VUV photodissociation of cationic alkylated PAHs and water-PAH complexes and formation of pentagonal carbon rings

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Studying the interaction of polycyclic aromatic hydrocarbon (PAH) molecules with VUV photons is necessary to better understand the evolution of the physical and chemical conditions in photodissociation regions (PDRs) associated with star forming regions. This interaction induces the well-known aromatic infrared band emission [1] but also leads to chemical evolution of the irradiated PAH population [2]. To approach the physical conditions which are found in PDRs, we used two setups to produce different cationic derivatives of PAHs in the gas phase and irradiate them with VUV photons.

Firstly, we studied the photoprocessing of alkylated PAHs with 10.5 eV photons, using the cryogenic ion trap PIRENEA [3] which produces a cold (≤ 30 K) and collisionless environment ($\leq 10^{-11}$ mbar). We show that these species have a higher fragmentation rate and a higher carbon to hydrogen loss compared to bare PAHs, in agreement with previous studies [4]. In addition, we suggest that the VUV photodissociation leads to the formation of species containing peripheral pentagonal cycles which are as stable as the bare PAH cations upon 10.5 eV irradiation [5].

Secondly, we studied the VUV photofragmentation of water-PAH complexes upon tunable VUV irradiation, relevant for PDRs, on the DESIRS beamline at SOLEIL. Previous studies have revealed a pathway leading to the incorporation of oxygen into PAHs via the formation quinones for example [6,7]. We studied $[(PAH-H)(H_2O)]^+$ and $[PAH(H_2O)]^+$ species which both led to similar main photoproduct families, involving the loss of CO+nH, O+nH and nH neutral fragments. We show the evolution of the branching ratio between these channels over the whole 4.5 eV to 13.6 eV range. In addition, we reveal that photoexcitation around the strong $\pi \to \pi^*$ transitions may induce the formation of pentagonal carbon rings such as suggested in the case of alkylated PAHs.

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