

Fragmentation dynamics of excited ionized polycyclic aromatic hydrocarbons

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Polycyclic aromatic hydrocarbons (PAHs) present an important interest in the fields of astrophysics and astrochemistry [1,2] since they are considered as a significant component of interstellar dust and gas. They are indeed responsible for the emission features detected in interstellar IR spectra of many galactic and extragalactic sources [2,3]. In the interstellar medium, PAH molecules are exposed to a variety of ionizing processes due to the presence of keV ions in solar and stellar winds. Therefore it is interesting to study the interaction of PAHs with low-energy ions [4-7]. Their fragmentation patterns provide information on their relative stability, which depends on the energy and charge transferred during the collision. Furthermore, previous works [8] showed that interstellar observations do not only come from single PAHs molecules, but also from photo dissociations of larger grains, which strongly evidences the existence of PAHs clusters [9]. The interaction of multiply charged ions with clusters of PAHs has been recently reported [7]. It was shown that these clusters have much higher tendencies to undergo fragmentation than other weakly bound clusters.

In this communication we present theoretical results obtained using the density functional theory. In particular we have studied the structure and stability of neutral and positively charged coronene (C₂₄H₁₂) as a prototype of PAH. We have first computed vertical and adiabatic ionization potentials with charges up to 6, which have been experimentally observed [6]. Dissociation energies for different channels involving hydrogen loss have been also computed: H, H⁺, H₂ and H₂⁺ loss channels have been considered. Finally, we have explored the potential energy surface of these fragmentation channels. We have analyzed the competition between direct H₂ fragmentation and sequential loss of two atomic hydrogen atoms and also between the loss of charged vs neutral hydrogen.

We present also in this communication our results concerning the fragmentation dynamics of singly charged clusters of pyrene. By means of molecular dynamics simulations at different levels of theory (DFT-TB, ADMP, CPMD and BOMD) we evaluate the stability of these clusters as a function of the internal excitation energy. We also compute the energy and charge redistribution inside the clusters and how the internal degrees of freedom may storage an excess of excitation energy.

References:

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