

Study (301)-(000) D₂O band in 10200 – 10450 cm⁻¹ spectral region

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ABSTRACT

Measurements of D₂O absorption spectra in the visible spectral region near 0.98 μm are performed using FT-spectrometer IFS-125M and Light-emitting diode (LED) as source of radiation. Water vapor spectrum has been obtained by averaging over 17136 scans recorded at 24 m optical path length, temperature 24 C and pressure of sample 27 mBar. Due to strong emission of LED source it was possible to achieve signal-to-noise ratio about 10⁴ and to record weak lines with intensities of 6 10⁻²⁷ cm/molecule. Comparisons with results of early works are made.

1. INTRODUCTION

The absorption spectra of water isotopologues are important for atmospheric applications and accurate determination of its potential energy and dipole moment functions. The spectra of different water isotopologues have been measured with high accuracy in a wide frequency region, ranging from infrared to microwave. Recently the IUPAC task group presents detailed reviews of the water vapor spectra [1-3]. The spectrum of D₂O in the range of 10 200-10 440 cm⁻¹ has been studied recently in [4] at a pressure of 2352 Pa, the optical path length of 105m, a spectral resolution of 0.02 cm⁻¹. More than 200 of vibrational-rotational lines with a value of the rotational quantum number J = 13 belonging to the 3ν₁+ν₃ vibrational-rotational band have been reported. Low signal to noise ratio (S/N = 100) does not allow to detect weaker lines and measure the intensity of the lines.

2. EXPERIMENT

The D₂¹⁶O absorption spectrum was recorded by a high resolution Fourier-transform spectrometer IFS-125M in the region 10 100-10 440 cm⁻¹ with an absorption path of 34.8 m and resolution of 0.03 cm⁻¹. White type multipass absorption cell with a basic length of 60 cm were used. Light-emitting diode (LED) EDEI-1LS3-R was applied as a source of radiation. Signal-to-noise ratio amounted to about 10⁴, which allowed to measure parameters of lines with intensity about 2*10⁻²⁷ cm/molecule[5-8]. Line positions and line intensities derived from the fitting were compared with Partridge-Sewenke calculation from [9] and with data obtained in previous work[4].

Table 1. Experimental conditions.

Spectral resolution	0.1 cm ⁻¹
Optical path length	34.8 m
Pressure	27 mBar
Temperature	24 ± 1 C
Signal-to-noise	about 10000

The overview of transmittance spectrum is shown in Fig. 1. It can be seen from Fig.1 that the maximum value of absorption in the spectral interval studied is only 0.0016 for strongest lines and it is tenths times less for very weak lines shown in the additional penal. The possibility of very weak line observation with small-size cell is provided by use of LED as source of light.

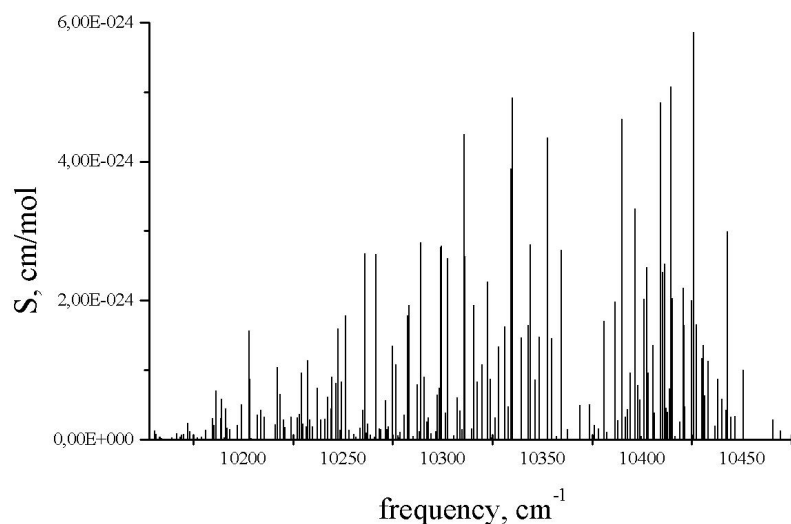


Fig.1.The absorption spectrum D₂O in 0.97 μm

Comparison of the experimental frequencies of the D₂O strong lines with the data of [4] and Partridge-Schwenke (PS) calculations is shown in Fig.2.

