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The chemistry of prebiotic N-containing compounds in the atmosphere of Titan and primitive Earth beyond a holistic approach

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How did life emerge from inanimate matter? The processes that led from complex organic molecules to the first self-replicating systems are no longer at play and we cannot easily reconstruct them because we do not have a geological record of the period when the transition from simple molecules to the very first forms of "life" have occurred. The presence of stable hydrosphere is considered as the first milestone in the timeline of the abiotic origin of life theory, with the second milestone being the massive accumulation of organic compounds necessary for the transition from organic chemistry to the biochemistry of life. But how Earth became so rich in complex organic molecules – up to the point that life spontaneously evolved from them - is still a matter of debate. At that stage, the abundance of liquid water, indeed, represents an obstacle for organic synthesis. Two theories have been suggested to solve this paradox, which are usually referred to as *endogenous synthesis* and *exogenous synthesis* scenarios [1]. But in both cases, prebiotic molecules (that is, molecules which are simple to be formed in abiotic processes but contain the functional groups typical of biological molecules or have the capability to easily evolve into them) are formed in gaseous media. Indeed, gas-phase prebiotic molecules have been observed in the upper atmosphere of Titan, the massive moon of Saturn, as well as in the interstellar clouds and cometary comae.

The comprehension of the chemical processes that lead from simple atomic/diatomic species to prebiotic complex chemicals is an important part of the study on the origin of life. The study of these preliminary steps might seem relatively simple compared to the characterization of the other unknown phenomena that have led to the first living organisms. Nevertheless, the formation mechanisms of many of the prebiotic molecules that we observe nowadays in proto-stellar clouds or comets/meteorites or planetary atmospheres are far from being understood, while a comprehension of those processes can certainly help to set the stage for the emergence of life to occur.

For this reason, in our laboratory we have started a systematic investigation of gas-phase reactions leading to simple prebiotic molecules within the Italian National Project of Astrobiology—Life in Space—Origin, Presence, Persistence of Life in Space, from Molecules to Extremophiles [2].

In particular, by combining an experimental and theoretical approach, we have investigated a series of bimolecular reactions under single collision conditions. The aim is to provide detailed information on the elementary reactions which are employed in photochemical models of planetary atmosphere and cometary comae [3]. In particular, we have investigated several reactive systems leading to the formation of nitriles (such as dicyanoacetylene) and imines (such as ethanimine), as well as reactive radicals that can further react in subsequent reactions. We have also investigated reactions involving nitrogen atoms and aromatic compounds (benzene, pyridine, toluene) to address the role of these compounds in the growth of N-containing aromatic compounds, a proxy of DNA and RNA bases. In this contribution, the main results concerning the reactions involving atomic nitrogen, N, or cyano radicals, CN, and cyanoacetylene, acrylonitrile, benzene, toluene and pyridine will be illustrated and the implications for prebiotic chemistry noted.

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[3] N. Balucani. Physics of Life Reviews 2020, 34–35, 136. DOI: 10.1016/j.plrev.2019.03.0061571-0645