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Ultrafast ionization and fragmentation dynamics of polycyclic aromatic hydrocarbons by XUV radiation

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Synopsis In the interstellar medium polycyclic aromatic hydrocarbon molecules (PAH) are exposed to strong ionizing radiation leading to complex organic photochemistry. We investigated these ultrafast fragmentation reactions after ionization of the PAHs phenanthrene, fluorene and pyrene at a wavelength of 30.3 nm using pump probe spectroscopy at a free electron laser. We observe double ionization and afterwards hydrogen abstraction and acetylene loss with characteristic time scales for the reaction processes below one hundred femtoseconds.

The interstellar medium (ISM) shows a surprisingly complex radiation driven organic chemistry. One important molecular species in the ISM are polycyclic aromatic hydrocarbons (PAHs). PAHs are very abundant in the galaxy with estimations from the characteristic IR emission bands showing up to 20% of carbon in the Milky Way exists in this form [1]. The harsh conditions in the ISM due to ionizing radiation cause complex fragmentation and isomerization reactions to take place in PAHs [2]. To explore these reaction processes on femtosecond timescales we performed pump probe experiments using the CAMP endstation [3] at the FLASH free electron laser facility. In our study, three PAHs fluorene, phenanthrene and pyrene were ionized by XUV radiation at 30.3 nm wavelength and the reaction dynamics was probed using laser pulses at 800 nm. Complex fragmentation patterns are observed for all three PAHs: multiple hydrogen and/or acetylene abstraction. Several fragmentation channels could be resolved by covariance mapping and characteristic timescales for the femtosecond decay process after ionization were retrieved.

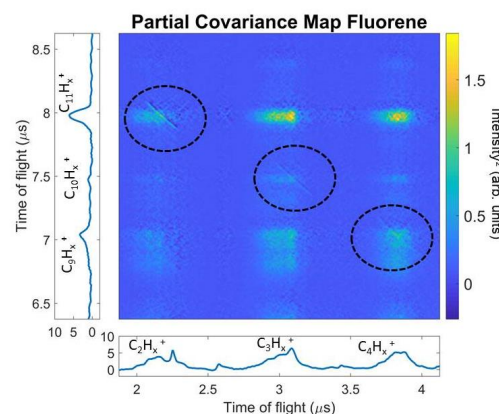


Figure 1. Partial covariance map of fluorene showing the two body fragmentation channels into C_xH_y and $C_{13-x}H_{10-y}$.

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