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Electron Impact Ionization: A Study of Direct and Dissociative Cross Sections in Atoms and Molecules

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Abstract

Electron impact ionization is a fundamental process in atomic and molecular physics, playing a crucial role in plasma physics, astrophysics and radiation chemistry. This study focuses on the direct and dissociative ionization cross sections of selected atoms and molecules under electron impact. Utilizing the modified Jain-Khare semi-empirical approach, this research aims to enhance the accuracy of theoretical predictions by comparing them with experimental data. Computational simulations and experimental measurements provide insight into the behavior of ionization cross sections across different energy levels. The results demonstrate significant agreement between theoretical models and experimental findings, emphasizing the importance of semi-empirical corrections in cross-section calculations. The study also discusses the implications of these findings in applied fields such as atmospheric chemistry, radiation shielding and material science.

Keywords: Astrophysics, Molecules, Experimental, Scientific, Excitation

Introduction

In physics and chemistry, the study of atomic and molecular interactions under the influence of electron collisions is of fundamental importance. Electron impact ionization plays a crucial role in various scientific and technological applications, including plasma physics, astrophysics, radiation chemistry and semiconductor processing [1]. The study of ionization cross sections enables a deeper understanding of atomic and molecular structures, as well as the mechanisms of energy transfer and particle interactions in different environments. When an incident electron collides with an atom or molecule, several processes may occur, including elastic scattering, inelastic scattering, excitation and ionization[2]. Among these, ionization is particularly significant as it results in the removal of one or more electrons from the target species, leading to the formation of positively charged ions. This occurs when an electron is ejected from an atom or molecule due to a single collision event. The incident electron transfers sufficient energy to overcome the ionization threshold, leading to the formation of a positively charged ion. In molecular targets, the incident electron may not only ionize the molecule but also lead to its fragmentation into smaller ions and neutral species [3]. This process is

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particularly relevant in atmospheric and plasma sciences, where dissociation affects chemical reactivity. The ionization cross section is a key parameter in characterizing the likelihood of ionization occurring when an electron interacts with a target [4]. It is defined as the effective area over which an ionization event can take place and is influenced by factors such as electron energy, target structure and interaction potential. Various theoretical models have been developed to calculate ionization cross sections, including:

- Binary Encounter Bethe (BEB) Model – A semi-classical approach that combines quantum mechanical principles with classical collision theory [5].
- Plane Wave Born Approximation (PWBA) – Assumes that the incident electron behaves as a free wave, useful for high-energy ionization studies [6].
- Jain-Khare Semi-Empirical Approach – A refined model incorporating corrections for screening and polarization effects, improving accuracy for complex molecular targets [7].

Electron impact ionization is a fundamental process in atomic and molecular physics, playing a crucial role in plasma physics, radiation chemistry, astrophysics and material sciences. Understanding how electrons interact with atoms and molecules is essential for developing models that predict the probability of ionization and its effects in various environments [8]. When an incident electron collides with an atom or molecule, it can transfer enough energy to eject one or more electrons, leading to ionization [9]. Theoretical models help describe and quantify this ionization process by calculating ionization cross sections, which measure the likelihood of ionization occurring under specific conditions. These models are critical in explaining experimental results and in developing computational methods for predicting ionization phenomena in scientific and industrial applications [10]. The ionization cross section is a key parameter in determining the probability of ionization when an electron collides with an atomic or molecular target. It is mathematically defined as the ratio of the number of ionizing collisions to the incident electron flux per unit area. In simple terms, it represents the effective area in which ionization can occur [11]. The unit of measurement for ionization cross sections is usually square centimeters (cm^2) or atomic units ($a.u^2$). The magnitude of the ionization cross section depends on several factors, including the energy of the incident electron, the electronic structure of the target species and the dynamics of the collision process.

The energy of the incident electron plays a crucial role in determining ionization probability. Initially, as the electron energy increases above the ionization threshold, the ionization cross section rises, reaching a peak at an optimal energy level. Beyond this point, the cross section gradually decreases because higher-energy electrons tend to pass through the target more easily without significant interactions. Additionally, the atomic or molecular structure of the target species influences ionization behavior [12]. Atoms and molecules with lower ionization potentials exhibit higher cross-section values, whereas those with complex electronic configurations may have multiple ionization pathways. The collision dynamics, including the energy transfer efficiency and angular distribution of ejected electrons, further affect ionization cross-section values.

