Total cross sections for the double ionization of oriented water molecule

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In this work, we present the theoretical total cross sections (TCS) for the double ionization of a single oriented water molecule by electron impact. These kind of reactions are of importance in several domains as for instance Radiotherapy. To simulate the damage provoked by the ionizing radiations, the living mater is frequently modeled as water. Our theoretical method are based on the first born approximation with a collisional system including an initial state composed by a projectile and a water target molecule described by a plane wave and an accurate one-centre molecular wave function [1], respectively, and a final state constituted by two ejected electron represented by a Coulomb wave and a scattered electron described by a plane wave. The contributions of each final state to the double ionization process, i.e., with target electrons ejected from similar and/or different molecular subshells, are studied. We have already study the strong dependence of the electron angular distribution on the orientation of the water molecule [2] and [3]. So, in this present work we demonstrate that the molecular orientation is still crucial when less differential double ionization cross sections are investigated, namely, in terms of secondary electron energy distributions, mean kinetic energy transfer and total cross sections.

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