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High sensitivity ICLAS of $H_2^{18}O$ in the 12,580–13,550 cm^{-1} transparency window

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ABSTRACT

High-sensitivity Intracavity Laser Absorption Spectroscopy (ICLAS) is used to measure the high resolution absorption spectrum of $H_2^{18}O$ between 12,580 and 13,550 cm^{-1}. This spectral region covers the $3\nu+\delta$ polyad of very weak absorption. Four isotopologues of water ($H_2^{18}O$, $H_2^{16}O$, $H_2^{17}O$, $HD^{18}O$) are found to contribute to the observed spectrum. Spectrum analysis is performed with the aid of variational calculations and allowed for assigning 1126 lines belonging to $H_2^{18}O$, while only 160 $H_2^{18}O$ lines are included in the HITRAN-2008 database. Altogether, 823 accurate energy levels of $H_2^{18}O$ are determined from transitions attributed to 26 upper vibrational states, 438 of them being reported for the first time. New information includes energy levels of four newly observed vibrational states of $H_2^{18}O$: (2 4 0), (1 4 1), (0 4 2) and (2 3 1) at 13,167.718, 13,212.678, 13,403.71 and 15,073.975 cm^{-1}, respectively. $H_2^{18}O$ transitions involving highly excited bending states like (1 6 0), (0 6 1), (0 7 1), (1 7 0), (0 9 0) and even (0 10 0) have been identified as a result of an intensity borrowing from stronger bands *via* high-order resonance interactions. Thirty-six new energy levels of $H_2^{17}O$, present with a 2% relative concentration in our sample, could be determined. The rotational structure of the (0 2 3) state of $HD^{18}O$ at 13,245.497 cm^{-1} is also reported for the first time.

1. Introduction

$H_2^{18}O$ is considered to be the fifth most contributor to the atmospheric absorption of solar radiation. Knowledge of the line positions and strengths of the $H_2^{18}O$ isotopologue is then of importance for an accurate atmospheric modeling. The exhaustive critical evaluation of all $H_2^{18}O$ rovibrational line positions and energy levels available in the literature was released by an international IUPAC-sponsored Task Group [1] and recently updated in Ref. [2]. It covers the 0–17,125 cm^{-1} range. Hereafter, we will call "IUPAC TG levels and transitions", the 5133 levels and 31,730 lines, which were critically evaluated and recommended in Refs. [1,2] for $H_2^{18}O$. In particular, the IUPAC-TG review showed a lack of high sensitivity investigations of the $H_2^{18}O$ spectrum in the high energy region above 12,500 cm^{-1} (see Fig. 3 of Ref. [1]).

The presently studied region (12,580–13,550 cm^{-1}) has been previously investigated by Bykov and co-workers [3] who analyzed the $H_2^{18}O$ enriched spectrum recorded between 11,300 and 13,600 cm^{-1} by Fourier-transform spectrometer (FTS) at the National Solar Observatory (Kitt Peak, AZ). These authors were able to obtain 315 accurate rotational energy levels for six interacting vibrational states by means of the effective Hamiltonian approach. Later, Tanaka et al. [4,5] used variational calculations to reanalyze these FTS spectra in the 12,400–14,520 cm^{-1} region covering the $3\nu+\delta$ and 4ν polyads. All the transitions of $H_2^{18}O$ provided in Ref. [5] were included into the HITRAN2004, 2008 [6,7] databases.

More recently, Intracavity Laser Absorption Spectroscopy (ICLAS) was used to investigate the 11,520–12,810 cm^{-1} [8] spectral region. Compared to FTS, ICLAS has the advantage of giving access to much weaker transitions with intensities as

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low as 5×10^{-28} cm/molecule, i.e. more than two orders of magnitude lower than previous FTS studies [3–5]. Rovibrational assignment based on results of high accuracy variational calculations [9–11] allowed 386 new energy levels belonging to 16 vibrational states to be derived from measurement of 1712 $H_2^{18}O$ transitions.

The present work is a continuation of this ICLAS investigation at higher energy. The same high sensitivity experimental setup was used to record the weak absorption spectrum in the 12,580–13,550 cm^{-1} region lying between the strong $2\nu_1+\nu_2+\nu_3$ and $3\nu_1+\nu_3$ bands at 12,116 and 13,795 cm^{-1}, respectively. The investigated region is known as one of the transparency windows of water vapor. Fig. 1 shows an overview of the $H_2^{18}O$ line list obtained in this work compared to the HITRAN-2008 line list and to the calculated line list of Ref. [11]. The gain is particularly significant in the wide 12,707–13,364 cm^{-1} interval where no $H_2^{18}O$ lines were previously reported. Note that we have recently performed a similar investigation [12] for the main isotopologue, $H_2^{16}O$, in the same transparency region, which is of particular interest for atmospheric applications, as it corresponds to the A-band of molecular oxygen used in measurements for radiative transfer purposes.

