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"Ionization Cross Sections Of Oxygen And Water Molecules For Modeling Electron-Induced Processes In Environmental And Astrophysical Media"

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Abstract
In this study, we present a theoretical evaluation of ionization cross sections for diatomic oxygen (O_2) and water (H_2O) molecules under electron impact using the Complex Scattering Potential–Ionization Contribution (CSP-ic) method, refined here as the Improved CSP-ic (ICSP-ic) approach. The ICSP-ic model offers a semi-empirical framework grounded in scattering theory to estimate total ionization cross sections, especially useful in the absence of extensive experimental data or for extending known data to higher energy ranges.
Calculations have been performed over a broad energy range (e.g., 10–2000 eV), covering the ionization threshold to well beyond the peak cross-section region. The obtained cross-section values are compared with available experimental data and existing theoretical models for validation. Our results show good agreement with known data and demonstrate the capability of the ICSP-ic method to reliably predict ionization behavior of small polyatomic and diatomic systems under electron impact. The insights from this study contribute to the growing database of cross sections critical for modeling atmospheric, astrophysical, and plasma environments where electron-molecule interactions play a pivotal role.

INTRODUCTION

Electron-molecule interactions, particularly electron impact ionization processes, play a crucial role in a wide range of natural and technological environments. Among the most significant molecular targets in such studies are oxygen (O_2) and water (H_2O) — both of which are abundant and chemically vital in Earth's atmosphere, biological systems, plasma devices, and space environments.

The ionization of O_2 and H_2O by energetic electrons is a fundamental process that governs the chemistry of the ionosphere and upper atmosphere, influencing auroral emissions, ozone layer dynamics, and atmospheric re-entry physics [1–3]. In plasma processing and plasma medicine, understanding the cross sections for electron-induced ionization is essential for modeling energy deposition and reactive species generation [4, 5]. Additionally, in radiation biology and radiation therapy, the secondary electrons produced by high-energy radiation can ionize water — the primary component of biological tissue — leading to molecular fragmentation and DNA damage through radical formation [6, 7]. Similarly, in astrophysical and planetary environments, both O_2 and H_2O are critical constituents whose ionization governs energy transport and ion chemistry [8].

Due to their importance, accurate evaluation of the total ionization cross sections (TICS) for these molecules is of high interest. Experimental data, though available in some energy ranges, often lack consistency or completeness across the full spectrum of incident electron energies. Therefore, theoretical approaches are widely employed to estimate or supplement the data. Among these, the Complex Scattering Potential – Ionization Contribution (CSP-ic) method, and its improved form, ICSP-ic, have emerged as reliable semi-empirical tools for computing electron impact ionization cross sections [9–11]. These models are particularly useful for targets where experimental data is sparse or difficult to obtain, as they incorporate physical scattering parameters and empirical ionization thresholds to produce robust energy-dependent cross sections.

In this study, we apply the ICSP-ic method to compute total ionization cross sections for O_2 and H_2O over a wide range of incident electron energies. The results are compared with available experimental and theoretical data to assess the model's accuracy and applicability. The findings provide valuable input for modeling electron-driven

processes in diverse environments, ranging from low-temperature plasmas to planetary atmospheres and radiation-affected biological systems.

In this section we report improved calculations of total ionization cross sections, Q_{ion}, for di and triatomic molecules (O_2, H_2O) on electron impact at energies from circa threshold to 2000 eV using the Improved Complex Spherical Potential – ionization contribution (ICSP-ic) method[12]. It involves the computation of ratio R_P in terms of the first electronic excitation energy (E_1), the ionization threshold (I) and energy at the peak of inelastic cross section (E_P) of the target. The computed R_P values for the present targets are listed in table 1 below.

Table 1: Properties of target along with values of R_P in the ICSP-ic method

Target	E_1 (eV) [81-89]	I (eV) [84,85]	E_P (eV)	R_P
O_2	8.40	12.07	80	0.66
H_2O	9.34	12.61	80	0.71

THEORETICAL METHODOLOGY

In the present study, we employ the Improved Complex Scattering Potential – Ionization Contribution (ICSP-ic) method to calculate the total ionization cross sections (Qion) of the O_2 and H_2O molecules due to electron impact over a broad energy range. This semi-empirical approach builds upon the foundational CSP-ic model, introducing refinements that enhance its predictive accuracy and physical grounding, particularly regarding the estimation of the key ratio parameter RP.

