

ULTRAFast DYNAMICS OF IONIZED MOLECULES AND MOLECULAR CLUSTERS IN THE GAS PHASE

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Abstract. Molecules and molecular clusters exposed to ionizing radiation can undergo numerous complex processes, leading to changes in their molecular and electronic structure. In the last years, we have studied the fragmentation dynamics of amino-acids and amino-acids derivatives induced by collisions with highly-charged ions, as well as the time-resolved photo-induced fragmentation dynamics of hydrocarbon derivatives. When these molecules are ionized and excited, they follow the so-called Coulomb explosion, where the charge splits in different fragments that repel each other after cleavage of bonds in the molecular backbone. However, other non-expected processes appear in competition, such as hydrogen migration [1,2], intramolecular charge transfer [3], isomerization [4], methyl roaming [5], etc. They occur in the cation and dication molecules, and take place within a few tens of femtoseconds to picoseconds. We have also determined the distribution of the energy deposited in the ionized molecule as a result of a collision with a highly-charged ion [6,7], which is the responsible for triggering the atomic reorganization. In the case of molecular clusters, in addition to the Coulomb explosion, ionizing radiation also induces intracluster reactions, producing molecular growth and leading to new ionized stable structures. In this context, we have shown the formation of peptide bonds in clusters of amino acids induced by collisions with alpha particles [8] and intermolecular reactivity in clusters of CO₂ [9] and in mixed clusters of NH₃ and H₂O [10] induced with soft X-ray radiation. A complete picture of the mechanisms underlying the dynamics was obtained using both experimental and theoretical state-of-the-art techniques. In this communication, comparison of the different processes, induced in the ionizing radiation and observed in the above-mentioned systems, will be presented and discussed. I will detail the joint theoretical and experimental strategy implemented in the last decade, which has allowed us to understand fundamental chemical processes of ionized molecules and clusters in the gas phase.

References

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