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First detection of cyanamide (NH$_2$CN) towards solar-type protostars


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ABSTRACT

 Searches for the prebiotically relevant cyanamide (NH$_2$CN) towards solar-type protostars have not been reported in the literature. We present here the first detection of this species in the warm gas surrounding two solar-type protostars, using data from the Atacama Large Millimeter/Submillimeter Array Protostellar Interferometric Line Survey (PILS) of IRAS 16293–2422 B and observations from the IRAM Plateau de Bure Interferometer of NGC 1333 IRAS2A. We also detected the deuterated and $^{13}$C isotopologs of NH$_2$CN towards IRAS 16293–2422 B. This is the first detection of NHDCN in the interstellar medium. Based on a local thermodynamic equilibrium analysis, we find that the deuteration of cyanamide ($\sim$1.7%) is similar to that of formamide (NH$_2$CHO), which may suggest that these two molecules share NH$_2$ as a common precursor. The NH$_2$CN/NH$_2$CHO abundance ratio is about 0.2 for IRAS 16293–2422 B and 0.02 for IRAS2A, which is comparable to the range of values found for Sgr B2. We explored the possible formation of NH$_2$CN on grains through the NH$_2$ + CN reaction using the chemical model MAGICKAL. Grain-surface chemistry appears capable of reproducing the gas-phase abundance of NH$_2$CN with the correct choice of physical parameters.

Key words. astrochemistry – astrobiology – ISM: molecules – stars: protostars – ISM: individual objects: IRAS 16293-2422 – ISM: individual objects: NGC 1333 IRAS2A

1. Introduction

Cyanamide (NH$_2$CN) is one of the rare interstellar molecules that contain two atoms of nitrogen. This species is thought to be relevant for prebiotic chemistry: in liquid water it may convert into urea, an important molecule in biological processes (e.g., Kilpatrick 1947). Its isomer carbodiimide (HNCCN) can be formed from NH$_2$CN in photochemically and thermally induced reactions in interstellar ice analogs (Duvernay et al. 2005). Molecules with the carbodiimide moiety ($\sim$NCN$\sim$) find use in various biological processes, among which the assembly of amino acids into peptides (see Williams & Ibrahim 1981 for an overview). Although this molecule has been detected in other galaxies, such as NGC 253 and M82 (Martin et al. 2006; Aladro et al. 2011), only two detections are mentioned in our Galaxy, in the massive star-forming regions Sgr B2 (Turner et al. 1975) and Orion KL (White et al. 2003).

Molecules formed early during the star formation process may be incorporated into comets or asteroids and delivered to planets during heavy bombardment periods, similar to that experienced by the young Earth (Raymond et al. 2004). Here, we report the detection of cyanamide towards two solar-type protostars, IRAS 16293–2422 (hereafter IRAS 16293) and NGC 1333 IRAS2A (hereafter IRAS2A). These two low-mass protostars are known to harbor a very rich chemistry in their inner regions (e.g., Bottinelli et al. 2004; Jørgensen et al. 2005). This can be explained by the thermal desorption of the numerous and complex species formed in the icy mantles of the grains. The detection presented in this work complements the list of molecules of prebiotic interest such as glycolaldehyde, formamide, and methyl isocyanate discovered in low-mass protostars (Jørgensen et al. 2012; Kahane et al. 2013; Maury et al. 2014; Coutens et al. 2015; Ligterink et al. 2017; Martín-Domènech et al. 2017). We also detected the deuterated form of cyanamide, NHDCN, for the first time in the interstellar medium.

2. Observations

To search for cyanamide, we used data obtained with the Atacama Large Millimeter/Submillimeter Array (ALMA) for
IRAS 16293 and with the IRAM Plateau de Bure Interferometer (PdBI) for IRAS2A.

The ALMA data are part of the Protostellar Interferometric Line Survey (PILS) program, a large spectral survey of IRAS 16293 observed in Cycle 2 between 329.1 and 362.9 GHz at a spatial resolution of about 0.5″ and a spectral resolution of ~0.2 km s⁻¹. The observations and their reduction are presented in Jørgensen et al. (2016). The data reach a sensitivity of about ~4–5 mJy beam⁻¹ km s⁻¹.

