Theoretical ionization and capture cross sections for DNA nucleobases impacted by light ions

C. Champion(a,b), H. Lekadir(a), M. E. Galassi(c), S. Incerti(b), O. Fojon(c), R. D. Rivarola(c) and J. Hanssen(a)

(a) Université Paul Verlaine-Metz, Laboratoire de Physique Moléculaire et des Collisions, Metz, France
(b) Université Bordeaux 1, CNRS/IN2P3, Centre d’Études Nucléaires de Bordeaux Gradignan, CENBG, Chemin du Solarium, BP120, 33175 Gradignan, France
(c) Instituto de Física Rosario, CONICET and Universidad Nacional de Rosario, Argentina

DNA lesions - and more particularly those involved in clustered damages - are nowadays considered of prime importance for describing the post-irradiation cellular survival. Indeed, these complex radio-damages may induce critical DNA lesions like double strand breaks whose relevance has been nowadays clearly identified in the radio-induced cellular death process. In these conditions further theoretical models as well as experimental data on ion-induced collisions at the DNA level remain still today crucial.

Until now experimental measurements on such biological systems remain scarce and are essentially limited to studies of mechanisms of radiation damage only explored at the mesoscopic scale and not at the single molecule (nanometric) scale. In this context, ionization and fragmentation of isolated gas-phase nucleobases have received only little interest and were essentially focused on the cross section determination for electron-induced collisions, the ion-induced collisions being rarely reported in the literature.

In this work, we will expose the three theoretical models - a first classical one based on a CTMC approach and two quantum mechanical ones, namely, a Coulomb Born and a continuum-distorted wave eikonal-initial-state (CDW-EIS) models - we have recently developed for predicting the single and multiple ionization and capture total cross sections for DNA bases impacted by heavy ions