

Ion-water collisions at intermediate energies

Clara Illescas^{*1}, L. F. Errea^{*}, L. Méndez^{*}, B. Pons[†] and I. Rabadán^{*}

^{*}Laboratorio asociado al CIEMAT de Física Atómica y Molecular en Plasmas de Fusión
Departamento de Química, módulo 13, Universidad Autónoma de Madrid
Madrid-28049, Spain

[†]CELI, Université de Bordeaux I - CNRS - CEA, 351 Cours de la Libération, 33405 Talence, France.

Synopsis We employ the independent event electron model in the framework of the classical trajectory Monte Carlo method to compute ionization and capture cross sections for one- and two- electron processes in collisions of H^+ , He^{2+} and C^{6+} with water molecules at intermediate impact energies. Subsequent fragmentation processes are also considered, as well as the differential cross sections for electron emission, of paramount importance for ion beam therapy.

We have studied the ionization and capture processes in collisions of H^+ , He^{2+} and C^{6+} with water molecules because of their relevance in the understanding of biological damage and in ion beam cancer therapy. We have employed an improved impact parameter-CTMC model [1] to calculate cross sections for one- and two-electron processes in the impact energy range $20 \leq E \leq 10000$ keV/amu. Our treatment is based on the assumption that the electrons evolve independently; therefore each electron moves in an effective field created by the nuclei and the remaining electrons. In order to describe the target anisotropy with respect to the impinging direction of the projectile, we use a three-center model potential to represent the interaction of the active electron with the H_2O^+ core

$$V_{\text{mod}} = V_O(r_O) + V_H(r_{H1}) + V_H(r_{H2}) \quad (1)$$

in contrast with our previous calculations which employed one-center (isotropic) potentials [2]. The evaluation of inelastic probabilities for the physical multielectron system, in terms of the mono-electronic ones, is performed by means of the IEVM [3].

As an example of our results, we display in Fig. 1 the cross sections for electron production and single capture plus transfer ionization as a functions of E . Good agreement is found with the experimental data [4]–[7] over the whole energy range.

Besides total cross sections, we will present at the conference the fragmentation cross sections associated to the capture and ionization pathways. Furthermore, special emphasis will be made on differential ionization cross sections of great importance for ion beam cancer therapy.

¹E-mail: clara.illescas@uam.es

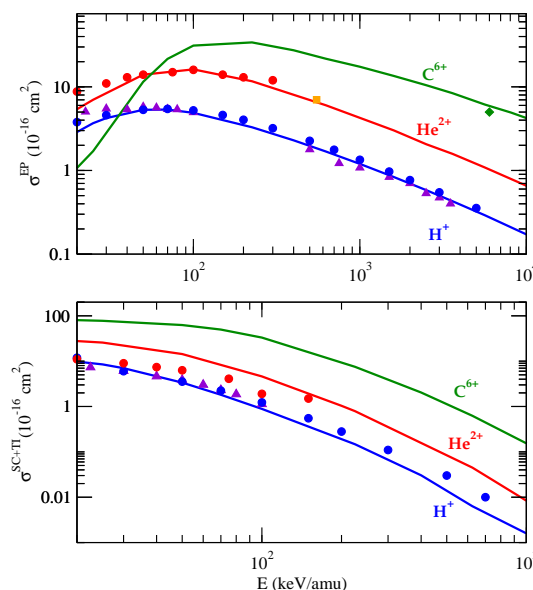


Figure 1. Cross sections for electron production (top) and single capture + transfer ionization (bottom) in ion-water collisions compared with experimental data of: (●) Rudd *et al.* [4]; (▲) Luna *et al.* [5]; (■) Rudolph and Melton [6]; (◆) Dal Cappello *et al.* [7].

References

- [1] C. Illescas *et al.*, 2011 *Phys. Rev. A* (submitted)
- [2] L. F. Errea *et al.*, 2007 *Phys. Rev. A* **76** 040701
- [3] D. F. S. Crothers and R. McCarroll, 1987 *J. Phys. B* **20** 2835
- [4] M. E. Rudd *et al.*, *Phys. Rev. A* **32** 2128
- [5] H. Luna *et al.*, 2007 *Phys. Rev. A* **75** 042711
- [6] P. S. Rudolph and C. E. Melton, 1966 *J. Chem. Phys.* **45** 2227
- [7] C. Dal Cappello *et al.*, 2009 *Nucl. Instr. and Meth. B* **267** 781