294.019	d
22	17	5	7611.189	d	9294.019	d
22	18	5	8021.164	d	9721.085	d
22	18	4	8021.164	d	9721.085	d
22	19	4	8450.371	d		
22	19	3	8450.371	d		
22	20	3			10632.566	d
22	20	2			10632.566	d
22	21	2	9366.836	d		
22	21	1	9366.836	d		
23	0	23	3652.398	d	5030.012	d
23	1	23	3652.398	d	5030.012	d
23	1	22	3938.265	d	5347.989	
23	2	22	3938.265	d	5348.017	
23	2	21	4195.052		5627.771	
23	3	21	4195.107		5627.642	
23	3	20	4423.568		5873.463	
23	4	20	4424.292		5874.594	
23	4	19	4619.446		6080.213	
23	5	19	4626.722		6091.177	
23	5	18	4768.576		6233.324	

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
23	6	18	4808.411		6286.414	
23	6	17	4878.296		6350.622	
23	7	17	4985.818		6479.813	
23	7	16	5004.291		6494.921	
23	8	16	5178.253		6690.747	
23	8	15	5180.822		6692.876	
23	9	15	5395.498		6927.921	
23	9	14	5395.765		6928.185	
23	10	14	5638.233		7190.978	
23	10	13	5638.455		7191.122	
23	11	13	5904.704		7476.729	
23	11	12	5904.816		7476.997	
23	12	12	6193.249		7784.920	
23	12	11	6193.282		7784.816	
23	13	11	6502.823		8113.377	
23	13	10	6502.860		8113.337	
23	14	10	6832.444	d	8463.318	
23	14	9	6832.444	d	8463.421	
23	15	9	7181.439	d	8829.215	d
23	15	8	7181.439	d	8829.215	d
23	16	8	7550.428	d	9216.976	d
23	16	7	7550.428	d	9216.976	d
23	17	7	7938.136	d	9620.066	d
23	17	6	7938.136	d	9620.066	d
23	18	6	8344.912	d		
23	18	5	8344.912	d		
23	20	4	9213.862	d		
23	20	3	9213.862	d		
23	21	3			11429.137	d
23	21	2			11429.137	d
24	0	24	3959.891		5334.785	
24	1	24	3959.891		5334.863	
24	1	23	4258.076		5667.067	
24	2	23	4258.081		5667.101	
24	2	22	4526.455		5959.349	
24	3	22	4526.485		5959.423	
24	3	21	4766.537		6217.584	
24	4	21	4766.968		6218.237	
24	4	20	4975.506		6438.692	
24	5	20	4980.108		6445.890	
24	5	19	5140.984		6608.881	
24	6	19	5170.049		6649.089	
24	6	18	5259.364		6732.807	
24	7	18	5350.860		6845.050	
24	7	17	5379.016		6868.741	
24	8	17	5542.104		7053.298	
24	8	16	5546.741		7058.249	
24	9	16	5756.701		7288.980	
24	9	15	5757.217		7289.506	
24	10	15	5996.865		7549.341	
24	10	14	5996.999		7549.555	
24	11	14	6260.933		7832.690	
24	11	13	6261.034		7833.146	
24	12	13	6547.199		8138.808	
24	12	12	6547.251		8138.644	
24	13	12	6854.498		8464.738	
24	13	11	6854.372		8464.716	
24	14	11	7181.611		8806.790	
24	14	10	7181.617		8807.590	
24	15	10	7528.079	d	9175.441	d

