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Unusual hydrogen and hydroxyl migration in the fragmentation of excited doubly-positively-charged amino acids in the gas phase

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Synopsis We present a combined experimental and theoretical study of the fragmentation of doubly-positively-charged amino acids in the gas phase. The combination of *ab initio* molecular dynamics simulations with ion-molecule collisions followed by multiple-coincidence mass spectrometric techniques, allows us to obtain a complete picture of the fragmentation dynamics. In addition to the expected Coulomb explosion, we have found evidence of hydrogen and hydroxyl-group migration processes, which leads to unusual fragmentation products.

Hadron therapy is radiation therapy using strongly interacting particles [1]. A better depth dose profile of the energetic ion beam (Bragg peak) has proven its superiority over gamma radiation for killing cancer cells selectively [2]. With the advent of these ion-beam cancer treatments [3,4], the interaction of biomolecules with ionising particles (X- rays, electrons, ions) in the gas phase has become a fundamental technique to investigate the radiation damage of biological tissues at the molecular level [5-7]. In biological tissues the damages produced in the biomolecules are not only caused directly by the particle-matter collision but also by radicals and secondary particles created after the fragmentation of different chemical species along the ionisation path [8,9]. This underlines the importance of a proper description of the fragmentation mechanisms after electron removal. Thus, studying the behavior of the amino acids after interaction with highly charged ions gives valuable information for the hadron therapy treatment based on ion beams.

In this communication we present recent results on fragmentation of small lineal amino acids, doubly-positively charged in the gas phase, $\text{NH}_2-(\text{CH}_2)_n-\text{COOH}$: $n=1$ glycine [10]; $n=2$ β -alanine [11] and $n=3$ γ -aminobutyric acid GABA [12]. Experimentally, we obtain the data in the gas phase for neutral molecules in collisions with low-energy highly charged ions. State-of-the-art multi-coincidence detection mass spectrometric techniques are used to determine the charge state of the molecule before fragmentation. The experimental data are analyzed by means of quantum chemistry calculations.

In particular, *ab initio* molecular dynamics simulations of the excited and charged species provide valuable information on the fragmentation mechanisms; further exploration of the potential energy surfaces with the density functional theory calculations allows us to obtain energetic and structural information on the most populated dissociation channels.

Our results [10-12] have shown that in competition with the expected Coulomb explosion, the doubly positively charged lineal amino acids present several de-excitation mechanisms. In particular, hydrogen migration and hydroxyl group migration that appear in the femtosecond timescale and lead to unusual fragmentation products.

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