Highly Reactive Molecular Ions in Laboratory and Space

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The number of discovered interstellar molecules and molecular ions grows exponentially due to new observation devices, especially space telescopes. Most of the interstellar species were detected in interstellar molecular clouds (IMCs) and give insights into the constitution of interstellar matter and its transformation to molecules.

Low temperatures in the region of 10 - 20 K and a high dilution of the species (comparable to ultra high vacuum) are the defining features of IMCs which enable very reactive molecules to survive long enough to be detected by spectroscopic methods. Consequently, a zoo of reactive molecules and molecular ions exists in the IMCs. Investigations on such species are challenging with respect to low temperature methods.

Our current research is focused on protonated small molecules. In some cases such molecular ions can be isolated or even prepared at low temperatures. We present our studies on protonated molecules like hydrogen cyanide (HCNH⁺), cyanogen (NCCNH⁺) and cyanoacetylene (HCCCNH⁺) which have been previously observed in IMCs.¹² Vibrational spectroscopic data and experimentally determined structures are discussed together with quantum chemically calculated values.

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² Haiges, R.; Baxter, A. F.; Goetz, N. R.; Axhausen, J. A.; Soltner, T.; Kornath, A. J.; Christe, K. O., Protonation of nitriles: isolation and characterization of alkyl- and arylnitrilium ions. Dalton Trans. **2016**, *45*, 8494-8499.