Long Path FTS Spectra of Deuterated Water Vapor: New Data for HDO Molecule in the 8800 – 9100 cm^{-1} Spectral Region

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Introduction

The long path (602.32 m) absorption spectra of deuterated water have been recorded in the 8800 – 11500 cm^{-1} spectral region. Spectra were recorded with resolution of 0.03 cm^{-1} and signal to noise ratio S/N from 2100 up to 3700. The total pressure of H_2O+HDO+D_2O mixtures was about 10 torr. Two spectra with different partial pressures of water species have been recorded. Table 1 lists the experimental conditions under which the spectra were taken. These spectra have been recently used to study of D_2O absorption in the 8800 – 9500 cm^{-1} region [1]. We use these spectra for analysis of HDO absorption in the 8800 – 9100 cm^{-1} because only 210 line positions were reported in Ref. [2]. Spectral region 9100 – 9500 cm^{-1} of HDO has been studied in Ref. [3].

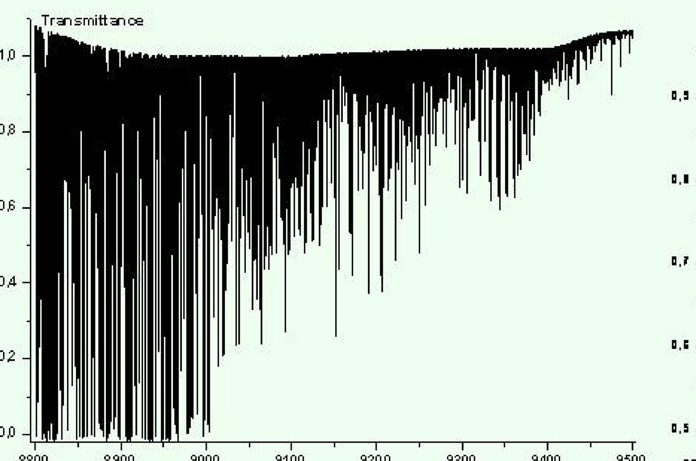

Fig.1. Overview of 98027 spectrum in the 8800-9100 cm^{-1} spectral range

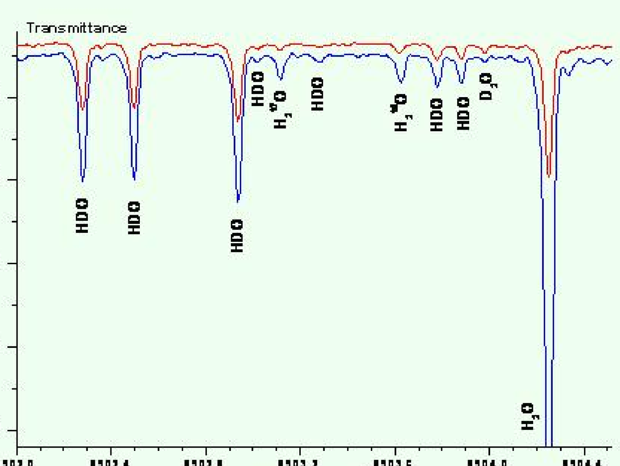

Fig.2. Example of experimental spectra at 8903 cm^{-1}

Table 1. Measurement conditions

Filename	98024	98027
Spectral range (cm^{-1})	8800–11500	8800–11500
Temperature (K)	293	293
Resolution (cm^{-1})	0.03	0.03
Path length (m)	602.32	602.32
Total pressure (torr)	9.956	9.877
P_{H2O} (torr)	0.327	1.713
P_{HDO} (torr)	2.216	4.829
P_{D2O} (torr)	7.413	3.335
Signal to noise ratio	2100÷3700	2100÷3700

