

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

This content has been downloaded from IOPscience. Please scroll down to see the full text.

2015 J. Phys.: Conf. Ser. 635 072079

(<http://iopscience.iop.org/1742-6596/635/7/072079>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

### Download details:

IP Address: 137.219.126.141

This content was downloaded on 24/02/2016 at 05:57

Please note that [terms and conditions apply](#).

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

J. de Urquijo<sup>1</sup>, M. Casey<sup>2</sup>, D. Konvalov<sup>2</sup>, M. J. Brunger<sup>3</sup>, G. Garcia<sup>4</sup>, Z. Petrovic<sup>5</sup> and R. D. White<sup>\*2</sup>

<sup>1</sup>Universidad Nacional Autónoma de México, Cuernavaca, Mor., Mexico

<sup>2</sup>College of Science, Technology and Engineering, James Cook University, Townsville, Australia

<sup>3</sup>Flinders University, Adelaide, South Australia

<sup>4</sup>CSIC, Madrid, Spain

<sup>5</sup>Institute of Physics, Belgrade, Serbia

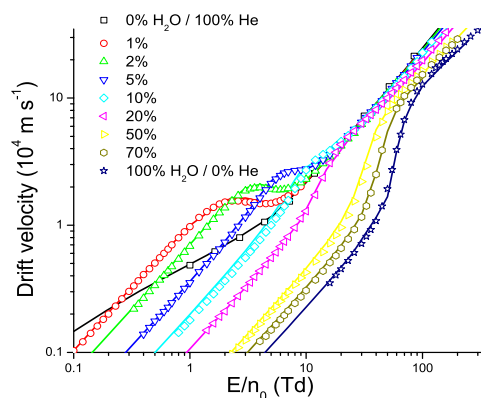
**Synopsis** The accuracy and completeness of electron impact cross-sections in water and tetrahydrofuran are assessed through comparison with experimental electron transport coefficients using the pulsed-Townsend experiment.

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/extrapolations. 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

tetrahydrofuran (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<sub>2</sub> 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)

\* E-mail: [Ronald.White@jcu.edu.au](mailto:Ronald.White@jcu.edu.au)

