Elucidating Fragmentation Pathways of Polycyclic Aromatic Hydrocarbons Using Covariance Analysis and the PImMS Camera

Polycyclic aromatic hydrocarbons (PAHs) are prominent organic molecules in the interstellar medium, accounting for 15% of the total carbon in the galaxy [1]. Experiments performed at the FLASH laser facility at DESY Hamburg replicated the naturally occurring high energy radiation incident on PAHs, leading to ionisation, dehydrogenation, fragmentation and isomerisation, with target molecules of pyrene, phenanthrene and fluorene.

The Pixel Imaging Mass Spectrometry (PImMS) camera was used to record the ion trajectories resulting from fragmentation of the charged PAH parent species [2]. Recoil frame covariance analysis is a relatively new technique that has been applied to other systems to track the dynamic changes in molecular vibrations and dissociations, and isolate different molecular isomers [3-5]. Applying covariance analysis to the PAH ion data has yielded direct evidence for multiple fragmentation pathways from the doubly-charge parent consistent with an initial fission into two monocations, followed by multiple neutral C2Hx losses.