High−Energy Chemistry of Formamide: A Simpler Way for Nucleobase Formation

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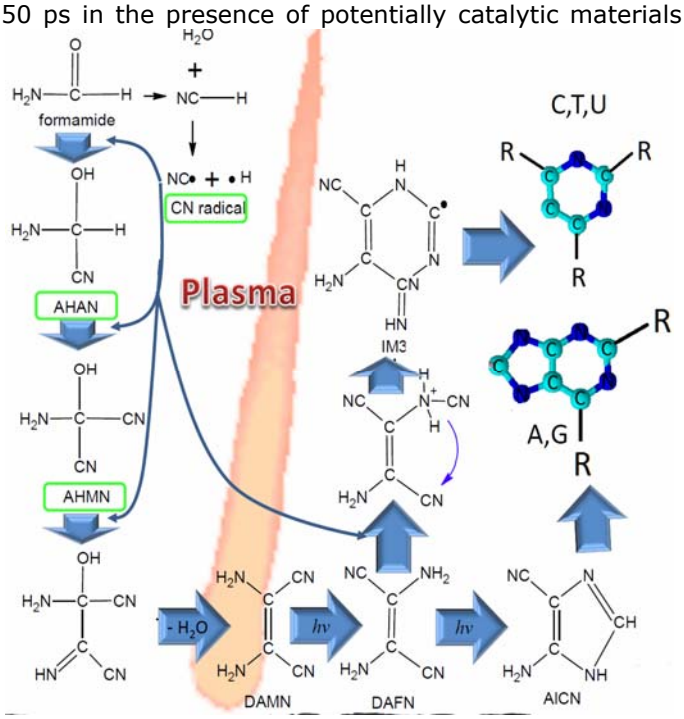
Formamide is common specie in the interstellar medium and can generate the ·CN radical and the CO molecule as the result of a high−energy event [1]. The ·CN radical and the CO molecule possess an abundance of rotational, vibrational and electronic states. Therefore, these two molecules are able to uniquely control the energy flow in a multistep reaction and exhibit a high reactivity towards nearly any type of molecule. The formation of nucleobases from formamide during a high−energy−density event, for example, the impact of an extraterrestrial body into the planetary atmosphere, was studied by irradiation of formamide ice and liquid samples with a high−power laser producing 150 J pulses with a duration of 350 ps in the presence of potentially catalytic materials (i.e., meteoritic material, clay, and titanium dioxide). Absorption FT−IR spectroscopy, time−resolved FT−IR emission spectroscopy of the glow discharge and GC−MS were used to study the dissociation of formamide into the simple molecular fragments HCN, H2O, HNCO, H_2, CO, and NH_3 and the unstable species HNC, ·CN, and ·NH, as well as the subsequent recombination reactions leading to the formation of nucleobases. Based on the experimental data, a kinetic and thermodynamic model was developed for the molecular dynamics of formamide dissociation. The possible reaction routes leading from the dissociation products to the nucleobases are discussed with respect to the available literature. In addition, using theoretical calculations, we propose a simple and original common reaction pathway for the formation of both pyrimidine and purine nucleobases involving ·CN radical chemistry (see Figure).



[1] M. Ferus, S. Civiš, A. Mládek, J. Šponer, L. Juha, and J.Šponer, *J. Am. Chem. Soc.*, 2012, 134 (51), pp 20788–20796

Acknowledgment: this work was funded by the Grant Agency of the Czech Republic (grant No. P208/10/2302).