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Infrared signature of linear carbon chains on Titan

A. Jolly (1), Y. Benilan (1), F. Kwabia-Tchana (1), L. Manceron (2), C. Nixon (3), N. A. Teanby (4), A. Fayt (5)

(1) LISA, Université Paris 7 et 12, 61 Av. du Général de Gaulle, 94010 Créteil Cedex, France. (2) Synchrotron SOLEIL, L'orme des Merisiers, Saint-Aubin-BP 48, 91192 Gif-sur yvette Cedex and LADIR, CNRS-U. Paris 6, 4, place Jussieu 75252, France. (3) Department of Astronomy, University of Maryland, College Park, MD 20742, USA. (4) School of Earth Sciences, University of Bristol, Wills Memorial Building, Queen's Road, BRISTOL BS8 1RJ, United Kingdom. (5) Laboratoire de Spectroscopie Moléculaire, Université Catholique de Louvain, Chemin du cyclotron 2, B-1348 Louvain-la-Neuve, Belgium

1. Introduction

The Composite Infrared Spectrometer (CIRS) on-board Cassini has recorded spectra in the far and mid-infrared since 2004 with a spectral resolution of up to 0.5 cm^{-1}. Mismatch between observed spectra and model spectra obtained from the available line lists has led us to study the spectroscopic parameters of HC_3N, C_4H_2 and more recently C_2N_2, the longest gas phase carbon chains observed so far on Titan. Band intensities, hot band intensities, and line lists were systematically verified by comparison with new laboratory spectra. Erroneous band intensities as well as an absence or shortage of hot band transitions in the line lists have been found leading to model-data mismatches and inaccurate quantifications.

Improvement in the spectroscopic parameters has led to the detection of isotopologues of ^{13}C and opens the way to the detection of ^{15}N isotopologues which abundances could give some clues to understand the origin and the evolution of Titan's atmosphere. Also, the higher accuracy of spectroscopic data used to model CIRS spectra should facilitate the search for longer carbon chains on Titan such as HC_5N, C_6H_2 and C_4N_2. Constraints on the abundances of such molecules would help to understand the complex chemistry taking place in Titan's atmosphere.

2. HC_3N

Our laboratory experimental study of HC_3N [1] has shown that band intensities had to be revised and that including hot bands was necessary to model the observed spectra. A new extended line list was obtained and due to the precision of the new spectroscopic data, ^{13}C isotopologues of HC_3N have been detected and quantified for the first time in the atmosphere of Titan using CIRS data [2]. The detection of the ^{15}N isotopologue of HC_3N was also considered but not possible at 663 cm^{-1} as the spectral resolution of CIRS was not sufficient to separate the nitrogen isotope band from the main band emission.

3. C_4H_2

The proportion of hot bands is even more important for C_4H_2 than for HC_3N and a new spectroscopic study was necessary to improve the CIRS spectral analysis. Laboratory experimental spectra of C_4H_2 were obtained between 193 and 296 K at 0.1 and 0.5 cm^{-1} resolution followed by a global analysis of all energy levels up to 1800 cm^{-1}. Low temperature spectra were used to reduce the contribution of the hot bands and to distinguish them from the isotopes. Taking into account all the hot bands, residuals due to the contribution of both ^{13}C isotopologues in the experimental spectra of C_4H_2 were analyzed for the first time. Using this new spectroscopic data, CIRS observations of C_4H_2 at 630 cm^{-1} in the mid infrared and at 220 cm^{-1} in the far infrared were well fitted giving coherent abundances [3]. Also, using very high signal to noise CIRS observations led to the first detection and quantification of ^{13}C isotopologues of C_4H_2 on Titan [4]. The $^{12}C/^{13}C$ isotopic ratio was found for both molecules to be in agreement with other measurements by Cassini and Huygens.

4. C_2N_2

C_2N_2 has only one observable signature at 234 cm^{-1} in the far infrared domain but it is a good chance to obtain a second measurement of the $^{14}N/^{15}N$ ratio in the atmosphere of Titan (following previous measurements of $HC^{15}N$) and consequently new constraints on the formation and the evolution of Titan's atmosphere. A complete new experimental study at various resolutions ranging from 0.002 to 0.5

cm^{-1}, made at the SOLEIL-AILES synchrotron facility has led to a new determination of the band intensities for NCCN and also for ^{15}NCCN. The high resolution study helped to perform a global analysis of all rotational levels up to about 2100 cm^{-1} leading to a new extended line list including for the first time ^{15}N and ^{13}C isotopic species. Figure 1 shows a very good agreement between laboratory spectra and calculated spectra using this new line list.

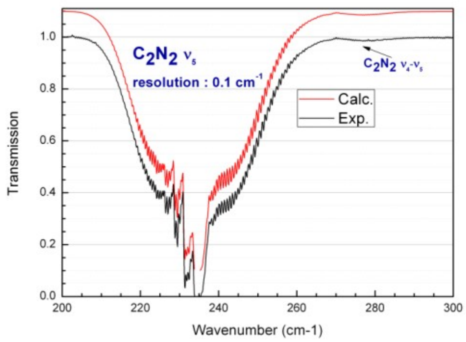

Figure 1: Calculated (shifted by 0.1 for clarity) and laboratory spectra of the ν_5 band of C_2N_2 at room temperature and at a resolution of 0.1 cm^{-1}.

Those new spectroscopic parameters give us now the possibility to search for ^{15}NCCN in Titan's atmosphere. Figure 2 presents a simulation, in Titan conditions, that is a temperature of 160 K and a ^{15}N abundance enhanced by a factor 4.5 compared to the terrestrial value according to the value found on Titan for HCN.

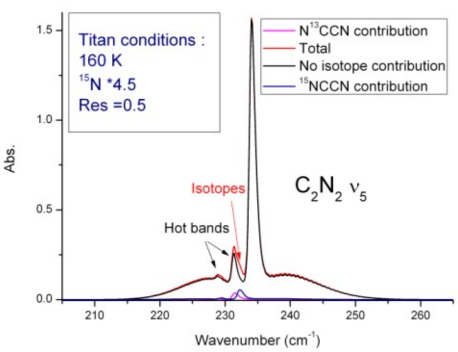

Figure 2: Calculated spectra of the ν_5 band of C_2N_2 showing the relative contribution of the isotopes and of the hot bands.

It shows a non negligible contribution of the isotopes close to the main hot bands wish are still visible even at 160 K.

References

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