High-Resolution Infrared Spectroscopy of DC$_3$N in the Stretching Region

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The perspectives opened by modern ground-based infrared facilities and the forthcoming James Webb Telescope mission have brought a great attention to the ro-vibrational spectra of simple interstellar molecules. In this view, and because of the lack of accurate spectroscopic data, we have investigated the infrared spectrum of deuterated cyanoacetylene (DC$_3$N), a relevant astrochemical species. The $v_1$, $v_2$, and $v_3$ fundamentals as well as their hot-bands were observed in the stretching region (1,500–3,500 cm$^{-1}$) by means of a Fourier transform infrared spectrometer. Supplementary measurements were performed at millimeter-wavelengths (243–295 GHz) with a frequency-modulation spectrometer equipped with a furnace, that allowed to probe pure rotational transitions in the investigated stretching states. Furthermore, since HC$_3$N is observed as by-product in our spectra and suffers from the same deficiency of accurate infrared data, its ro-vibrational features have been analyzed as well. The combined analysis of both rotational and ro-vibrational data allowed us to determine precise spectroscopic constants that can be used to model the infrared spectra of DC$_3$N and HC$_3$N. The importance of accurate molecular data for the correct modeling of proto-planetary disks and exoplanetary atmospheres is then discussed.

Keywords: cyanoacetylene, interstellar: matter, rovibrational spectroscopy, spectral analysis, infrared spectroscopy

1 INTRODUCTION

Interstellar DC$_3$N was first discovered in the dark cloud TMC-1 (Taurus Molecular Cloud 1) through the observation in emission of its $J = 5 – 4$ rotational transition lying at nearly 42.2 GHz (Langer et al., 1980). Subsequently, deuterated cyanoacetylene has been extensively observed in cold molecular clouds, such as L1498, L1544, L1521B, L1400K, and L1400G (Howe et al., 1994), as well as in the hot cores of the high-mass star-forming regions Orion KL and Sagittarius B$_2$(N) (Esplugues et al., 2013; Belloche et al., 2016). Recently, DC$_3$N has been employed to investigate the evolutionary stage of massive star-forming regions: Rivilla et al. (2020) detected the emission of DC$_3$N ($J = 11 – 10$ transition) in a sample of 15 sources containing both cold and warm high-mass star-forming cores, and acquired the first emission map of DC$_3$N in the high-mass proto-cluster IRAS 05358+3543.
The astrophysical relevance of DC$_3$N is related both to the ubiquitous presence of its parent species (HC$_3$N) in Space and to its deuteration. Indeed, the study of interstellar D-containing molecules provides important information on the properties and the evolution of star-forming regions (see, e.g., Ceccarelli et al., 2014, and references therein), and is a key tool to follow the chemical history of the materials which eventually enter into the composition of planetary bodies.

On a general ground, the identification of an interstellar molecule is achieved through the detection of its rotational and/or vibrational spectral features (McGuire, 2018). In recent years, the observations of molecules in the interstellar medium (ISM) has prospered thanks to the development of new high-sensitivity telescopes operating at a wavelength range spanning from centimeter to micrometer. The Atacama Large Millimeter/sub-millimeter Array (ALMA) is one of the best facility for the observation of molecular signatures in a variety of astrophysical objects, including remote galaxies and planets. With ten different bands (from 0.32 to 3.6 mm) ALMA covers a spectral window wherein most of the rotational transitions fall, allowing to probe a multiplicity of chemical (light and medium-sized molecules) and excitation conditions (gas temperature).

