

# Ionization of the water molecule by electron and positron impact

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**Abstract.** Theoretical cross-sections for the ionization of the water molecule by electron and positron impact are presented. The calculations were performed in the framework of the simpler CPE and two distorted-wave models, ES and TS, by employing Gaussian wavefunctions for the description of the target. We found good agreement with the experiment, especially for higher impact energies.

## 1. Introduction

Water has a large practical importance in collision processes with positron and electron beams. Because a large percentage of living tissue is water, all medical diagnosis and treatment methods need precise cross section data for the water molecule in collision with charged particles. These collisions play an important role also from the viewpoint of other research fields like astrophysics or chemistry.

The interaction of water with positron and electron projectiles, has received significant attention in the last years. Both experimental [1, 2, 3] and theoretical [4, 5, 6], total cross-sections have been reported for the positron-water scattering process. Other experiments have measured positronium-water total cross sections [3] and even double-differential cross-sections [7] for the ionization of H<sub>2</sub>O by positron impact. Unfortunately, there are no experimental data for the direct ionization of the water molecule by positron impact. For electron impact ionization, experimental data [8, 9, 10, 11] exist even for the direct ionization process.

Previously we have calculated cross-sections for the direct ionization of several molecules by positron impact, like H<sub>2</sub> [12], N<sub>2</sub> [13], O<sub>2</sub> [14], CO, CO<sub>2</sub> [15], CH<sub>4</sub> [16]. Later, we have refined [17] and extended [18] our calculations to the ionization of the studied molecules by electron impact. These studies were based on the simple CPE (Coulomb plus plane waves with full energy range) and the more complex distorted-wave models, ES (Electron Screening) and TS (Total Screening). In each case, the initial state of the active electron was described by Gaussian-type wavefunctions.

In this paper we extend our calculations to the direct ionization of the water by electron and positron projectiles. The obtained results are compared with the existent experimental data [8, 9, 10, 11], the theoretical results of [19], and the DWBA (Distorted-Wave Born Approximation) calculations of Champion et al. [20] in the case of electron impact ionization. Champion et al. [20] have employed the Slater-type functions of Moccia [21] for the description of the initial state of the target molecule. They have considered each molecular orbital as a linear

combination of Slater-type functions, all centered at a common origin, i. e. the oxygen atom. They have employed plane waves for the description of the incident and scattered particles, while the ejected electron was represented by a distorted-wave.

## 2. Theory

The present calculation for the water molecule follows closely the method employed in the case of the CH<sub>4</sub> [16], since both are nonlinear molecules. Here, we give a brief overview of the main steps of the theory.

The triple differential cross-section for the ionization of a molecular target by electron or positron impact may be written as

$$\frac{d^3\sigma}{d\hat{\mathbf{k}}_f d\hat{\mathbf{k}}_e dE_e} = \sum_r \frac{(2\pi)^4}{E_i} |f_t^r|^2, \quad (1)$$

where the sum runs over all occupied molecular orbitals. In (1) the continuum wave functions were normalized in energy, and the energy is expressed in Rydbergs.  $E_i$  denotes the impact energy, while  $E_e$  stands for the energy of the ejected electron.  $\hat{\mathbf{k}}_f$  and  $\hat{\mathbf{k}}_e$  stand for the angles of the momenta of the scattered and ejected particles, respectively. For a positron projectile the total scattering amplitude,  $f_t^r$ , coincides with the  $f_d^r$  direct amplitude, while for electron projectiles the inclusion of the exchange effects lead to

$$|f_t^r|^2 = |f_d^r|^2 + |f_{ex}^r|^2 - \alpha |f_d^r| |f_{ex}^r|. \quad (2)$$

Here  $f_{ex}^r$  is the exchange amplitude, while  $\alpha$  is a phase factor [22]. The direct and the exchange amplitudes may be written as

$$f_d^r = \langle \phi_f(\mathbf{r}_1) \phi_e(\mathbf{r}_2) | V(r_{12}) | \phi_i(\mathbf{r}_1) \phi_b^r(\mathbf{r}_2) \rangle \quad (3)$$

$$f_{ex}^r = \langle \phi_e(\mathbf{r}_1) \phi_f(\mathbf{r}_2) | V(r_{12}) | \phi_i(\mathbf{r}_1) \phi_b^r(\mathbf{r}_2) \rangle, \quad (4)$$

where  $\phi_i$ ,  $\phi_e$  and  $\phi_f$  are the wave functions of the incident, ejected and scattered particles, respectively. In order to make the calculations tractable, these wave functions were expanded in terms of the partial waves. In the direct amplitude  $\mathbf{r}_1$  is the position vector of the projectile and  $\mathbf{r}_2$  gives the position of the active electron, while in the exchange amplitude the states of the scattered and the ejected particles are exchanged.  $\phi_b^r$  stands for the initial state (orbital) of the active electron. We have taken into account the following orbitals of the water molecule:  $2a_1$ ,  $1b_2$ ,  $3a_1$  and  $1b_1$  with the corresponding ionization potentials (in atomic units): 1.26805, 0.61744, 0.45300 and 0.39122. The molecular orbitals are constructed as linear combination of the O and the two H Gaussian orbitals:

$$\phi_b^r(x, y, z) = C_O^r \phi_O^r(x, y, z) + \sum_{i=1}^2 C_{H_i}^r \phi_{H_i}^r(x - x_i, y - y_i, z - z_i). \quad (5)$$