Data reduction and assignment

Fig. 1 shows a general view of water absorption in the 8800 – 9100 cm^{-1} region. About 2050 lines have been measured in this region. More than 1860 lines were assigned to five water species. Practically all lines of $H_2{}^{16}O$ (708 lines), $H_2{}^{18}O$ (66 lines) and $H_2{}^{17}O$ (31 lines) have been assigned using well known literature energy levels [4-7]. The lines correspond to D_2O transitions were assigned in Ref. [1]. More than 650 transitions of HDO molecule have been assigned to rotation-vibration bands correspond to 8 upper vibrational states: (012), (041), (060), (121), (150), (201), and (310). The assignment of transitions has been done using literature experimental energy levels and calculated water linelist based on variational calculations using PES [8] and DMS [9] (PS calculation). This linelist is available on http://spectra.iao.ru.

Determination of experimental energy levels of HDO molecule and confirmation of lines assignment was made using the RITZ code as well as in our previous studies of D_2O molecule [10, 11]. For this purpose we use all available line positions from microwave to visible region, including data of Refs. [2, 3, 12], and observed in this study.

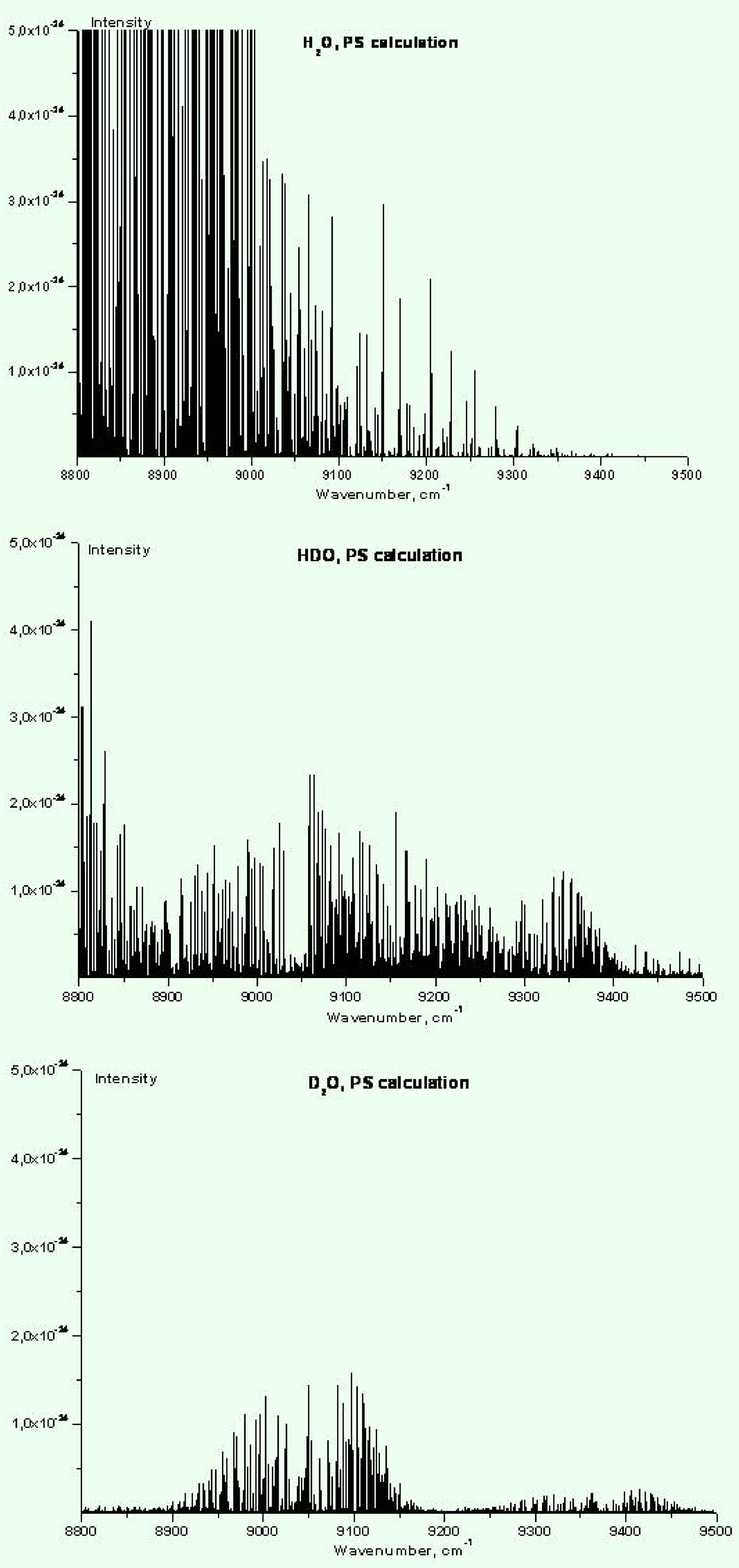

Fig.3. Calculated spectra of H_2O, HDO and D_2O in the 8800–9100 cm^{-1} spectral range