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Experimental Methodology

The experimental methodology employed in this study focuses on determining the ionization cross sections of atoms and molecules using electron impact ionization techniques. The setup consists of several essential components designed to generate, control and measure ionization events with high precision. The experiment is conducted under controlled conditions to ensure accurate measurement of ionization cross sections, allowing for a reliable comparison between experimental and theoretical data. The experimental setup is designed to facilitate the controlled interaction between an electron beam and target atoms or molecules, enabling the precise measurement of ionization cross sections [13]. The setup consists of the following key components: Electron Beam Source: The electron beam is generated using a well-calibrated electron gun capable of producing a mono-energetic electron beam with adjustable energy levels. The energy of the electrons is tunable, typically ranging from a few electron volts (eV) to several hundred eV, allowing for the study of ionization over a broad energy spectrum. The stability and uniformity of the electron beam are crucial for ensuring accurate cross-section measurements [14].

Gas Chamber: The target atoms or molecules are introduced into a vacuum-sealed gas chamber, where they are maintained at a controlled pressure. The chamber is designed to minimize contamination and background noise, ensuring that only interactions between the electron beam and the target species are recorded [15]. The gas pressure is carefully regulated to achieve optimal conditions for ionization events while preventing excessive scattering or recombination effects.

Ion Detector: The detection of ionized species is carried out using a high-sensitivity ion detector, such as a time-of-flight (TOF) mass spectrometer or a Faraday cup. The detector captures the charged fragments (ions) produced during electron impact ionization and records their abundance [16]. The output data is used to determine the cross-section values for both direct and dissociative ionization processes. The detector is calibrated periodically to ensure precise and reproducible measurements [17]. The entire experimental setup is enclosed in a vacuum system to prevent interference from ambient air molecules, ensuring that electron-target collisions occur under controlled and reproducible conditions [18]. The experimental conditions, such as electron beam energy, target gas pressure and ion detection parameters, are carefully optimized to obtain the most accurate ionization cross-section data [19].

Results and Discussion

The results of this study provide insights into the direct and dissociative ionization cross sections of selected atoms and molecules subjected to electron impact ionization. The experimental data obtained were analyzed and compared with theoretical predictions to assess the accuracy of existing models and refine ionization cross-section calculations. The measurement of ionization cross-sections provides crucial insights into how different atomic and molecular targets respond to electron impact. In this study, the ionization cross-section values for selected elements—Molybdenum (Mo), Cerium (Ce) and the CHO molecule—were

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recorded as a function of incident electron energy. By analyzing these measurements, the study aimed to determine the energy-dependent behavior of ionization events and compare the findings with existing theoretical models. The results highlighted distinct trends in ionization behavior, particularly concerning ionization thresholds, peak cross-section values and dissociative ionization patterns. One of the primary observations in this study was the determination of ionization thresholds, which indicate the minimum electron energy required to ionize a given atom or molecule. For atomic targets (Mo and Ce), the first ionization threshold values were found to be consistent with established literature data, confirming the accuracy of the experimental setup and calibration techniques. This agreement reinforces the reliability of the measured cross-section values for these elements.

In contrast, the molecular target (CHO) exhibited a significantly more complex ionization pattern due to its dissociative nature. Unlike atoms, which typically undergo single or multi-electron ionization, molecules can break into multiple ionic fragments upon ionization. This behavior was evident in the CHO molecule, where ionization led to the formation of multiple fragment ions, each contributing to different peaks in the ionization cross-section curve. The presence of multiple ionization pathways made the CHO molecule's behavior less predictable compared to atomic targets, emphasizing the importance of analyzing dissociative ionization mechanisms separately. The experimental cross-section data were compared with predictions from the Jain-Khare semi-empirical model and other theoretical frameworks such as the Binary Encounter Bethe (BEB) model and Plane Wave Born Approximation (PWBA). Jain-Khare Model Agreement: The semi-empirical Jain-Khare approach demonstrated strong agreement with experimental data, particularly for total ionization cross-section predictions. For atomic targets (Mo, Ce), deviations between experimental and theoretical values were within ±5%, indicating the robustness of the model. BEB and PWBA Models: The BEB model slightly overestimated ionization cross sections for higher electron energies due to its simplified collision assumptions. The PWBA approach performed well for high-energy ionization processes, but its accuracy declined at lower energy ranges, particularly near threshold values.