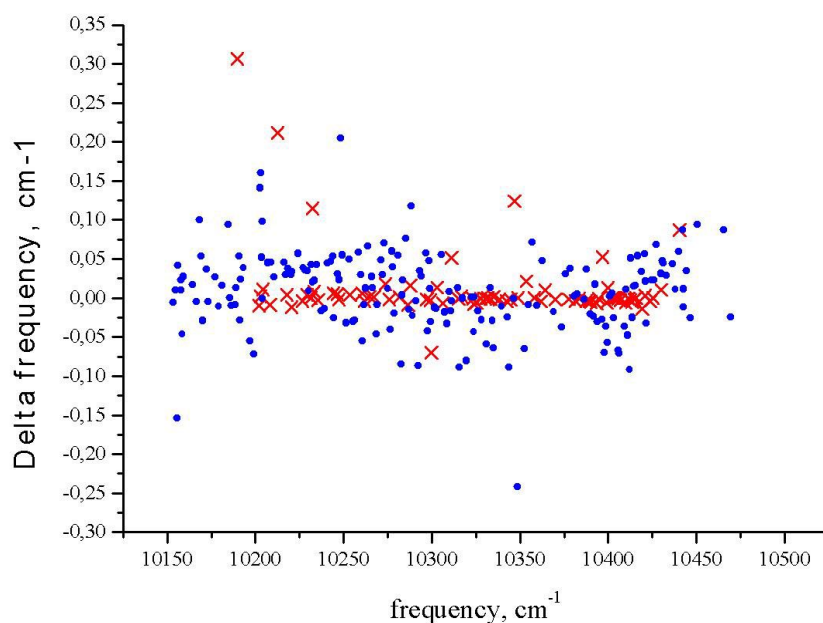


Fig.2. Differences between the experimental line positions (ν^{OBS}) and data of [4] (crosses) and PS(circles)

Table 2. Part of the D₂O spectrum in 10189-10153 cm⁻¹ range

ν , cm ⁻¹	S, cm/mol	N[4], cm ⁻¹	N(PS), cm ⁻¹	S(PS), cm/mol	V	V	V	J'	K'a	K'c	J	Ka	Kc
10157,5589	3,750E-26		10157,470	4,309E-26	3	0	1	11	4	8	12	4	9
10157,7322	1,797E-28		10157,722	2,306E-28	3	1	1	8	6	3	9	6	4
10157,8167	1,655E-26		10157,831	1,058E-26	3	0	1	5	2	4	6	4	3
10158,0050	4,256E-26		10157,982	1,078E-27	2	3	1	6	6	1	6	6	0
10158,3449	2,546E-26		10158,323	3,147E-28	0	4	2	9	1	8	8	2	7
10158,5199	3,553E-26		10158,566	2,447E-26	3	0	1	10	6	4	11	6	5
10159,0655	3,066E-26		10159,124	4,568E-26	3	0	1	10	6	5	11	6	6
10159,2564	2,093E-26		10159,229	2,659E-28	4	0	0	14	2	13	14	3	12
10159,3485	7,668E-26		10159,335	8,952E-26	2	2	1	1	1	1	2	1	2
10164,4324	2,683E-26		10164,415	2,104E-26	4	0	0	5	4	2	6	5	1
10164,6394	3,292E-26		10164,624	6,907E-27	3	0	1	7	1	6	8	3	5
10166,7691	8,600E-26		10166,774	9,310E-26	3	0	1	10	5	6	11	5	7
10168,0016	7,402E-26		10167,975	6,770E-26	2	2	1	0	0	0	1	0	1
10168,5662	4,297E-26		10168,466	6,620E-26	3	0	1	11	3	8	12	3	9
10168,7120	4,276E-26		10168,846	1,540E-26	3	0	1	9	7	3	10	7	4
10169,1293	6,669E-26		10169,076	5,204E-26	3	0	1	11	3	9	12	3	10
10170,1015	1,554E-25		10170,155	9,810E-26	3	0	1	13	0	13	14	0	14
10170,1792	7,824E-26		10170,208	3,176E-26	3	0	1	5	2	3	6	4	2
10170,2317	6,642E-26		10170,215	7,866E-26	3	0	1	11	2	9	12	2	10
10172,2437	2,353E-25		10172,207	4,833E-26	3	0	1	12	1	11	13	1	12
10172,6248	6,793E-26		10172,638	3,602E-26	0	4	2	11	5	7	12	2	10
10173,3160	1,255E-25		10173,321	9,931E-26	2	2	1	2	1	2	2	1	1
10176,9737	9,342E-26		10177,028	1,210E-27	3	0	1	14	1	13	14	3	12
10177,0900	2,523E-26		10177,063	8,157E-26	3	0	1	9	6	3	10	6	4
10178,9451	5,779E-26		10178,989	3,534E-26	4	0	0	11	1	11	12	2	10
10179,1998	4,398E-26		10179,210	1,991E-26	4	0	0	4	4	0	5	5	1
10180,6861	7,354E-26		10180,675	7,749E-26	2	2	1	6	3	4	6	3	3
10181,3220	1,370E-25		10181,306	9,433E-26	2	2	1	3	2	2	3	2	1
10183,8386	2,316E-25		10181,814	3,917E-27	3	2	0	5	0	5	4	1	4
10184,5993	3,051E-25		10184,505	3,342E-26	2	2	1	8	4	5	8	4	4
10184,6693	2,459E-25		10184,694	1,626E-25	3	0	1	9	5	4	10	5	5
10185,5532	2,069E-25		10185,553	1,774E-25	2	2	1	2	2	0	2	2	1
10185,7877	3,445E-25		10185,780	1,851E-25	2	2	1	3	2	1	3	2	2
10186,3181	7,017E-25		10186,328	1,594E-25	3	0	1	10	3	8	11	3	9
10187,5050	6,299E-25		10187,429	2,321E-25	3	0	1	11	1	10	12	1	11
10188,7501	3,108E-25		10188,759	3,844E-26	2	2	1	6	3	3	6	3	4

