Absolute cross sections for production of molecular dications by electron impact

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Although doubly charged molecular ions are possibly a crucial factor for the understanding of physical-chemical processes in energized media, such as planetary atmospheres, plasma environments and the human body when submitted to radiotherapy treatments, little is known regarding the absolute cross sections for the dication production in symmetric molecules, due to the intrinsic impossibility of separating moieties with the same mass to charge ratio in a time of flight spectrum [1,2].

Besides, the mechanisms and pathways for dications formation and possible stability are still not known, raising the question if post-collisional processes play a significant role and – if that is the case – what would their relevance be for the production of these metastable species. In this work, the following symmetric molecular dications were investigated: nitrogen, oxygen, benzene and ethylene. In order to disentangle the dication from the fragment representing the breakup of the molecule in two equal parts (e.g. N2++ and N+), the DETOF technique was employed. The DETOF technique allows one to identify different kinetic energy distributions present in recoil ions – since the fragmented molecules acquire kinetic energy in the fragmentation process and dications retain their original Maxwell-Boltzmann velocity distribution, its identification becomes straightforward [3].

It was found that nitrogen and oxygen molecules present pure, very contrasting features. We found that the nitrogen dication is produced mainly via a double direct ionization process, where both electrons are removed in the same collisional process, while the oxygen dication is formed predominantly by an inner valence shell ionization, followed by an Auger decay, with no indication whatsoever of direct double ionization leading to the stable dication [4]. The carbon containing molecules studied, ethylene [5] and benzene, both present contributions from both direct double ionization and Carbon K-shell ionization followed by Auger decay to each dication production, and their relative proportions were obtained, with respect to their dependency with the impact energy.

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