Combined experimental and theoretical investigation of reactions involving atomic/diatomic radicals and leading to N-containing organic molecules in extra-terrestrial environments

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Life is based on organic molecules containing a bunch of elements other than carbon and hydrogen, among which the most relevant ones are nitrogen and oxygen. More specifically, nitrogen is present in most amino acids and in the nucleobases, which can certainly be described as the main molecular bricks of life as we know it. For this reason, the presence of N-containing organic molecules of some complexity in extra-terrestrial environments arouses the interest of the scientific community. The characterization of their abundance and distribution in star-forming regions or in the bodies of the Solar System (comets, asteroids, moons, and planets) as well as of their formation mechanisms can help in understanding the origin of life on Earth or in addressing the possibility that other planets or moons harbour life.

In our laboratory, we have undertaken a systematic investigation of bimolecular reactions involving nitrogen atoms or cyano radicals and organic compounds. In particular, we have investigated 1) the reactions of cyano radicals with cyanoacetylene and cyanoethylene, two abundant nitriles that have been observed in star forming regions, comets and the atmosphere of Titan (the massive moon of Saturn) and 2) the reactions of the first electronically excited state of atomic nitrogen (the metastable ^{2}D state) with aliphatic hydrocarbons (methylacetylene and allene), nitriles (cyanoacetylene and cyanoethylene), and aromatic compounds (benzene, pyridine and toluene). We have employed the crossed molecular beam technique with mass spectrometric detection to derive the reaction mechanisms and product branching ratios. All the experiments have been complemented by dedicated electronic structure calculations of the underlying potential energy surface and RRKM estimates of the product branching ratios.

In most cases, the main reaction products are molecules or radicals containing one or more N-atoms with a significant prebiotic potential. Implications for the chemistry of the atmosphere of Titan, cometary comae as well as interstellar objects will be noted.

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