Journal of Physics: Conference Series **635** (2015) 032044 doi:10.1088/1742-6596/635/3/032044

Ionization and electron capture cross sections for single and multiple electron removal from H_2O by Li^{3+} impact

H. Luna[†1], W. Wolff [†], A. C. Tavares*, E C Montenegro[† 2], T. Pausz[$], M. Murakami[§], H. J. Lüdde[$], M. Horbatsch[§], and T. Kirchner[§3]

[*] Departamento de Física, Pontifícia Universidade Católica do Rio de Janeiro, 22451-900, Rio de Janeiro, RJ, Brazil
[†] Instituto de Física, Universidade Federal do Rio de Janeiro, 21941-972, Rio de Janeiro, RJ, Brazil
[$] Institut für Theoretische Physik, Goethe-Universität, D-60438 Frankfurt, Germany
[§] Department of Physics and Astronomy, York University, Toronto, Ontario, Canada M3J 1P3

Synopsis We report experimental and theoretical ionization and single electron capture cross sections for single, double and triple electron removal from H_2O by Li^{3+} with energies ranging from 0.75 to 5.8 MeV. Single electron removal is dominant for ionization, while double electron removal is dominant for electron capture. For the one- and two-electron removal cases, the calculations based on time-dependent orbital propagation in density functional theory show good agreement with experiment for the two collision channels studied.

The quality of theoretical calculations of ionization and charge exchange processes when multiply charged ions collide with molecules cannot be assessed based on measurements of the produced ions alone, as is the case for atomic targets. This follows since the relationship between the observed ionic fragments and the distribution of primary vacancies, either single or multiple, is not straightforward. A better check is achieved from a finer selection of the measured ionic fragments by discriminating the collision events that produced either one, two or more ions. If this measurement is differential in the final projectile charge state, a quite stringent comparison with theory can be made.

In this work we report experimental and theoretical ionization and single-electron capture cross sections for single, double and triple electron removal from water by Li^{3+} with energies ranging from 0.75 to 5.8 MeV. The experiment was carried out selecting both the final charge state of the projectile and the ejected fragments in coincidence to obtain cross sections associated with ionization and electron capture channels [1]. The ionic fragments and the emitted electrons produced under single-collision conditions were collected by a time-of-flight spectrometer with single-hit (e.g. $OH^+ + H^0$) and double-hit events (e.g. $OH^+ + H^+$) properly discriminated.

The theoretical framework is a continuation of previous work [2]. The molecular orbitals from a self-consistent field calculation are represented in an atomic oxygen basis and propagated with the basis generator method. This can be achieved for a limited number of molecular orientations, but should be sufficient for the generation of reliable total cross sections.

The measured and calculated cross sections for single, double, and triple electron removal from water are shown in Figure 1.

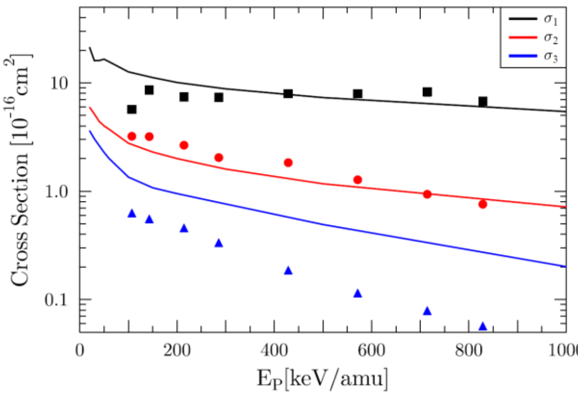

Figure 1. Cross sections for single, double, and triple electron removal from water by Li^{3+} impact.

These cross sections σ_j for removal of j electrons represent a relatively inclusive property, and should be predicted reliably by the theoretical method. We observe that for j=1,2 and impact energies above 100 keV/amu the agreement between theory and experiment is good. For j=3 the theory overestimates the measured data by a factor of two and more. Given that j matches the initial charge state of the projectile this overestimation is perhaps unexpected. Also unexpected is the different fall-off with projectile energy which would indicate a possible breakdown of the independent-electron model for this charge state. More detailed comparisons on the level of final projectile-charge-state-specific cross sections will be shown at the conference.

References

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[1] E-mail: : hluna@if.ufrj.br
[2] E-mail: : montenegro@if.ufrj.br
[3] E-mail: tomk@yorku.ca