SPECTROSCOPIC PROBING OF LOW-TEMPERATURE ION-MOLECULE REACTIONS

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Polycyclic aromatic hydrocarbons (PAHs) are abundant in many regions of the Universe, representing a major reservoir for cosmic carbon. However, their formation pathways in cold regions of space, such as dense molecular clouds and Titan's atmosphere, remain elusive despite the recent advances in the detection of aromatic molecules there[a]. Astronomical observations show that astrochemical models significantly underestimate the abundance of these aromatic molecules, indicating that efficient formation pathways, such as ion-molecule reactions involving aromatic ions and hydrocarbon neutrals, are likely missing in the existing models.
In our work, we use a cryogenic 22-pole ion trap apparatus[b] to study ion-molecule reactions at low temperature, and to structurally identify ionic reactants, reaction intermediates and products in-situ employing infrared-predissociation (IRPD) and infrared multiple-photon dissociation (IRMPD) spectroscopy using the infrared free-electron lasers at the FELIX Laboratory. We reveal efficient low-temperature formation pathways towards PAHs and related species via exothermic ion-molecule reactions. The experimental approach combines kinetic and spectroscopic studies, and unambiguously identifies key reaction intermediates, and, in the case of the reaction of pyridine$^+$ with acetylene, the final nitrogen-containing PAH product ion quinolizinium$^+$.[c] These studies not only reveal competing formation pathways relevant in cold astronomical environments, but also deliver a variety of information to verify in-silico potential energy surfaces, astronomical models, and to guide infrared observations.

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[a] B.A. McGuire et al., Science 359, 202 (2018); B.A. McGuire et al., Science 371, 1265 (2021); J. Cernicharo et al., A&A 649, L15 (2021)

[b] P. Jusko, S. Brünken, O. Asvany, S. Thorwirth, A. Stoffels, L. van der Meer, G. Berden, B. Redlich, J. Oomens, and S. Schlemmer, Faraday Discuss. 217, 172 (2019)

[c] D.B. Rap, J.G.M. Schrauwen, A.N. Marimthu, B. Redlich, and S. Brünken, Nat. Astron. 6, 1059 (2022)