# Modeling electron and energy transfer processes in collisions between ions and Polycyclic Aromatic Hydrocarbon molecules

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Polycyclic Aromatic Hydrocarbons (PAHs) are believed to be an important component of the interstellar medium (ISM) [1]. Until now, the heating of PAHs in such environments has been assumed to be predominantly due to UV-absorption, where they subsequently cool down by IR-emission or statistical fragmentation through H-loss or $C_2H_2$-loss processes. However, collisions between keV ions and PAHs have gained recent interest [2, 3, 4, 5], as they may for instance be important in the processing of PAHs in shocks driven by supernova explosions. In this work we have used two models which describe interactions where the PAHs may be ionized and moderately heated in distant collisions or strongly heated in penetrating ion collisions, respectively.

In the first model an over-the-barrier approach was used to describe distant electron transfer collisions [6]. In order to take the orientation dependent polarization effects into account, the PAHs were modeled as infinitely thin and perfectly circular conducting disks. We calculate the absolute charge exchange cross-sections for a selection of planar almost circular PAHs (pyrene $C_{14}H_{10}$, coronene $C_{24}H_{12}$ and circumcoronene $C_{54}H_{18}$). The relative ionization cross-sections obtained from the model were found to compare favorably with the corresponding experimental results.

In the second model, we use well-known expressions for nuclear [7] and electronic stopping [2] processes to describe penetrating collisions. Here, we incorporate the actual molecular structures obtained from Density Functional Theory calculations. We have calculated the stopping energies as a function of PAH size and centre-of-mass energy, and for different collision partners. The model results suggest that non-statistical fragmentation processes, i.e. single atom knock-outs due to nuclear stopping processes, may be important for astrophysically relevant collision systems (He+PAH collisions at 100 eV centre-of-mass energies). This is consistent with recent experimental results from Stockholm University. Such collisions may thus induce highly reactive species with unsaturated carbon atoms, which is not possible in statistical processes following, for example UV-absorption. These types of collisions may therefore be an important initial step in molecular growth processes, as have been recently demonstrated in collisions between alpha particles and clusters of fullerenes carried out at the ARIBE facility in Caen, France.

References:
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