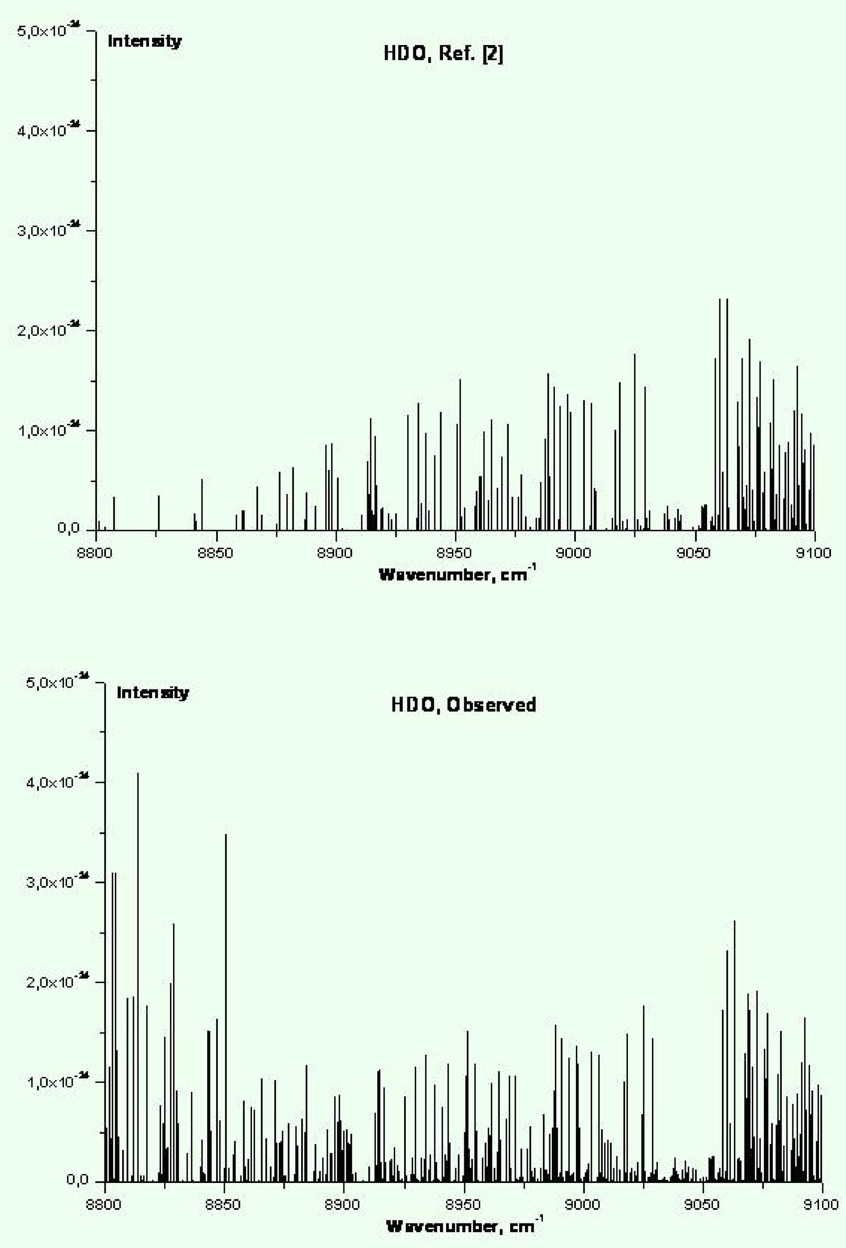

Fig. 4. Observed lines of HDO in Ref. [2] (upper panel) and in this study (lower panel)

Results and comparison with literature data

Our study of HDO absorption in the 8800–9100 cm^{-1} region allows us to assign more than 440 lines for the first time and to complete the sets of rotational energy levels of several vibrational states. Table 2 contains a comparison of the rotational levels deduced from this study with the most complete previous data sets [3, 12]. Columns 5, 6, 13 and 14 contain our experimental energies with their uncertainties. Columns 7 and 15 contain experimental energies from [12] (for the (012) state) and [3] (for the (070), (041) and (201) states). δE (Columns 8 and 16) are discrepancies between energies of two sets in 10^{-4} cm^{-1} units.

Table 2. Comparison of experimental rotational levels of the (012), (070), (041) and (201) states of HDO

