# Study (301)-(000) $D_2O$ band in 10200 – 10450 $см^{-1}$ spectral region

Sinitsa L.N.[a,b], Serdukov V.I.[a], Scherbakov A.P. [a] A.S.Sergeeva[b], M.O.Miheenko[b]

[a]V.E. Zuev Institute of Atmospheric Optics SB RAS, 1, Academician Zuev square, Tomsk, 634021, Russia;
[b]National Research Tomsk State University, 36, Lenina Avenue, Tomsk, 634050, Russia.

**Key word:** water vapor spectra, visible spectral region, $D_2O$ line positions and intensities, Fourier spectrometer.

## 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 $10^4$ 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 $\mathbf{3\nu_1+\nu_3}$ 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 $D_2{}^{16}O$ 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 $см^{-1}$. 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 $10^4$, 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-Scwenke 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 |

21st International Symposium on Atmospheric and Ocean Optics: Atmospheric Physics,
edited by G. G. Matvienko, O. A. Romanovskii, Proc. of SPIE Vol. 9680, 968000
 · doi: 10.1117/12.2206020

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.

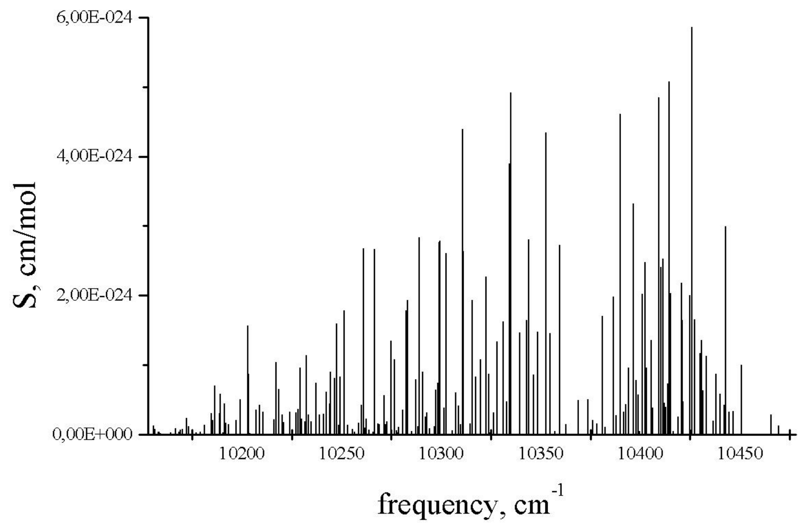


Fig.1.The absorption spectrum $D_2O$ in 0.97 μm

Comparison of the experimental frequencies of the $D_2O$ strong lines with the data of [4 ] and Partridge-Schwenke (PS) calculations is shown in Fig.2.

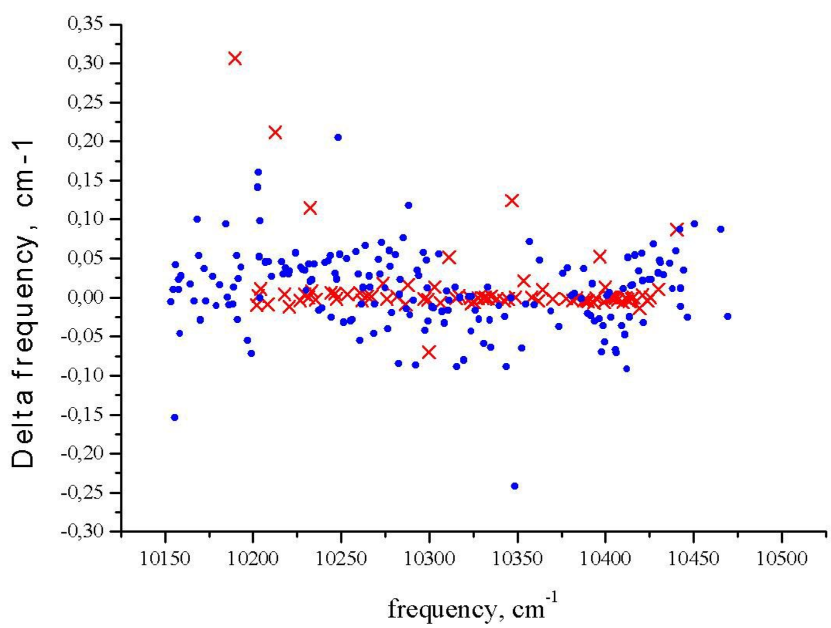


Fig.2. Differences between the experimental line positions ($v^{OBS}$) and data of [4 ] (crosses) and PS(circles)

