National Aeronautics and Space Administration

Modeling observations of complex organic molecules in dense photodissociation regions under various UV & X-ray field strengths

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Objectives: Our objective was to make fiduciary chemistry models and predict the observables of (Complex Organic Molecules) COMs toward molecular clouds with dense photodissociation regions (PDRs) in high-mass star-forming regions. We carried out COM simulations of molecular clouds irradiated by UV and X-rays with varying intensities. With the results of the chemistry models, we generated near- and mid-IR spectra showing spectral features of COM ices. We analyzed the chemistry models to determine major pathways to COMs, and determined which COMs could be targeted by JWST observations.

Background: Key goals of NASA missions such as JWST, SPHEREx and TESS are to find evidence of complex organic, prebiotic, and biotic molecules in the Universe. The main reservoir of complex organic molecules (COMs) is thought to be the icy mantles that are present on dust grains in the dense interstellar medium. We have generated the first set of comprehensive models to describe the chemistry of COMs in such regions, and have used the results to predict the observational spectra of COMs ices.

Approach and Results: The Meudon PDR code was used to generate the structure (density and temperature profiles) of a number of 1-D PDRs. This code is not able to model the ice composition and we pass the calculated structure to our COMs chemistry code (Nautilus, Ruaud et al. 2018) which includes chemistry from simple atomic particles to glycine formation in ice and gas under interstellar conditions. To create observables of COM ices in NIR and MIR, we used the Hyperion radiative transfer code.

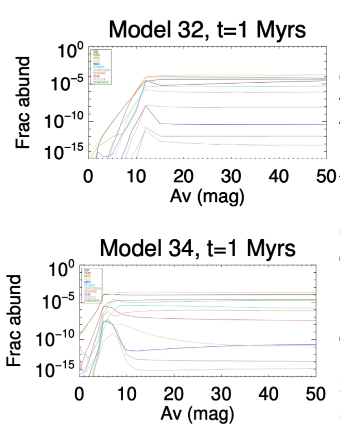
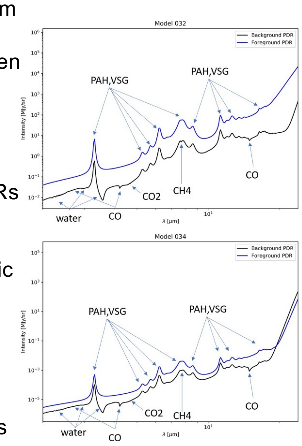


Figure 1: The ice compositions depend on the physical structure of the PDR Model 32 has an incident UV field of 100x that in Model 34. The location of the peak of COM abundances is different in the two models, and the types of molecules formed are different, with HCOOH more abundance in Model 32 and CH_3NH_2 in Model 34.

Figure 2: Spectra derived from the models in Figure 1. The black lines denote spectra when the photodissociation regions (PDRs) are on the far side of the cloud from the observer while the blue lines show spectra of the clouds with PDRs being on the near side of the observer. All of the spectra show emissions from polycyclic aromatic hydrocarbons and very small dust grains. The black lines show absorption features of various molecules against bright near- and mid-infrared background emissions from PDRs.



We find general trends in the composition of ices with both temperature and UV field.

- COMs form most abundantly in cool regions (< 20 K), with the exception of HCOOH which can form in large quantities at temperatures up to 40K.
- COMs in the ices are only present in regions where the UV has been attenuated.
- A few of the COMs have abundances that show a weak correlation with the local UV field, e.g. CH_2CHCN forms best in regions where the local UV flux is between 10^{-3} and 10^{-1} G_0. HCOOH and CH_3OH prefer a weaker local UV field of < 10^{-3} G_0.

Significance/Benefits to NASA/JPL: These results are relevant to JWST obsertions of COMs in ices and to the SPHEREx mission which will search for organics in ices across the galaxy, and to the PRIMA concept being developed at JPL.

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