The PdBI data of the low-mass protostar IRAS2A were obtained with the WIDEX correlator in the framework of several programs (V010, V05B, W00A, and X060). The data reduction of each dataset is described in Coutens et al. (2014, 2015) and Persson et al. (2014). They cover the spectral ranges 223.5–227.1, 240.2–243.8, and 315.5–319.1 GHz with a spectral resolution of 1.95 MHz (~1.8–2.6 km s⁻¹). The angular resolution is about 1.2″ × 1.0″ at 225 GHz, 1.4″ × 1.0″ at 242 GHz, and 0.9″ × 0.8″ at 317 GHz. The rms are ~5–6 mJy beam⁻¹ km s⁻¹ or lower.

The spectroscopic data used here for cyanamide and its ¹³C isotopolog come from the spectroscopic catalogs Jet Propulsion Laboratory (JPL, Pickett et al. 1998; Read et al. 1986) and Cologne Database for Moleculer Spectroscopy (CDMS, Müller et al. 2001, 2005; Kraańicki et al. 2011). The spectroscopy of NHDCN was studied by Kisiel et al. (2013). Carbodiimide spectroscopic information comes from the CDMS (Birk et al. 1989; Jabs et al. 1997).

3. Results

The CASSIS² software was used to search for and identify the lines of NH₂CN and its isotopologs towards IRAS 16293 and IRAS2A. Synthetic spectra were produced and compared with the observations to identify the lines. Potential blending with other species from the CDMS or JPL catalogs was checked. Column densities were determined assuming local thermodynamic equilibrium (LTE), which is reasonable for the inner regions of low-mass protostellar envelopes owing to their very high densities (≥10¹⁰ cm⁻³). Jørgensen et al. (2016).

3.1. Analyses of cyanamide and carbodiimide

For the binary IRAS 16293, 11 unblended lines of the main cyanamide isotopolog are detected towards source B (see Fig. 2) at the full-beam offset position analyzed in previous studies (Coutens et al. 2016; Lykke et al. 2017; Ligerink et al. 2017). No clear detection could be obtained towards IRAS 16293 A, where the lines are broader (≥2 km s⁻¹). Maps indicate that the emission of this species arises from the warm inner regions around the B component (see Fig. 1), similarly to other complex organic molecules (Baryshev et al. 2015; Jørgensen et al. 2016). This species also appears to be strongly affected by absorption against the strong continuum similarly to formamide (Coutens et al. 2016, see their Fig. 1). The deep absorptions at the continuum peak and half-beam offset positions are clearly seen for all the lines (see Fig. B.1). Although a LTE model with a lower excitation temperature of 100 K is in relatively good agreement with the observations (see Fig. 2), a temperature of 300 K is a more appropriate fit. This is consistent with the temperature derived for other species with high binding energies such as glycolaldehyde, ethylene glycol, and formamide (see discussion in Jørgensen et al. 2018). At the full-beam offset position, a column density of (7 × 10¹³ cm⁻²) is derived for an excitation temperature of 300 K (≥5 × 10¹³ cm⁻² for 100 K) and a source size of 0.5″. It should be noted that this column density can only be considered as a lower limit because of the absorption components that could lower the emission contribution of the line profile. The higher value of the column density of NH₂CN is confirmed by the analysis of the ¹³C isotopolog (see Sect. 3.2).

Three bright and unblended lines of cyanamide are also detected towards NGC 1333 IRAS2A (see Fig. 3). An excitation temperature of ~130 K and a source size of ~0.5″ were derived from the analysis of other complex organics towards this source by Coutens et al. (2015). Based on these parameters, an LTE model with a column density of 2.5 × 10¹⁴ cm⁻² is in very good agreement with the observations. An excitation temperature of 300 K does not properly reproduce the lines. No other line is missing in the spectral range covered by our data. Based on this model, we can confirm the detection of this molecule by comparing our predictions with the list of lines observed in the spectral range 216.8–220.4 GHz covered by the CALYPSO program (Maury et al. 2014). Among the six brightest lines, five of them are in agreement with the presence of unidentified lines detected by Maury et al. (2014; see Table A.5). The last one is blended with a NH₂CHO line. Maps confirm that the molecule is emitting within the warm inner regions of the source (see Fig. 1).