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
24	15	9	7528.079	d	9175.441	d
24	16	9	7894.226	d		
24	16	8	7894.226	d	9558.701	
24	17	8	8278.846	d		
24	17	7	8278.846	d		
24	18	7	8682.347	d		
24	18	6	8682.347	d		
24	19	6	9104.665	d		
24	19	5	9104.665	d		
25	0	25	4279.321		5651.141	
25	1	25	4279.320		5651.555	
25	1	24	4589.759		5997.975	
25	2	24	4589.762		5998.035	
25	2	23	4869.569	d	6302.605	
25	3	23	4869.569	d	6302.679	
25	3	22	5120.929		6572.948	
25	4	22	5121.170		6573.279	
25	4	21	5342.191		6807.427	
25	5	21	5345.054		6812.044	
25	5	20	5523.459		6994.663	
25	6	20	5543.933		7024.132	
25	6	19			7128.614	
25	7	19	5729.143		7224.271	
25	7	18	5770.084		7258.859	
25	8	18	5920.136		7433.214	
25	8	17	5928.097		7438.777	
25	9	17	6132.213			
25	9	16	6133.163		7665.121	
25	10	16	6369.613		7921.830	
25	10	15	6369.775			
25	11	15	6631.188		8202.490	
25	11	14	6631.319		8203.137	
25	12	14	6915.017		8506.605	
25	12	13	6915.132		8506.267	
25	13	13			8829.914	
25	13	12			8829.871	
25	14	12	7544.584	d	9170.915	
25	14	11	7544.584	d	9171.232	
25	15	11			9535.491	
25	15	10			9535.481	
25	16	10	8251.751		9915.396	d
25	16	9	8251.683		9915.396	d
25	17	9	8633.244	d		
25	17	8	8633.244	d		
26	0	26	4610.681		5980.020	d
26	1	26	4610.695		5980.020	d
26	1	25	4933.236		6340.678	
26	2	25	4933.225		6340.881	
26	2	24	5224.284		6657.395	
26	3	24	5224.285		6657.482	
26	3	23	5486.675		6939.529	
26	4	23	5486.816		6939.677	
26	4	22	5719.617		7186.554	
26	5	22	5721.398		7189.433	
26	5	21	5915.732			
26	6	21	5929.711		7410.985	
26	6	20	6060.513		7537.166	
26	7	20	6120.538			
26	7	19	6177.083			
26	8	19	6311.976		7824.851	

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
26	8	18	6325.097		7834.413	
26	9	18	6521.824		8052.206	
26	9	17	6523.580			
26	10	17	6756.370			
26	10	16	6756.649			
26	11	16	7015.293			
26	11	15	7015.471			
26	12	15	7296.663			
26	12	14	7296.823			
26	13	14	7599.052			
26	13	13	7599.055			
27	0	27	4953.766	d	6320.332	d
27	1	27	4953.766	d	6320.332	d
27	1	26	5288.457		6694.723	
27	2	26	5288.452		6695.133	
27	2	25	5590.581	d	7023.628	
27	3	25	5590.566	d	7023.788	
27	3	24	5863.717		7317.341	
27	4	24	5863.808		7317.265	
27	4	23	6107.851		7575.770	
27	5	23	6108.923		7577.429	
27	5	22	6317.700			
27	6	22	6327.007			
27	6	21	6478.228			
27	7	21	6524.436			
27	7	20	6598.915			
27	8	19	6737.922			
27	9	19	6925.321			
27	9	18	6928.513			
27	10	18	7156.989			
27	10	17	7157.462			
27	11	17	7413.162			
27	11	16	7413.377			
27	12	16	7691.922			
27	12	15	7692.139			
27	13	15	7992.035			
27	13	14	7991.856			
27	14	14	8311.383	d		
27	14	13	8311.380	d		
28	0	28	5308.590	d	6672.286	d
28	1	28	5308.590	d	6672.286	d
28	1	27	5655.240		7061.489	
28	2	27	5655.231		7061.055	
28	2	26	5968.269	d	7401.298	
28	3	26	5968.269	d	7401.602	
28	3	25	6251.986		7706.042	
28	4	25	6252.026		7706.222	
28	4	24	6506.866		7976.087	
28	5	24	6507.530		7976.999	
28	5	23	6729.440			
28	6	23	6735.531			
28	6	22	6906.086			
28	7	22	6940.441			
28	8	21	7136.548			
29	0	29	5675.066	d	7035.849	d
29	1	29	5675.066	d	7035.849	d
29	1	28			7438.591	
29	2	28			7438.726	
29	2	27	6357.327	d	7790.198	
29	3	27	6357.327	d	7791.556	

TABLE 2—*Continued*

J	K_a	K_c	(000)		(010))	
29	3	26	6651.376			
29	4	26	6651.410			
29	4	25	6916.640			
29	5	25	6917.028			
29	5	24	7151.108			
29	6	24	7155.008			
30	0	30			7411.070	d
30	1	30			7411.070	d
30	2	28	6757.643	d		
30	3	28	6757.643	d		
30	3	27	7061.823			
30	4	27	7061.832			
30	4	26	7337.012			
30	5	26	7337.253			

