Calculation of FDCS for the low and intermediate energy electron impact ionization of water molecules

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Synopsis Fully differential cross sections (FDCS) results for the electron impact ionization of water molecules taking place from $1b_1$, $1b_2$ and $2a_1$ orbitals are presented. The FDCS calculations have been performed in second Born approximation.

Fully differential cross sections (FDCS) for molecular ionization by electron impact, normally referred to as (e, 2e), represents a powerful tool to study the electronic structure of molecules as well as to examine the fundamental interaction between continuum electrons and molecules. Over the last few decades, there have been many theoretical and experimental studies performed for the (e, 2e) process with molecular targets. However most of these studies were for high incident-energy electron impact ionization of molecules [1].

Water molecule is the third most abundant molecule on the earth and is therefore of great importance in numerous multi-disciplinary research fields like radiobiology where it is commonly used as surrogate of the living matter [2, 3]. The knowledge of the collision dynamics of low-energy electrons with biological systems remain crucial so as to develop robust numerical models of charged particle tracking in biological matter.

Recently Singh et al. [4] reported fully differential cross section results for the electron and positron impact ionization of $3a_1$ orbital of the water molecule. We present in this communication the results of fully differential cross sections (FDCS) for the electron impact single ionization taking place from $1b_1$, $1b_2$ and $2a_1$ orbital of water molecule. We calculate FDCS for the ionization of water molecule in second order distorted wave Born approximation formalism in the low and intermediate energy ranges. We compare and discuss the salient features of FDCS observed for ionization taking place from different molecular orbitals of water.

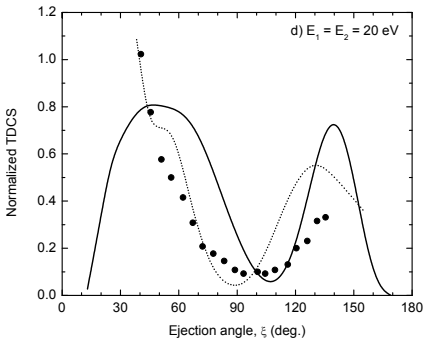

Figure 1: Triply differential cross sections for the electron impact ionization of the $3a_1$ molecular state of the water molecule in coplanar symmetric kinematics (*i.e.* $\phi_1 = 0$; $\phi_2 = 180^0$ and $\xi_1 = \xi_2 = \xi$) at incident electron energy 40 eV above the ionization potential (IP~15 eV). The solid line represents the second Born distorted wave Born approximation while the dotted line refers to the molecular distorted wave (MDW) approximation [5].

References

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