We also searched for carbodiimide, HNCCNH, which is not detected with an upper limit of 3 × 10¹⁵ cm⁻² towards IRAS 16293 B. Based on the non-detection of the HNCCNH line at 223.7918 GHz, we derived a similar upper limit for IRAS2A. The non-detection of carbodiimide is not really surprising since the upper limits are high and this isomer is known to be less stable than cyanamide.

3.2. Analyses of the deuterated and ¹³C isotopologs of cyanamide

The ¹³C and deuterated isotopologs of NH₂CN were searched for towards both sources. Eight unblended lines of NHDCN were identified towards the full-beam offset position of IRAS 16293 B (see Fig. 4). This marks the first detection of this isotopolog in the interstellar medium. Although the lines are faint, we can confirm that all the features are real after checking the spectra at the half-beam position (where the lines are brighter). Additional lines are present, but are not included here as they are blended with other species. A few other lines do not appear as

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¹ http://youngstars.nbi.dk/PILS/
² CASSIS has been developed by IRAP-UPS/CNRS (http://cassis.irap.omp.eu/).
and 100 K are in red and blue, respectively. The detection of NH$_2$CN with other species at the same frequency. A column density of $3 \times 10^{13}$ cm$^{-2}$ is obtained for an excitation temperature of 300 K. The detection of NH$_3$CN is less straightforward. Three lines can be attributed to this isotopolog (see Fig. 5). One of them (361.997 GHz) may be blended with an unknown species since its flux is higher than predicted by the LTE model. Based on the analysis of the NH$_3$CN isotopolog and the lower contribution of the absorptions. The D/H of NH$_2$CN corrected for statistics, i.e., divided by 2) is 1.7%, assuming a standard reaction CN + H$_2$ → HCN + H has been proposed (Smith et al. 2004), the theoretical study of Talbi & Smith (2009) suggests that the production of NH$_2$CN involves large internal barriers, with HCN and NH$_2$ being the likely products. An experimental study by Blitz et al. (2009) confirms that this reaction proceeds exclusively to HCN + NH$_2$. Electronic recombination of NH$_2$CN$^+$ may produce NH$_3$CN, but the only apparent way to form this ion is through protonation of NH$_2$CN itself. An alternative source of NH$_2$CN is thus required to explain our observations. Cyanamide could be formed on grain surfaces through the addition of NH$_3$CN and CN radicals. The possible formation of formamide from the same precursor NH$_3$ (Fedoseev et al. 2016) could explain the similarity of these two species in terms of deep absorption against the strong continuum and the similar deuteration of the two species towards IRAS 16293 B.

To test this hypothesis we ran MAGICKAL, a three-phase chemical kinetics model (Garrod 2013), modified with the grain-surface back-diffusion correction of Willis & Garrod (2017). The model uses a network based on that of Belloche et al. (2013), in which dissociative recombination of NH$_2$CN$^+$ was assumed to produce NH$_3$CN in 5% of cases. The reaction NH$_3$ + CN → NH$_2$CN was added to the grain/ice chemical network, and NH$_2$CHO lines covered by our data suggests a column density of about $1.2 \times 10^{16}$ cm$^{-2}$ assuming a similar excitation temperature of 130 K. This is in agreement with the value determined by Taquet et al. (2015). The ratio of NH$_2$CN-to-NH$_2$CHO is consequently about 0.02, an order of magnitude lower than for IRAS 16293 B.

The NH$_2$CN-to-NH$_2$CHO ratios derived for the low-mass protostars are similar to the range of values found in Sgr B2 (Belloche et al. 2013, see Table 1). The NH$_2$CN-to-NH$_2$CHO ratio in Orion KL seems to be higher ($\sim$0.4–1.5, White et al. 2003). This value is, however, more uncertain since it was obtained using only one line of NH$_2$CHO and assuming different excitation temperatures for the two molecules.

