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

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Abstract. Triply differential cross sections for the electron induced ionization of the 3a₁ and 1b₁ orbitals of the water molecule are calculated within the distorted wave Born approximation. The distorted wave functions are numerically calculated by modelling both the initial and the final channels whereas single-center Slater type wave functions are used for describing the molecular target. A good agreement with the existing experimental data is obtained.

1. Introduction
Charged particle impact ionization of targets (atoms / ions / molecules) is an important fundamental collision process that plays a significant role in many areas as diverse as plasma physics, astrophysics, atmospheric modelling, discharge physics and radiobiology. Extensive theoretical and experimental investigations have been carried out to understand the electron impact single ionization (i.e. (e, 2e) processes) of various targets [1-6]. Being able to provide the information about momentum vectors of final state continuum electrons, the (e, 2e) processes are very important in understanding the dynamical behavior of quantum mechanical systems and also provide the stringent tests of the theoretical models. Accurate cross sections for H₂O target ionization by electron impact are very important for the understanding of the complex interactions involved in the bimolecular processes. Water molecule is the most abundant molecule on the earth and has attracted much attention over the years. It is of great importance in numerous multi-disciplinary research fields like radiobiology. Almost 80% water is contained in the human body and other biological material, which makes water an ideal test case to investigate processes occurring in the human body. For example, energetic and angular distributions resulting from electron-induced collisions with water molecules are commonly used in charged particle track structure codes for modelling the radio-induced damages in biological samples [7]. Besides, the low-energy electrons - abundantly produced in the high-energy radiations and commonly used in radiotherapy treatment planning - have been now a days clearly identified of prime importance in particular since the observation of their crucial role in lethal cellular lesion induction [8]. Under these conditions, the knowledge of the collision dynamics of such low-energy electrons with biological systems remain crucial so as to develop robust numerical models of charged particle tracking in biological matter.

In the present study, we report the results of our calculation of triply differential cross sections for electron impact ionization of the 3a₁ and 1b₁ molecular orbital of the H₂O in coplanar symmetric...
kinematics within the distorted wave Born approximation (DWBA) including post-collision interaction (PCI). We briefly outline the theoretical model and compare our TDCSs to measurements \[9\] in coplanar symmetric kinematics for incident electron energies 20 eV above the ionization potential of the \(3a_1\) molecular state and 20 eV, 40 eV and 60 eV above ionization potential of \(1b_1\) molecular state of water.

2. Theory
The electron impact single ionization process on \(H_2O\) molecule is expressed as
\[
e^- + H_2O \rightarrow H_2O^+ + e^- + e^-
\] (1)
The triply differential cross section for the ionization process of water molecule as in Eq.(1) may be written as
\[
\frac{d^3\sigma}{d\Omega_1 d\Omega_2 d\Omega_1} = (2\pi)^4 \frac{k_1 k_2}{k_0} \sum_{av} |T(k_1, k_2, k_0)|^2
\] (2)
where \(k_0, k_1\) and \(k_2\) are the momenta of incident, scattered and ejected particles, respectively. The elements \(d\Omega_1 = \sin \xi_1 d\xi_1 d\phi_1\) and \(d\Omega_2 = \sin \xi_2 d\xi_2 d\phi_2\) denote the solid angle for the scattered and the ejected electron, respectively, whereas the energy interval of the ejected electron is represented by \(dE\). In the coplanar symmetric geometry used here, \(k_0, k_1\) and \(k_2\) are in the same plane \((\phi_1 = \phi_2 = 0^0)\) while the scattering and ejection angles are taken as equal \((\xi_1 = \xi_2)\). The incident electron energy \(E_0\) is defined by the relation \(E_0 = E_1 + E_2 + IP\), where \(E_1\) and \(E_2\) refer to the energies of the two outgoing electrons while IP denotes the ionization potential of the orbital of water molecule. Let us note that Eq.(2) includes a sum over final and average over initial magnetic and spin-state degeneracy.

The first-order term in DWBA is given by
\[
f_{BL} = \frac{1}{Z f_1^2} \left\langle \chi_1^{(-)}(k_1, r_1) \chi_2^{(-)}(k_2, r_0) \right| - \left( \frac{Z}{f_1} - \frac{1}{|r_1 - r_0|} \right) \left| \psi_1(r_0) \chi_0^{(+)}(k_0, r_1) \right\rangle,
\] (3)
\(Z\) refers to the charge of the ionized target (here \(Z = 1\)). \(\chi_0^{(+)}(k_0, r_1)\) is the distorted wave function used for describing the incident particle while \(\chi_1^{(-)}(k_1, r_1)\) and \(\chi_2^{(-)}(k_2, r_0)\) refer to the distorted wave functions used for the two outgoing particles. \(\psi_1(r_0)\) is the initial bound state wave function which is approximated as the orientation averaged molecular wave function for the respective orbital of water molecule.

The target molecular orbitals are here expressed in terms of Slater-like functions all centered at a common origin \(i.e.\) the heaviest atom, and are written as
\[
\psi_1(r_0) = \sum_{j=1 N_i} a_j \Phi_{n_i l_j m_{ij}}(r),
\] (4)
Where \(N_i\) is the number of Slater orbitals \(\Phi_{n_i l_j m_{ij}}(r)\) and \(a_j\) the weight of each atomic component
\[
\Phi_{n_i l_j m_{ij}}(r) = R_{n_i l_j m_{ij}}(\vec{r}) Y_{l_j m_{ij}}(\hat{r})
\] (5)
with the radial part \(R_{n_i l_j m_{ij}}(\vec{r})\) of each atomic orbital given by
Let us note that in Eq. (5), \( \hat{r} \) designates the solid angle direction. All the needed parameters and quantum numbers are taken from Ref. [10]. The distorted wave function used for describing the incident particle is generated in the equivalent local ground-state potential of the water molecule while the distorted wave functions used for modelling the outgoing particles are generated in the equivalent local ground-state potential of the residual ion. Moreover, let us add that all along the current calculations reported here we have made a careful check to ensure that the cross sections converge satisfactorily. Finally, let us note that the spin-averaged static-exchange potential of Furness and McCarthy [11] as modified by Riley and Truhlar [12] has been used for the case of electron-induced ionization. We have included PCI in our DWBA calculations using the Ward-Macek factor \( M_{\text{ei}} \) [13].

