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Measurements of positions, strengths and self-broadened widths of H_2O from 2900 to 8000 cm^{-1}: line strength analysis of the 2nd triad bands

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Abstract

High-resolution spectra of H_2O were recorded with a Fourier-transform spectrometer covering H_2O transitions from 2900 to 8000 cm^{-1}. Over 13,000 absorptions were measured to determine line positions, strengths and self-broadened half-width coefficients. The $H_2{}^{16}O$ line strengths of the (0 3 0)–(0 1 0), (1 1 0)–(0 1 0), (0 1 1)–(0 1 0) and (0 3 0)–(0 0 0), (1 1 0)–(0 0 0), (0 1 1)–(0 0 0) bands were fitted to a quantum mechanical model which involves the interactions between the (0 3 0), (1 1 0), and (0 1 1) vibrational states. Also fitted were experimental strengths of the hot bands; (1 2 0)–(0 1 0) and (0 2 1)–(0 1 0). The model includes 14 dipole matrix elements for B- and A-type transitions. The measured line positions were used along with hot water emission measurements (for the (0 3 0), (0 4 0), and (0 5 0) states of $H_2{}^{16}O$) in an analysis to obtain high-accuracy energy level values in the (0 3 0), (1 1 0), (0 1 1), (0 4 0), (1 2 0), (0 2 1), (2 0 0), (1 0 1), (0 0 2), and (0 5 0) vibrational states of $H_2{}^{16}O$ and the (1 1 0) and (0 1 1) states of $H_2{}^{17}O$. Also included were measurements and analysis of self-broadened half-widths for over 4700 absorptions between 4405 and 7729 cm^{-1}. The results from this investigation provide new information for the noted $H_2{}^{17}O$ bands and present a more accurate representation of the measured $H_2{}^{16}O$ bands.

Keywords: H_2O; Infrared; Laboratory; Spectroscopy

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1. Introduction

This investigation follows a study [1] in which ground state and "hot" band transitions of $H_2{}^{16}O$, connecting the triad: (0 2 0), (1 0 0), and (0 0 1), were measured and analyzed. The present work involves a similar analysis of measured line positions and strengths of the (0 3 0)–(0 1 0), (1 1 0)–(0 1 0), and (0 1 1)–(0 1 0) bands in the 2.7 μm region and the (0 3 0)–(0 0 0), (1 1 0)–(0 0 0), and (0 1 1)–(0 0 0) bands in the 1.9 μm region. The $H_2{}^{16}O$ line strengths were analyzed with a quantum mechanical model using perturbation theory which involves interactions between the hot bands in the 2.7 μm region and interactions between the ground state bands in the upper spectral region. Also included in this study were measurements of self-broadened half-widths for over 4700 H_2O absorptions between 4405 and 7729 cm^{-1}, and $H_2{}^{17}O$ transitions in the (1 1 0)–(0 0 0) and (0 1 1)–(0 0 0) bands. Also treated with a quantum model were measurements between 4961 and 5649 cm^{-1} of line strengths of two $H_2{}^{16}O$ hot bands: (0 2 1)–(0 1 0) and (1 2 0)–(0 1 0).

Previous studies relevant to this work are the above noted paper [1] and several others [2–36] listed in chronological order of publication date. These include the study of the interacting states, (0 3 0), (1 1 0), and (0 1 1) by Camy-Peyret and Flaud [4] and line strength measurements of $H_2{}^{16}O$ by Toth et al. [11] for medium to strong transitions in the 5000–5750 cm^{-1} region and calculations of strengths of the ground state bands of the triad by Camy-Peyret et al. [8]. Toth et al. [9] reported measured line positions of $H_2{}^{18}O$ and $H_2{}^{17}O$ in the region between 5030 and 5640 cm^{-1} while Chevillard et al. [16] measured and analyzed line positions and strengths of $H_2{}^{18}O$ between 4400 and 6100^{-1}. Results from other studies that were applied here include the $H_2{}^{16}O$ levels of the (0 1 1) state given by Flaud et al. [5] and the (0 2 1), (1 0 1), (1 1 1) states given by Camy-Peyret et al. [7]. Measured positions of the (0 3 0)–(0 2 0) and (0 4 0)–(0 3 0) bands given by Polyansky et al. [26] and Zobov et al. [29] were used here to derive energy level values of the (0 3 0) and (0 4 0) $H_2{}^{16}O$ states. Mikhailenko et al. [33] measured the 4200–6260 cm^{-1} region of which 2351 lines were assigned to the second triad of $H_2{}^{16}O$. Smith et al. [34] measured the 5000–10,000 cm^{-1} region and obtained line strengths that were about 15–20% higher than given in the HITRAN 2000 edition [35] for the 2ν (1.4 μm) and $2\nu + \delta$ (1.14 μm) bands.

An earlier study by the present author, Toth [22], presented experimental results for line positions and strengths of $H_2{}^{16}O$ covering the 5750–7965 cm^{-1} region and listed energy level values for the (0 4 0), (1 2 0), (0 2 1), (2 0 0), (1 0 1), and (0 0 2) vibrational states. A comparison with the present work shows that in some cases, the line strengths were under estimated by as much as 20% in the earlier work, and the listing was not as comprehensive. The earlier study [22] involved over 3750 measured absorptions whereas over 4400 $H_2{}^{16}O$ lines were measured in the present study for the 5750–8000 cm^{-1} region.

Other studies include measurements of $H_2{}^{18}O$ and $H_2{}^{17}O$ between 6600 and 7640 cm^{-1} [23] and measurements of $H_2{}^{18}O$ from 5900 and 8000 cm^{-1} [18]. Tennyson et al. [31] presented a large compilation of vibration–rotation energy level listings which covered the ground state to levels in the u.v. The work was aided by measurements from many sources.

2. Experiment

The spectra were recorded using the Fourier transform spectrometer (FTS) located in the McMath Solar facility at the Kitt Peak National Observatory. The experimental conditions for