TABLE 3
Experimental Term Values in cm^{-1} for the (020) and (030) Vibrational States of HDO

J	K_a	K_c	(020)		(030)	
6	0	6	3089.126	a	4451.759	b
6	1	6	3092.811	a	4456.083	b
6	1	5	3154.965	a	4519.117	b
6	2	5	3186.626	a	4555.954	b
6	2	4	3206.336	a	4575.059	b
6	3	4	3291.072	a	4672.403	b
6	3	3	3292.976	a	4674.109	b
6	4	3	3425.685	a	4825.009	b
6	4	2	3425.748	a	4825.057	b
6	5	2	3594.668	a	5015.533	b
6	5	1	3594.669	a	5015.534	b
6	6	1	3795.879	a	5240.158	d
6	6	0	3795.879	a	5240.158	d
7	0	7	3185.579	a	4548.066	b
7	1	7	3187.760	a	4550.724	b
7	1	6	3268.346	a	4632.882	b
7	2	6	3292.830	a	4662.303	b
7	2	5	3324.490	a	4693.313	b
7	3	5	3401.218	a	4782.865	b
7	3	4	3405.847	a	4786.940	b
7	4	4	3535.818	a	4935.425	b
7	4	3	3536.047	a	4935.606	
7	5	3	3704.195	a	5125.396	b
7	5	2	3704.199	a	5125.400	b
7	6	2	3904.897	a	5349.536	d
7	6	1	3904.898	a	5349.536	d
7	7	1	4135.476	a	5604.348	d
7	7	0	4135.476	a	5604.348	d
8	0	8	3294.197	a	4656.481	b
8	1	8	3295.443	a	4658.062	b
8	1	7	3395.168	a	4760.389	b

[a] From Toth (18).
[b] From Toth (21).
[c] Level reassigned from Toth (21).
[d] Levels treated as degenerate.

TABLE 3—*Continued*

J	K_a	K_c	(020)		(030)	
8	2	7	3413.012	a	4782.755	b
8	2	6	3459.535	a	4828.795	b
8	3	6	3526.894	a	4908.896	b
8	3	5	3536.354	a	4917.294	b
8	4	5	3661.860	a	5061.768	
8	4	4	3662.525	a	5062.297	
8	5	4	3829.486	a	5251.033	b
8	5	3	3829.508	a	5251.051	b
8	6	3	4029.533	a	5474.554	d
8	6	2	4029.533	a	5474.554	d
8	7	2	4259.517	a	5728.796	d
8	7	1	4259.517	a	5728.796	d
8	8	1	4517.274	a	6010.901	d
8	8	0	4517.274	a	6010.901	d
9	0	9	3415.036	a	4777.040	b
9	1	9	3415.732	a	4777.960	b
9	1	8	3534.570	a	4900.782	b
9	2	8	3546.853	a	4916.961	b
9	2	7	3610.681	a	4980.608	b
9	3	7	3667.776	a	5050.239	b
9	3	6	3684.868	a	5065.595	
9	4	6	3803.790	a	5204.030	b
9	4	5	3805.449	a	5205.350	b
9	5	5	3970.574	a	5392.467	c
9	5	4	3970.645	a	5392.524	c
9	6	4	4169.791	a	5615.242	
9	6	3	4169.790	a	5615.242	
9	7	3	4399.060	a	5868.765	d
9	7	2	4399.060	a	5868.765	d
9	8	2	4656.109	d	6150.151	d
9	8	1	4656.109	d	6150.151	d
9	9	1	4939.118	d	6457.181	d
9	9	0	4939.118	d	6457.181	d
10	0	10	3548.148	a	4909.788	b
10	1	10	3548.530	a	4910.315	b
10	1	9	3685.981	a	5053.412	b
10	2	9	3694.020	a	5064.591	b
10	2	8	3777.003	a	5148.026	b
10	3	8	3823.522	a	5206.573	
10	3	7	3851.399	a	5231.952	
10	4	7	3961.528	a	5362.130	
10	4	6	3965.184		5365.038	
10	5	6	4127.477	a	5549.718	
10	5	5	4127.688	a	5549.876	
10	6	5	4325.684	a	5771.521	d
10	6	4	4325.686	a	5771.521	d
10	7	4	4554.094	d	6024.234	d
10	7	3	4554.094	d	6024.234	d
10	8	3	4810.320	d	6304.800	d
10	8	2	4810.320	d	6304.800	d
10	9	2	5092.462	d	6610.936	d
10	9	1	5092.462	d	6610.936	d
10	10	1	5399.039	d	6940.950	d
10	10	0	5399.039	d	6940.951	d
11	0	11	3693.560	a	5054.751	b
11	1	11	3693.768	a	5055.050	b
11	1	10	3849.171	a	5217.919	b
11	2	10	3854.222	a	5225.344	b
11	2	9	3957.464	a	5330.063	
11	3	9	3993.756	a	5377.525	

