DAMOP19-2019-000558

Abstract for an Invited Paper
for the DAMOP19 Meeting of
the American Physical Society

An independent-atom-model-based description of ion collisions with complex biomolecules[1]

TOM KIRCHNER[2], York University

Collisions with biomolecules have generated a lot of interest and scientific activity lately, in large parts because of their relevance in a number of applications, specifically in the context of ion-beam cancer therapy. For ion-impact collisions, both experimental and theoretical efforts have largely focused on relatively small systems, such as DNA nucleobases and their precursors. While on the experimental side the technique of electrospray ionization holds the promise to make a systematic investigation of more complex systems feasible [1], it does not look like ab-initio theoretical methods can be pushed to deal with a much larger number of target nuclei and electrons anytime soon. There is therefore a role to be played by (sophisticated) modeling. This talk will report on our recent progress in this area. We have developed an independent-atom-like model that is capable of dealing, in principle, with arbitrarily large target systems. It is based on a geometrical interpretation of a cross section as an effective area composed of overlapping circular disks which represent the cross sections of the atomic constituents of the system under study. The latter are calculated using a well-tested time-dependent density-functional theory framework, and a pixel-counting method is used to carry out the effective-area calculation for any target molecule orientation of interest [2,3]. Orientation-averaged proton-impact net ionization and electron transfer cross sections will be presented for a number of target systems ranging from structural analogues of DNA building blocks, such as pyrimidine and purine, to a select set of amino acids and nucleotides. We will also discuss a recent extension of the model that allows for *multiple*-ionization calculations. [1]D. Egorov *et al.*, J. Phys.: Conf. Series **635**, 112083 (2015). [2]H. J. Lüdde *et al.*, Eur. Phys. J. D **70**, 82 (2016). [3]H. J. Lüdde *et al.*, Eur. Phys. J. B **91**, 99 (2018).

[1]Work supported by NSERC, Canada.

[2]The work presented has been carried out in collaboration with Hans Jürgen Lüdde (Goethe University Frankfurt) and Marko Horbatsch (York University).