

Classical calculation of total and differential cross sections for electron capture and ionization in proton - molecule collisions

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Synopsis The Classical Trajectory Monte Carlo method is applied to treat proton collisions with N₂, CO and CH₄ at collision energies $25 < E < 2.5 \times 10^3$ keV. The calculation employs model potentials to describe the interaction of the active electron with the molecular core. General good agreement with available experimental data is found.

In previous works [1, 2, 3], we have developed a method to treat ionization and capture processes in ion-molecule collisions at energies above 25 keV/amu, where close-coupling methods become cumbersome. The method assumes straight-line ion trajectories. The independent electron approximation is employed to describe the process, and the active electron motion takes place in a model potential, which includes the electron interaction with the target and projectile cores (see [2]). We have employed the Classical Trajectory Monte Carlo (CTMC) method [4], where the electronic state is described by a classical density. In our calculation a density is associated to the motion of electron initially described by each molecular orbital of the target. Initially, each density is given by a microcanonical distribution, obtained as explained in [2].

The electron densities after the collision yield the one-electron capture p^{cap} and ionization p^{ion} probabilities, and a many-electron interpretation is then applied to obtain the corresponding probabilities for the many-electron system. In particular, we have applied an interpretation based on the so-called independent event model (see [5] and references therein). The experiments report values of electron production cross sections (they include contributions from single ionization, double ionization and transfer ionization), and net capture probability, which includes transfer ionization. The corresponding probabilities are calculated in the form:

$$P^{\text{ep}} = 2 \sum_{i=1}^N p^{\text{ion}}, P^{\text{cap}} = 2 \sum_{i=1}^N p^{\text{cap}} \quad (1)$$

As an illustration, we show in figure 1 the calculated cross section for electron production and net capture for H⁺ + N₂ and H⁺ + CO col-

lisions. It can be noted the general good agreement with the experimental data of ref. [6] with some discrepancies in the energy region near the maximum of the ionization cross section, which are probably due to the well-known limitation of microcanonical initial distributions, to describe the tail of the spatial quantal distribution.

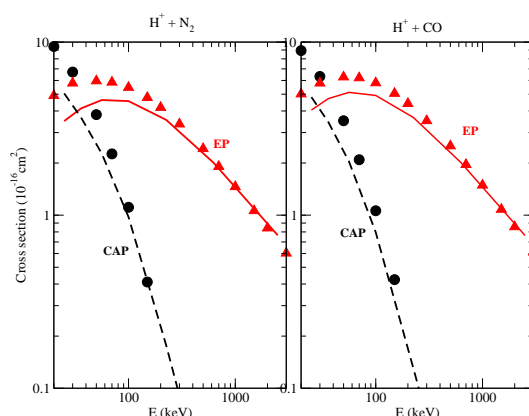


Figure 1. Electron production (EP) and electron capture (CAP) total cross sections in H⁺ + N₂ and H⁺ + CO collisions compared with the experimental data of Rudd *et al.* [6].

References

- [1] L. F. Errea, *et al* 2007 *Phys. Rev. A* **76** 040701
- [2] H Getahun *et al.* 2010 *Eur. J. Phys. D* **60** 45
- [3] L. F. Errea, *et al* 2011 *Phys. Rev. A* (submitted)
- [4] R. Abrines and I. C. Percival 1966 *Proc. Phys. Soc.* **88** 873
- [5] L. A. Wehrman *et al* 1996 *J. Phys. B* **29** 5831
- [6] M. E. Rudd, T. V. Goffe, and A. Itoh 1985 *Phys. Rev. A* **32** 2128

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