### 3. Results and Discussion

The TDCSs calculations have been performed in doubly symmetric coplanar to perpendicular kinematics with equal outgoing electron energies and polar angles, namely, \( E_1 = E_2 \) and \( \varphi_1 = \varphi_2 = \varphi \) at incident energies, namely, 20 eV above the ionization potential (IP) of the \( 3a_1 \) molecular state (IP ~ 15 eV) of the water molecule. The TDCSs for electron impact ionization of the water molecule are reported in Figure 1 as a function of the symmetric scattering angle \( \varphi \). The solid line represents the DWBA calculations including post collision interaction (PCI). We compare our results with the recent measurements of Nixon et al. (solid circles) [9]. All the theoretical and experimental data are independently normalized.

**Figure 1**: Triply differential cross sections for the electron impact ionization of the \( 3a_1 \) molecular state of the water molecule from coplanar symmetric to perpendicular kinematics (i.e. \( \varphi_1 = 0 \); \( \varphi_2 = 180^0 \) and \( \varphi_1 = \varphi_2 = \varphi \)) at incident electron energy 20 eV above the ionization potential (IP ~ 15 eV). The solid line represents the distorted wave Born approximation results. The solid circles represent the experimental data [9].
In the cases of coplanar ionization reported in Fig. 1a, we observe that the experimental data show a peak at forward scattering angles \( (\xi < 90^\circ) \) and a small one at backward scattering angle \( (\xi > 90^\circ) \). The coplanar differential cross section exhibits a forward peak and a backward peak due to single electron-electron binary collision and double scattering mechanism respectively [14]. We observe that the ratio of forward to backward scattering peak decreases as the ionization takes place from coplanar to perpendicular plane geometry.

![Graph](image)

Figure 2: Triply differential cross sections for the electron impact ionization of the 1b_1 molecular state of the water molecule in coplanar symmetric kinematics \( (i.e. \phi_1 = 0 ; \phi_2 = 180^\circ \) and \( \xi_1 = \xi_2 = \xi \) ) at several incident electron energies: (a) 20 eV (b) 60 eV and (c) 40 eV above the ionization potential (IP=12.6 eV). The solid line represents the distorted wave Born approximation results while the solid circles are the experimental data [9].
A reasonable agreement is observed between our theoretical predictions and the available experimental data with some discrepancies in terms of magnitude as well as position for the forward and backward scattering peaks. In Figure 2, we present the results of our calculation of TDCS for the electron impact ionization taking place from 1b₁ molecular orbital of water. These calculations have been done at the 20 eV, 40 eV and 60 eV above ionization potential (IP = 12.6 eV) of the 1b₁ molecular orbital of water in the coplanar symmetric geometry. A dominant forward scattering peak is observed for all the above cases reported in Figure 2 in the measurements as well as our theoretical results. Overall good agreement is obtained between our results and experimental data. As reported recently [15], more calculations including higher order effects may be useful to describe the collision dynamics of water molecule at these low and intermediate energies.

4. Conclusions
Electron impact triply differential cross sections have been calculated in the distorted wave Born approximation formalism for the coplanar to perpendicular plane ionization of the 3a₁₁ orbital of water molecule as well as for the coplanar ionization of 1b₁ orbital of water molecule at the low and intermediate energies. A mixed degree of agreement with the experimental data has been obtained and post collisional interaction has been found to be significant for the ionization of water molecule. Present attempt is useful to understand the delicate collision dynamics of water molecule and more theoretical efforts are required to make clear understanding of the complex reaction mechanism.

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5. References
[1] McCarthy I E and Weigold E (1976) Phys. Rep. C27 275.
[2] Lahmam-Bennani A (1991) J. Phys. B: At. Mol. Opt. Phys. 24 2401.
[3] Byron Jr F W and Joachain C J (1989) Phys. Rep. 179 211.
[4] Purohit G, Singh P, Patidar V, Azuma Y, and Sud K K (2012) Phys. Rev. A 85, 022714.
[5] Nakel W and Whelan C T (1999) Phys. Rep. 315 409.
[6] Bray I (2002) Phys. Rev. Lett. 89 273201.
[7] Champion C, Le Loirec C, and Stosic B (2012) Int. J. Radiat. Biol.88 62-65.
[8] Boudaiffa B, Cloutier P, Hunting D, Huels M A and Sanche L (2000) Science 287 1658.
[9] Nixon K L, Murray A J, Al-Hagan O, Madison D H, and Ning C (2010) J. Phys. B: At. Mol. Opt. Phys.43, 035201.
[10] Moccia R (1964) J. Chem. Phys. 40, 2186.
[11] Furness J B and McCarthy I E (1973) J. Phys. B6, 2280.
[12] Riley M E and Truhlar D G (1975) J. Chem. Phys.63, 2182.
[13] Ward S J and Macek J H (1994) Phys. Rev. A49, 1049.
[14] Zhang X, Whelan C T and Walters H R J (1990) J. Phys. B: At. Mol. Opt. Phys. 23, L509.
[15] Singh P, Purohit G, Champion C and Patidar V (2014) Phys. Rev. A 89, 032714.