Table 2. Part of the $D_2O$ 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 $D_2O$ with the intensities of lines of PS work is shown in

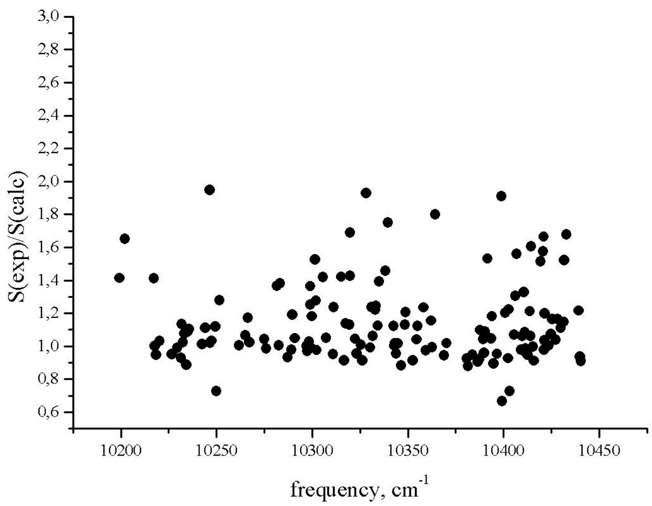


Fig.3.Comparison of the experimental intensities of strong lines of $D^2O$ with the intensities of lines of PS work

Table 3. Water lines mistakenly referred to $D_2O$ 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 $D_2O$ 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 $D_2O$ 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 $1.2\times10^{-7}$ $cm^{-1}$. The majority of lines in the registered spectra was assigned to the $3\nu_1+\nu_3$ $D_2O$ band.

## ACKNOWLEDGEMENTS

The work was supported in part by RFBR (Grant №13-03-98023) and Program of FI SB RAS № II.10.1.

## References

[1] J. Tennyson, P.F. Bernath, L.R. Brown, et all, “IUPAC critical evaluation of the rotational-vibrational spectra of water vapor. Part II. Energy levels and transition wavenumbers for $HD^{16}O$, $HD^{17}O$, and $HD^{18}O$”, JQSRT, **111**, 2160-2184 (2010)

[2] J. Tennyson, P.F. Bernath, L.R. Brown, et all, “IUPAC critical evaluation of the rotational-vibrational spectra of water vapor. Part I. Energy levels and transition wavenumbers for $H_2{}^{17}O$ and $H_2{}^{18}O$ “, JQSRT, **110**, 573-596 (2009)

[3] J. Tennyson, P.F. Bernath, L.R. Brownet all, “IUPAC critical evaluation of the rotational-vibrational spectra of water vapor. Part IV: Energy levels and transition wavenumbers for $D_2{}^{16}O$, $D_2{}^{17}O$, and $D_2{}^{18}O$ “, JQSRT, **142**, 93-108 (2014)

[4] O. N. Ulenikov, Shui-Ming Hu, E. S. Bekhtereva, et all, “High-Resolution Fourier Transform Spectrum of $D_2O$ in the Region Near 0.97 μm “, J.Mol.Spectrosc. 8433 (2001).

[5] V.I. Serdyukov, L.N. Sinitsa, S.S.Vasil’chenko, **“**Highly sensitive fourier transform spectroscopy with led sources “, J.Mol.Spectrosc. **290** ( 1), 13-17 (2013)

[6] V.I.Serdyukov, L.N.Sinitsa, S.S.Vasil’chenko, B.A.Voronin, “High-Sensitive Fourier-Transform Spectroscopy with Short-Base Multipass Absorption Cells,” Atmospheric and Oceanic Optics 26(4), 329–336 (2013).

[7] V.I. Serdyukov, ”New possibility of highly sensitive molecular absorption spectra”, Atmospheric and Oceanic Optics 26(9), 817-821 (2013)

[8] S. S. Vasil’chenko, V. I. Serdukov, L. N. Sinitsa, ”Spectral system for measuring gaseous atmospheric components with a fiber-optic tracking system, and certain analysis results of atmospheric spectra”, Atmospheric and Oceanic Optics 26(4), 240-246 (2013)