Journal of Molecular Spectroscopy xxx (2016) xxx–xxx

Contents lists available at ScienceDirect

Journal of Molecular Spectroscopy

journal homepage: www.elsevier.com/locate/jms

The water vapour continuum in near-infrared windows – Current understanding and prospects for its inclusion in spectroscopic databases

Keith P. Shine [a,*], Alain Campargue [b,c], Didier Mondelain [b,c], Robert A. McPheat [d], Igor V. Ptashnik [e], Damien Weidmann [d]

[a] Department of Meteorology, University of Reading, Earley Gate, Reading RG6 6BB, UK
[b] Univ. Grenoble Alpes, LIPhy, F-38000 Grenoble, France
[c] CNRS, LIPhy, F-38000 Grenoble, France
[d] Space Science and Technology Department, Rutherford Appleton Laboratory, Chilton, Didcot, Oxon OX11 OQX, UK
[e] Spectroscopy Division, Zuev Institute of Atmospheric Optics SB RAS, 1 Akademichesky Av., Tomsk 634055, Russia

ARTICLE INFO

Article history:
Received 15 December 2015
In revised form 22 March 2016
Accepted 19 April 2016
Available online xxxx

Keywords:
Water vapour
Absorption continuum
MT_CKD model
Water dimer

ABSTRACT

Spectroscopic catalogues, such as GEISA and HITRAN, do not yet include information on the water vapour continuum that pervades visible, infrared and microwave spectral regions. This is partly because, in some spectral regions, there are rather few laboratory measurements in conditions close to those in the Earth's atmosphere; hence understanding of the characteristics of the continuum absorption is still emerging. This is particularly so in the near-infrared and visible, where there has been renewed interest and activity in recent years. In this paper we present a critical review focusing on recent laboratory measurements in two near-infrared window regions (centred on 4700 and 6300 cm^{-1}) and include reference to the window centred on 2600 cm^{-1} where more measurements have been reported. The rather few available measurements, have used Fourier transform spectroscopy (FTS), cavity ring down spectroscopy, optical-feedback – cavity enhanced laser spectroscopy and, in very narrow regions, calorimetric interferometry. These systems have different advantages and disadvantages. Fourier Transform Spectroscopy can measure the continuum across both these and neighbouring windows; by contrast, the cavity laser techniques are limited to fewer wavenumbers, but have a much higher inherent sensitivity. The available results present a diverse view of the characteristics of continuum absorption, with differences in continuum strength exceeding a factor of 10 in the cores of these windows. In individual windows, the temperature dependence of the water vapour self-continuum differs significantly in the few sets of measurements that allow an analysis. The available data also indicate that the temperature dependence differs significantly between different near-infrared windows. These pioneering measurements provide an impetus for further measurements. Improvements and/or extensions in existing techniques would aid progress to a full characterisation of the continuum – as an example, we report pilot measurements of the water vapour self-continuum using a supercontinuum laser source coupled to an FTS. Such improvements, as well as additional measurements and analyses in other laboratories, would enable the inclusion of the water vapour continuum in future spectroscopic databases, and therefore allow for a more reliable forward modelling of the radiative properties of the atmosphere. It would also allow a more confident assessment of different theoretical descriptions of the underlying cause or causes of continuum absorption.

© 2016 The Authors. Published by Elsevier Inc. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

1. Introduction

Spectroscopic catalogues for atmospheric applications (notably GEISA [1] and HITRAN [2]) have reported the rotational and rotational–vibrational spectral line parameters across visible, infrared and microwave wavelength regions, as well as some cross-section data on broadband absorbers and collision-induced absorption [3]. However, they have not yet included information relevant to the water vapour continuum which pervades these same spectral regions. Instead, the default description of the water vapour continuum has generally been the semi-empirical Clough–Kneizys–Davies (CKD) continuum and its successor Mlawer–Tobin–CKD (MT_CKD) (see especially [4,5]). CKD and MT_CKD have

* Corresponding author.
E-mail address: k.p.shine@reading.ac.uk (K.P. Shine).

http://dx.doi.org/10.1016/j.jms.2016.04.011
0022-2852/© 2016 The Authors. Published by Elsevier Inc.
This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

been widely used in atmospheric radiative transfer codes for applications including numerical weather prediction, climate modelling and remote sensing.

For understanding radiative fluxes in the Earth's atmosphere, it is the continuum in the windows between the dominant features in the water vapour spectrum (the pure rotational lines, at wavelengths less than 20 μm, and the many rotational–vibrational bands) that is of most significance. Within the main absorbing regions, continuum absorption is generally dominated by spectral-line absorption, with some exceptions. Although it may be of lesser importance in determining fluxes, the in-band continuum holds important clues as to the continuum's physical origin [6–8].

Historically, most attention has focused on the mid-infrared (800–1250 cm^{-1}, 8–12 μm) window (see [9] for references), which has a major influence on radiative fluxes (e.g. [10–12]), especially in atmospheres with high absolute humidity. To a lesser extent, the window centred on 2600 cm^{-1} (about 3.85 μm) has also been the subject of many studies (e.g. [13–16]). More recently, attention has begun to focus on several shorter wavelength near-infrared windows (which we define here to be 2500–14,300 cm^{-1} (0.7–4 μm)) where, prior to the year 2000, there were hardly any measurements. These windows are of atmospheric importance because they contain significant fluxes of solar radiation (e.g. [17]). They are also widely used for satellite-based sensing of gaseous abundances, notably carbon dioxide and methane (e.g. [18–20]), and cloud and surface properties (e.g. [21,22]).