**4. Discussion**

The formation routes of NH$_2$CN have only been marginally explored. According to the Kinetic Database for Astrochemistry (KIDA, Wakelam et al. 2012), there are no known gas-phase mechanisms capable of its production. While the reaction CN + NH$_2$ → HCN + H has been proposed (Smith et al. 2004), the theoretical study of Talbi & Smith (2009) suggests that the production of NH$_2$CN involves large internal barriers, with HCN and NH$_2$ being the likely products. An experimental study by Blitz et al. (2009) confirms that this reaction proceeds exclusively to HCN + NH$_2$. Electronic recombination of NH$_2$CN$^+$ may produce NH$_3$CN, but the only apparent way to form this ion is through protonation of NH$_2$CN itself. An alternative source of NH$_2$CN is thus required to explain our observations. Cyanamide could be formed on grain surfaces through the addition of NH$_3$CN and CN radicals. The possible formation of formamide from the same precursor NH$_3$ (Fedoseev et al. 2016) could explain the similarity of these two species in terms of deep absorption against the strong continuum and the similar deuteration of the two species towards IRAS 16293 B.

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For IRAS2A, an upper limit of $5 \times 10^{13}$ cm$^{-2}$ is derived for NHDCN, leading to a D/H of $\lesssim 10\%$. The $^{13}$C isotopolog also presents an upper limit of $5 \times 10^{13}$ cm$^{-2}$, which is equivalent to a $^{13}$C/H of $\lesssim 5\%$.

**3.3. Abundances of cyanamide**

Based on the analysis of the NH$_3$CN isotopolog and the lower limit of the H$_2$ column density derived by Jørgensen et al. (2016), for IRAS 16293 B we get an abundance of NH$_2$CN with respect to H$_2$ of $\lesssim 2 \times 10^{-10}$ at 60 AU from source B. The NH$_3$CN/NH$_2$CHO abundance ratio is about 0.2.

Using the H$_2$ column density derived by Taquet et al. (2015, $5 \times 10^{13}$ cm$^{-2}$) for IRAS2A, the abundance with respect to H$_2$ is about $5 \times 10^{-11}$. A simple analysis of the most optically thin...
the gas-phase reaction between CN and NH$_2$ was adjusted per Talbi & Smith (2009) and Blitz et al. (2009). The physical model used here is very similar to that described by Belloche et al. (2017), in which a cold collapse to high density is followed by a temperature increase to 400 K; here, a final density $n_f = 6 \times 10^{10}$ cm$^{-3}$ was assumed to better represent the density structure of IRAS 16293 B (Jørgensen et al. 2016).

The model results (for an intermediate warm-up timescale) are shown in Fig. 6 for both NH$_2$CN and NH$_2$CHO. NH$_2$CNis seen to be produced at a temperature of $\sim 30$ K on the grain surfaces, desorbing into the gas at higher temperatures. The model underproduces the amount of gas-phase NH$_2$CN, showing a peak fractional abundance with respect to H$_2$ of $6.7 \times 10^{-12}$ that is nevertheless well maintained to a temperature of 300 K and beyond. The low NH$_2$CN abundance in the gas-phase is caused primarily by underproduction on the dust grains; at the high density used in the model, the rapid accretion of H and H$_2$ onto grain surfaces makes hydrogenation of the NH$_2$CN radicals much more competitive with the reaction that produces NH$_2$CN. This competition becomes important for gas densities greater than $\sim 10^9$ cm$^{-3}$. We therefore also present a model with a lower final density of $n_f = 1.6 \times 10^9$ cm$^{-3}$ (corresponding to the density of the envelope between the two protostars in IRAS 16293, Jacobsen et al. 2018), intended to represent the approximate conditions of the gas while at a temperature of 30 K (see Fig. 6). This model produces an NH$_2$CN fractional abundance of $3.7 \times 10^{-10}$, a value very close to the detected value. However, the resulting NH$_2$CN:NH$_2$CHO peak abundance ratio of 0.0011 is still lower than the observed values in both IRAS2A ($0.002$, and IRAS 16293 ($0.2$). This may be due to the possible overproduction of NH$_2$CHO, related to uncertainties in the efficiency of formation of that molecule, which is still a matter of debate, particularly for the gas-phase mechanism (e.g., Barone et al. 2015; Song & Kästner 2016); our model assumes...
only a grain-surface/ice formation route. The difficulty in reproducing the observed NH$_2$CN abundance at the high densities determined for the source highlights the necessity for future models of hot-core/corino chemistry to treat the rising density and temperature in such cores concurrently, rather than as a two-stage process, so that the gas densities are appropriate at the key temperatures at which many molecules are formed.