$v_1v_2v_3$	J	K_a	K_c	E_{obs} (cm^{-1})	dE	E_{BBN} (cm^{-1})	δE	$v_1v_2v_3$	J	K_a	K_c	E_{obs} (cm^{-1})	dE	E_{obs} (cm^{-1})	δE
012	6	0	6	8910.4091	8	8910.4085	6	012	13	0	13			9821.7166	
012	6	1	6	8912.1343	8	8912.1340	3	012	13	1	13			9821.7284	
012	6	1	5	8972.4958	10	8972.4951	7	012	13	1	12			9991.2692	
012	6	2	5			8991.7122		012	13	2	12			9991.7312	
012	6	2	4	9014.7579	8	8991.7582	-3	012	13	2	11	10130.6120	12		
012	6	3	4	9074.2978	8	9074.2987	-9	012	13	3	11	10137.3321	12	10137.3342	-21
012	6	3	3	9077.4584	10	9077.4588	-4	012	13	3	10	10228.5517	12		
012	6	4	3	9178.0548	10	9178.0556	-8	012	13	4	10	10266.7375	12		
012	6	4	2	9178.1941	8	9178.1934	-7	012	13	4	9			10303.2292	
012	6	5	2	9309.1527	10	9309.1455	72	012	13	5	9	10398.2137	14		
012	6	5	1	9309.1527	20	9309.1482	45	012	13	5	8	10404.7758	10		
012	6	6	1	9466.9366	12	9466.9364	2	012	13	6	8	10549.4133	12		
012	6	6	0	9466.9364	12	9466.9380	-16	012	14	0	14			10000.3884	
012	7	0	7			9004.2525		012	14	1	14			10000.3944	
012	7	1	7	9005.1549	8	9005.1580	-31	012	14	1	13			10184.1156	
012	7	1	6	9082.3103	8	9082.3089	14	012	14	2	13			10184.3510	
012	7	2	6	9095.6908	8	9095.6903	5	012	14	2	12	10338.6594	14	10338.6593	1
012	7	2	5	9131.6942	6	9131.6940	2	012	14	3	11	10453.3569	18	10453.3339	230
012	7	3	5	9183.0890	8	9183.0869	21	012	14	4	10	10533.5518	22		
012	7	3	4	9190.3691	8	9190.3695	-4	012	14	5	9	10627.8435	22		
012	7	4	4	9287.1539	8	9287.1561	-22	012	14	6	8	10767.7380	22		
012	7	4	3	9287.6455	8	9287.6467	-12	012	15	0	15			10191.1124	
012	7	5	3	9417.6177	10	9417.6182	-5	012	15	1	15			10191.1153	
012	7	5	2	9417.6314	10	9417.6307	7	012	15	3	13	10560.2887	18		
012	7	6	2	9574.8856	10	9574.8892	-36	012	15	3	12	10689.8379	20		
012	7	6	1	9574.8867	8	9574.8894	-27	012	15	4	12	10709.0620	18		
012	7	7	1	9757.5135	12	9757.5134	1	012	15	4	11	10779.8778	20		
012	7	7	0	9757.5135	14	9757.5134	1	012	15	5	10	10870.0191	34		
012	8	0	8	9110.1566	10	9110.1562	4	012	16	0	16			10393.8352	
012	8	1	8	9110.6149	12	9110.6154	-5	012	16	1	16			10393.8410	
012	8	1	7			9204.5172		012	16	1	15			10605.6074	
012	8	2	7	9213.1532	8	9213.1537	-5	012	16	3	14	10790.0150	22		
012	8	2	6	9264.5966	6	9264.5939	27	012	16	3	13	10937.2366	32		
