Low energy elastic and electronically inelastic electron scattering from biomolecules

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Reactions initiated by collisions with low-energy secondary electrons has been found to be the prominent mechanism toward the radiation damage on living tissues through DNA strand breaks. Now it is widely accepted that during the interaction with these secondary species the selective breaking of chemical bonds is triggered by dissociative electron attachment (DEA), that is, the capture of the incident electron and the formation of temporary negative ion states [1,2,3]. One of the approaches largely used toward a deeper understanding of the radiation damage to DNA is through modeling of DEA with its basic constituents (nucleotide bases, sugar and other subunits). We have tried to simplify this approach and attempt to make it comprehensible at a more fundamental level by looking at even simple molecules. Studies involving organic systems such as carboxylic acids, alcohols and simple five-membered heterocyclic compounds are taken as starting points for these understanding. In the present study we investigate the role played by elastic scattering and electronic excitation of molecules on electron-driven chemical processes. Special attention is focused on the analysis of the influence of polarization and multichannel coupling effects on the magnitude of elastic and electronically inelastic cross-sections. Our aim is also to investigate the existence of resonances in the elastic and electronically inelastic channels as well as to characterize them with respect to its type (shape, core-excited or Feshbach), symmetry and position. The relevance of these issues is evaluated within the context of possible applications for the modeling of discharge environments and implications in the understanding of mutagenic rupture of DNA chains. The scattering calculations were carried out with the Schwinger multichannel method (SMC) [4] and its implementation with pseudopotentials (SMCPP) [5] at different levels of approximation for impact energies ranging from 0.5 eV to 30 eV.

References

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