Recent results for electron and photon scattering from biomolecules and molecules of technological significance

M J Brunger¹

¹College of Science and Engineering, Flinders University, GPO Box 2100, Adelaide, S.A. 5001, Australia

Over the last decade our international team have largely been concentrating on measuring cross sections for electron and photon scattering from biomolecules such as water, tetrohydrofuran (THF), tetrahydrofurfural alcohol (THFA), pyrimidine and 1,4-benzoquinone (pBQ) and for 'techno-molecules' such as phenol, furfural, thiophene and the primary alcohols methanol, ethanol, 1-propanol and 1-butanol (see e.g. [1]). Specifically, at Flinders University we have focussed on measuring differential cross sections (DCSs) and integral cross sections (ICSs) for vibrational-mode and electronic-state excitation for electrons with energies in the range 15-50 eV (e.g. for THF, THFA, pyrimidine, pBQ, phenol and furfural). This work has been strongly supported by Schwinger Multicannel (SMC) calculations by the Brazilian group. In Madrid measurements have concentrated on the total cross sections (TCSs) for biomolecules such as pyrimidine and pBQ and for the techno-molecules furfural and thiophene using a magnetically confined electron beam and the Beer-Lambert law. Theory using their IAM-SCAR+I method has also been undertaken. At Juiz de Fora partial and total ionisation cross sections and TCSs for the primary alcohols have been measured, while in Mexico transport coefficients have been experimentally determined for pure H₂O, THF and THFA and mixtures of those species with standard gases such as helium, argon and N₂. In conjunction with transport simulations from James Cook University, they represent a very good cross check for the validity of the underlying cross section data base used in those simulations. Finally, in Aarhus absolute photo absorption cross sections have been measured for phenol, pBQ, furfural and thiophene with synchrotron radiation and using the Beer-Lambert law to set the absolute scale.

A small selection of our more recent results from the above investigations will be presented at the meeting.

[1] Brunger MJ 2017 Int. Rev. Phys. Chem. 36 333

Acknowledgements

This work would not have been possible without the input of Darryl Jones, Laurence Campbell, Ron White, Luca Chiari, Marco Lima, Cristina Lopes, Márcio Bettega, Roma da Costa, Márcio Varella, Gustavo García, Paulo Limão-Vieira, Filipe Ferreira da Silva, Nykola Jones, Søren Hoffmann, Jaime de Urquijo, Jimena Gorfinkiel and Oddur Ingólfsson, as well as many other friends and colleagues overs the years. Funding from the Australian Research Council through grants such as DP1600102787 and DP180101655 is also gratefully acknowledged.