On the other hand, the observation of vibrational signatures of interstellar molecules is comparatively more difficult due to the limited transparency of the Earth atmosphere in the Mid- and Far-infrared regions. Despite the fact that a number of powerful telescopes are equipped with state-of-the-art high-resolution ($R > 50,000$) infrared spectrographs (e.g., CRIRES at ESO Very Large Telescope, TEXES at NASA IR Telescope facility), still the identification of vibrational features of species different from the main tracers (H$_2$O, CH$_4$, HCN, NH$_3$, etc.) remains challenging due to a combination of signal weakness, line overlap, and contamination by stratospheric OH lines. In this context, a future important contribution is expected from the James Webb Space Telescope (JWST), to be launched in October 2021 as a follow-on mission of the Hubble Space Telescope. Located outside the Earth atmosphere, JWST will allow for the observation of high-sensitivity wideband infrared spectra with its on-board infrared spectrographs. The Mid-Infrared Instrument (MIRI) covers continuously the 5–28 μm region at mid resolution ($R \sim 3,000$) with four bands (Banks et al., 2008), while NIRSPEC is designed to pinpoint the shorter wavelength range (1.8–5.2 μm). Such facilities will provide a full spectral overview of the sources, thus allowing to sample simultaneously the complete vibrational manifold of the molecular targets: i.e., the bending region below 12 μm already excited in the warm gas ($T < 500$ K), and the C-H stretching region around 3 μm, characterised by high excitation energies ($E/k \sim 4,000$ K) and useful to probe the inner (AU-sized) parts of proto-planetary disks and the atmospheres of hot exoplanets.

The laboratory spectroscopic knowledge of DC$_3$N over the full spectral range of interest for astronomy is, however, not homogeneous. While the rotational spectrum of DC$_3$N has been accurately studied and it is well suited to guide astronomical observations at millimeter wavelengths, a detailed knowledge of its infrared spectrum is limited to the spectral range between 200 and 1,100 cm$^{-1}$ (Melosso et al., 2020). At higher frequencies, only low-accuracy spectroscopic data are available in the literature (Mallinson and Fayt, 1976). The same applies to the MIR spectrum of HC$_3$N above 1,000 cm$^{-1}$, for which the ro-vibrational bands were recorded either at low resolution of 0.025 and 0.050 cm$^{-1}$ (Mallinson and Fayt, 1976) or in a narrow spectral interval (Yamada et al., 1980; Yamada and Winnewisser, 1981; Yamada et al., 1983). Such patchy results were due mainly to the type of instrumentation employed, i.e., Ebert-type and Diode-laser spectrometers. Currently, these limitations are easily overcome by Fourier-transform infrared (FTIR) spectrometers, which offers the possibility of recording high-resolution ro-vibrational spectra in a wide frequency range.

To fill the lack of information described above, in this work we report on a comprehensive investigation of the high-resolution MIR spectra of DC$_3$N and HC$_3$N, obtained using FTIR spectroscopy. In addition, the pure rotational spectra in some vibrational excited states of DC$_3$N have been recorded in order to determine highly-accurate spectroscopic parameters. The new assignments of the IR and millimeter-wave spectra were combined into a single global fit from which a consistent set of spectroscopic constants has been determined. The analysis of DC$_3$N provides a highly-precise rest-frequency catalog useful for astronomical observations.

## 2 EXPERIMENTAL DETAILS

The DC$_3$N sample was prepared as recently reported in Melosso et al. (2020).

### 2.1 Fourier-Transform Infrared Interferometer

Infrared spectra of DC$_3$N and HC$_3$N were recorded in the 1,500–3,500 cm$^{-1}$ range with a Fourier-Transform Bomem DA3.002 interferometer (Stoppa et al., 2016; Tamassia et al., 2020). In the present work, the spectrometer was equipped with a KBr beam-splitter, a Globar source, a liquid-nitrogen InSb detector, and a multipass cell whose absorption-pathlength was set to 8 m. Two spectra were recorded in the 1,500–3,500 cm$^{-1}$ region using different pressures of DC$_3$N, namely 16 and 32 Pa, at a nominal resolution of 0.004 cm$^{-1}$. Both of them were obtained from the co-addition of 140–200 scans, for a total integration time of 13–18 h. The frequency axis of the spectra was calibrated by using some 50 transitions of H$_2$O and CO$_2$ as references, whose wavenumbers were taken from the HITRAN database (Gordon et al., 2017). On average, the calibration residuals are about 5 × 10$^{-3}$ cm$^{-1}$. The HC$_3$N absorptions were also detected in the same spectra with a good signal-to-noise ratio (S/N) because of the hydrogen-deutrium (H/D) exchange occurring in the multipass cell. The line-center frequencies were retrieved with PGOPHER (Western, 2017) using the maximum intensity of the lines and their uncertainty is assumed to be 4 × 10$^{-3}$ cm$^{-1}$ in all cases.
2.2 Frequency-Modulation Millimeter/Submillimeter-Wave Spectrometer