TABLE 3—*Continued*

J	K_a	K_c	(020)		(030)	
11	3	8	4035.537	a	5416.346	
11	4	8	4134.914	a	5535.919	
11	4	7	4142.173	a	5541.765	
11	5	7	4300.205		5722.771	
11	5	6	4300.743		5723.160	
11	6	6	4497.212		5943.435	
11	6	5	4497.234		5943.453	
11	7	5	4724.597	d	6195.163	
11	7	4	4724.597	d	6195.164	
11	8	4	4979.884	d	6474.798	
11	8	3	4979.884	d	6474.798	
11	9	3	5261.060	d	6779.960	d
11	9	2	5261.060	d	6779.960	d
11	10	2	5566.586	d	7108.852	d
11	10	1	5566.586	d	7108.852	d
11	11	1	5895.293	d	7460.204	d
11	11	0	5895.293	d	7460.204	d
12	0	12	3851.280	a	5211.937	b
12	1	12	3851.391	a	5212.106	b
12	1	11	4024.142	a	5394.190	
12	2	11	4027.219	a	5398.980	
12	2	10	4151.015	a	5525.707	
12	3	10	4177.912	a	5562.713	
12	3	9	4236.551	a	5617.859	
12	4	9	4323.706		5725.215	
12	4	8	4336.861		5735.733	
12	5	8	4488.727		5911.820	
12	5	7	4489.966		5912.591	
12	6	7	4684.378		6130.957	
12	6	6	4684.447		6130.998	
12	7	6	4910.560		6381.545	
12	7	5	4910.562		6381.547	
12	8	5	5164.766	d	6660.119	
12	8	4	5164.766	d	6660.124	
12	9	4	5444.871	d	6964.188	
12	9	3	5444.871	d	6964.189	
12	10	3	5749.250	d	7291.935	d
12	10	2	5749.250	d	7291.935	d
12	11	2	6076.692	d	7641.921	d
12	11	1	6076.692	d	7641.921	d
12	12	1	6426.289	d	8013.230	d
12	12	0	6426.289	d	8013.230	d
13	0	13	4021.296	a	5381.322	b
13	1	13	4021.354	a	5381.423	b
13	1	12	4210.990	a	5582.254	
13	2	12	4212.824	a	5585.279	
13	2	11	4356.753	a	5734.016	
13	3	11	4375.881	a	5761.719	
13	3	10	4453.505		5835.820	
13	4	10	4527.591		5929.705	
13	4	9	4549.511		5948.035	
13	5	9	4692.963		6116.181	
13	5	8	4695.583		6118.087	
13	6	8	4887.169		6334.060	
13	6	7	4887.336		6334.173	
13	7	7	5111.967		6583.309	
13	7	6	5111.965		6583.317	
13	8	6	5364.940		6860.666	
13	8	5	5364.962		6860.702	
13	9	5	5643.861	d	7163.574	d

