„Recommended" Cross Sections for Electron Collisions with Molecules

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Closer and closer deadlines for the peaceful use of thermonuclear energy [1] and recent discoveries in astrochemistry [2] triggered a renewed interest in electron-molecule scattering. A series of papers is under publication by our group, starting from CH_4, C_2H_4, NF_3 to nitrogen oxides (NO, N_2O, NO_2). Differently from earlier works, now the inquiry moves from total cross sections [3] into processes that are responsible for the energy-loss in plasmas, i.e. total and partial ionization, electronic and vibrational excitation, and rotational excitation and de-excitation. Comprehensive comparisons have been done.

The main novelty of our approach is the extensive referring to the theory. The UK R-Matrix code (and the Quantemol package) proved to be the most versatile tool to calculate elastic cross sections both in molecules dominated at low energies by resonances like NF_3 [4] and in polar targets like H_2O [5]. The R-Matrix codes allowed also to evaluate electronic excitation in nitrogen oxides (work in progress). For validation of total ionization cross sections we use with success the Born-Bethe binary encounter model [6]; however, application of this model to partial ionization cross sections [4] still requires some experimental input.

Further consistency of the proposed sets is obtained by comparison of cross sections from beam techniques with data derived from swarm experiments, both for pure and (what is even more stringent) mixed gases [7]. "Recommended" cross sections are prepared possibly for all partial processes, in a wide (0.01-1000 eV) energy range. An extensive discussion of the methodology will be given at the Seminar.

References

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