Calculations of Electron Impact Ionization Cross Sections for Molecular Targets: Ionospheric and Other Applications

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This presentation aims at a two-fold purpose. First we highlight our quantum mechanical approach for calculating
total cross sections (CS) for ionization of various atoms and molecules induced by the impact of energetic electrons. We then indicate the implications and applications of these (microscopic) ionization CS in various bulk media, ranging from ionospheres to ices and other solids.

The microscopic calculation of electron-molecule ionization CS rests on our quantum mechanical approximations discussed in [1-3]. Briefly, the electron-target system is represented in a complex spherical potential to determine elastic scattering CS (Qel) and inelastic scattering CS (Qinel) at different electron energies Ei. The inelastic CS of the target molecule contain ionization CS (Qion), and our theoretical method [1-3] successfully deduces the required Qion from our calculated Qinel. It has been demonstrated in our recent papers that the present theoretical method yields reliable Qion for a number of molecules like H2, N2, O2 etc (in their ground as well as excited electronic states), and many polyatomic molecules.

An attempt can be made to incorporate this valuable and well published quantum mechanical cross section Qion results in treating electron interactions with realistic systems, such as ionospheres and atmospheres of various planets on one hand, and different solids on the other. Therefore, we have applied micro to macro approach with Qion as our theoretical input. The resulting macroscopic cross sections in (length)-1 generated for a particular bulk medium are employed to find other important quantities such as Mean Free Path of electrons, ionizing collision frequency and ionization rate coefficients.

For a medium with identical N molecules per unit volume, the macroscopic ionization CS Σ ion as a function of Ei
is defined by

$$\Sigma ion\ (Ei) = N.\ Qion\ (Ei) \quad (1)$$

The Mean free path Λion (Ei) is the inverse of Σ ion (Ei). present calculations are carried out on the ionization
induced by energetic electrons in different ionospheric regions, considering the appropriate constituent species.
Mean free paths are also separately calculated for solids and icy materials, in particular H2O (ice).
Detailed results will be presented at the conference AOGS-2010.

References:
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