Here,  $x_i$ ,  $y_i$  and  $z_i$  are the coordinates of the hydrogen atoms. We have obtained the Gaussian orbitals as contractions of Gaussian-type functions. As in the case of the methane molecule [16], the multi-centre molecular orbitals were expanded in terms of the spherical harmonics

$$\phi_b^r(\mathbf{r}_2) = \sum_{l_b\mu} C_{l_b\mu}^r(r_2) Y_{l_b\mu}(\hat{\mathbf{r}}_2), \quad (6)$$

where the expansion coefficients may be expressed as

$$C_{l_b\mu}^r = \int d\hat{\mathbf{r}}_2 Y_{l_b\mu}(\hat{\mathbf{r}}_2) \phi_b^r(\mathbf{r}_2). \quad (7)$$

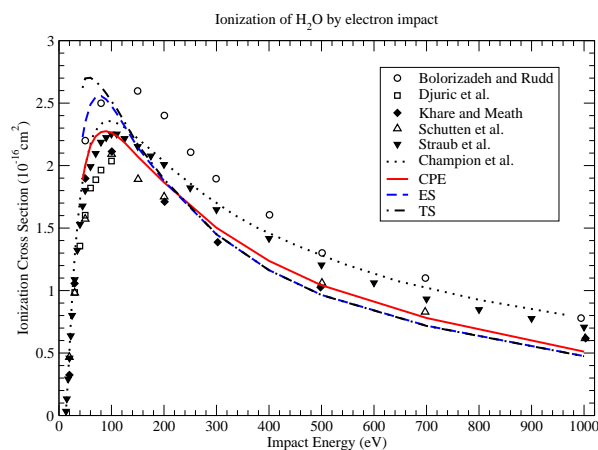
In order to calculate the ionization cross section, one has to integrate the differential cross-section (1) over the angles of the scattered and ejected electron as well as the energy of the ejected electron. Further, the cross-section is averaged over all molecular orientations.

We have calculated the cross-sections for the ionization of the H<sub>2</sub>O molecule in the framework of three models developed earlier, the CPE, ES and TS models. The CPE [23] is a simple model, which uses Coulomb or plane waves for the description of the free particles. The ES and TS are distorted-wave models. The distorted-waves were calculated by solving the radial Schrödinger equation in the field of a spherically averaged potential created by the nuclei and the electrons of the target. The ES model employs the distorted-wave description for the ejected electron, while the TS model uses the distorted-wave formalism for the description of all free particles. Details about the calculational method and these models were given in papers [17] and [18].

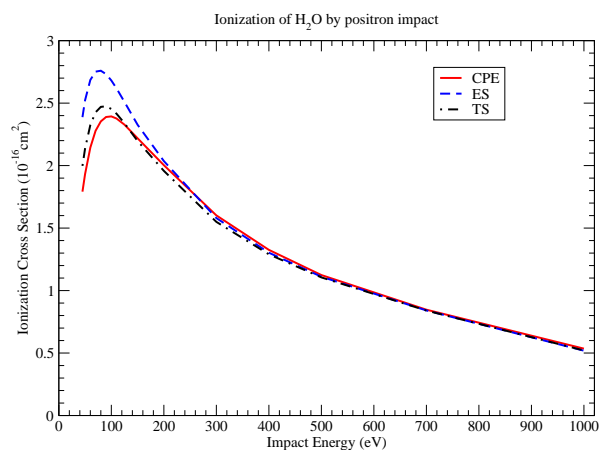
### 3. Results and discussions

We present the results for the direct ionization of the H<sub>2</sub>O molecule in Figures 1-2 and Tables 1-2, respectively.

Fig. 1 shows the integrated cross-sections for the direct ionization of the water molecule by electron impact, determined in the framework of the CPE, ES and TS models. Our calculations are compared with various experimental data [8, 9, 10, 11] and the theoretical results [19] and [20].



**Figure 1.** Cross-sections for the direct ionization of the H<sub>2</sub>O molecule by electron impact, calculated in the framework of the CPE, ES and TS models, compared with the measurements of [8, 9, 10, 11] and the theoretical results [19] and [20].



**Figure 2.** Cross-sections for the direct ionization of the H<sub>2</sub>O molecule by positron impact, calculated in the framework of the CPE, ES and TS models. At the date of the study there were no experimental data for the direct ionization of this target.