TABLE 3—*Continued*

J	K_a	K_c	(020)		(030)	
13	9	4	5643.861	d	7163.574	d
13	10	4	5946.981	d	7490.065	d
13	10	3	5946.981	d	7490.065	d
13	11	3	6273.070	d	7838.575	d
13	11	2	6273.070	d	7838.575	d
13	12	2	6621.146	d	8208.206	d
13	12	1	6621.146	d	8208.206	d
13	13	1	6990.499	d	8599.229	d
13	13	0	6990.499	d	8599.229	d
14	0	14	4203.589	a	5562.927	
14	1	14	4203.613	a	5562.982	
14	1	13	4409.821	a	5782.226	
14	2	13	4410.895	a	5784.103	
14	2	12	4574.064		5954.206	
14	3	12	4587.080		5974.167	
14	3	11	4685.335		6069.247	
14	4	11	4746.182		6149.058	
14	4	10	4780.039		6177.898	
14	5	10	4912.775		6336.283	
14	5	9	4917.900		6340.039	
14	6	9	5105.553		6552.689	
14	6	8	5105.951		6552.949	
14	7	8	5328.760		6800.405	
14	7	7	5328.778		6800.438	
14	8	7	5580.359		7076.506	
14	8	6	5580.361		7076.482	
14	9	6	5857.987	d	7378.061	d
14	9	5	5857.987	d	7378.061	d
14	10	5	6159.757		7703.206	d
14	10	4	6159.741		7703.206	d
14	11	4	6484.356	d	8050.141	d
14	11	3	6484.356	d	8050.141	d
14	12	3	6830.839	d	8417.949	d
14	12	2	6830.839	d	8417.949	d
14	13	2	7198.305	d	8807.787	d
14	13	1	7198.305	d	8807.787	d
14	14	1	7587.022	d	9215.047	d
14	14	0	7587.022	d	9215.047	d
15	0	15	4398.133	a	5756.723	
15	1	15	4398.144	a	5756.685	
15	1	14	4620.707	a	5994.169	
15	2	14	4621.328	a	5995.322	
15	2	13	4802.663		6185.804	
15	3	13	4811.219		6199.696	
15	3	12	4930.919		6317.066	
15	4	12	4979.068		6382.887	
15	4	11	5027.996		6425.431	
15	5	11	5147.962		6571.788	
15	5	10	5157.261		6578.695	
15	6	10	5339.468		6786.789	
15	6	9	5340.341		6787.367	
15	7	9	5560.912		7032.879	
15	7	8	5560.968		7032.852	
15	8	8	5810.921		7307.404	
15	8	7	5810.935		7307.400	
15	9	7	6087.162		7607.569	
15	9	6	6087.161		7607.554	
15	10	6	6387.476		7931.301	d
15	10	5	6387.476		7931.301	d
15	11	5	6710.528	d	8276.553	d
15	11	4	6710.528	d	8276.553	d

TABLE 3—*Continued*

J	K_a	K_c	(020)		(030)	
15	12	4	7055.295	d	8642.442	d
15	12	3	7055.295	d	8642.442	d
15	13	3	7420.797	d	9030.968	d
15	13	2	7420.797	d	9030.968	d
15	14	2	7807.703	d	9435.691	d
15	14	1	7807.703	d	9435.691	d
15	15	1	8213.975	d	9860.164	d
15	15	0	8213.975	d	9860.164	d
16	0	16	4604.889	a	5962.595	
16	1	16	4604.895	a	5962.616	
16	1	15	4843.687		6218.156	
16	2	15	4844.048		6218.862	
16	2	14	5042.533		6428.599	
16	3	14	5047.993		6437.996	
16	3	13	5189.148		6578.216	
16	4	13	5225.805		6630.897	
16	4	12	5292.562		6690.038	
16	5	12	5398.267		6822.431	
16	5	11	5414.029		6834.354	
16	6	11	5588.862		7036.262	
16	6	10	5590.624		7037.456	
16	7	10	5808.391			
16	7	9	5808.515		7280.540	
16	8	9	6056.728			
16	8	8	6056.729			
16	9	8	6331.399			
16	9	7	6331.338			
16	10	7	6629.985		8174.291	
16	10	6	6630.093		8174.284	
16	11	6	6951.509	d		
16	11	5	6951.509	d		
16	12	5	7294.505	d	8881.623	d
16	12	4	7294.505	d	8881.623	d
16	13	4	7657.897	d	9268.805	
16	13	3	7657.897	d	9268.725	
16	14	3	8042.931	d	9670.878	d
16	14	2	8042.931	d	9670.878	d
16	15	2	8446.768	d	10092.855	d
16	15	1	8446.768	d	10092.855	d
16	16	1	8870.284	d		
16	16	0	8870.284	d		
17	0	17	4823.826	d	6180.624	d
17	1	17	4823.826	d	6180.624	d
17	1	16	5078.784		6454.221	
17	2	16	5079.003		6454.638	
17	2	15	5293.768		6682.573	
17	3	15	5297.188		6688.802	
17	3	14	5459.125		6851.657	
17	4	14	5485.970		6892.335	
17	4	13	5572.703		6970.837	
17	5	13	5663.264		7087.895	
17	5	12	5688.369		7107.258	
17	6	12	5853.563			
17	6	11	5856.961			
17	7	11	6071.108			
17	7	10	6071.366			
17	8	10	6317.517			
17	8	9	6317.555			
17	9	9	6590.166			
17	9	8	6590.521			
17	10	8	6887.482			

