Search for neutral and multiply charged coronene in the interstellar medium: a theoretical study

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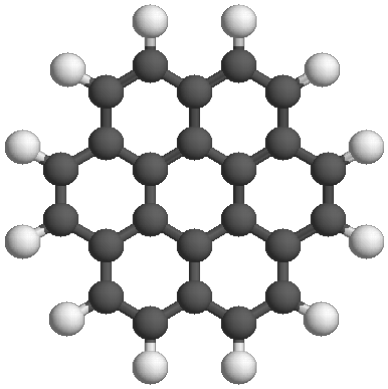
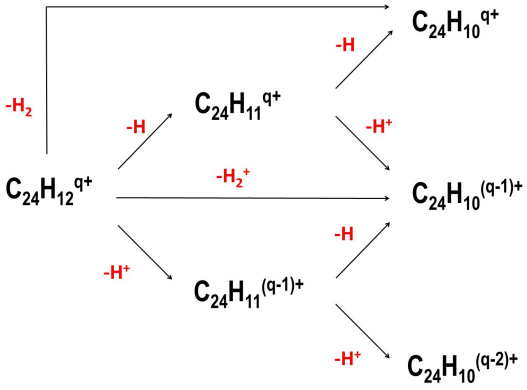
It is now widely accepted that polycyclic aromatic hydrocarbons (PAHs), both neutral and ions are present in many galactic and extragalactic environments [1, 2, 3, 4]. In particular, they have been suggested as the best candidates for the carriers of strong infrared emission (also known as "undefined infra-red bands" (UIR)) observed in many regions of the interstellar medium (ISM) [5, 6, 7]. From the flux of the UIR bands, it has been possible to estimate that interstellar PAHs are (one of) the most abundant molecules in the space, contributing up to the 20% of the cosmic carbon [8]. However, because of their environment, these molecules are exposed to continuous radiation and are subject to fragmentation as described by Leger and coworkers [9]. Several studies in the laboratory have been devoted to address this topic. Recent experiments based on the collision of PAHs with KeV ions (He^{2+},O^{3+} and Xe^{20+}) have shown that the most predominant fragmentation channels in general correspond to the loss of H, H_2 and acetylene molecule C_2H_2.[10, 11] The competion between the H and H_2 channels is of particolar interest since several authors have evidenced that PAHs can play an important role in the formation of H_2 in photodissociation regions of the ISM [12, 13].

In this seminar, I will present recent theoretical results based on density functional theory calculations. In particular we have studied the structure and stability of neutral and positively charged coronene $C_{24}H_{12}$ as an archetypal of PAHs. We have first computed vertical and adiabatic ionization potentials with charge up to 9. Dissociation energies for different channels involving hydrogen loss (H, H^+, H_2 and $H_2{}^+$) have been also computed. Finally, we have explored the potential energy surface of these fragmentation channels. We have analysed the competition between direct H_2 fragmentation and sequential loss of two atomic hydrogens and also between the loss of charged vs neutral hydrogen (see figure below).





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