

Formation of the simplest amide in molecular clouds: formamide and its derivatives in interstellar ice analogs upon VUV irradiation

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Formamide has been astronomically identified in various star-forming regions and comets, suggesting the simplest amide might have a cold origin in interstellar molecular clouds before a star formed. Solid-state studies in the laboratory have proven the possible NH_2CHO formation in interstellar ice upon (non-)energetic processing at cryogenic temperatures.^{1,2,3} However, it is under debate whether one of the proposed formation mechanisms via radical-radical recombination reactions forming interstellar large organic molecules is still valid in an abundant H_2O environment.⁴ This work, for the first time, aims at verifying the formation of NH_2CHO and its chemical derivatives in $\text{CO}:\text{NH}_3$ ice mixtures with or without H_2O triggered by the cosmic ray induced secondary vacuum UV photons (mainly H_2 emission bands at ~ 160 nm). The goal of this study is to reveal a potential chemical network involving the three abundant molecules H_2O , CO , and NH_3 in interstellar ice and underpin the formation of complex organic molecules (COMs) in H_2O -rich ice mantles.

Three selected interstellar ice analogs, including $\text{H}_2\text{O}:\text{CO}:\text{NH}_3$ (10:5:1), $\text{CO}:\text{NH}_3$ (4:1), and $\text{CO}:\text{NH}_3$ (0.6:1), were studied in an ultra-high vacuum chamber at 10 K. Fourier-transform infrared spectroscopy (FTIR) was used to monitor in situ the initial and newly formed species as a function of photon fluence. The infrared spectral identifications are complementarily secured by a temperature-programmed desorption (TPD) experiment combined with a quadrupole mass spectrometer. The experimental results show that the UV photolysis of $\text{CO}:\text{NH}_3$ ice mixture mainly leads to the NH_2CHO formation with its chemical derivatives, including isocyanic acid (HNCO) and cyanate (OCN^-). The formation kinetics suggest a strong dependency on the initial ice composition; the highest production yield of NH_2CHO is observed in the H_2O -rich ice mixture. The proposed reaction network (Fig. 1) and its astronomical relevance are further discussed.

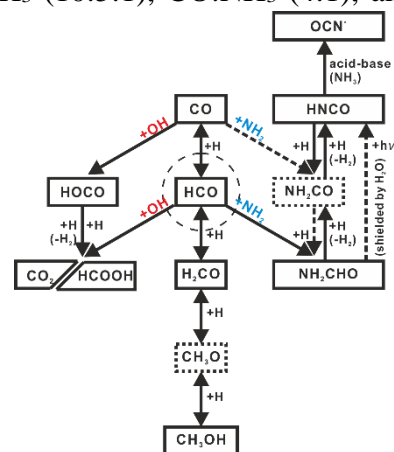


Figure 1. Proposed reaction diagram linking simple interstellar molecules at 10 K upon UV photons impact.

¹ Jones BM, Bennett CJ, Kaiser RI. Mechanical studies on the production of formamide (H_2NCHO) within interstellar ice analogs. *ApJ*. **2011**, 734(2), 78.

² Dulieu F, Nguyen T, Congiu E, et al. Efficient formation route of the prebiotic molecule formamide on interstellar dust grains. *MNRAS Letter*. **2019**, 484(1), L119.

³ Haupa KA, Tarczay G, Lee YP. Hydrogen abstraction/addition tunneling reactions elucidate the interstellar $\text{H}_2\text{NCHO}/\text{HNCO}$ ratio and H_2 formation. *J. Am. Chem. Soc.* **2019**, 141(29), 11614.

⁴ Enrique-Romero J, Rimola A, Ceccarelli C, et al. Reactivity of HCO with CH_3 and NH_2 on water ice surfaces. a comprehensive accurate quantum chemistry study. *ACS Earth and Space Chemistry*. **2019**, 3(10), 2158.