TABLE 3—*Continued*

J	K_a	K_c	(020)		(030)	
17	10	7	6887.748			
17	11	7	7207.185		8773.701	
17	11	6	7207.183		8773.684	
17	12	6	7548.568	d		
17	12	5	7548.568	d		
17	13	5	7909.580	d		
17	13	4	7909.580	d		
17	14	4	8292.651	d		
17	14	3	8292.651	d		
17	15	3	8693.918	d		
17	15	2	8693.918	d		
17	16	2	9114.763	d		
17	16	1	9114.763	d		
17	17	1	9553.977	d		
17	17	0	9553.977	d		
18	0	18	5054.907	d	6410.733	d
18	1	18	5054.907	d	6410.733	d
18	1	17	5325.981		6702.406	
18	2	17	5326.073		6702.645	
18	2	16	5556.514		6947.844	
18	3	16	5558.617		6951.889	
18	3	15	5740.213		7136.553	
18	4	15	5759.595		7167.029	
18	4	14	5867.250		7266.800	
18	5	14	5942.614			
18	5	13	5980.165			
18	6	13	6133.408			
18	6	12	6139.572			
18	7	12	6349.142			
18	7	11	6349.565			
18	8	11	6593.183			
18	8	10	6593.387			
18	9	10	6864.234			
18	9	9	6864.827			
18	10	9	7159.668			
18	10	8	7159.394			
18	11	7	7477.528			
18	12	7	7816.054	d		
18	12	6	7816.055	d		
18	13	6	8175.745	d		
18	13	5	8175.745	d		
18	14	5	8556.839	d		
18	14	4	8556.839	d		
18	15	4	8955.350	d		
18	15	3	8955.350	d		
18	16	3	9373.426	d		
18	16	2	9373.426	d		
18	17	2	9809.778	d		
18	17	1	9809.778	d		
18	18	1	10258.304	d		
18	18	0	10258.304	d		
19	0	19	5298.092	d	6652.504	
19	1	19	5298.092	d	6652.646	
19	1	18	5585.278		6962.716	
19	2	18	5585.329		6962.827	
19	2	17	5830.849		7224.509	
19	3	17	5832.122		7227.091	
19	3	16	6032.024		7432.226	
19	4	16	6044.858		7454.531	
19	4	15	6176.016		7576.713	
19	5	15	6235.871			
19	5	14	6288.926			
19	6	14	6428.113			
19	6	13	6438.720			
19	7	13	6641.838			
19	7	12	6643.079			
19	8	12	6884.063			
19	8	11	6884.128			
19	9	11	7152.897			
19	9	10	7152.522			
19	10	10	7446.587			
19	10	9	7446.117			
19	11	9	7762.375			
19	11	8	7762.359			
19	12	8	8099.137			
19	12	7	8099.137	a		
19	13	7	8456.368	d		
19	13	6	8456.368	d		
20	0	20	5553.322	d	6906.757	
20	1	20	5553.322	d	6906.824	
20	1	19	5856.631		7235.211	
20	2	19	5856.645		7235.160	
20	2	18	6116.857		7512.665	
20	3	18	6117.619		7514.248	
20	3	17	6334.436		7738.131	
20	4	17	6342.986		7754.482	
20	4	16	6496.337		7899.724	
20	5	16	6542.561			
20	5	15	6613.810			
20	6	15	6737.434			
20	6	14	6754.659			
20	7	14	6950.001			
20	7	13	6951.936			
20	8	13	7189.485			
20	9	12	7456.101			
20	9	11	7455.924			
21	0	21	5820.577		7172.861	
21	1	21	5820.616		7172.929	
21	1	20	6140.014		7519.627	
21	2	20	6140.037			
21	2	19	6414.528		7812.473	
21	3	19	6414.949		7813.166	
21	3	18	6647.595			
21	4	18	6653.128			
21	4	17	6827.262			
21	5	17	6862.266			
21	6	16	7060.912			
21	6	15	7087.217			
21	7	15	7272.515			
21	7	14	7276.268			
21	8	14	7508.776			
21	8	13	7510.086			
21	10	12	8064.452			
21	10	11	8063.861			
22	0	22	6099.713		7450.882	
22	1	22	6099.802		7451.331	
22	1	21	6435.418		7816.239	
22	2	21	6435.483		7815.555	
22	2	20	6723.891			
22	3	20	6724.127			
22	3	19	6971.579			
22	4	19	6975.122			

