Nitrogen bearing species in massive star forming regions

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Abstract. Recent observations revealed that there is a difference in the spatial distribution of both nitrogen and oxygen bearing species towards massive star forming regions. These differences can be explained under different temperature regimes in hot cores. In this study, we attempt to model the chemistry of few nitrogen species; namely, vinyl cyanide (CH_2CHCN), ethyl cyanide (CH_3CH_2CN), and formamide (NH_2CHO), using gas-grain chemical models. A special attention is given to the role and efficiency of surface chemistry as it is suggested to play one of the main key roles in manufacturing these species.

Keywords. Astrochemistry, stars: formation, stars: low-mass, ISM: abundances, ISM: molecules

1. Introduction

The interstellar medium is chemically rich and varied due to the diversity in the physical conditions of the different interstellar regions. To-date, more than 200 species with a wide range of complexity have been detected in many astrophysical regions and many of these species are now considered as characteristic of these regions (e.g. Tielens 2013 and CDMS†).

Molecules that contain more than 6 atoms are called complex or large molecules (Herbst & van Dishoeck 2009). Complex organic molecules (COMs) have been the subject of several studies while studies paid less attention to N-bearing COMs. Recent surveys of star forming regions (SFRs) showed their richness in large O- and N- bearing species (e.g. Bottinelli *et al.* 2004; Bisschop *et al.* 2007; Fontani *et al.* 2007; Suzuki *et al.* 2016, and references there in). The most recent observations by (Suzuki *et al.* 2018) towards eight massive SFRs showed that they are rich in CH_3OH, $HCOOCH_3$, CH_3OCH_3, $(CH_3)_2CO$, CH_3CHO, CH_3CH_2CN, CH_2CHCN, and NH_2CHO. The interstellar nitrogen chemistry was not the scope of many studies as the attention was paid more to oxygen- and carbon-based chemistry. For this reason and given the some recent observations of some large nitrogen species by Suzuki *et al.* (2018), we were motivated to conduct this study in order to shed light on the general trend of the chemistry of N-bearing molecules in hot cores around massive SFRs.

Gas-grain chemical models were used to understand the chemical evolution of a sample of large nitrogen-bearing molecules (e.g. CH_3CH_2CN, CH_2CHCN, and NH_2CHO) in a typical hot core. We focus on the role of grain chemistry in the formation of these species and the time evolution of their fractional abundances. Details of the chemical model and network are given in section 2 while in section 3 we discuss and present the results obtained.

† https://www.astro.uni-koeln.de/cdms/molecules

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Table 1. Initial elemental abundances and physical conditions utilized in this study.

Initial abundances[a]		Physical parameters[b]	
Helium	8.50×10^{-2}	Core density (cm^{-3})	1×10^{7}
Carbon	2.69×10^{-4}	Core temperature (K)	$150-300$
Oxygen	4.90×10^{-4}	Core radius (pc)	0.03
Nitrogen	6.76×10^{-5}	[†]Depletion	full

† The gas is considered fully depleted if more than 90% of the abundance of
its gaseous species are involved into grain surface reactions.
References: (a) Asplund *et al.* 2009, (b) Awad *et al.* 2010

2. Chemical model

The chemical evolution of the species, in question, was studied using UCL_CHEM which is a real-time-dependent gas-grain astrochemical model†. Details of the code are published elsewhere (e.g. Viti *et al.* 2004; Holdship *et al.* 2017).

Briefly, we follow the time evolution of a cold, atomic, diffuse (400 cm^{-3}) gas that undergoes a free-fall collapse, at a constant temperature of 10 K, following Rawlings *et al.* (1992). This collapsing phase (Ph-I) ends when the core reaches a final density that is often treated as a free parameter. In this study, the density is adopted to be $\sim 1 \times 10^{7}$ cm^{-3} to represent a typical hot core. During this stage, the chemistry takes place both in the gas-phase and on grain surfaces where species stick effectively to grain surfaces enabling surface chemistry to occur. By the end of the collapsing phase, the warming up phase (Ph-II; second phase of the computations) starts to mimic the heating up of the medium due to the stellar UV radiation from the new star. In this case, the core temperature gradually increases (with a specific temperature profile; see Viti *et al.* 2004; Awad *et al.* 2010 for details), causing the mantle species to evaporate and enrich the gas. The chemistry occurs both in the gas and on grains, however freeze out reactions are neglected due to the high temperature of the core ($\sim$ 150 K) during this stage.

The chemical network includes all the gas-phase reactions from UMIST ratefile 2012 (McElroy *et al.* 2013) except for NH$_2$CHO where both chemical reactions and rate coefficients (α, β, and γ) were taken from KIDA ratefile 2014 (Wakelam *et al.* 2015). The surface chemistry is based on the hydrogenation of the species including two-body reactions such as radical-radical reactions as proposed by Garrod *et al.* (2008). Thermal and non-thermal desorption mechanisms are included as outlined by (Collings *et al.* 2003b, 2004; Viti *et al.* 2004; Roberts *et al.* 2007). All desorption energies were updated following Wakelam *et al.* (2017). Table 1 lists the initial physical and chemical conditions of the reference model (RM) of this work. Panel (a) in Fig. 1 shows the fractional abundances of the three N-species as computed in the RM.

