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Ionization of complex biomolecules studied with an independent atom model including geometric screening corrections[1]

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A thorough understanding of the radiation damage of biological tissue begins with data for the fundamental ionization processes of molecules in the gas/vapor phase. A growing body of experimental and theoretical work for photon, electron and heavy-particle impact is addressing this need. This talk focuses on ion-impact collisions and reports on cross-section results for target molecules such as water and the DNA/RNA nucleobases adenine and uracil obtained from independent-atom-model (IAM) based calculations. In the simplest version of the IAM the ionization or electron transfer cross sections of the atoms that make up the molecule are added up. We have recently shown that this naive Bragg additivity rule can be significantly improved by taking the overlapping nature of effective cross-sectional areas into account [1]. A pixel counting method is used to calculate the overlaps and the model is referred to as IAM-PCM. It is demonstrated that IAM-PCM net ionization results for projectile charges Q=2,3 can be reproduced by scaled proton-impact (Q=1) cross sections over a wide range of collision energies. We also show how based on this scaling model the available experimental data can be reduced to effective Q=1 cross sections and present a comparison of those results with proton impact data [2].

The work presented in this paper has been carried out in collaboration with Hans Jürgen Lüdde (Goethe University Frankfurt) and Marko Horbatsch (York University).1] H. J. Lüdde *et al.*, Eur. Phys. J. D **73**, 249 (2019). [2] H. J. Lüdde *et al.*, Phys. Rev. A (accepted for publication).

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