TABLE 3—*Continued*

J	*K_a*	*K_c*	(020)	(030)	
22	4	18	7169.329		
22	5	18	7194.425		
22	5	17	7308.237		
22	6	17	7398.144		
22	6	16	7436.726		
23	0	23	6390.891	7740.686	
23	1	23	6390.998	7740.803	
23	1	22	6742.804		
23	2	22	6742.966		
23	2	21	7044.892		
23	3	21	7044.949		
23	3	20	7306.531		
23	4	20	7308.736		
24	0	24	6693.846	8042.550	d
24	1	24	6693.943	8042.658	d
24	1	23	7062.126		
24	2	23	7063.575		
24	2	22	7377.377		
24	3	22	7377.530		
24	3	21	7652.538		
24	4	21	7653.801		
24	4	20	7881.869		
25	0	25	7008.773		
25	1	25	7008.797		
25	1	24	7392.866		
25	2	24	7393.400		
25	2	23	7721.393		
25	3	23	7721.804		
25	3	22	8009.664		
26	0	26	7335.478		
26	1	26	7335.497		
26	1	25	7736.133		
26	2	25	7736.662		
27	0	27	7673.981		
27	1	27	7674.006		

TABLE 4

Experimental Term Values for the (040) Vibrational State of HDO

J	*K_a*	*K_c*	E / cm^{-1}
1	0	1	5435.6068
1	1	0	5465.0623
2	0	2	5466.4376
2	1	1	5499.5585
3	0	3	5511.8399
3	1	3	5530.7079
3	1	2	5551.0726
3	2	2	5620.0923
3	2	1	5621.7228
3	3	1	5802.9254
3	3	0	5802.9551
4	0	4	5571.0447
4	1	4	5585.5093
4	2	3	5681.7361
4	2	2	5686.4474
5	0	5	5643.1421
5	1	5	5653.5189
5	1	4	5703.6235
5	2	4	5758.3228
5	2	3	5768.6395
6	0	6	5727.4602
6	1	6	5734.4833
6	1	5	5803.5002
6	2	5	5849.5472
7	0	7	5823.6422
7	1	7	5828.1982
7	1	6	5918.0485
7	2	5	5985.9790
7	3	5	6149.7993
7	3	4	6153.3642
7	4	4	6320.5506
8	0	8	5931.5867
8	1	8	5934.4373
8	1	7	6046.2411
8	2	7	6074.5291
8	2	6	6120.4486
9	0	9	6051.3254
9	1	9	6053.0712
9	2	8	6207.5327
9	2	7	6271.1832
9	3	7	6417.2246
9	0	9	6051.3254
9	1	9	6053.0712
9	2	8	6207.5327
9	2	7	6271.1832
9	3	7	6417.2246
10	0	10	6182.9611
10	1	10	6184.0147
10	1	9	6339.7061
10	2	8	6504.9100
10	4	7	6747.7909
10	4	6	6749.9688
11	1	11	6327.1599
11	1	10	6503.6295
11	2	10	6583.8419
11	4	8	6921.7836
11	1	11	6327.1599
11	1	10	6503.6295
11	2	10	6583.8419
11	4	8	6921.7836
12	0	12	6482.0818
12	1	12	6482.4608
12	0	12	6482.0818
12	1	12	6482.4608
13	0	13	6649.6576
13	1	13	6649.8965

4. CONCLUSIONS

We present the first hot emission spectrum of HDO. This spectrum is very dense since it contains many lines belong to H_2O and D_2O as well as HDO. HDO lines have been identified by comparison with other hot emission spectra. The HDO transitions have been analyzed resulting in the assignment of many hot pure rotational transitions, bending hot bands linking states up to the previously unobserved (040) bending state, and vibrational difference bands.

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