Pure rotational transitions of DC$_3$N were recorded in three high-energy vibrational states by means of a frequency-modulation (FM) millimeter/submillimeter-wave spectrometer (Melosso et al., 2019a; Melosso et al., 2019b). Briefly, the primary radiation source is a Gunn oscillator working in the W band (80–115 GHz), whose frequency is stabilized and modulated in a phase-lock loop. Higher frequencies are obtained by coupling the Gunn diode with passive frequency-multipliers (doublers and triplers). The detection system is constituted by a Schottky barrier diode connected to a lock-in amplifier set at twice the modulation frequency (2f detection scheme). However, in order to observe rotational transitions belonging to vibrational states with energies between 1,900 and 2,400 cm$^{-1}$, a new experimental set-up has been tested. A 1.5 m long quartz absorption cell has been surrounded by a homogeneous S/N ratio for a wide range of values to account for these different band intensities, and to obtain spectral recordings were performed employing various pressure values. The effective absorption-path was at least 1.8 m. For the present measurements, the temperature furnace was set to 700°C, while a small flow (~1 Pa) of DC$_3$N was ensured inside the cell. The accuracy of the retrieved frequencies is estimated to be around 30 kHz.

3 ANALYSIS AND RESULTS

3.1 Theoretical Background

DC$_3$N is a closed shell linear molecule which possesses seven vibrational modes: four stretching modes ($v_1, v_2, v_3, v_4$; $\Sigma$ symmetry) and three doubly-degenerate bending modes ($v_5, v_6, v_7$; $\Pi$ symmetry), all of being infrared-active. The low-lying vibrational states ($v_4, v_5, v_6, v_7$) as well as some of their overtone and combination states have been extensively analyzed in a previous paper (Melosso et al., 2020). In the present work, we focus on the fundamental transitions of the $v_1, v_2, v_3$ stretching modes, and their hot bands ($v_1 + v_2 - v_7$, $v_2 + v_7 - v_2$, and $v_3 + v_7 - v_3$), which all lie in the MIR region. Since the corresponding bands of HC$_3$N, formed in the absorption cell by isotopic exchange, are visible in the same spectra, we analyzed them as well. A more extended analysis of the HC$_3$N data through a global fit including a large number of rotational and ro-vibrational transitions is currently being completed.

The effective Hamiltonian employed in this work to analyze the ro-vibrational transitions mentioned above (both DC$_3$N and HC$_3$N) and to retrieve the spectroscopic parameters was already described in Bizziocchi et al. (2017). Since the present study focuses on the analysis of three stretching states ($\Sigma$ symmetry) and their $v_7$ associated hot bands, the Hamiltonian can be simplified as:

$$ H = H_{ro} + H_{l-type} $$

(1)

where $H_{ro}$ is the ro-vibrational Hamiltonian and $H_{l-type}$ describes the $l$-type interaction between $l$ sub-levels of the excited bending states.

