Electron impact cross-sections for biomolecules – completeness and self-consistency via swarm analysis

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Synopsis The accuracy and completeness of electron impact cross-sections in water and tetrahydrofuran are assessed through comparison with experimental electron transport coefficients using the pulsed-Townsend experiment.

The determination of a comprehensive set of electron-biomolecule cross-sections is fundamental to understanding electron-induced processes arising in plasma medicine and radiation damage modelling. Formulation of complete sets is generally based on a critical assessment of available experimental `beam' studies and theoretical calculations, and interpolations/extropolations. Issues of completeness and accuracy of cross-section sets arise.

Swarm experiments provide one of the key discriminating tests on the accuracy and completeness of cross-section sets. In swarm experiments, excess electrons under the action of an applied electric field are passed through a gas of known temperature and pressure. Measured currents are interpreted in terms of transport coefficients such as drift velocities, diffusion coefficients, and ionization/attachment rates. Various energy regimes of the cross-sections can be preferentially accessed by varying the electric field which modifies the velocity distribution of the electrons. Through comparison of measured transport coefficients with those calculated from transport theory/ simulation, one can assess the ability of the cross-section set to accurately treat particle, momentum, and energy balance. Cross-section degeneracy (i.e., different sets of cross-sections can produce the same field dependence of the transport coefficients) is an issue. Additional handles to assess the degeneracy, accuracy and completeness of the cross-section set can be through measurements in admixtures with well known cross-sections which can considerably modify the distribution function.

In this presentation we report on recent swarm measurements in the biomolecules of water and tetrahydrafuran (THF) using the pulsed-Townsend technique of the de Urquijo group. We present and assess the consistency of cross-section sets for water and THF (in various admixtures) through a comparison of calculated transport coefficients using a multi-term Boltzmann equation solution with the available experimental swarm measurements provides a discriminating test on consistency and accuracy of the cross-section sets. Sample results for electron transport in gaseous water/helium mixtures are presented in Figure 1 [1]. Further results will be presented for water/Ar mixtures and THF/N_2 mixtures.

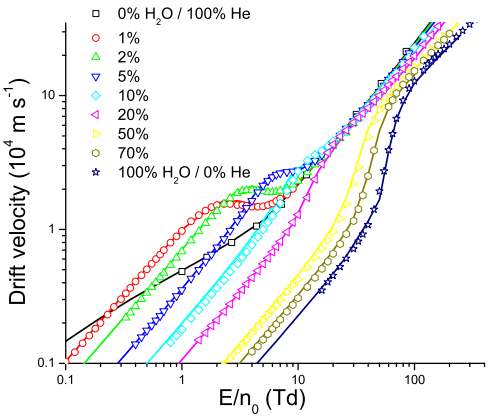

Figure 1. Comparison of experimental and calculated drift velocities for electrons in gaseous water/Ar mixtures.

References

[1] J. de Urquijo, E. Basurto, a M. Juárez, K. F. Ness, R. E. Robson, M. J. Brunger, and R. D. White (2014) *J. Chem. Phys.* **141**, 014308 (2014)

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