Improved diode laser spectrometer for ortho/para ratio measurements in water vapor

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Abstract

The main isotopomer of water – H216O is a mixture of two nuclear spin isomers. The sum of nuclear spins of hydrogen atoms could be either equal to 1 in ortho molecule or equal to 0 in para molecule. Each spin isomer has its own system of rovibrational levels. Optical transitions between levels of different spin isomers are strongly forbidden. Number of ortho isomer molecules is three times greater than number of para isomer molecules in the thermal equilibrium state at room temperature.

Earlier it was shown that TDLS is a good technique for ortho/para ratio measurements in water vapor [1,2]. Interest to this kind of measurements is connected with probable medicine application of para-enriched water (NMR-tomography).

In our previous report a DL-spectrometer designed for ortho/para ratio measurement was demonstrated [2]. In this work improved spectrometer is presented. Optical part of the spectrometer consists of DFB laser with fiber output (1.392 μ m), gas cell (20 cm long) and detector (germanium photodiode). Such kind of diode laser and so simple optical scheme give an opportunity to minimize the influence of interference of direct and scattered light beams. For the same purpose the windows of the gas cell are tilted with respect to axes of laser beam. The detector window is tilted too.

Spectral lines of ortho-water (7181.15578; 7182.20911; 7183.01579) and of para-water (7182.94962) were chosen for the measurements [3].

The spectrometer was tested in experiments with pure water vapor in the pressure range of 0.01 - 10 torr. The effect of selective sorption of ortho and para spin isomers of water was demonstrated.

[1] A.I. Nadezdinskii, P. M. Omarova. J. Mol. Spectr., v.170, p.27 (1995).

[2] C.L.Malugin, T.Yu.Moskalev A.I. Nadezhdinskii, Ya.Ya. Ponurovskii, D.B. Stavrovskii

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[3] L. S. Rothman et al, The HITRAN molecular spectroscopic database, *JQSRT*, vol. **82**, numbers 1–4, 15 November–15 December (2003). http://cfa-www.harvard.edu/hitran//

Ortho and para spin-isomers of water

 \mathbf{S}_1 \mathbf{S}_1 **Ortho-water Para-water** $S_1 + S_2 = 1$ $S_1 + S_2 = 0$ **Equilibrium ratio is 3:1 at room temperature**

Absorption spectrum of 101 – 000 H_2O band in the vicinity of 1.392 μ



Simulated by SPECTRA Information System (http://spectra.iao.ru/en/home/)

General view of the initial spectrometer



General view of the improved spectrometer



Inner view of diode laser module



Electrical Block-scheme



Experimental spectra of 'ortho' and 'para' water lines



Initial spectrum

Developed spectra with the Gauss functions approximation



Selective sorption of ortho and para spin isomers of water.





Stages of the experiment

- 1 pumped cell is filling with water vapor passing throw the adsorbent (charcoal)
- 2 pumping of the cell is switching on, pumping rate is aligning
- 3 passing of water vapor from the tube with adsorbent throw the cell under pumping
- 4 pumping is switching off, filling of the cell with water vapor passing throw the adsorbent
- 5 input of the tube with adsorbent is closed, pumping is switching on
- 6 the process after 1 minute heating of the tube with adsorbent by hot air
- 7 one more 1 minute heating of the tube
- 8 pumping of the cell is switching off
- 9 output of the tube with adsorbent is closed, the cell is filling with water vapor passing throw the pumping tube