For the purpose of this study, we updated the surface chemistry network to account for the formation of large N-bearing molecules by including the following surface hydrogenation pathway from Charnley *et al.* (2004)

$$HC_3N + 2H \rightarrow CH_2CHCN + 2H \rightarrow CH_3CH_2CN \qquad (1)$$
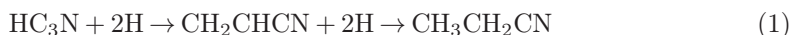
and the radical-radical reactions (2) and (3) from Garrod *et al.* (2008) and Shivani *et al.* (2014), respectively

$$NH_2 + HCO \rightarrow NH_2CHO, \text{ and} \qquad (2)$$

$$CH_2 + HCCN \rightarrow CH_2CHCN \qquad (3)$$

Reaction (3) was studied by performing quantum chemical calculations and found to be viable and efficient. The influence of including these reactions to the network was studied by running the RM without these route (Model M1); see panel (b) in Fig. 1.

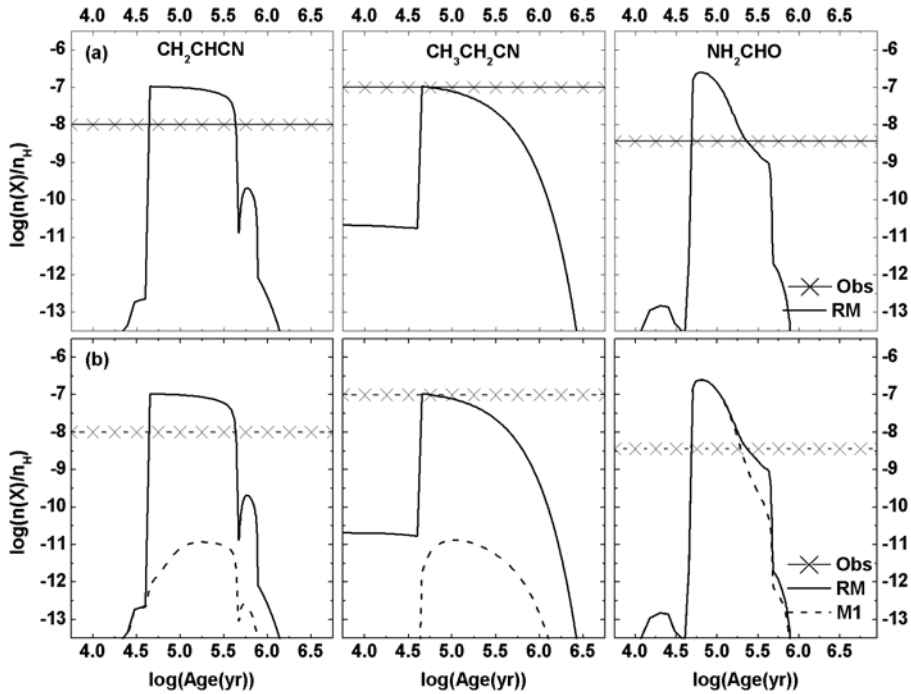† The code is available publicly online at https://uclchem.github.io/

Figure 1. The time evolution of N-bearing species in a typical 15 M⊙ hot core. The top panel, (a), shows the results of the RM while the bottom panel, (b), illustrates the role of surface chemistry by comparing the RM calculations (solid line) to those of model M1 (dashed line) where the three surface formation routes are omitted (see section 2 for details). Observations taken from Suzuki *et al.* (2018) are denoted by the straight (⨯⨯) lines, parallel to the X-axis.

3. Results and Discussion

In this section we present and discuss our preliminary results on the general trend of the chemical evolution of the selected large nitrogen species; CH_2CHCN, CH_3CH_2CN, and NH_2CHO. As shown in the top panel of Fig. 1 the RM is able to reproduce the observed amount of CH_3CH_2CN and CH_2CHCN up to a factor of ~ 7 while it is overestimating the amount of NH_2CHO by around 2 orders of magnitude. In order to understand the role of surface chemistry on the abundances of these molecules, we ran model M1 in which we removed the three routes included in the updated network of the RM. Panel (b) of Fig. 1 shows a comparison between the results of RM (solid line) and M1 (dash line). It is clear that formamide (NH_2CHO) is the least affected by the inclusion of surface formation route. The initial chemical analysis of the molecules showed that the code is probably overestimating the abundance of the parent of the species, HNCO, but further investigation is needed before concluding.

On the other hand, the abundances of CH_2CHCN and CH_3CH_2CN were highly affected by the inclusion of the related surface routes even when CH_2CHCN became over abundant. We found that the formation of CH_2CHCN via the radical-radical reaction (CH_2 + HCCN) proposed by Shivani *et al.* (2014) is very effective while the hydrogenation of HC_3N is less efficient. The enhanced abundance of this molecule is probably due to the high abundance of one of its parent molecules. Further analysis and tests are required to reach a final conclusion. We also found a correlation between the two cyanide complexes that represents a parent/daughter correlation.

4. Concluding remarks

This paper outlines the preliminary results of the modeling of the nitrogen chemistry in massive star forming regions using the gas-grain chemical models, UCL_CHEM. The results showed that both vinyl and ethyl cyanide are more affected by the inclusion of surface chemistry while formamide was not affected at all. The reason for this finding is probably that our model is over estimating the abundance of the parent molecule; NHCO.

The model was successful in reproducing the observed abundances of CH_2CHCN and CH_3CH_2CN up to a factor of 7 for the former. We found a strong correlation between the two species characterised as a parent/daughter correlation. Further analysis is required to fully understand the behaviour of the set of species selected for this study.

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