H_2O single ionization by light particle-impact: fully differential cross sections

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E Acebal[1] * and S Otranto[1]

[1]Instituto de Física del Sur (IFISUR), Departamento de Física, Universidad Nacional del Sur (UNS), CONICET, Av. L. N. Alem 1253, B8000CPB-Bahía Blanca, Argentina

Synopsis Fully differential cross sections for the single ionization of the $1b_1$ and $3a_1$ orbitals of H_2O by electron- and positron-impact are calculated by means of the CDW-EIS model at an impact energy of 81 eV. A proper average procedure over molecular orientations is performed. Main differences between positron- and electron-impact are observed for coplanar geometries in the binary structures. In addition, an enhancement of the binary region and a decrease of the recoil lobe are observed for positron-impact.

Over the last decades, radiation therapy is becoming one of the most common modes of cancer treatment. This increases the importance of studying the dynamics of ionization radiation with living tissue. In this sense, the ionization of the water molecule (H_2O) by particle-impact has become of great interest since this single compound represents up to sixty percent of the human body.

Fully differential cross sections (FDCS), in this sense, provide the most exhaustive test for state-of-the-art theoretical models and a clear challenge for current experimental setups.

Recently, a complete kinematically study of the single ionization of the two most outer valence orbital of H_2O by electron-impact at 81 eV has been reported [1]. The theory under use was based on the DWBA, and the authors concluded that higher-order terms in the projectile –target interaction might be relevant at this impact energy based on the discrepancies observed with the experimental data. Subsequently, in a previous work, we analysed those data with the CDW-EIS model [2] and found good overall agreement with the reported data.

In this work, we focus ourselves on the influence of the projectile charge sign in the single ionization of the $1b_1$ and $3a_1$ orbitals of H_2O. Fully differential cross sections were calculated by means of the CDW-EIS model and contrasted after a proper averaged procedure over molecular orientations.

In Figure 1, we compare positron- and electron-impact results for one of the four geometries reported for the scattering plane. It can be seen how the recoil lobe is decreased for positron-impact. We also observe a maximum among the direction of $\boldsymbol{k}_1$, which is slightly suggested for electron projectiles but no fully apparent. These features obey to the post-collisional interaction. The same situation stands for the four geometries reported.

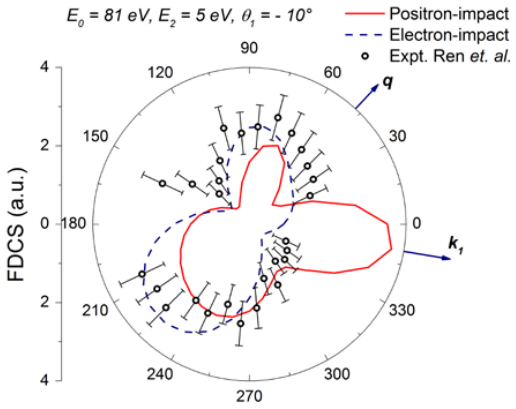

Figure 1. FDCS for positron- (solid line) and electron- (dashed line) impact ionization of H_2O, for the scattering plane *xz*. Cross sections represent the sum of $1b_1$ and $3a_1$ orbitals. Experimental data for electron-impact from Ref. [1] scaled to the present theoretical results.

In addition, we present FDCS for electron- and positron-impact ionization of the $1b_1$ and $3a_1$ orbitals of H_2O, for the denominated semi-perpendicular and full perpendicular plane. In these cases, similar structures are observed with an enhancement of the binary region and a decrease of the recoil lobe for positron-impact.

References

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* E-mail: emiliano.acebal@uns.edu.ar