012	8	3	6	9306.9426	8	9306.9430	-4	012	16	4	13	10949.8954	32		
012	8	3	5	9321.1836	8	9321.1895	-59	012	16	4	12	11040.6547	32		
012	8	4	5	9412.0314	6	9412.0318	-4	012	16	5	12	11095.0698	32		
012	8	4	4	9413.4373	8	9413.4374	-1	012	17	3	14	11195.3906	40		
012	8	5	4	9541.7737	8	9541.7745	-8								
012	8	5	3	9541.8329	8	9541.8339	-10								
012	8	6	3	9698.3531	20	9698.3588	-57	070	5	0	5	9311.8556	12		
012	8	6	2	9698.3531	10	9698.3585	-54	070	9	1	9	9764.1949	10		
012	8	7	2	9880.4135	10	9880.4148	-13								
012	8	7	1	9880.4135	12	9880.4148	-13	041	0	0	0	9032.1034	12		
012	9	0	9	9228.1781	8	9228.1784	-4	041	1	0	1	9047.5966	8		
012	9	1	9	9228.4040	8	9228.4054	-14	041	1	1	1	9089.1683	10		
012	9	1	8			9338.5104		041	1	1	0	9092.9769	10		
012	9	2	8			9343.7269		041	2	0	2	9078.2603	10		
012	9	2	7	9412.3985	8	9412.4010	-25	041	2	1	2	9116.2360	8	9116.2352	8
012	9	3	7	9445.4754	6	9445.4755	-1	041	2	1	1	9127.3945	8		
012	9	3	6	9469.9214	8	9469.9212	2	041	3	0	3	9123.4292	8		
012	9	4	6	9552.5963	10	9552.6052	11	041	3	1	3	9156.9438	8	9156.9572	-134
012	9	4	5	9556.0268	8	9556.0264	4	041	3	1	2	9178.8292	8		
012	9	5	5	9681.6655	6	9681.6655	0	041	3	2	2	9245.7606	12	9245.7607	-1
012	9	5	4	9681.8644	6	9681.8648	-4	041	3	2	1	9250.0243	8	9250.0222	21
012	9	6	4	9837.3766	8	9837.3785	-19	041	3	3	1	9362.2016	8	9362.2007	11
012	9	6	3	9837.3804	8	9837.3740	64	041	3	3	0	9362.2368	8	9362.2373	-5
012	9	7	3	10018.7262	24	10018.7274	-12	041	4	0	4	9182.0380	8		
012	9	7	2	10018.7262	12	10018.7275	-13	041	4	1	4	9211.1045	8	9211.1067	-22
012	9	8	2	10224.1584	16	10224.0627	957	041	4	1	3	9246.9579	8	9246.9491	88
012	9	8	1	10224.1584	14	10224.0627	957	041	4	2	3	9307.2053	10		
012	10	0	10			9358.3473		041	4	2	2	9313.2991	8	9313.2991	0
012	10	1	10			9358.4578		041	4	3	2	9424.3166	12	9424.3165	1
012	10	2	10			9484.0968		041	4	3	1	9424.5038	8	9424.5038	0
012	10	2	9	9487.1473	10	9487.0912	561	041	4	4	1	9641.8567	8	9641.8567	0
012	10	2	8			9573.9222		041	4	4	0	9641.8622	8	9641.8589	33
012	10	3	8	9598.2054	8	9598.2053	1	041	5	1	5	9278.4664	8	9278.4454	210
012	10	3	7	9636.0412	10	9636.0334	78	041	5	1	4	9331.3856	8	9331.3790	66
