HCN adsorption and reactivity on cosmic silicates

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Hydrogen cyanide (HCN) has been receiving an increasing attention as a possible precursor of life since when J. Orò synthesized adenine from a solution of HCN and ammonia. [1] Since HCN molecules are widespread in the interstellar medium and the products of their polymerization (including purines) have been detected on meteoritic fragments, [2] the scientific community is now investigating the possible pathways for the oligomerization of HCN in cosmic environments to form molecules of prebiotic interest. In this sense, the gas phase oligomerization of HCN is hindered by high energetic barriers which cannot be overcome at the conditions of a molecular cloud. [3] In the condensed phase, instead, more promising results were obtained, thanks to a more feasible acid-base chemistry. [4]

For these reasons, the surfaces of cosmic silicates in interstellar and interplanetary dust grains, cometary nuclei, asteroids and planetary systems, may play a fundamental role in this type of chemistry. Moreover, it has been recently demonstrated that the surfaces of silicates, among the primary components of dust grains cores, are able to catalyze the oligomerization of HCN to adenine. [5]

In this work, we studied by mean of atomistic simulations the adsorption and the reactivity of HCN molecules on different model surfaces of the crystalline pure Mg-silicate (forsterite). We computed the structures and relative adsorption energies of 16 adsorption complexes, together with the energetic barriers for 5 cases of dimerization of two adsorbed molecules to form the dimer iminoacetonitrile ($H_2C_2N_2$). We observed that, thanks to the acid-base properties of its surfaces, [6] forsterite is able to efficiently deprotonate HCN molecules, hence triggering the polymerization process, and to stabilize the transition states of iminoacetonitrile formation. Most cases show favorable energetic barriers and, according to a kinetic analysis, the reaction is likely to take place at the conditions proper of proto-planetary disks and planetesimals formation, while it results to be hindered in molecular clouds.

References

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