In the ro-vibrational part, the diagonal elements of the Hamiltonian can be expressed as:

$$ \langle l_Y + 2, k \pm 2 | H_{l-type} | l_Y, k \rangle = \frac{1}{4} \{ q_7 + q_7 f(J + 1) + q_{7l} f(J + 1)^2 \} \times \sqrt{(v_7 \pm l_Y)(v_7 \pm l_Y + 2)} \times \sqrt{f_{s+}(J, k)} $$

(3)

The functions $f(J, k)$ and $f_{s+}(J, k)$ appearing in the equations above are defined as follows:

$$ f(J, k) = f(J + 1) - k^2, $$

(4)

$$ f_{s+}(J, k) = \prod_{p=1}^{n} (J + 1) - [k \pm (p - 1)](k \pm p). $$

(5)

3.2 Spectral Features

The stretching bands $v_1$, $v_2$, and $v_3$ are located between 1,900 and 3,400 cm$^{-1}$ (2.9–5.3 μm), for both DC$_3$N and HC$_3$N. An overview of the vibrational bands recorded in this work is provided in Figure 1. By inspecting this figure, it is evident that all the twelve bands observed and analyzed show the typical contour of $\Sigma - \Sigma$ or $\Pi - \Pi$ bands of a linear rotor, thus presenting well-defined P and R branches, but no Q branch.

While the absolute intensities of DC$_3$N bands are quite similar to each other ($v_1 = 81$ atm$^{-1}$ cm$^{-2}$, $v_2 = 50$ atm$^{-1}$ cm$^{-2}$, and $v_3 = 39$ atm$^{-1}$ cm$^{-2}$ Bénilan et al., 2006), the situation is different for HC$_3$N ($v_1 = 249$ atm$^{-1}$ cm$^{-2}$, $v_2 = 41$ atm$^{-1}$ cm$^{-2}$, and $v_3 = 8$ atm$^{-1}$ cm$^{-2}$ Jolly et al., 2007), with an overall variation of more than one order of magnitude. Furthermore, the hot-bands analyzed in this work ($v_1 + v_7 - v_7$, $v_2 + v_7 - v_2$, and $v_3 + v_7 - v_3$) are nearly three times weaker than the corresponding fundamental bands because of the Boltzmann factor at room temperature (the energy of the $v_7 = 1$ state is 221.8 cm$^{-1}$). As stated in Section 2.1, spectral recordings were performed employing various pressure values to account for these different band intensities, and to obtain a homogeneous S/N ratio for a wide range of J values.

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1 Tamassia et al., 2021, in preparation
In addition to the infrared measurements, pure rotational spectra of three vibrational excited states of DC$_3$N were recorded between 243 and 295 GHz using the spectrometer described in Section 2.2. In detail: some $J + 1 \rightarrow J$ rotational transitions have been observed for the $v_3 = 1$, $v_2 = 1$, and $v_1 = v_7 = 1$ states, with $J$ ranging from 28 to 34. Both $v_3 = 1$ and $v_2 = 1$ are Π states and their rotational spectra appear like a sequence of (almost) equally-spaced lines, while the $v_1 = v_7 = 1$ state has a Σ symmetry, thus showing a series of doublets due to the $l$ type resonance.

3.3 Analysis of the Spectra

The analysis of the ro-vibrational and pure rotational spectra has been performed with the aid of the PGOPHER program (Western, 2017) and the CALPGM suite (Pickett, 1991). Initially, more than 1500 ro-vibrational transitions of DC$_3$N belonging to the fundamental bands $v_1$, $v_2$, and $v_3$ and to their hot-bands $v_1 + v_7 - v_7$, $v_2 + v_7 - v_7$, and $v_3 + v_7 - v_7$ were assigned, and they include high-$J$ transitions up to $J = 110$. However, not all the ro-vibrational transitions assigned could be incorporated in the fit with the estimated experimental accuracy. In particular, the $v_2 + v_7 - v_7$ hot-band exhibited some deviations from our modelling, especially for transitions with $J$ between 10 and 15. To check and correct possible misassignments, we have also employed the Loomis-Wood for Windows (LWW) program package for symmetric-top molecules (Łodyga et al., 2007), which revealed no errors in our assignments, through both the graphical diagrams and the Ground State Combination Differences (GSCDs) method. Possible perturbations due to a nearby state are therefore plausible. However, the identification of the perturbing state is not feasible at these energies because of the very large number of unknown ro-vibrational levels. Since a complete treatment of all the anharmonic resonances is beyond the goal of this work, an effective approach has been adopted and lines showing the largest deviations (10 in total) were removed from the analysis. The comparison between the simulation based on our analysis and the observed $v_2 + v_7 - v_7$ ro-vibrational transitions is shown in Figure 2, together with the corresponding Loomis-Wood plot.

