Spectrum of $HD^{16}O$ for investigation of the terrestrial planets atmospheres

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Infra-red spectroscopy represents one of the remote sensing methods for determining the $HD^{16}O$ contents in the atmospheres of planets, and the results obtained are interpreted using the HITRAN and GEISA databases (DB) adapted for studies in the Earth atmosphere. Unfortunately, these databases are incomplete: there are gaps in wavenumbers and intensities depending on the spectral region, while the line shape parameters represent averaged values or entirely missing. Unlike Earth, atmospheres of Mars and Venus consist, mainly, of the carbon dioxide, CO_2 (~96%), and have different range of the pressure and temperature variations, which complicates the use of available DB. Recently, a number of papers dealing with the line broadening of water vapor and its isotopologues in the CO_2 atmosphere have been published (see, for example, [1]). These studies, however, involved specific spectral regions and were not generalized on the total spectral range.

This paper is aimed at generation of the complete absorption linelist of $HD^{16}O$ isotopologue assigned for modeling its spectrum in the atmospheres of Earth, Mars, and Venus in the 0 -26000 cm^{-1} spectral region. The linelist includes line shape parameters caused by self-, CO_2 -, and air – broadening, as well as the temperature dependence coefficients. This list is based on the $HD^{16}O$ variational linelist known as VTT (Voronin, Tennyson, Tolchenov [2]). Application of the VTT linelist made already it possible to refine the water vapor contents at Venus' surface by taking into account the previously unknown weak absorption bands of $HD^{16}O$ in the 1.05-1.2 μm region [3]. Self – and air – broadening parameters were taken from [4].

The rovibrational labeling established in [5], as well as that provided by the spectra.iao.ru database was used to label majority of VTT lines stronger than 10^{-25} cm/molecule. Reliable rotation - vibration labeling allowed to calculate the linewidths more accurately. VTT line positions were changed, where possible, on the differences between the experimental upper and lower energy levels using the energy levels set from [5].

Calculations of the $\gamma(HD^{16}O\text{-}CO_2)$ depending on the complete set of rotation-vibration quantum numbers have been performed using semi-empirical approach [6], which has been widely used earlier for calculations of the broadening coefficients for different kind of mixtures: H_2O -N_2 (O_2, H_2O), O_3-N_2(O_2), CO_2- N_2 (O_2, N_2O), see, for example [7].

VTT linelist as well as estimates of the line shape parameters $\gamma(HD^{16}O\text{-}HD^{16}O)$ and $\gamma(HD^{16}O$–air) are published on ftp://ftp.iao.ru/pub/VTT/ and http://www.exomol.com/. Estimates of the isotope composition of water vapor for Earth, Venus, and Mars (normalized to unit) will also be presented in poster. Data on $\gamma(HD^{16}O\text{-}CO_2)$ as well as the temperature dependence coefficients in case of $HDO\text{-}CO_2$ broadening are available from the authors on request.

The study was partly supported by the RFBR (№ 11-02-93112-CNRS) and RAS programs №3.9 and 22.2.

[1] R.R. Gamache, A.L. Laraia, J.Lamouroux *Icarus*, **2011,** *213,* 720.
[2] B. Voronin et al., *Monthly Notices of the Royal Astronomical Society,* **2010,** *402*, 492.
[3] Bezard B., Fedorova A. et.al., *Icarus,* 2011, 216, 173-183.
[4] B.A. Voronin, N.N.Lavrentieva, et al., *Atmospheric and Oceanic Optics,* **2012,** *25*(1), 27.
[5] J. Tennyson et al., *J. Quant. Spectrosc. Radiat. Transfer.* **2010.** *111(15),* 2160.
[6] A. Bykov, N. Lavrentieva, L.Sinitsa, *Molecular Physics,* **2004,** *102*, 1706.
[7] J. Buldyreva, N. Lavrentieva, *Molecular Physics*, **2009,** *107*, 1527.