Kinetic energy release of fragments from electron impact dissociation of the molecular hydrogen ion

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Synopsis We calculate the kinetic energy release distributions of fragments produced in electron-impact dissociation of the vibrationally excited molecular hydrogen ion. Results are presented for a number of dissociative excitation transitions and ionisation. Agreement with experiment is good.

Data for dissociative processes in molecular scattering is vital in many fields, including atmospheric physics and plasma modelling. Electron-impact dissociation of molecular ions produces fragments with a kinetic energy release (KER) distribution. This distribution corresponds to transitions to the vibrational continuum and is the fragments single differential cross section. KER from e-H_2^+ scattering affects the energy balance in fusion plasmas, and contributes to heating and depletion of planetary atmospheres. H_2^+ is also the simplest molecule and provides a convenient starting point for developing KER models.

Using the convergent close-coupling (CCC) method [1] we performed adiabatic nuclei approximation calculations of e-H_2^+ scattering to obtain excitation T-matrices, and excitation and ionisation cross sections as a function of internuclear distance. The KER distributions were obtained from the CCC collision data using a number of techniques that are discussed and their results compared.

We present in Fig. 1 the KER distributions for electron scattering from a hot H_2^+ molecule calculated using the electronic ground state vibrational population measured by Von Busch and Dunn (BD) [2] for a number of electronic transitions for incident electron energies from 30 to 500 eV. The sum of the KER distributions (from dissociative excitation and ionisation processes) is weighted according to the BD vibrational distribution and the Franck-Condon (FC) factors [3]. We find that the majority contribution is from transitions to the $2p\sigma_u$ and $2p\pi_u$ states and dissociative ionisation. The low energy KER region of the distribution proved to be highly sensitive to the inclusion of higher vibrational states and the choice of target vibrational population.

Comparison with the first-order model of El Ghazaly et. al. [4] have been conducted and the importance of the approximations made in their work is discussed. We find a reasonably good agreement of the CCC KER calculations with the experiment [4].

In future work we plan to extend the model to the dissociation of H_2 and then more complicated molecules, particularly those of relevance to the modelling of fusion and industrial plasmas.

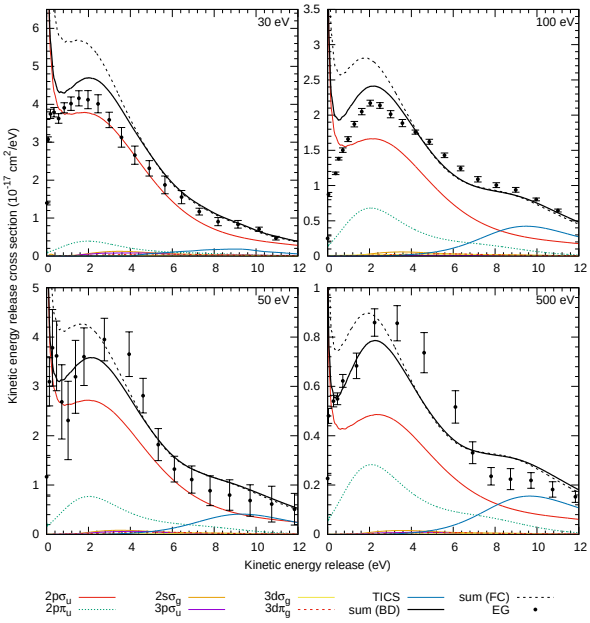

Figure 1. KER distributions for 30, 50, 100 and 500 eV incident electron energies. The KER for individual electronic transitions are shown for the vibrational population measured by Von Busch and Dunn (BD) [2]. The KER summed over electronic transitions are shown for the BD and Franck-Condon (FC) distributions. Experiment (EG) is due to El Ghazaly et. al. [4]

References

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