

## Water vapour line assignments in the 9250–26 000 $\text{cm}^{-1}$ frequency range

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### Abstract

Line parameters for water vapour in natural abundance have recently been determined for the 9250–13 000  $\text{cm}^{-1}$  region [M.-F. Mérienne, A. Jenouvrier, C. Hermans, A.C. Vandaele, M. Carleer, C. Clerbaux, P.-F. Coheur, R. Colin, S. Fally, M. Bach, J. Quant. Spectrosc. Radiat. Transfer 82 (2003) 99] and the 13 000–26 000  $\text{cm}^{-1}$  region [P.-F. Coheur, S. Fally, M. Carleer, C. Clerbaux, R. Colin, A. Jenouvrier, M.-F. Mérienne, C. Hermans, A.C. Vandaele, J. Quant. Spectrosc. Radiat. Transfer 74 (2002) 493] using a high-resolution Fourier-transform spectrometer with a long-path absorption cell. These spectra are analysed using several techniques including variational line lists and assignments made. In total, over 15 000 lines were assigned to transitions involving more than 150 excited vibrational states of  $\text{H}_2^{16}\text{O}$ . Twelve new vibrational band origins are determined and estimates for a further 16 are presented.

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### 1. Introduction

Understanding the rotation–vibration spectrum of water is central to constructing reliable models of the transmission of light through our atmosphere. Yet, particularly at the higher frequencies crucial for many atmospheric processes, this spectrum remains difficult to both characterise and interpret. Recently, some of

us [1–3] have collaborated in a series of experiments to characterise the line parameters of water using a high-resolution Fourier-transform spectrometer with a long-path absorption cell. These studies, which considered the ranges 9250–13 000  $\text{cm}^{-1}$  and 13 000–26 000  $\text{cm}^{-1}$ , covered the entire visible region as well as extending into the near-infrared. The spectra were recorded by the Bruxelles-Reims groups and are collectively referred to as BR below.

A considerable number of previous laboratory measurements have been made of the near-infrared [4–8] and visible [7–10] wavelength spectra of water vapour in natural isotopic abundance. The complexity of weak

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rotation–vibration spectrum of water at these wavelengths has encouraged the development of assignment procedures based on variational nuclear motion calculations [11,12]. These have been widely applied to the spectrum of water vapour at near-infrared and visible wavelengths [13–19]. The result has been a considerable advance in our understanding of the spectroscopy of water in these regions, see [20] for example.

The new Fourier-transform spectra contained 7061 lines in the 9250–13000  $\text{cm}^{-1}$  and 9353 lines in the 13000–26000  $\text{cm}^{-1}$  region, although, as discussed below, these lines contain a number of blends. Quantum number assignments for these transitions were based simply on the analysis of other spectra discussed above. However, since the new systematic spectra have already been included in the 2003 edition of the GEISA database [22] and is being prepared for inclusion in the 2004 edition of HITRAN [21], it is important that as complete and correct as possible set of assignments are made to these. In this work, we present a comprehensive analysis of the line assignments performed using a variety of methods but largely based on line lists generated using variational nuclear motion calculations. One advantage of analysing the present spectra is the broad spectral range studied which significantly reduces problems with edge effects when searching for combination differences. However, for convenience, much of the analysis was performed separately for the 9250–13000, 13000–16000, and 16000–26000  $\text{cm}^{-1}$  regions, and these three regions will be considered separately below.

## 2. Experimental details

Detailed descriptions of the experimental setup and procedures have been given previously [2,15]. Briefly, the absorption spectra of water vapour were recorded using a high-resolution Fourier-transform Spectrometer (Bruker IFS120M) coupled to two White multiple-reflection cells of 5 and 50 m base path. The combination of two light sources (high-pressure Xenon arc and tungsten halogen) and two detectors (Si and GaP-diode) coupled to optical filters enabled us to cover the spectral region from 27000 to 8000  $\text{cm}^{-1}$  in three overlapping ranges. Spectra with an absorption path of 600 m and a resolution of 0.06  $\text{cm}^{-1}$  (15 cm MOPD) were recorded in the near-UV and visible regions using the Xenon arc lamp. A resolution of 0.03  $\text{cm}^{-1}$  (MOPD of 30 cm) and absorption paths of 100 and 600 m were chosen to re-

cord the visible-NIR region using the tungsten halogen lamp. The temperature inside the cell was measured with three platinum wire thermometers which gave a ‘room temperature’ value of  $292 \pm 3$  K. Table 1 summarises the spectra analysed here.

The co-addition of some 2000–4000 interferograms, leading to measurement times of 12–24 h, proved sufficient to get a signal-to-noise ratio (expressed as the maximum signal amplitude divided by twice the root-mean-square noise amplitude) better than 2500. The spectra were wavenumber calibrated using the  $\text{I}_2$  visible spectrum. Pressure was measured with an MKS Baratron type manometer. Pure water vapour spectra were measured at various pressures from 6 to 18 hPa into the absorption cell. Additional spectra were recorded after adding  $\text{N}_2$  or dry-air in the cell in four steps up to about 800 hPa, in order to measure the pressure effect on the lines shape and position. Data concerned with the line profiles have been presented previously [1–3] and are not re-analysed here.

Spectral line positions and other parameters were determined by fitting the lines with a Voigt profile using the procedure discussed previously [1–3]. The spectrum was treated in two separate regions: 9250–12896 and 13184–25232  $\text{cm}^{-1}$ . No transitions were observed above this frequency. The gap between 12896 and 13184  $\text{cm}^{-1}$  was found to contain no  $\text{H}_2\text{O}$  lines although some transitions which could be assigned to the  $\text{O}_2$  A-band and to HDO were observed.

The experimental line list contains 7061 lines in the 9250–12896  $\text{cm}^{-1}$  region and 9353 between 13184 and 25232  $\text{cm}^{-1}$ . In practise, particularly at lower frequencies, some of these lines are blends of more than one transition so the assigned line list presented here is somewhat longer. On the other hand, we have chosen to be more conservative than the original work of [1] in the higher-frequency region, and to remove from the final list a set of very weak lines, which could have been misidentified. Similarly, about 25 lines around 14500  $\text{cm}^{-1}$  have been identified as probably due to transitions of  $\text{O}_2$ . The  $\text{O}_2$  lines are listed in Table 2 and have been removed from our final line list.

## 3. Line assignments

Line assignments were performed in both London and Tomsk and iterated until an agreed set of parameters was obtained. The main means of assignment was

Table 1  
Summary of experimental spectra analysed

Region	Wavenumber ( $\text{cm}^{-1}$ )	Lamp	Detector	Resolution ( $\text{cm}^{-1}$ )	Path (m)
Near-UV–VIS	27000–17000	Xe	GaP	0.06	600
VIS	23000–10000	Xe	Si	0.06	600
VIS–NIR	15500–8000	W	Si	0.03	100 and 600

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