It may be observed that our CPE model provides a good agreement with the measurements of Schutten et al. [10] and the results of Khare and Meath [19], respectively. The agreement is especially good for impact energies higher than 200 eV. In this energy range our results are slightly lower than the measurements of Bolorizadeh and Rudd [8] and Straub et al. [11]. The calculated cross-section of Champion et al. [20] agree well with the measurements of Straub et al. [11], but is higher than the cross-sections of [9, 10, 19]. In the region of the peak, the CPE results are a slightly higher than the measurements of Djuric et al. [9], Schutten et al. [10] and

the calculated cross-sections of Khare and Meath [19], but still are in reliable agreement with the data of Straub et al. [11]. However, the peak of the CPE model is slightly shifted to lower energies. The ES and TS models provide good agreement with the data of [10] and [19] but overestimate these results at the region of the peak. It seems that the approximation introduced by spherically averaging the real potential created by the nuclei and electrons of the target is not suitable in this case, where the CPE model, which uses simple Coulomb potentials, provide better results. For energies higher than 200 eV the distorted-wave models give lower values for the cross-section than the measured data of [8] and [11] and the theoretical calculations of [20].

The results obtained within the CPE, ES and TS models for the ionization of the water molecule by positron projectiles are presented in Fig. 2. There are no experimental data for the direct ionization process of this target. The obtained cross-sections for electron and positron projectiles show similar values. Nevertheless, the cross-sections for positron impact are slightly higher than for electron projectiles, except for the TS model. In the region of the peak, the distorted-wave models ES and TS show higher values than the CPE model, similarly as in the case of the electron cross-section. For impact energies higher than 200 eV the positron cross-sections calculated in the framework of the different models seem to merge. It will be interesting to compare these results with the experimental measurements expected in the near future [24].

An analysis of the contributions to the total cross section of the different orbitals taken into account and the contributions coming from the different terms of the expansion on  $l_b$  is provided in Table 1 for electron projectiles and in Table 2 for positron projectiles.

**Table 1.** Partial ionization cross-sections (in  $10^{-16}$  cm<sup>2</sup>) calculated in the framework of the ES model for an electron projectile of 50 eV impact energy.

Orbital	$l_b$				Total Orbital
	0	1	2	3	
$2a_1$	$9.67 \times 10^{-2}$	$4.49 \times 10^{-4}$	$7.47 \times 10^{-5}$	$3.36 \times 10^{-5}$	0.097
$1b_2$	0	0.64	$1.07 \times 10^{-2}$	$6.52 \times 10^{-4}$	0.651
$3a_1$	0.10	0.22	$7.22 \times 10^{-3}$	$6.10 \times 10^{-4}$	0.327
$1b_1$	0	1.24	$9.08 \times 10^{-3}$	$1.89 \times 10^{-4}$	1.249
Total $l_b$	0.196	2.100	0.027	$1.48 \times 10^{-3}$	2.324

**Table 2.** Partial ionization cross-sections (in  $10^{-16}$  cm<sup>2</sup>) calculated in the framework of the ES model for a positron projectile of 50 eV impact energy.

Orbital	$l_b$				Total Orbital
	0	1	2	3	
$2a_1$	$7.71 \times 10^{-2}$	$4.98 \times 10^{-4}$	$9.51 \times 10^{-5}$	$2.94 \times 10^{-5}$	0.077
$1b_2$	0	0.750	$1.18 \times 10^{-2}$	$8.24 \times 10^{-4}$	0.762
$3a_1$	0.106	0.246	$7.68 \times 10^{-3}$	$6.42 \times 10^{-4}$	0.360
$1b_1$	0	1.308	$1.23 \times 10^{-2}$	$1.03 \times 10^{-4}$	1.320
Total $l_b$	0.183	2.304	0.031	0.001	2.52

The tables list the contributions for an impact energy of 50 eV, in the case of the ES model. In each case, for large  $l_b$  values the contributions are less important than for smaller  $l_b$  values. This is the reason why we have neglected the  $l_b > 3$  terms. As Tables 1 and 2 show, the first molecular orbital ( $2a_1$ ) taken into account has mainly a spherical character (the  $l_b = 0$  term is dominant), the contributions from higher order terms are negligible. In the case of the  $1b_2$  and the  $1b_1$  orbitals the  $l_b = 1$  term is dominant, therefore the orbitals show a mainly dipole character. For the  $3a_1$  orbital, both the monopole ( $l_b = 0$ ) and dipole ( $l_b = 1$ ) terms contribute significantly to the cross section.

#### 4. Conclusions

The ionization of the water molecule by electron and positron impact was investigated. We found a fair agreement between the experimental data and our results. Particularly, the good agreement with the measurements provided by the simpler CPE model is impressive. It seems that in the region of the peak, our distorted-wave models overestimate the experimental results for electron impact ionization. Nevertheless, for higher impact energies the agreement is good. The cause of the discrepancy may be the spherical nature of the potential employed to calculate the distorted-waves.

Although there are no measurements for the ionization of the water by positron impact, we found similar values for positron and electron cross-sections. In both cases, our distorted-wave models provide higher values than the CPE in the region of the peak. However, the positron cross-sections are slightly higher than for electron cross-sections, except for the TS model.

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