012	10	4	7	9708.6976	8	9708.6954	22	041	5	2	4	9383.6218	8	9383.6227	-9
012	10	4	6	9715.9768	8	9715.9772	-4	041	5	2	3	9396.9488	10	9396.9477	11
012	10	5	6	9837.3105	10	9837.3116	-11	041	5	3	3	9502.0200	8	9502.0199	1
012	10	5	5	9837.8854	10	9837.8851	3	041	5	3	2	9502.8005	8	9502.7995	10
012	10	6	5	9991.9739	10	9991.9684	55	041	5	4	2	9720.2237	8	9720.2235	2
012	10	6	4	9992.0005	10			041	5	4	1	9720.2896	8	9720.2907	-11
012	10	7	4	10172.4582	10	10172.4593	-11	041	5	5	1	9916.2354	8	9916.2354	0
012	10	7	3	10172.4563	12	10172.4593	-30	041	5	5	0	9916.2369	12	9916.2344	25
012	10	8	3	10377.1156	14			041	6	0	6	9347.5998	10		
012	10	8	2	10377.1141	12			041	6	1	6	9358.7038	6	9358.7026	12
012	11	0	11			9500.6711		041	6	1	5	9431.2239	10		
012	11	1	11			9500.7193		041	6	2	5	9474.6786	8	9474.6785	1
012	11	1	10			9641.3408		041	6	2	4	9497.2367	8	9497.2284	83
012	11	2	10			9642.9955		041	6	3	4	9595.3986	6	9595.3971	15
012	11	2	9	9746.9849	10	9747.9899	-50	041	6	3	3	9597.5802	10	9597.5801	1
012	11	3	9	9764.7466	10	9764.7446	20	041	6	4	3	9814.2772	8	9814.2756	16
012	11	3	8	9818.6124	8	9818.6178	-54	041	6	4	2	9814.5580	8	9814.5579	1
012	11	4	8	9880.0145	10	9880.0154	-9	041	6	5	2	10010.0205	8	10010.0194	11
012	11	4	7	9893.7923	10	9893.7946	-23	041	6	5	1	10010.0205	8	10010.0210	-5
012	11	5	7	10008.7279	8	10008.7245	34	041	6	6	1	10243.0113	12	10243.0112	1
012	11	5	6	10010.1460	8	10010.1471	-11	041	6	6	0	10243.0113	14	10243.0113	0
012	11	6	6	10162.1709	10	10162.1650	59								
012	11	6	5	10162.2496	10	10162.2468	28	201	11	2	9	10137.4993	8		
012	11	7	5	10341.6226	14			201	12	2	11	10211.8069	12		
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012	12	1	12			9655.1606		201	12	4	8	10459.7884	12		
012	12	1	11			9810.3647									
012	12	2	11			9811.2539									
012	12	2	10	9933.7029	14	9933.7027	2								
012	12	3	10	9944.5836	12	9944.5849	-13								
012	12	3	9	10016.5473	10	10016.5440	33								
012	12	4	9	10066.1824	10	10066.1802	22								
012	12	4	8	10089.6428	10										
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012	12	5	7	10198.9093	10										
012	12	6	6	10348.2162	10										
012	12	7	5	10526.2355	16										

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