Abstract Submitted
for the GEC11 Meeting of
The American Physical Society

Computational studies of inelastic electron-molecule scattering processes with the Quantemol-N system BRENT WALKER, JONATHAN TENNYSON, University College London and Quantemol Ltd. — Data for cross-sections of electron-molecule scattering processes is an important ingredient in the study of plasmas, especially in undertaking reactor scale computer simulations of industrial plasmas. Such cross-section data can be obtained computationally from first principles, where a highly successful and accurate approach is the **R**-matrix method. In the **R**-matrix method, to approach the quantum-mechanical problem of the electron molecule interaction, space is divided into two regions: the *inner* region, in which the (complicated) $N + 1$ electron problem of the interaction between the scattering electron and the N electron molecule is solved in detail; and the *outer* region, where a much simpler scattering problem is solved. We report on recent developments in the *Quantemol-N* package – which provides an expert system interface to the state-of-the-art UK Molecular R- matrix codes – for taking account of *inelastic* electron- molecule scattering processes. The electron-impact processes we will focus on are: (1). dissociative attachment; (2). impact ionization; and (3). electron impact excitation/dissociation. Example calculations will be presented. We will also illustrate how data obtained from calculations of such inelatic scattering processes has been incorporated into reactor-scale plasma simulations at Quantemol Ltd.

Brent Walker
University College London and Quantemol Ltd.

Date submitted: 15 Jul 2011 Electronic form version 1.4