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New line intensity measurements for $^{12}C_2H_2$ around 7.7 μm and HITRAN format line list for applications

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ABSTRACT

Absolute intensities of 467 lines are measured in 9 bands of the 7.7 μm spectral region of the $^{12}C_2H_2$ molecule, with an average accuracy of 5%. For each band, the vibrational transition dipole moment squared and Herman–Wallis coefficients are obtained in order to model the rotational dependence of the transition dipole moment squared. These results are used to calculate a line list for atmospheric or astrophysical applications. Merged in the line list set up in a previous work for the 8 strongest bands around 7.7 μm [5], these new data give now a quasi-exhaustive view of the $^{12}C_2H_2$ spectrum in the involved spectral region.

1. Introduction

The 7.7 μm spectral region of acetylene $^{12}C_2H_2$ is known mainly since the extensive work of assignment performed by Kabbadj et al. [1] in 1991. As far as line intensities are concerned, accurate absolute values were obtained by Vander Auwera [2] in 2000 for the $(\nu_4+\nu_5)^0_+$ and $(\nu_4+\nu_5)^2$ cold bands, and then by Jacquemart et al. [3] and Lepère et al. [4] for the $(\nu_4+\nu_5)^0_+$ band. A more detailed bibliography has been given in Ref. [5]. This spectral region corresponds to the $\Delta P=2$ sequence of vibrational transitions [6], P being a pseudo-quantum number equals $5\nu_1+3\nu_2+5\nu_3+\nu_4+\nu_5$, 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 in the ground electronic state. As the spectral region around 7.7 μm is of interest for astrophysical applications (see, e.g., Ref. [7]), it has been important to increase the knowledge of line intensities in order to improve databases [8,9], which contained data only for the $(\nu_4+\nu_5)^0_+$ band, issued from Ref. [3]. Thus, in a previous work [5], we measured 414 line intensities in 8 hot bands around 7.7 μm, and set up a line list from these results. In the present paper, we report line intensities obtained in the 9 remaining bands assigned by Kabbadj et al. [1].

The studied bands are gathered in Table 1. We have adopted the same notations as in Ref. [5]. A given value of P is assigned to a given set of interacting vibrational states, named polyad or cluster. Then, polyads are noted $\{P\nu_5\}$. 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

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Table 1
List of the bands observed by Kabbadj et al. [1] in the ΔP=2 series of transitions of $^{12}C_2H_2$ around 7.7 μm and studied in this paper.

Band	Center[a]	Upper level[b]	Polyad[b]	Symmetry
$\nu_2-\nu_5^1$	1245.140	$010(00)_+^0$	$\{3\nu_5\}$	$\Sigma_g{}^+ \leftarrow \Pi_u$
$(\nu_4+3\nu_5)_+^0-2\nu_5^0$	1308.686	$000(13)_+^0$	$\{4\nu_5\}$	$\Sigma_u{}^+ \leftarrow \Sigma_g{}^+$
$(\nu_4+3\nu_5)^2-2\nu_5^2$	1310.182	$000(13)^2$	$\{4\nu_5\}$	$\Delta_u \leftarrow \Delta_g$
$(2\nu_4+2\nu_5)^2\ \mathrm{II}-(\nu_4+\nu_5)^2$	1318.652	$000(22)^2$ II	$\{4\nu_5\}$	$\Delta_g \leftarrow \Delta_u$
$(2\nu_4+2\nu_5)_+^0-(\nu_4+\nu_5)_+^0$	1319.942	$000(22)_+^0$	$\{4\nu_5\}$	$\Sigma_g{}^+ \leftarrow \Sigma_u{}^+$
$(2\nu_4+2\nu_5)_-^0-(\nu_4+\nu_5)_-^0$	1320.638	$000(22)_-^0$	$\{4\nu_5\}$	$\Sigma_g{}^- \leftarrow \Sigma_u{}^-$
$(3\nu_4+\nu_5)^2-2\nu_4^2$	1328.019	$000(31)^2$	$\{4\nu_5\}$	$\Delta_u \leftarrow \Delta_g$
$(3\nu_4+\nu_5)_+^0-2\nu_4^0$	1330.206	$000(31)_+^0$	$\{4\nu_5\}$	$\Sigma_u{}^+ \leftarrow \Sigma_g{}^+$
$(\nu_4+2\nu_5)^1\ \mathrm{I}-\nu_5^1$	1336.644	$000(12)^1$ I	$\{3\nu_5\}$	$\Pi_g \leftarrow \Pi_u$