COMPLEX OPTICAL POTENTIAL FRAMEWORK

The electron-molecule interaction is described within the fixed-nuclei approximation, and the system is modeled using a spherically symmetric complex optical potential (SCOP):

$$\mathbf{V_{opt}(Ei, r) = V_R(Ei, r) + iV_I(Ei, r)}$$

Here, the real part V_R includes:
- Static potential V_{st}, derived at the Hartree-Fock level,
- Exchange potential V_{ex}, and
- Polarization potential V_p, accounting for short-range correlation and long-range polarization effects.

The imaginary part V_I corresponds to the absorption potential V_{abs}, representing the flux loss into all inelastic channels. It is based on the non-empirical, quasi-free model proposed by Staszewska et al., and depends on target charge density, incident energy, and a threshold parameter **Δ**, which varies with energy to accommodate excitation at low energies and ionization at higher energies.

CALCULATION OF CROSS SECTIONS

The Schrödinger equation is solved numerically via partial wave analysis using the Numerov method, yielding complex phase shifts for the SCOP. These are used to calculate:
- Elastic cross section $Q_{el}(E_i)$
- Inelastic cross section $Q_{inel}(E_i)$, from which the total cross section is given by:

$$\mathbf{Q_T(E_i) = Q_{el}(E_i) + Q_{inel}(E_i)}$$

Since ionization cross section is not directly extractable, the ICSP-IC method partitions the inelastic component as:

$$\mathbf{Q_{inel}(E_i) = \Sigma Q_{exc}(E_i) + Q_{ion}(E_i)}$$

To estimate Q_{ion}, a ratio function is defined:

$R(E_i) = Q_{ion}(Ei) / Q_{inel}(E_i) = 1 - f(U)$

$f(U) = C1 * (C2 / (U + a) + \ln(U)/U)$, where $U = Ei/I$

Parameters C1, C2, a are computed using the following boundary conditions:
- $R = 0$ for $Ei \leq I$

- R = RP at $E_i = E_P$ (peak of Qinel)
- $R \rightarrow 1$ as $E_i \rightarrow \infty$

For detail Theoretical Methodology you can refer [12]

RESULTS AND DISCUSSION

The computed total ionization cross sections for present targets are plotted in figures 1-2 respectively along with other experimental and theoretical results available in the literature as a function of incident energy.

O_2 and H_2O

Both O_2 and H_2O are perhaps the most important and ubiquitous biologically important molecules for the growth and sustenance of biological systems. In nature, free oxygen is produced by the light-driven splitting of water during oxygenic photosynthesis. Molecular dioxygen, O_2, is essential for cellular respiration in all aerobic organisms. Oxygen is used in mitochondria to help to generate adenosine triphosphate (ATP) during oxidative phosphorylation [13]. The water content of the human body is about 60% by weight. Any radiation that penetrates the human body produces secondary electrons, with appreciable kinetic energy, that will subsequently interact with water to liberate free radicals e.g., OH which lead to various biological effects in the human body. Electron interactions with water have therefore been studied extensively although there remain several questions as to the magnitude of many cross sections [14].

Table 2: Total ionization cross sections, Q_{ion} (Å^2) for O_2 and H_2O.

E_i (eV)	O_2	H_20
15	0.09	0.04
20	0.41	0.31
30	1.08	1.05
40	1.61	1.62
50	1.94	1.95
60	2.19	2.13
70	2.37	2.22
80	2.50	2.28
90	2.59	2.29
100	**2.65**	**2.30**
200	2.49	1.96
300	2.20	1.58
400	1.94	1.35
500	1.74	1.17
600	1.59	1.04
700	1.45	0.94
800	1.33	0.85
900	1.24	0.78
1000	1.16	0.71
2000	0.69	0.43

Here, the calculated total cross sections on electron impact ionization for H_2O and O_2 are the updates of the previous results [14,15]. Total ionization cross sections for O_2 are measured by Rapp and E. Golden [16] and Krishnakumar and Srivastava [17]. Theoretically Q_{ion} for O_2 are reported by only two groups, Kim et al [18] and Deutsch et al [19]. In the case of H_2O, there is theoretical study for Q_{ion} by Kim et al [20] and experimental study by Straub et al [21].

