

Exploring the Ion Chemistry of Small Polycyclic Aromatic Hydrocarbons with Coincidence Spectroscopy

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Polycyclic aromatic hydrocarbon (PAH) molecules have been postulated to be key species in astrochemistry. This proposal has motivated numerous laboratory studies to advance our understanding of the formation and evolution of these species in space and their impact on the physics and chemistry of interstellar and circumstellar environments. In particular, PAHs absorb UV photons from stars, which can lead to their photoionization and dissociation and therefore limit their survival in astrophysical environments. Molecular H₂ is the most prolific molecular species found in the interstellar medium (ISM). Whereas it has been long recognized that H₂ is formed on dust grains, investigation of the involved mechanisms is still a very active subject of research. One popular theory is that polycyclic aromatic hydrocarbons (PAH) may play a role in the formation of H₂ by acting as catalysts. Atomic hydrogen would adsorb onto the surface of the molecules, thus hydrogenating the PAHs, prior to the desorption of H₂. This reaction channel demonstrates the importance of investigating the energetics of not only PAHs but modified PAHs as well, such as hydrogenated species.

In this presentation, we have explored the photoionization and subsequent unimolecular dissociation of small PAH molecules ranging from naphthalene, anthracene and pyrene as well as two dihydrogenated species 1,2-dihydronaphthalene and 9,10-dihydrophenanthrene using the imaging photoelectron photoion coincidence apparatus at the Swiss Light Source. RRKM modeling of the competitive dissociation pathways provides reliable reactions energetics and entropies that agree with reactions mechanisms derived from calculations and tandem mass spectrometry.

Not only does the derived data from the above experiments allow speculation on the stability and chemical role of PAHs in the interstellar environment, they have also been used as standard systems to probe the reliability of modeling the dissociation of these systems by collision-induced dissociation mass spectrometry. A brief summary of these results will also be presented in this presentation.

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