Line intensities of $^{12}C_2H_2$ in the 1.3, 1.2, and 1 μm spectral regions

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ARTICLE INFO

ABSTRACT

Intensities of about 320 lines of the $^{12}C_2H_2$ molecule, belonging to 7 parallel bands, are measured in the 1.3, 1.2, and 1 μm spectral regions, with a mean accuracy around 3% or 7% depending on the spectral region. Vibrational transition dipole moment squared values and Herman-Wallis coefficients are obtained for each band, in order to model the rotational dependence of the transition dipole moment squared, except for the $v_1+v_3+2v_4^0$ band at 7732.78 cm^{-1} that exhibits an unusual rotational dependence because of a strong ℓ-type resonance. HITRAN format line lists are set up for applications.

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1. Introduction

The near infrared spectral range being very important in the field of optical communications, $^{12}C_2H_2$ was one of the molecules chosen to furnish wavenumber reference standards in this range. Towards this goal Vander Auwera et al. [1] published absolute wavenumbers of acetylene lines in the 1.4, 1.3, 1.2, and 1 μm spectral regions. In a previous work [2], we measured acetylene line intensities in the 1.4 μm region. The present paper reports the results of line intensity measurements in the three remaining regions of interest, namely around 1.3, 1.2, and 1 μm.

First of all, let us recall the notations used throughout this paper. According to Refs. [3,4], we will denote P the pseudo-quantum number equal to $5v_1+3v_2+5v_3+v_4+v_5$, where v_1, v_2, v_3, v_4, and v_5 are the quantum numbers associated with the normal modes of vibration of the molecule in the ground electronic state. A given value of P is assigned to a given set of interacting vibrational states, named polyad or cluster, polyads being also denoted $\{Pv_5\}$. To label the vibrational levels, we will use the notations of Plíva [5,6]: vibrational levels will be noted $v_1\ v_2\ v_3\ (v_4\ v_5)^\ell \pm r$, 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 ($r = I$ for the highest energy level), inside the set of states having the same vibrational symmetry, and coupled by ℓ-type resonances. With these notations, the vibrational states and bands involved in this work are listed in Table 1. They concern

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Table 1
List of the bands observed in the $\Delta P = 12$, 13, and 15 series of transitions of $^{12}C_2H_2$ between 7600 and 9900 cm^{-1}.

Band	Center[a]	Upper level[b]	Polyad[c]	Symmetry	N[d]	%[e]	$PJ_{max}-RJ_{max}$[f]
$\nu_1+\nu_3+2\nu_4^0$	7732.78	$101(20)_+^0$	$\{12\nu_5\}$	$\Sigma_u^+ \leftarrow \Sigma_g^+$	38	3	23–21
$\nu_1+\nu_2+\nu_3$	8512.06	$111(00)_+^0$	$\{13\nu_5\}$	$\Sigma_u^+ \leftarrow \Sigma_g^+$	58	3	31–30
$\nu_1+2\nu_2+(\nu_4+\nu_5)_+^0$	8556.60	$120(11)_+^0$	$\{13\nu_5\}$	$\Sigma_u^+ \leftarrow \Sigma_g^+$	33	3	25–25
$3\nu_3$	9639.87	$003(00)_+^0$	$\{15\nu_5\}$	$\Sigma_u^+ \leftarrow \Sigma_g^+$	61	7	33–33
$\nu_1+\nu_2+\nu_3+2\nu_4^0$	9668.17	$111(20)_+^0$	$\{15\nu_5\}$	$\Sigma_u^+ \leftarrow \Sigma_g^+$	33	7	25–25
$2\nu_1+\nu_3$	9835.18	$201(00)_+^0$	$\{15\nu_5\}$	$\Sigma_u^+ \leftarrow \Sigma_g^+$	54	7	29–29
$3\nu_3+\nu_4^1-\nu_4^1$	9602.66	$003(10)^1$	$\{16\nu_5\}$	$\Pi_u \leftarrow \Pi_g$	42	7	26–18