Total ionization cross sections for O_2 and H_2O are tabulated in the table 2. They are also presented in figures 1 – 2 as a function of incident electron energy with other experimental and theoretical investigations available in the literature.

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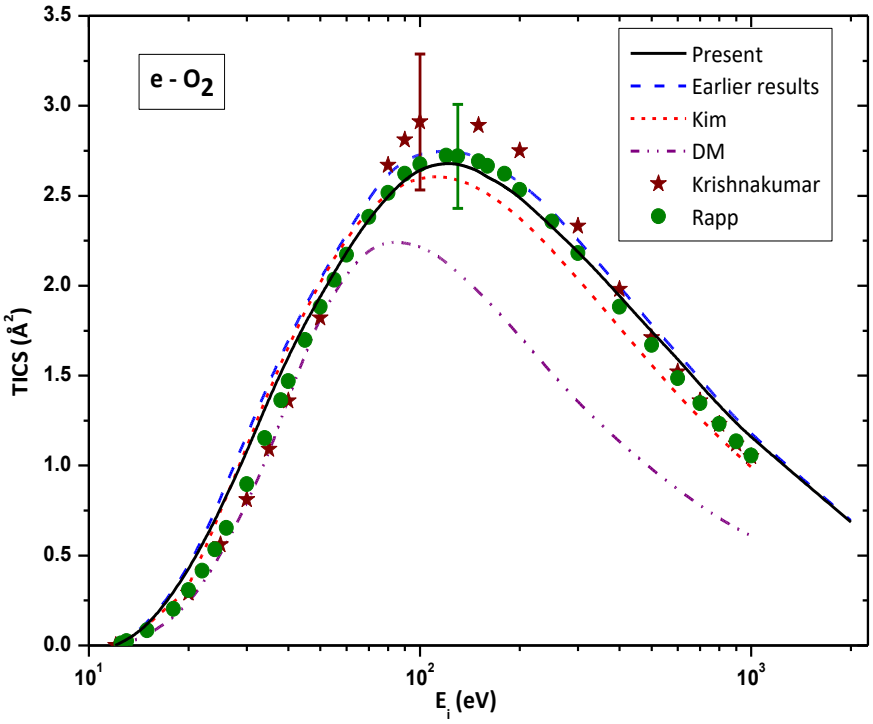

Figure 1: Total Ionization Cross Sections, Q_{ion}, for e – O_2 scattering in Å^2.

Solid line → Present results with new CSP-ic method; Dashed line → Earlier results with old CSP – ic method [15]; Short dashed line → Kim et al [18]; Dashed dot dot line → Deutsch et al [19]; Stars →Krishnakumar and Srivastava [17]; Filled Circle → Rapp and Englander-Golden [16].

Figure 1 shows the comparison of e – O_2 scattering. For e –O_2 scattering the present results do not differ much from the earlier results [15] and they agree very well with experimental values of Rapp et al[16] throughout the reported values. The present values are slightly lower than the experimental values of Krishnakumar and Srivastava [17] especially near the peak but well within their experimental uncertainty. The theoretical values of Kim et al [18] are in good accord with present values throughout the energy range. The theoretical values of Deutsch et al[19] are in good accord till 40 eV beyond which they are exceedingly lower compared to all other reported data [17,18]. The peak value of the cross section is around 100 eV for all reported data except for DM data for which the peak is around 80 eV.

