Low-energy positron and electron scattering from tetrahydrofuran and 3-hydroxy-tetrahydrofuran

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Abstract
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Synopsis We present new cross section results from a joint experimental and theoretical investigation into low-energy positron and electron scattering from two targets of biological interest, namely tetrahydrofuran and 3-hydroxy-tetrahydrofuran. We compare and discuss the total, elastic and inelastic cross sections for these species in the light of potential positron and electron-induced damage in biomolecular systems.

We present recently measured and computed cross sections for low-energy positron collisions with the structurally related molecules tetrahydrofuran (THF) [1] and 3-hydroxy-tetrahydrofuran (3H-THF) [2]. Those two species represent suitable models for the sugar rings contained in the phosphate-deoxyribose backbone structure of the nucleic acids [3, 4]. As the knowledge of the impact cross sections is essential for charged-particle track simulations, studying those compounds can assist us in shedding more light on the effects of positron and electron-induced damage in biological media.

Total, positronium formation, elastic differential and inelastic integral cross sections have been measured at selected energies in the range 1-190 eV using the buffer-gas trap and positron beam spectrometer at the Australian National University [5] with an energy resolution of 60-100 meV.

Total, inelastic and elastic integral, as well as elastic differential cross sections have also been computed at energies between 1 and 1000 eV within the Independent Atom Model and using the Screening Corrected Additivity Rule formalism [6]. In addition, electron-impact cross sections have also been calculated in order to explore the different role that positrons and electrons play in the low-energy scattering dynamics for those species.

References

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Figure 1. Comparison of the present experimental and theoretical total cross sections for positron scattering from THF and 3H-THF.

We also compare the present cross sections for THF and 3H-THF in order to examine how small changes in the molecular structure (that can lead to quite different physico-chemical properties) can affect the scattering process for those systems.