10188,9058	1,233E-25		10188,853	1,076E-25	1 2 2	10 2 8	11 3 9
10189,0579	5,881E-25		10189,045	1,131E-25	3 0 1	10 2 8	11 2 9
10189,8218	7,935E-26	10189,515	10189,845	1,228E-25	2 2 1	4 3 1	4 3 2

Comparison of the experimental intensities of strong lines of D₂O with the intensities of lines of PS work is shown in

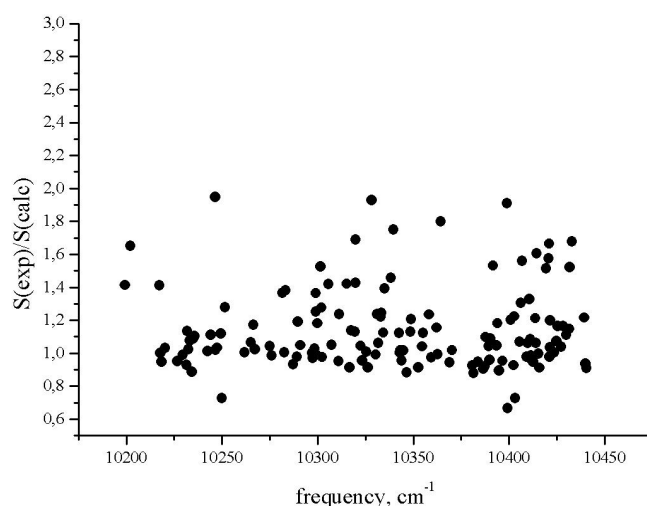


Fig.3.Comparison of the experimental intensities of strong lines of D₂O with the intensities of lines of PS work

Table 3. Water lines mistakenly referred to D₂O in [4], cm⁻¹

10219.571	10260.326	10260.398	10284.420	10311.903	10314.541
10315.027	10320.896	10342.172	10365.108	10374.890	10385.962
10394.218	10397.562	10397.679	10405.014	10405.127	10425.588
10433.574	10434.224	10434.381	10435.301	10436.972	10437.578

CONCLUSIONS

A detailed information on the absorption of D₂O in the spectral range 10 150 to 10 450 cm⁻¹ was obtained. The line parameters (positions and intensities) were determined for a large number of the D₂O rotation-vibration lines. Owing to the use of high luminescence LED sources with the path length of 24 m, it was made possible to achieve an absorption sensitivity of 1.2×10^{-7} cm⁻¹. The majority of lines in the registered spectra was assigned to the 3ν₁+ν₃ D₂O band.

ACKNOWLEDGEMENTS

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