[a] Rough values of band centers, in cm^{-1}, compiled from [1].
[b] Upper vibrational level.
[c] Polyad to which the upper vibrational level belongs.
[d] Number of line intensities measured in each band.
[e] Estimated mean accuracy of measured line intensities.
[f] Maximum J values of the lines whose intensity could be measured, in P and R branches.

the sequences of vibrational transitions $\Delta P = 12$, 13, and 15, corresponding to the 1.3, 1.2, and 1 μm spectral regions, respectively. Six cold bands of the $\Sigma_u^+ \leftarrow \Sigma_g^+$ type are presented, and one hot band of the $\Pi_u \leftarrow \Pi_g$ type.

An exhaustive bibliography being given in Ref. [1], we will recall here only some references useful for our purpose. As far as line position measurements and spectroscopic analysis are concerned, one should refer mainly to Refs. [1,7–15]. For intensity data, one can refer to the following works. Around 1.3 μm, Moriwaki et al. [9] gave measured intensity values for five P lines of two bands. Around 1.2 μm, Kou et al. [11] gave relative observed and calculated values for the vibrational transition dipole moment squared of four bands. Similar data were given by Abbouti Temsamani et al. [15]. Around 1 μm, Smith and Winn [8] gave relative observed intensity data for three bands. Herman et al. [10] gave the results of measurements and calculations for the vibrational transition dipole moment squared of three bands. Some similar observed and calculated values were also given in [15] for more bands. All these works show that intensity data are very scarce, and that most of them are relative band intensity values or similar data of average accuracy. In the following, we will rely on the results of Abbouti Temsamani [16] who gave values of vibrational transition dipole moments squared for five of the bands we studied around 1.2 and 1 μm. This author estimated the precision and the accuracy of his results to be 5% and 15%, respectively, due to the uncertainties on the temperature and mainly on the pressure measurements. Though intensities of individual lines are not reported in Ref. [16], those results will be useful for comparison purpose.

Using Fourier transform spectra, we have measured absolute intensities for 319 lines belonging to 7 bands around 1.3, 1.2, and 1 μm. Their mean accuracy is about 3% and 7% depending on the spectral region. Section 2 of the paper will be devoted to the experimental conditions and to the measurements. The results will also be given in this section. In Section 3, the data reduction and the calculation of line lists for applications will be discussed.

2. Line intensity measurements

2.1. Experimental details

To study C_2H_2 between 7600 and 9900 cm^{-1}, 9 spectra have been obtained with the rapid scan Bruker IFS 120 HR interferometer of the Laboratoire de Dynamique, Interactions, et Réactivité (LADIR, Paris). Experimental conditions are gathered in Table 2. These spectra were already used to study C_2H_2 around 1.4 μm [2], together with other spectra recorded at the Groupe de Spectrométrie Moléculaire et Atmosphérique (GSMA, Reims). Let us recall that the Bruker was equipped with a Globar source, CaF$_2$ beam splitter, and an InSb detector. 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 on the temperature measurements has been estimated to be ± 0.5 K. The pressure of the gas was measured with a capacitive MKS Baratron manometer with an accuracy estimated to be about $\pm 0.5\%$. Each scan among at least 390 recorded for every spectrum has then been individually transformed to a spectrum using the Fourier transform procedure included in the Bruker software OPUS package [17], selecting a Mertz phase error correction [18,19]. In the spectral regions studied in the present work, the SNR is not as good as around 1.4 μm, and it decreases towards high wavenumbers, leading to less accurate line intensities (see Table 1).

2.2. Method of measurement and results

To derive line intensities from the spectra, a multispectrum fitting (MSF) procedure [20] was used in the following conditions. As in Ref. [2], the absorption coefficient of the lines was calculated as a Voigt profile. The Doppler-width is