In conclusion, the detection of cyanamide towards IRAS 16293 B and IRAS2A indicates that this species can be formed early in solar-type protostars. If it survives during the star formation process until its incorporation into comets or asteroids, these objects could then deliver it to planets, which may enable the development of life. Searches for this species in the coma of comets could shed further light on this possibility. Theoretical and experimental studies as well as more detailed chemical models are needed to confirm the formation of NH$_2$CN through the grain-surface pathway NH$_2$ + CN. It would also be interesting to investigate whether this mechanism is sufficient to explain the large-scale emission of NH$_2$CN in galaxies.

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Raymond, S. N., Quinn, T., & Lunine, J. I. 2004, Icarus, 168, 1
Taquet, V., & Smith, I. W. M. 2009, Phys. Chem. Chem. Phys., 11, 8477
### Appendix A: Tables with detected lines of NH$_2$CN and its isotopologs

#### Table A.1. Detected lines of NH$_2$CN towards IRAS 16293 B with ALMA.

<table>
<thead>
<tr>
<th>Transition (N, K$_A$, K$_C$, v)</th>
<th>Frequency (MHz)</th>
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<th>$A_{ij}$ (s$^{-1}$)</th>
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#### Table A.2. Detected lines of NH$_2$CN towards IRAS2A with PdBI.

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#### Table A.3. Detected lines of NHDCN towards IRAS 16293 B with ALMA.

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#### Table A.4. Detected lines of NH$_3^{13}$CN towards IRAS 16293 B with ALMA.

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<td>18 4 15 1–17 4 14 1</td>
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<td>460.9</td>
<td>4.55 x 10$^{-3}$</td>
<td>111</td>
</tr>
<tr>
<td>18 4 14 1–17 4 13 1</td>
<td>359154.9</td>
<td>460.9</td>
<td>4.55 x 10$^{-3}$</td>
<td>111</td>
</tr>
<tr>
<td>18 1 17 0–17 1 16 0</td>
<td>361997.1</td>
<td>179.6</td>
<td>5.01 x 10$^{-3}$</td>
<td>111</td>
</tr>
</tbody>
</table>

#### Table A.5. Unidentified lines from (Maury et al. 2014; their Table 1) that can be assigned to NH$_2$CN. These data have a spectral resolution of 3.9 MHz (∼5.3 km s$^{-1}$).

<table>
<thead>
<tr>
<th>Rest frequency (MHz)</th>
<th>Frequency of the U-line (MHz)</th>
</tr>
</thead>
<tbody>
<tr>
<td>218461.8</td>
<td>No U-line but blending with NH$_2$CHO at 218459 MHz</td>
</tr>
<tr>
<td>219441.6</td>
<td>219441</td>
</tr>
<tr>
<td>219474.0</td>
<td>219474</td>
</tr>
<tr>
<td>219719.7</td>
<td>219719</td>
</tr>
<tr>
<td>219893.8</td>
<td>219892</td>
</tr>
<tr>
<td>220126.6</td>
<td>220126</td>
</tr>
<tr>
<td>220127.9</td>
<td>220126</td>
</tr>
</tbody>
</table>
Appendix B: Spectra of NH$_2$CN observed with ALMA at different positions towards IRAS 16293 B

Fig. B.1. Spectra of the unblended lines of NH$_2$CN detected with ALMA towards IRAS 16293 B at the full-beam offset position (left), at the half-beam offset position (middle), and at the peak continuum position (right). The best-fit model for $T_{\text{ex}} = 300$ K at the full-beam offset position is shown in red in the left panels. The identification of the other lines is indicated in blue. The dashed lines in the middle and right panels indicate the average velocity of the absorptions, 3.8 km s$^{-1}$. The dotted lines show the level 0.
Fig. B.1. continued.