Electron molecule collision calculations: a primer

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Synopsis Electron-molecule collisions are important in a variety of natural processes ranging from lightning to the the chemistry of the interstellar medium, and drive technological plasmas which underpin much of modern industry. This tutorial will discuss the variety of process that occur following an electron collusion appropriate methods for computing cross sections for different electron energy regimes.

There is a great demand for electron molecule collision cross sections driven by the desire to model key process both natural and technological. This demand is largely being met by theory given the difficulty and expense of experiments which also find it difficult to probe key processes ranging from electron impact rotational excitation of molecular ions (important for models of interstellar medium spectra) to electon collisions with open shell molecules (radicals) which form an important driver in cold (molecular) plasmas.

Appropriate methods for treating electron molecule collisions depend on the kinetic energy of the impacting electron. Broadly these can be divided into the low energy regime where the electron has insufficient energy to the ionize the target molecule; the high energy regime (above about 50 eV) where simplified treatments often yield excellent results and the challenging intermediate energy regime which straddles the ionization regime. There is also the case the high energy relativistic regime but this is only important in special circumstances such as cosmic ray ionization.

While some processes such as electron impact ionization can be treated using simplified (semi-empirical) procedures; generally detailed scattering calculations are required to obtain energy-dependent cross sections. In the low energy regime so-called resonances, where the scattering electron is temporarily trapped in a quasi-bound state, provide prominant structures in the cross sections and drive much of the processes. In this regime procedures such as close-coupling bear some similarities with quantum chemistry calculations, albeit with the need to treat processes lying in the continuum. At high energies, electron collisions can often be treated using procedures based on perturbation theory such the Born approximation. At intermediate energy quasi-complete treatments such as the convergent close-coupling or R-matrix with pseudo states have been demonstrated to give excellent results, although so far their application has been restricted to collisions with simple (few electron) molecular targets.

This tutorial lecture will discuss the various processes that can result from electron collisions with molecules and methods available for their study. Attendees will be given a temporary licence to the QEC (Quantemol electron collisions) expert system [1] which drives the UK molecular R-matrix code UKRmol+ [2] to allow them to explore performing electon – molecule collision calculations.

References

[1] Cooper B *et al.*, 2019 *Atoms*, **74** 97
[2] Masin Z, Benda J, Gorfinkiel JD, Harvey AG and Tennyson J, 2020 *Computer Phys. Comms.*, **249**, 107092

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