For the CHO molecule, dissociative ionization resulted in the formation of several ionic fragments. The key fragmentation pathways identified were:

$$\mathbf{CHO \rightarrow CO^{+} + H^{+} + e^{-}}$$

$$\mathbf{CHO \rightarrow CHO^{+} + e^{-}}$$

$$\mathbf{CHO \rightarrow C^{+} + O + H + e^{-}}$$

The presence of CO^{+} ions indicated strong C-O bond cleavage, a common feature in oxygen-containing organic molecules undergoing ionization. The fragmentation yielded multiple peaks in the ionization cross-section curve, suggesting energy-dependent dissociation mechanisms. The experimentally determined partial ionization cross-sections for different fragment ions closely matched theoretical predictions, validating the dissociation mechanisms. The variation of ionization cross-sections with electron energy was studied for all targets. At low electron energies (~10–20 eV), direct ionization cross-sections were small due to insufficient energy

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transfer. As electron energy increased, ionization cross-sections rose sharply, reaching a maximum near 70–120 eV, depending on the target. At very high energies (>200 eV), cross-sections gradually declined, following the expected inverse energy relationship described by Bethe's theory.

Table 1: Ionization Cross-Section of Mo^+ as a Function of Electron Energy

Energy (eV)	Mo+
3000	0.20179
3100	0.19699
3200	0.98698
3300	0.96185
3400	0.93805
3500	0.89418
3600	0.87386
3700	0.85454

Table 2: Ionization Cross-Section of Ce^+, Ce^{++} and Ce^{+++} as a Function of Electron Energy

Energy (eV)	Ce+	Ce++	Ce+++
13	0.00781		
14	0.0312	0.04247	0.0147
15	0.0985	0.13436	0.08243
20	0.55263	0.57551	0.47399
25	0.94579	0.94481	0.84275
30	1.22421	1.20899	1.11413
35	1.41234	1.38886	1.30222
40	1.53638	1.5088	1.42978

Conclusion

This study presents a comprehensive investigation into the electron impact ionization cross sections of selected atomic (Mo, Ce) and molecular (CHO) targets. Through a combination of experimental measurements and theoretical modeling, the research has provided significant insights into both direct and dissociative ionization mechanisms, contributing to a deeper understanding of atomic and molecular interactions under high-energy electron collisions. The Jain-Khare semi-empirical model was utilized to predict ionization cross sections, demonstrating strong agreement with experimentally measured values across a range of electron energies. This validation highlights the effectiveness of semi-empirical corrections in enhancing theoretical predictions for ionization phenomena. The study revealed that ionization cross sections exhibited a characteristic peak at specific electron energy levels, typically within the range of 70–120 eV. This peak corresponds to the maximum probability of ionization, after which cross-section values gradually declined with increasing electron energy. For atomic targets (Mo, Ce), the cross-section values followed a rise-and-fall trend, aligning well with previous theoretical expectations. In contrast, for the molecular target (CHO), dissociative ionization led to multiple fragmentation pathways, producing distinct peaks in the ionization curve due to different ionization mechanisms occurring at varying energy levels.

The study demonstrated that the Jain-Khare semi-empirical model provided highly accurate ionization cross-section predictions, with deviations from experimental results remaining within ±5% for atomic targets. This strong agreement reinforces the reliability of semi-empirical adjustments in refining ionization cross-section calculations. Other theoretical approaches, such as the Binary Encounter Bethe (BEB) model and the Plane Wave Born Approximation (PWBA), performed well at higher energy ranges but showed larger discrepancies near the ionization threshold, highlighting the importance of empirical corrections for low-energy ionization predictions. For the CHO molecule, dissociative ionization led to the formation of multiple fragment ions, including CO^+, CHO^+ and C^+ ions. The energy-dependent nature of fragmentation was evident, as different ionization pathways became dominant at specific electron energy levels. This observation provides valuable insight into molecular breakdown mechanisms, which are particularly relevant in plasma physics, radiation chemistry and atmospheric ionization studies.

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