Photochemistry of Pyrimidine in Astrophysical Ices: Formation of Nucleobases and Other Prebiotic Species

Michel Nuevo[1,2,*], Scott A. Sandford[1], Christopher K. Materese[1,2], and Stefanie N. Milam[3]

[1]*NASA Ames Research Center, Moffett Field, CA 94035, USA*
[2]*SETI Institute, Mountain View, CA 94043, USA*
[3]*NASA Goddard Space Flight Center, Greenbelt, MD 20771, USA*
*e-mail: michel.nuevo-1@nasa.gov

Nucleobases are *N*-heterocycles that are the informational subunits of DNA and RNA. They are divided into two molecular groups: pyrimidine bases (uracil, cytosine, and thymine) and purine bases (adenine and guanine). Nucleobases have been detected in meteorites,[1,2] and their extraterrestrial origin confirmed by isotopic measurements.[3] Although no *N*-heterocycles have ever been observed in the ISM,[4,5] the positions of the 6.2-μm interstellar emission features suggest a population of such molecules is likely to be present.[6] However, laboratory experiments have shown that the ultraviolet (UV) irradiation of pyrimidine in ices of astrophysical relevance such as H_2O, NH_3, CH_3OH, CH_4, CO, or combinations of these at low temperature ($\leq$ 20 K) leads to the formation of several pyrimidine derivatives including the nucleobases uracil[7,8,9] and cytosine,[8] as well as precursors such as 4(3*H*)-pyrimidone and 4-aminopyrimidine.[7,8,9] Quantum calculations on the formation of 4(3*H*)-pyrimidone and uracil from the irradiation of pyrimidine in pure H_2O ices are in agreement with their experimental formation pathways.[10] In those residues, other species of prebiotic interest such as urea as well as the amino acids glycine and alanine could also be identified.[8,9] However, only very small amounts of pyrimidine derivatives containing CH_3 groups could be detected, suggesting that the addition of methyl groups to pyrimidine is not an efficient process. For this reason, the nucleobase thymine was not observed in any of the samples.[9] In this work, we study the formation of nucleobases and other photo-products of prebiotic interest from the UV irradiation of pyrimidine in ices containing H_2O, NH_3, CH_3OH, and CO, mixed in astrophysical proportions.

References

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