[a] Band centers, in cm^{-1}, have been compiled from Ref. [1].
[b] For each band, the upper vibrational level and the polyad to which it belongs have been quoted.

Table 2
Main experimental conditions of the spectra recorded around 7.7 μm using the rapid-scan interferometer in Paris (LADIR).

Commercial sample (Air Liquide Alphagaz)			
Natural C_2H_2	97.760% of $^{12}C_2H_2$		
Stated purity	99.55%		
Maximum path difference	180 cm		
Unapodized FWHM resolution	$\approx 2.8\times10^{-3}\ cm^{-1}$		
Spectrum number	Total pressure (hPa) ±0.5%[a]	Absorbing path (cm) ±1 cm[a]	Temperature (K) ±0.5 K[a]
1	7.585	2015	297.15
2	2.283	2015	296.45
3	1.254	2015	297.15
4	0.8185	2015	297.85
5	0.4283	2015	298.35
6	0.1971	2015	298.95

[a] Absolute uncertainty (excess digits are given as a guide).

quantum number associated with the degenerate bending mode t, ± being the symmetry type for Σ vibrational states (ℓ=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. Section 2 of the paper recalls the experimental conditions and the measurement procedure, the data reduction is explained in Section 3, and the last section recalls how we have proceeded to set up a line list for databases.

2. Experimental details and measurement procedure

The 6 spectra used in this work are the same as in Ref. [5]. They have been recorded with the rapid scan Bruker IFS 120 HR interferometer of the LADIR (Laboratoire de Dynamique Interactions et Réactivité) in Paris. The main experimental conditions are gathered in Table 2. The temperature of the gas in the cell was recorded via four platinum probes at different places inside the cell. Pressures were measured using two full scale ranges MKS Baratrons (10 and 100 Torr manometers) with an accuracy of 0.5%. Details on the experimental conditions and wavenumber calibration are given in Section 2 of Ref. [5].

The same multispectrum procedure as in Ref. [5] was used to deduce line intensities from the spectra, following a method already described [10]. A Voigt profile was used to calculate the absorption coefficient of the lines, the Doppler-width being kept fixed at its theoretical value, and the baseline is adjusted as a polynomial of the second degree around each studied line. Because of the relatively low pressures, the self-broadening coefficients were fixed at the values calculated according to Ref. [11], and the self-shifting coefficients were fixed at zero. Finally, 467 line intensities have been measured in 9 bands with an average accuracy estimated around 5%. Note that the uncertainty can attain 10% or more for weak lines or overlapped ones. Results obtained for selected bands are given in Table 3. The full list of results is given in Supplementary material.

3. Data reduction

Let us recall the equations needed to reduce experimental data. For each line intensity $S(T_0)$ obtained from the multispectrum fitting procedure, in cm molecule^{-1} for pure $^{12}C_2H_2$ (i.e., for a sample containing 100% of $^{12}C_2H_2$) at the standard temperature T_0=296 K, we use the following formula to deduce the transition dipole moment squared $|R|^2$, in D^2 (1 debye=$3.33,546\times10^{-30}$ C m)

$$S(T_0) = (1/4\pi\varepsilon_0)(8\pi^3/3hc)[g''\nu_0/g_V Q(T_0)]|R|^2 L(J,\ell) \times \exp(-hcE''/kT_0)[1-\exp(-hc\nu_0/kT_0)], \qquad (1)$$