In order to illustrate some of the issues that will have to be resolved before the water vapour continuum can be included in some form on spectroscopic databases, this paper particularly focuses on 2 of these windows, centred on about 6300 and 4700 cm^{-1} (1.6 and 2.1 μm). In these windows there have been a number of recent laboratory measurements which have highlighted important characteristics of the continuum absorption but also revealed significant and, as yet, unresolved disagreements. The nature of these disagreements, and prospects for future progress in resolving these, will be discussed with mention of the situation in other windows where appropriate.

2. Some characteristics of the water vapour continuum

2.1. Definitions

Since the work of Bignell [13] it has been clearly recognised that there are two distinct components to the water vapour continuum: (i) a self-continuum, which is interpreted as the interaction between water vapour molecules (such as collisions or the formation of some bound complex) and whose strength scales closely with the vapour pressure squared and (ii) a foreign-continuum, due to interaction of water vapour with other molecules, and most importantly molecular nitrogen and oxygen when considering the Earth's atmosphere. The foreign-continuum depends linearly on the water vapour pressure and on the foreign gas pressure.

As a result, the continuum absorption coefficient of water vapour in air, α_{WC}, is the sum of the self (WCS) and foreign (WCF) contributions so that

$$\alpha_{WC}(\nu,T) = \alpha_{WCS}(\nu,T) + \alpha_{WCF}(\nu,T) = \frac{1}{k_B T} C_S(\nu,T) P_{H_2O}^2 + \frac{1}{k_B T} C_F(\nu,T) P_{H_2O} P_F \quad (1)$$

where k_B is the Boltzmann constant, T is temperature, P_{H_2O} and P_F are the water vapour and foreign gas (here air) partial pressures, respectively, and C_S and C_F represent the self- and foreign-continuum cross-sections, respectively, at a given temperature T, following the definition in Burch and Alt [14]. In the standard units adopted in this field, C_S and C_F are reported in cm^2 $molec^{-1}$ atm^{-1}, α_{WC} is in cm^{-1}, P_{H_2O} and P_F are in atm, T is in K and $k_B = 1.36 \times 10^{-22}$ atm $molec^{-1}$ cm^3 K^{-1}. Note that for comparison, the MT_CKD values of C_S and C_F [5], which are normalised to the number density at 1 atm and 296 K, should be multiplied by the factor $296/T$ (e.g. [23]).

Most, but not all (see Sections 3.1 and 3.2), available measurements of the self-continuum cross-section show a strong negative temperature dependence. By contrast, within measurement and analysis uncertainties, the foreign continuum appears independent of temperature in the range from about 300 to 430 K (see Section 3.3).

There is no unambiguous way of defining the water vapour continuum, and separating it from smoothly varying line absorption. However, some operational definition is needed to enable comparison between observations and to allow implementation of the continuum in radiative transfer codes. The most widespread definition is that used by CKD and MT_CKD [4,5]. The line absorption is defined as the purely Lorentzian-broadened profile calculated above its value at 25 cm^{-1} from line centre. All line absorption further than 25 cm^{-1} from line centre, as well as the 25 cm^{-1} "pedestal" on which the line sits, is assumed to be part of the continuum (see Fig. 1 of [4]). At any wavenumber, the continuum is thus defined as the observed absorption that cannot be accounted for by line-by-line calculations using this assumed line profile for all lines within 25 cm^{-1} of that wavenumber. Using this definition, the derived continuum is not independent of the spectral line database used to derive it, and indeed should be updated as new information on water vapour lines (including all isotopologues) becomes available. However, in the near-infrared bands, the pedestal itself accounts for only 5–7% of the continuum, and it is much less important (around 1%) within the window regions (e.g. [24]) which are the focus here.

2.2. Theoretical overview

Since this paper focuses on the observational evidence for the characteristics of the water vapour continuum, we largely sidestep the issue of the underlying physical cause, or causes, of the water vapour continuum absorption, which remains a vigorously debated area; greater confidence, stemming from a larger set of independent, cross-validated, experimental data is essential to judge the success, or otherwise, of theoretical explanations, and to guide new developments. Nevertheless, a brief overview will help frame the discussion. Up to now, there have been broadly two main "competitor" explanations for the continuum, which should not be seen as mutually exclusive. Some history of the development of these ideas can be found in Ref. [9].

The first explanation is far-wing theory. The CKD and MT_CKD descriptions have been based on the semi-empirical adjustment to the Lorentz line shape of water vapour lines; the adjustment was derived so as to fit available observations of the continuum mostly at wavenumbers less than 2200 cm^{-1}. The resulting lineshape was then applied at all wavenumbers. In CKD, this adjustment led to both a super-Lorentzian component in the near-wing regions (10–100 cm^{-1} from line centre) with a sub-Lorentzian component beyond; the sub-Lorentzian component therefore dominates in the windows [4]. In MT_CKD, the super-Lorentzian component was replaced by a "weak interaction term" where the weak interaction is between a water vapour molecule with another molecule (which could itself be water vapour) [5]. A quite different approach to far-wing line theory has been presented by Ma et al. [25,26], which has a more *ab initio* basis,

Download English Version:

https://daneshyari.com/en/article/5414213

Download Persian Version:

https://daneshyari.com/article/5414213

Daneshyari.com