The analysis of the other five bands was instead rather straightforward and satisfactory, with the Hamiltonian of Eqs 1–3 able to well reproduce all experimental data within their nominal uncertainty. The quality of the band analyses can be inferred from the root-mean-square (rms) errors of the fits, which are reported in Table 1.

The spectroscopic constants determined from the preliminary analysis of the six bands of DC$_3$N were used to predict its pure rotational spectrum in the $v_3 = 1$, $v_2 = 1$, and $v_1 = v_7 = 1$ states, which are the three lowest energy states among those investigated in this work. A total of 21 pure rotational transitions, which do not suffer from contamination of nearby lines, have been successfully recorded and then added to the data-set in order to improve the accuracy of the spectroscopic parameters determined in the fit. It should be pointed out that, although the analysis of the $v_3$ band gave no hint of perturbations (as evident from its LWW plot in Figure 3) and the fit has a rms error as low as $3.4 \times 10^{-4}$ cm$^{-1}$, the rotational transitions recorded in the $v_3 = 1$ state show deviations about 10 times larger than the expected error, i.e., around 300 kHz. Once again, a plausible
explanation is that the $v_3 = 1$ state is involved in an anharmonic interaction with one or more vibrational states close in energy, but such perturbation is moderately weak and hidden in the larger uncertainty of the infrared data. Nonetheless, despite these somewhat large residuals, the inclusion of pure rotational lines reduces the uncertainty of the derived spectroscopic parameters by up to a factor of 3. The upper states spectroscopic parameters determined from the combined analysis of rotational and ro-vibrational transitions are collected in Table 2. The spectroscopic constants of the ground and $v_7 = 1$ states, i.e., the lower levels involved in the current analysis, were kept fixed at the values determined in our previous global analysis (see Tables 4, 5 in Melosso et al., 2020).

As far as HC$_3$N is concerned, being a side-product of our spectral recording, we limited the analysis to its infrared spectrum. With the only exception of a few small deviations involving blocks of 2–3 consecutive $J$ levels, no evident perturbations were observed during the assignment procedure and/or at the fitting stage. Overall, for HC$_3$N, 1221 different lines were assigned to the $v_1$, $v_2$, and $v_3$ fundamental bands and their corresponding hot bands originating from the $v_7 = 1$ state. Similarly to DC$_3$N, the vibrational energies $G_v$ and the

