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Ionization and fragmentation of cold clusters of PAH molecules: collisions with keV ions

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Synopsis We report on collisions between atomic ions and pure, loosely bound, clusters of Polycyclic Aromatic Hydrocarbon (PAH) molecules. We find that charge and excitation energy is distributed on the cluster constituents before break-up which mostly leads to emissions of intact, excited, singly charged monomers. Surprisingly, collisions with highly charged ions lead to hotter monomers than collisions with ions in low charge states. Small PAH clusters fragment promptly when singly ionized while clusters of more than 13 or 5 molecules may remain intact for anthracene or coronene clusters, respectively.

We present results on collisions between atomic ions (keV energies and low and high charge states) and pure, internally cold, clusters of the Polycyclic Aromatic Hydrocarbon (PAH) molecules anthracene C\textsubscript{14}H\textsubscript{10} [1], pyrene C\textsubscript{16}H\textsubscript{10}, fluoranthen C\textsubscript{16}H\textsubscript{10}, triphenylene C\textsubscript{18}H\textsubscript{12}, and coronene C\textsubscript{24}H\textsubscript{12}. These clusters are loosely bound and as the binding energy is roughly 0.1 eV per carbon atom ring, the binding energy for e.g. the anthracene dimer is about 0.3 eV (anthracene has three hexagonal rings). For all clusters we find that charge and excitation energy, which initially are induced locally in the clusters close to the ion trajectories, is distributed on the individual PAH molecules before the clusters break apart and that the most probable fragment then always is a singly charged, initially intact, PAH monomer. Anthracene clusters containing up to about 13 molecules are found to fragment promptly even when only singly ionized by He\textsuperscript{+} or Xe\textsuperscript{20+} ions while larger such clusters may remain intact on microsecond timescales. Clusters of larger PAH molecules (coronene C\textsubscript{24}H\textsubscript{12} c.f. Fig. 1) may be singly ionized without fragmentation in collisions with He\textsuperscript{2+} already when they contain six molecules as we measure kinetic energies of the corresponding cluster ions to be very low (≤ 1 meV). For anthracene clusters, we surprisingly find that collisions with highly charged ions lead to emission of much hotter singly charged anthracene monomers than collisions with ions in low charge states. Highly charged ions are known to remove electrons from targets at much larger distances than ions in lower charge states and would thus be expected to give less heating. However, as charge is distributed before fragmenta-

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\textbf{Figure 1.} Mass-to-charge spectra of coronene clusters, \{C\textsubscript{24}H\textsubscript{12}\}_k, in collision with He\textsuperscript{2+}. Labels denote the size of the measured cluster. The insets are zoom-ins of the j/q region from 4-25, where j is the cluster size after the reaction.

References

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