Chemical modelling of N-bearing COMs in star-forming regions

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Abstract. The study of complex organic molecules, and more specifically those of prebiotic interest, is important to understand the chemical richness of star-forming regions. The chemistry of nitrogen bearing molecules such as formamide or methyl isocyanate is poorly constrained. We study different chemical pathways to form and destroy these molecules from both the gas phase and grain surface chemistry. From comparison with observations of four different relevant astrophysical regions, we show that both the gas phase and grain surface chemistry are required to explain the observed abundances of these species.

**Keywords.** astrochemistry, molecular processes, ISM: molecules

1. Introduction

Complex organic molecules (COMs), and more specifically nitrogen-bearing COMs, are of great interest for their potential role in prebiotic chemistry (Saladino *et al.* 2012). Several COMs have been detected in comets (Crovisier *et al.* 2004, Goesmann *et al.* 2015), including species such as formamide (NH_2CHO, Biver *et al.* 2014).

Detailed modelling of the chemistry of N-bearing COMs in star-forming regions such as pre-stellar cores (L1544) and hot corinos (IRAS16293–2422) are needed to fully characterise the main formation and destruction routes of these species, establishing their expected abundances, and compare them to available observations. This study focuses on the study of 3 important N-bearing COMs: isocyanic acid (HNCO and its isomers), formamide (NH_2CHO) and methyl isocyanate (CH_3NCO).

2. Chemical modelling and results

The chemistry of N-bearing COMs in the ISM, and of its precursors, is highly uncertain under the physical conditions found in pre-stellar cores or low-mass proto-stars. We have used the gas-grain chemical code UCLCHEM (Holdship *et al.* 2017) to model the chemistry of N-bearing COMs in these regions. We have updated UCLCHEM with processes such as surface diffusion (Hasegawa *et al.* 1992), chemical reactive desorption (Minissale *et al.* 2016) and reaction-diffusion competition (Garrod & Pauly 2011; Ruaud *et al.* 2015) to study the formation of N-bearing complex organics in those regions.

The chemical network of formamide and methyl isocyanate are highly uncertain. In this study, we have included several possible chemical formation and destruction route of formamide and methyl isocyanate. To test their chemical pathways, we have confronted the result given by UCLCHEM with observations of these species in the proto-typical

415
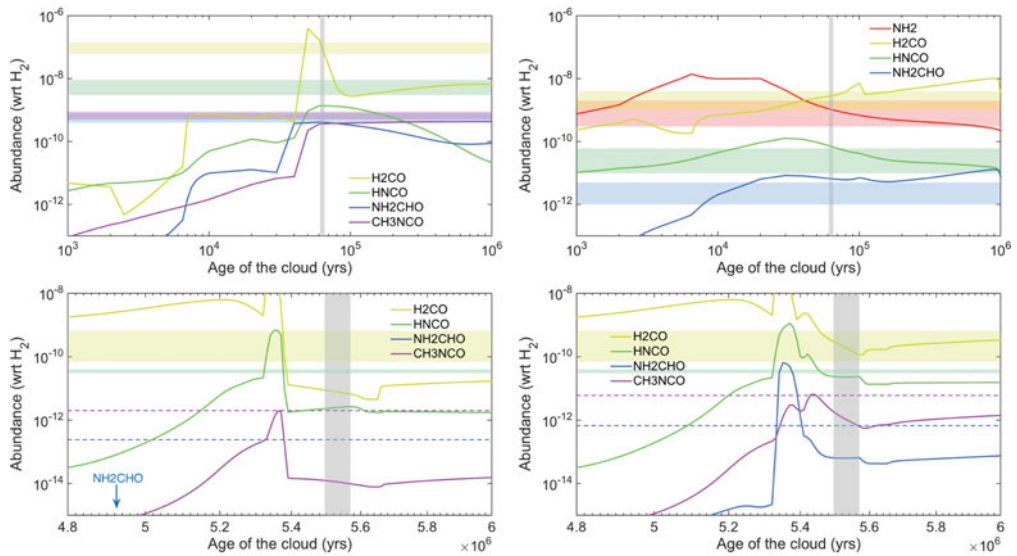
Figure 1. *Top panels:* Modelled abundances from UCLCHEM for the hot corino (left) and the cold envelope (right) of IRAS16293–2422. The grey vertical area shows the best agreement for an age of $\sim(6–7)\times10^4$ yrs. *Bottom panels:* Modelled abundances from UCLCHEM for the core centre (left) and the methanol peak (right) of L1544. The grey vertical area shows the best agreement for an age of $\sim(5.5–5.6)\times10^6$ yrs. This age corresponds to $\sim(2–3)\times10^5$ yrs after the end of the contraction. Coloured areas and dashed lines represent observations errors bars and upper limits, respectively.

low-mass proto-star IRAS16293–2422. We have modelled the hot corino ($T_{kin}=250\,K$, $n_H=5\times10^8\,cm^{-3}$) and the cold envelope ($T_{kin}=20\,K$, $n_H=2\times10^6\,cm^{-3}$) of the source using a 3-steps chemical modelling: initial diffuse cloud ($T_{kin}=10\,K$, $n_H=100\,cm^{-3}$) followed by a collapse and a warming-up phase.

We have also used recent observations toward the pre-stellar core L1544 to test the chemical network. Jiménez-Serra *et al.* (2016) reported several observational constraints for various N-bearing COMs (including NH_2CHO and CH_3NCO) in both the core centre and the *methanol peak* (Bizzocchi *et al.* 2014) of L1544. The physical conditions of these two regions are respectively: $T_{kin}=10\,K$, $n_H=5\times10^6\,cm^{-3}$ and $T_{kin}=10\,K$, $n_H=4\times10^5\,cm^{-3}$ using a 2-steps chemical modelling: initial diffuse cloud followed by a contraction phase of the core (collapse).

The results for these four regions is shown in Fig. 1. We obtain a good agreement between the observed abundances and the predicted values, for all four regions. In our network, formamide is mainly formed via gas-phase reactions at low temperature ($\sim$10-20 K) and from both grain surface and gas phase chemistry at higher temperature ($\gtrsim$50 K). Methyl isocyanate is equally formed from both the grain surface and the gas phase, even though it is destroyed efficiently on the grain surface to form N-methylformamide, as suggested by Belloche *et al.* (2017).

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