Cross-sections of molecules important to lighting plasmas using the R-Matrix method

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The R-Matrix method, first introduced by Wigner to study nuclear reactions dominated by the formation of a compound state, relies on the division of configuration space into two distinct regions: the inner region, containing the compound nucleus and including electron correlation effects, and the external region, corresponding to various possible reactions prior to and after the reaction, utilising a long-range multipole potential. There is a crucial need for balance between the neutral target and the anionic parts of the calculation. This can be achieved throught the manual selection of wavefunctions for both, and allows the method to deal with excited electronic states. As such care must be taken in producing a suitable neutral 'target' model. The method has been extended for electron-atom scattering and electron-molecule scattering, leading to the further development of a treatment for electron-diatomic scattering and electron-polyatomic systems [1], which utilise Slater type and Gaussian type orbitals respectively. There have been a number of review articles covering the development of this method, the most recent being by Tennyson [2].

The UK R-matrix package has been applied widely to a number of electron-scattering systems. These include both charged and neutral species, ranging in size from electron-atom up to electron scattering off uracil [3]. Calculations have also taken place at low (below ionization) and intermediate (around ionization) scattering energies, as well as being used as a method for positron-molecule scattering [4]. Currently the package is undergoing development as part of the UKRMol project.

The computer software Quantemol-N has been created to act as an expert system for users of the R-Matrix method for electron-molecule scattering [5]. By streamlining the set-up of calculations using a step-by-step 'wizard' interface, inexperienced users can apply the R-matrix method in order to calculate data such as electron impact cross-sections with ease. The software is now used as a tool for carrying out R-matrix calculations, both in academia and industry.

In recent years the demand for molecular cross-sections has been growing in the field of lighting physics. People have examined molecules like N_2 for lighting, (for which detailed electron impact studies are available [6]), with limited success.This is mainly due to the losses associated with vibrational states. A fundamental understanding concerning the limitations of using molecules for generating radiation is becoming increasingly valuable. This modelling is critical to aid in the search for suitable species to use in molecular lighting, which have to be at least as efficient and have similar radiative properties as the current generation mercury bulbs. Failiure to find the correct molecules will prevent a decrease in the use of the poisonous mercury. By theoretical modelling of molecular plasmas and production of cross-sections, the radiation properties may be obtained. Recent work has started to look at heavy molecule plasmas containing GaI in a multi-scale, non-empirical approach [7] and experimentally [8]. Here we use the R-Matrix method as implemented in the Quantemol-N expert system to model the electron-impact cross-sections for potentially important lighting-plasma molecules, with results including N_2 and O_2 to be presented at the conference.

Reference

[1] L.A. Morgan et. al., 1997, J. Phys. B; At. Mol. Opt. Phys., 30, 4087-4096
[2] J. Tennyson, 2010, Physics Report, doi:10.1016/j.physrep.2010.02.001
[3] A. Dora et. al., 2009, J. Chem. Phys., 130, 164307
[4] K.L. Baluja et. al., 2007, J. Phys. B; At. Mol. Opt. Phys., 40, 3515-3524

[5] J. Tennyson et. al., 2007, J. Phys. Conf. Series 86, 012001
[6] M. Tashiro & K. Morokuma, 2007, Phys. Rev. A. 75, 1, 012720
[7] S. Adamson et. al., 2007, J. Phys. D; Appl. Phys., 40, 3857-3881
[8] D. Smith et. al., 2007, J. Phys. D; Appl. Phys., 40, 3842-3856