GEC15-2015-000423

Abstract for an Invited Paper
for the GEC15 Meeting of
the American Physical Society

An independent-atom-model description of ion-molecule collisions including geometric screening corrections[1]

TOM KIRCHNER[2], York University

A simple way of calculating charged-particle-induced electron removal cross sections for molecular targets consists in adding up atomic cross sections for all the atoms that make up the molecule. This procedure is commonly referred to as Bragg's additivity rule (AR) and is based on the independent-atom model, in which the molecule is viewed as a collection of (undistorted) atoms. The AR works well at sufficiently high collision energies, where the atomic cross sections tend to be small. For electron-molecule collisions several extensions of the AR have been proposed to make it applicable to lower impact energies, where the atomic cross sections are large and the AR results in an overestimation of the experimental data. One such extension is the so-called screening-corrected additivity rule (SCAR) [1]. For each atomic cross section σ_A in the AR a weight factor $0 \leq s_A \leq 1$ is introduced to account for the partial screening of the atoms due to the geometrical overlap of the σ_A's when viewed from the incident electron. The weight factors are determined heuristically and are interpreted as orientation-averaged screening coefficients. In this contribution, we propose a similar model for net ionization and electron transfer in heavy-particle collisions, but in contrast to the SCAR model the weight factors do depend on the orientation of the molecule relative to the projectile beam direction. For a given geometry we construct a space-filling-like model of the molecule by surrounding each atom A by a sphere of radius $r_A = \sqrt{\sigma_A/\pi}$. The weight factors in the SCAR-like cross section formula are determined as those fractions of the σ_A's that are visible for an observer that moves with the impinging projectile. The procedure is repeated for a number of molecular orientations, and total cross sections that can be compared with experimental data are obtained by averaging over all orientations. The atomic cross sections are calculated by using the two-center basis generator method [2], while the molecular geometry information that enters the calculation of the screening coefficients is taken from the literature. In my talk, I will explain the model in more detail and will present total cross section results for proton collisions from a number of targets ranging from diatomic molecules such as H_2 and CO to intermediate-size hydrocarbons such as butane.

[1] F. Blanco *et al.*, Phys. Lett. A **374**, 4420 (2010).
[2] M. Zapukhlyak *et al.*, J. Phys. B **38**, 2353 (2005).

[1]Work supported by NSERC, Canada.
[2]In collaboration with Hans Jürgen Lüdde, Goethe University Frankfurt and Marko Horbatsch, York University.