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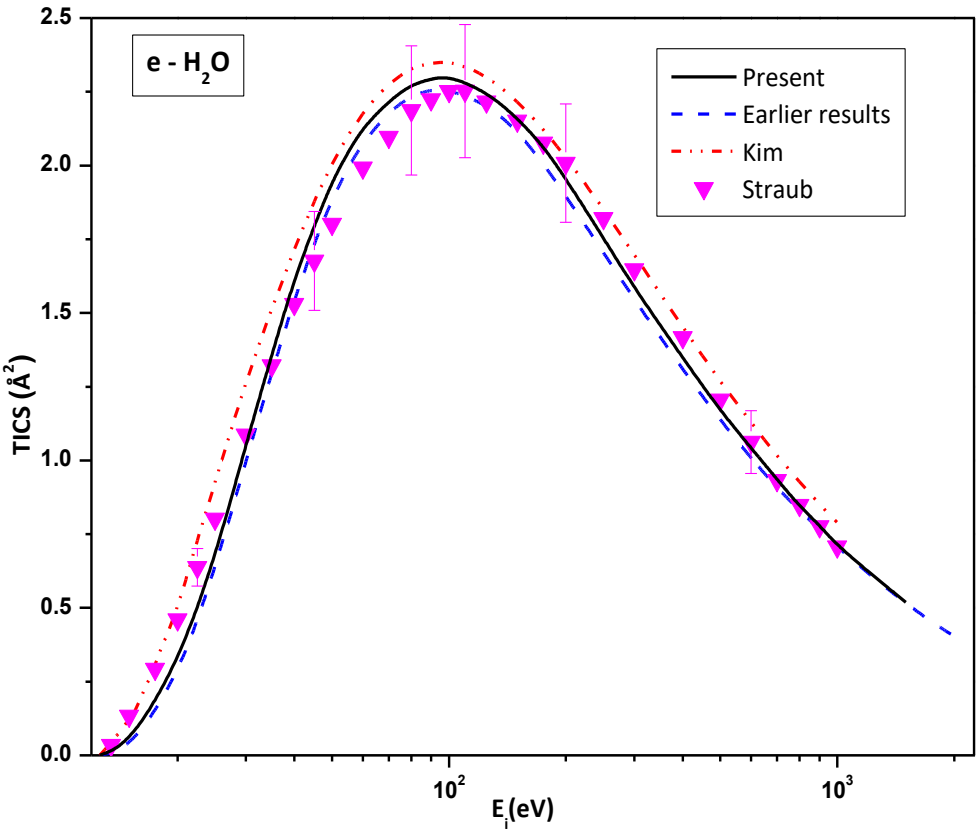

Figure 2: Total Ionization Cross Sections, Q_{ion}, for e–H_2O scattering in Å^2.

Solid line → present results with new CSP-ic method; Dashed line → Earlier results with old CSP – ic method [14]; Dash dot dot line → Kim et al [20]; Solid down triangles → Straub et al [21].

In case of H_2O (Figure 2), again the present results are very close to earlier [14] values. The present data compare very well with experimental values of Straub et al[21] and theoretical values of Kim et al [20] throughout the given range. The peak of the ionization cross sections is around 100 eV for all the reported data.

In general comparing the curves for e – O_2 and e – H_2O it can be noticed that both the curves show peak at around 100 eV and their ionization threshold are also very near, 12.07 eV for O_2 and 12.61 eV for H_2O. Also, comparing the maximum value of the cross sections it is 2.65 Å^2 and 2.30 Å^2 for O_2 (16 electrons) and H_2O (10 electrons).

CONCLUSION

In this study, we have successfully applied the Improved Complex Scattering Potential – Ionization Contribution (ICSP-ic) method to evaluate the total ionization cross sections for O_2 and H_2O molecules over a broad range of incident electron energies. The ICSP-ic model builds upon the original CSP-ic approach by introducing a more physically grounded estimation of the key parameter R_P, based on target-specific excitation and inelastic processes. This refinement enhances the model's consistency and predictive capability.

The calculated ionization cross sections show trends consistent with physical expectations, including the correct onset at the ionization threshold, a rise toward a peak, and a gradual fall-off at higher energies. These results are found to be in good agreement with available experimental and theoretical data, validating the effectiveness of the ICSP-ic model for small molecular targets like O_2 and H_2O.

Given the fundamental importance of these molecules in atmospheric chemistry, plasma environments, astrophysical media, and radiation biology, the cross section data obtained here provide a valuable input for

modeling electron-driven processes in diverse scientific and technological contexts. Moreover, the success of the ICSP-ic method in capturing ionization dynamics of such key molecular systems underscores its potential applicability to a broader range of molecular targets, including radicals and bio-relevant species.
Future work may involve extending this approach to compute differential or partial ionization cross sections, or coupling it with plasma modeling tools to study energy deposition and ion production rates in complex media.

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