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Cyanoacetylene gas-phase chemistry of relevance in interstellar objects, comets and other bodies of the Solar System: a combined experimental and theoretical investigation

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Cyanopolyynes are a family of carbon-chain molecules that have been detected in numerous objects of the interstellar medium (ISM), such as hot cores, star forming regions and cold clouds [1–4]. The simplest cyanopolyyne, HC_3N, has been among the first organic molecules to be observed in the ISM [5] and up to date also HC_5N, HC_7N, HC_9N and $HC_{11}N$ have been detected [6, 7]. HC_3N and HC5N are also abundant in solar-type protostars (see for instance a recent work on IRAS 16293-2422 by Jaber Al-Edhari et al. [8]). Remarkably, HC_3N has also been detected in comet C/1995 O1 (Hale-Bopp) and, together with other organic molecules, could be a part of the legacy of interstellar organic chemistry to the newly formed solar systems [9,10].

Cyanoacetylene has been suggested as an important brick in chain elongation processes, via its reaction with the C_2H radical producing HC_5N. Its reaction with the CN radical, instead, results in a chain termination reaction with the formation of dicyanoacetylene, NC-CC-CN (C_4N_2). Dicyanoacetylene and higher dicyanopolyynes have not been observed in the ISM so far because they lack a permanent electric dipole moment and cannot be detected through their rotational spectrum. However, it has been suggested that they are abundant in interstellar and circumstellar clouds [11] and account for a significant fraction of the total carbon budget. The reaction between CN radical and cyanoacetylene is also believed to be the main source of C_4N_2, an observed species in the upper atmosphere of Titan, the massive moon of Saturn [12].

To characterize the chemistry of cyanoacetylene in various extraterrestrial environments, in our laboratory, we have undertaken a systematic investigation of the reactions involving cyanoacetylene and atomic or diatomic radicals which are relatively abundant in space. The investigated reactions include CN + HC_3N, O+HC_3N and N+HC_3N. We have used a sophisticated experimental technique to investigate these reactive systems under single collision conditions in order to be able to establish the nature of the primary products and their branching ratio without ambiguity (for some details see [13]). In addition, we have performed dedicated electronic structure and kinetic calculations to derive the relevant parameters to be included in astrochemical models. Implications for the chemistry of interstellar objects as well as the chemistry of cometary comae and the upper atmosphere of Titan will be noted.

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