Abstract for an Invited Paper
for the DAMOP06 Meeting of
The American Physical Society

Electron-impact ionization and dissociative ionization of biomolecules[1]

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Oxidative damages by ionizing radiation are the source of radiation-induced damages to human health. It is recognized that secondary electrons play a role in the damage process, particularly important is the damage of DNA by electrons, potentially leading to mutagenesis. The damage can be direct, by creating a DNA lesion, or indirect, by producing radicals that attack the DNA. Molecular-level study of electron interaction with DNA provides information on the damage pathways and dominant mechanisms. This investigation focuses on ionization and dissociative ionization (DI) of DNA fragments by electron-impact. For ionization we use the improved binary-encounter dipole (iBED) model [W.M. Huo, Phys. Rev. A64, 042719-1 (2001)]. For DI it is assumed that electron motion is much faster than nuclear motion, allowing DI to be treated as a two-step process and the DI cross section given by the product of the ionization cross section and dissociation probability. The ionization study covers DNA bases, sugar phosphate backbone, and nucleotides. An additivity principle is observed. For example, the sum of the ionization cross sections of the separate deoxyribose and phosphate fragments is in close agreement with the C_3'- and C_5'-deoxyribose-phospate cross sections, differing by less than 5%. The result implies that certain properties of the DNA, like the total ionization cross section, are localized properties and an additivity principle may apply. This allows us to obtain properties of a larger molecular system built up from the results of smaller subsystem fragments. The DI of guanine and cytosine has been studied. For guanine, a proton is produced from the channel where the ionized electron originates from a molecular orbital with significant charge density along the N(1)-H bond. The interaction of the proton with cytosine was also studied.

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