| Species | Band | Sub-band | $J_{max}$ | Freq. Range (cm$^{-1}$) | Lines | rms error ($10^{-4}$ cm$^{-1}$) |
|---------|------|----------|-----------|--------------------------|-------|-------------------------------|
| DC$_3$N | $v_1$ | $\Sigma - \Sigma$ | 110 | 2,577–2,635 | 189 | 3.5 |
|         | $v_2$ | $\Sigma - \Sigma$ | 105 | 2,215–2,275 | 199 | 3.6 |
|         | $v_3$ | $\Sigma - \Sigma$ | 110 | 1,932–1,995 | 219 | 3.4 |
|         | $v_1 + v_7 - v_7$ | $\Pi - \Pi$ | 100 | 2,579–2,632 | 269 | 6.3 |
|         | $v_2 + v_7 - v_7$ | $\Pi - \Pi$ | 91 | 2,220–2,271 | 284 | 20.3 |
|         | $v_3 + v_7 - v_7$ | $\Pi - \Pi$ | 97 | 1,943–1,990 | 292 | 4.1 |
| HC$_3$N | $v_1$ | $\Sigma - \Sigma$ | 91 | 3,298–3,352 | 174 | 5.0 |
|         | $v_2$ | $\Sigma - \Sigma$ | 91 | 2,243–2,296 | 161 | 4.0 |
|         | $v_3$ | $\Sigma - \Sigma$ | 87 | 2,050–2,102 | 169 | 3.7 |
|         | $v_1 + v_7 - v_7$ | $\Pi - \Pi$ | 78 | 3,301–3,348 | 225 | 6.0 |
|         | $v_2 + v_7 - v_7$ | $\Pi - \Pi$ | 93 | 2,249–2,294 | 240 | 4.3 |
|         | $v_3 + v_7 - v_7$ | $\Pi - \Pi$ | 71 | 2,052–2,096 | 252 | 4.0 |
Rotational constants $B_v$ were determined with high precision for all the six vibrational excited states. Accurate values for the centrifugal distortion constant $D_v$ and the $l$-type doubling constant $q_l$ were derived as well. Table 3 lists the complete set of upper state spectroscopic parameters used in the final fit, while the quality of the analysis is demonstrated by the low rms error achieved for each band (see Table 1). Also in this case, the spectroscopic constants of the ground and $v_7 = 1$ states were kept fixed at the values determined in our previous global analysis (see Table 5 in Bizzocchi et al., 2017).

The fit output files containing the assigned transitions, their wavenumbers, and the residual errors for each band are provided as Supplementary Material.
4 DISCUSSION AND CONCLUSION

Nowadays, the improvement of the ground-based infrared facilities (e.g., CRIRES + at VLT) and the perspectives opened by the forthcoming JWST telescope (with MIRI and NISPEC instruments) have brought a considerable interest to the ro-vibrational spectrum of simple interstellar molecules, both at low and high wavenumbers. In particular, the possibility of probing the inner portions of young proto-planetary disks where the material is funneled into the planetary formation zone and—at later stages—to directly observe the atmospheres of the mature exoplanets, makes the stretching spectral interval (1,500–3,500 cm$^{-1}$) of particular interest due to its selectivity to the high gas temperatures typical of these regions. In this context, a detailed knowledge of the associated hot bands is as important as that of the fundamentals. In high excitation conditions, many vibrational states are significantly populated and the corresponding satellite features are able to make up a considerable amount of the retrieved flux. Hot bands are thus critical to accurately model the shape of the band profile and to retrieve reliable column densities. The laboratory detection of accurate infrared spectra is therefore essential to guide such astronomical investigations. Prior to our investigation, the knowledge of the mid-infrared spectra of DC$_3$N and HC$_3$N (Melosso et al., 2020) and Fayt (1976), and are consistent with the most recent two orders of magnitude more accurate than those from Mallinson and Fayt (1976; Bénilan et al., 2006; Jolly et al., 2007). Future studies will focus on these subjects.

As a final remark, the high-temperature rotational spectroscopy experimental technique presented in this work can be successfully applied to future investigations of the vibrational excited states of molecules relevant to astrophysics and possessing only highly-energetic vibrations, such as water or other small species.

DATA AVAILABILITY STATEMENT

The original contributions presented in the study are included in the article/Supplementary Material, further inquiries can be directed to the corresponding author.

AUTHOR CONTRIBUTIONS

MM, FT, and CP contributed to conception and design of the study; JG synthesized the sample; MM, FT, and LD set-up the experiments; NJ, MM, FT, and EC recorded the spectra; NJ prepared the figures; MM organized the tables; NJ, MM, and FT performed the analysis; NJ wrote the first draft of the article with the help of MM and CP; MM, LB, and CP wrote sections of the article; DF contributed to the discussion on the astronomical applications. All authors contributed to article revision, read, and approved the submitted version.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fspas.2021.656295/full#supplementary-material.
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Conflict of Interest: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

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