



Contents lists available at ScienceDirect

Journal of Quantitative Spectroscopy & Radiative Transfer

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

The IR spectrum of $^{12}\text{C}_2\text{H}_2$: Line intensity measurements in the 1.4 μm region and update of the databases

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ARTICLE INFO

Article history:

Received 26 June 2008

Received in revised form

9 October 2008

Accepted 11 October 2008

Keywords:

Acetylene

Infrared

Vibro-rotational transitions

Line parameters

Databases

ABSTRACT

Spectroscopic data are noticeably enriched in six spectral regions of the main isotopologue $^{12}\text{C}_2\text{H}_2$ of the acetylene molecule, namely, in the regions around 3, 2.2, 1.9, 1.7, 1.5, and 1.4 μm . Among these regions, only those at 3 and 1.5 μm were already presented partly in the databases. The results of line intensity measurements, performed for the first time in the 1.4 μm region, are given. Data available in the literature, or obtained in the present work, are compiled to set up line lists usable for applications in the quoted spectral regions. On the whole, 5748 new lines pertaining to 65 bands can be added to the databases.

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1. Introduction

A review of the acetylene spectroscopic parameters in the HITRAN database was given in a paper by Jacquemart et al. [1] in 2003. Last issues of databases are HITRAN 2004 [2] and GEISA 2003 [3,4]. HITRAN 2004 was enriched by the results of El Hachtouki and Vander Auwera [5] in the 1.5 μm region, which is an important spectral domain since it occurs in the emission range of telecom diode lasers. In the beginning of 2007, new line lists were added in the HITRAN database as update, in the 3.8 and 2.5 μm regions where line intensity measurements had been done [6,7]. Despite these important improvements, databases are far from to be updated. Indeed, other recent line intensity measurements have been performed but have not yet been put in the appropriate form to be included in databases. Five spectral regions of acetylene are thus concerned, the regions at 3 [1,8,9], 2.2 [10], 1.9 [11], 1.7 [11], and 1.5 μm [12,13]. The goal of this work is to set up

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line lists in these five regions, usable for atmospheric or astrophysical applications. Data existing in databases have been completed, using band-by-band effective models based on polynomial adjustments of line positions and intensities. The aim of such lists is to help for current applications, not to propose a complete synthetic spectrum that more powerful models will be able to produce in some years. A sixth spectral region, at 1.4 μm , has been also investigated in the present work. More than 230 line intensities have been measured in this region, and a line list has also been produced to be put in databases. Section 2 of the paper reports results obtained around 1.4 μm from Fourier transform spectra recorded both at GSMA (Reims) and at LADIR (Paris). Section 3 presents in details the content of the line lists and how they have been set up in each spectral region. In the Conclusion we list the data of atmospheric and astrophysical interest which still have to be added to databases. In the remaining of the paper, databases refer specifically to the HITRAN and GEISA databases.

2. $^{12}\text{C}_2\text{H}_2$ line intensity measurements in the 1.4 μm spectral region

2.1. Introduction

The 1.4 μm spectral region of $^{12}\text{C}_2\text{H}_2$ concerns the $\Delta P = 11$ sequence of vibrational transitions. According to [14] and [15], we have noted P the pseudo-quantum number equals to $5\nu_1+3\nu_2+5\nu_3+\nu_4+\nu_5$, where ν_1 , ν_2 , ν_3 , ν_4 , and ν_5 are the quantum numbers associated with the normal modes of vibration of the molecule. A given value of P is assigned to a given set of interacting vibrational states, named polyad or cluster. Polyads are also noted $\{P\nu_5\}$. In this frame, global vibration and vibration–rotation analysis were performed [16–19]. Throughout this paper, we will use the vibrational notations of Plíva [20,21] adopted in the HITRAN database [2,22]. Thus, vibrational levels are noted $\nu_1 \nu_2 \nu_3 (\nu_4 \nu_5)^\ell \pm r$, with $\ell = |\ell_4 + \ell_5|$, ℓ_t being the vibrational angular momentum quantum number associated with the degenerated bending mode t , \pm being the symmetry type for Σ vibrational states ($\ell = 0$), and r a roman numeral indicating the rank of the level, by decreasing energy value ($r = J$ for the highest energy level), inside the set of states having the same vibrational symmetry, and coupled by ℓ -type resonances. The last work performed on the 1.4 μm spectral region is that of Vander Auwera et al. [23], who measured absolute line wavenumbers in four cold bands and deduced spectroscopic parameters for the involved vibrational levels. Their work was undertaken mainly to help metrological applications in the field of optical fiber communication systems. The accuracy of the measured wavenumbers is between 0.0003 and 0.006 cm^{-1} depending on the line. As far as line intensities are concerned, no data have been published to our knowledge, except for a prediction of band intensities for two bands around 7200 cm^{-1} , by Abbouti Tamsamani et al. [24]. Note that databases do not contain any data for $^{12}\text{C}_2\text{H}_2$ around 1.4 μm .

The four cold bands observed by Vander Auwera et al. [23], and that we also observed in our spectra, are listed in Table 1. Since these perpendicular bands are all of $\Pi_u \leftarrow \Sigma_g^+$ type, they exhibit the same structure with a strong Q-branch and a 3:1 intensity alternation ratio, according to odd:even J , J being the rotational quantum number of the lower level.

2.2. Experimental details

To study the C_2H_2 1.4 μm spectral region, 15 spectra were obtained with the GSMA (Reims) step-by-step interferometer [25,26]. Experimental conditions are gathered in Table 2. The apparatus was used with a tungsten radiation source, SiO_2 splitting and mixing plates, InSb detectors, and CaF_2 cell windows. Pressures were measured using two full scale ranges MKS Baratron (10- and 100-Torr manometers) with an accuracy of 0.5%. Spectra number 1–10 of Table 2 had already been used to study the 1.5 μm region [12,13], whereas spectra number 11–15 are new spectra recorded with a shorter length cell, in order to better observe strong lines around 7200 cm^{-1} .

Nine additional spectra were obtained with the rapid scan Bruker IFS 120 HR interferometer of the LADIR (Paris). Experimental conditions are gathered in Table 3. This interferometer was equipped with a Globar source, CaF_2 beam splitter, an InSb detector, and an optical filter covering the 500–12 500 cm^{-1} spectral region. The whole optical path was under vacuum and a multipass cell of 1-m base length was used. The cell was equipped with KCl windows. The temperature of the gas in the cell was recorded via four platinum probes at different places inside the cell. The uncertainty

Table 1

List of the bands observed in the $\Delta P = 11$ series of transitions of $^{12}\text{C}_2\text{H}_2$ around 1.4 μm

Band	Center ^a	Upper level	Polyad ^b	Symmetry	Nb lines ^c
$2\nu_1 + \nu_5^1$	7417.57	200(01) ¹	{11 ν_5 }	$\Pi_u \leftarrow \Sigma_g^+$	74
$\nu_1+\nu_2+(2\nu_4+\nu_5)^1$	7229.45	110(21) ¹	{11 ν_5 }	$\Pi_u \leftarrow \Sigma_g^+$	41
$2\nu_3 + \nu_5^1$	7219.37	002(01) ¹	{11 ν_5 }	$\Pi_u \leftarrow \Sigma_g^+$	64
$\nu_1 + \nu_3 + \nu_4^1$	7142.67	101(10) ¹	{11 ν_5 }	$\Pi_u \leftarrow \Sigma_g^+$	54

^a Rough values of band centers, in cm^{-1} , compiled from [23].

^b Polyad to which the upper vibrational level belongs.

^c Number of line intensities measured in the present work.

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