Knockout driven reactions in porphyrin molecules and butadiene clusters

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Recent studies on collisions between energetic ions/atoms and PAHs, fullerenes or their clusters have demonstrated the importance of prompt atom knockout in Rutherford-like scattering for molecular processing [1]. Such processes may lead to molecular growth, due to the formation of highly reactive fragments that very efficiently form new covalent bonds with surrounding molecules [1]. This type of energetic processing can be of importance for, e.g., the origin and evolution of complex molecules in space [2].

Here we present the modeling of keV-ion impact on butadiene clusters [3] and of collisions between tetraphenyl-porphyrin (TPP) ions and Ne or He atoms at 50-80 eV center-of-mass collision energies [4]. We have performed classical Molecular Dynamics simulations to model entire collision sequences, i.e. the initial knockout event and the subsequent fragmentation or molecular growth processes inside molecular clusters. Figure 1 shows a comparison between experimental and simulated mass spectra for collisions with butadiene clusters. The spectra clearly suggest the presence of molecular growth within the clusters and that this is driven by prompt carbon knockouts. We are currently investigating possible secondary fragmentation pathways, specific to collisions with atoms or ions, by means of density functional theory based methods.

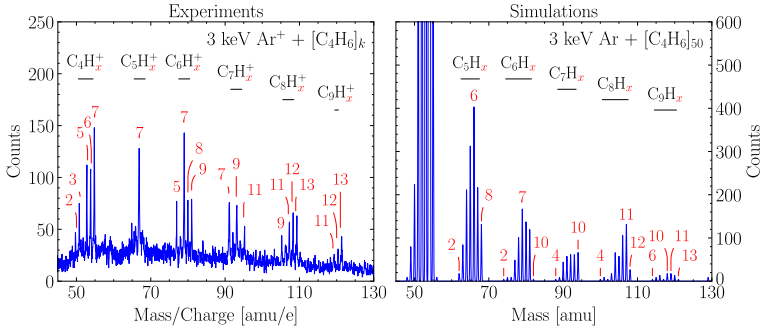

Fig.1 Experimental (left) and simulated (right) mass spectra for collision of C_4H_6 cluster with Ar^+.

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