2. Experimental details and line list construction

The ICLAS spectrum was recorded in successive 14 cm^{-1} wide spectral window separated by about 10 cm^{-1} (see Refs. [8,13,14] for details). The wavenumber calibration of each of these individual spectra requires: (i) The correction of the non-linear dispersion of the grating spectrograph,

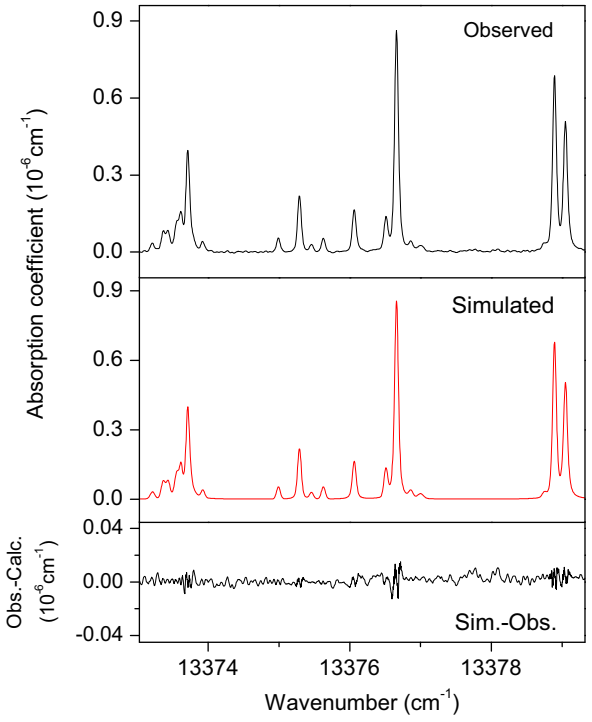

Fig. 2. Line profile simulation of the ICLAS spectrum of $H_2^{18}O$ in a spectral section around 13,376 cm^{-1}. The spectrum of a highly ^{18}O enriched sample of water was recorded with a pressure of 11.8 Torr and an equivalent pathlength of about 24 km. The lower panel shows the residuals of the line profile simulation obtained with a Voigt profile.

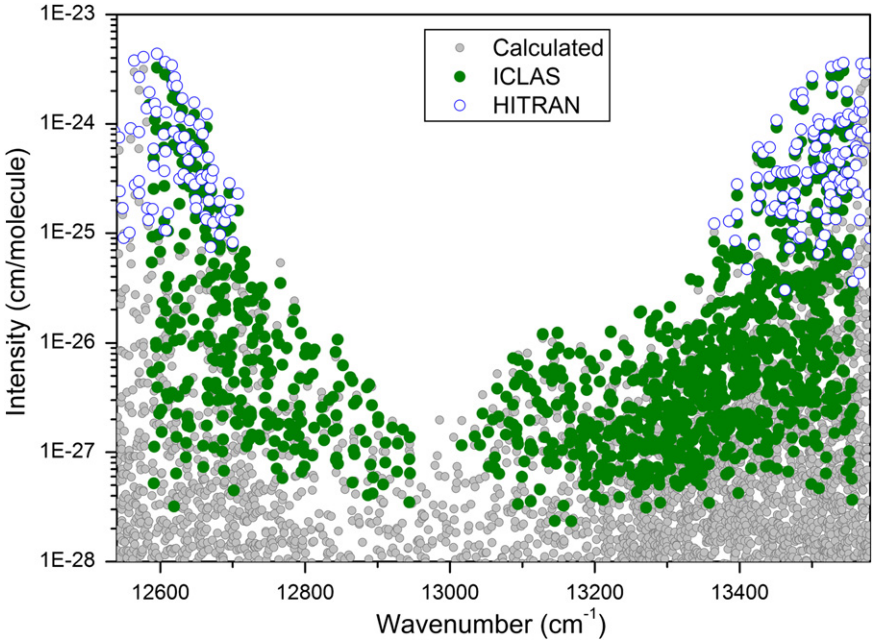

Fig. 1. Overview comparison of the $H_2^{18}O$ spectrum between 12,550 and 13,550 cm^{-1} showing the data available in the HITRAN-2008 database [7], the ICLAS observations and the results of the variational calculations [11].