



Research Article

# Electron-Induced Ionization of the Boron Monochloride Molecule

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## Abstract

In the present study, the electron impact ionization characteristics of the (BCl) molecule have been investigated using the semi-empirical Jain–Khare formalism. The total ionization cross sections have been calculated over a wide range of incident electron energies from ionization threshold to 5000eV. In addition to the total ionization cross sections, the optical oscillator strength distribution has been evaluated, as it represents an important input parameter governing the dipole interaction effect in molecular ionization processes. Furthermore, the ionization rate coefficients have been determined by combining the calculated cross sections with the appropriate electron energy Maxwell-Boltzmann distribution, which is particularly relevant for plasma applications.

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**KEYWORDS:** Total ionization cross sections, Oscillator strength, ionization rate coefficients, Jain-Khare semi-empirical approach.

## 1. INTRODUCTION

Electron–molecule collision processes have been a subject of sustained interest in atomic and molecular physics due to their fundamental role in understanding the interaction of charged particles with matter. Among these processes, electron impact ionization is particularly significant, as it governs the production of ions and free electrons in gaseous systems and directly influences plasma behaviour, gas discharge phenomena, atmospheric chemistry, and plasma-assisted material processing technologies. Accurate ionization data are therefore essential for reliable modelling of such environments, since they affect reaction rates, energy transfer mechanisms, and charge balance in plasmas [1-3]. In addition to ionization cross sections, other related quantities such as optical oscillator strength and ionization rate coefficient play an important role in describing electron–molecule interactions. It is widely used in semi-empirical ionization models, including the Jain–Khare formalism, to account for the energy-dependent behavior of ionization cross sections [4]. The oscillator strength represents the probability of electronic transitions within a molecule and is a key parameter in determining dipole interaction contributions to ionization processes [5]. Accurate oscillator strength data are therefore essential for obtaining physically meaningful ionization cross sections. Here, ionization rate coefficients are derived from ionization cross sections by incorporating the electron energy distribution. It provides a direct measure of the rate at which ionization occurs in plasma environments and is particularly relevant for plasma diagnostics and kinetic modelling. While ionization cross sections describe the probability of ionization for a given electron energy, the ionization rate coefficient links this probability to realistic plasma conditions, making it a crucial parameter in applied plasma studies. Despite their importance, experimental measurements of electron impact ionization cross sections, oscillator strengths, and ionization rate coefficients are often difficult to obtain for molecular targets. Experimental challenges arise due to molecular complexity, multiple fragmentation channels, and the chemical reactivity or instability of many molecules [6-7]. Consequently, for many molecular systems of technological relevance, reliable experimental data remain scarce or unavailable. This has led to increased reliance on theoretical and semi-empirical models, which provide an effective alternative for estimating ionization-related quantities over a wide range of incident electron energies [8-9]. Boron monochloride (BCl) is a boron-containing molecule of interest in plasma-assisted material processing, chemical vapour deposition, and semiconductor fabrication environments. In such plasma systems, boron halides often appear as reactive intermediates and significantly influence plasma chemistry and surface reactions [10]. However, detailed information on electron impact ionization cross sections, oscillator strength, and ionization rate coefficients for the BCl molecule is very limited in the existing literature. This lack of data limits accurate plasma modelling of boron–chlorine systems and underscores the need for reliable theoretical investigations. Among the available semi-empirical approaches, the Jain–Khare formalism has been successfully applied to several atomic and molecular targets. This model combines the

Bethe theory, which is valid in the high-energy region, with Mott-type binary collision contributions that dominate at intermediate energies, enabling the calculation of ionization cross sections over a wide energy range [11]. The formalism also incorporates oscillator strength distributions, making it suitable for studying molecular ionization processes where dipole interactions are important [12]. In the present work, the electron impact ionization characteristics of the BCl molecule have been investigated using the semi-empirical Jain–Khare formalism [4, 13-17]. The total ionization cross section and oscillator strength have been calculated, and the ionization rate coefficient has been evaluated by combining the cross-section data with the Maxwell-Boltzmann distribution [18-19]. The obtained results are analyzed and compared with available theoretical data reported in the literature. The objective of this study is to assess the applicability of the Jain–Khare formalism to the BCl molecule and to provide a consistent set of ionization parameters that may be useful for theoretical studies and plasma modelling applications.

## 2. Theoretical Model and Inputs:

Several theoretical approaches have been developed to calculate electron impact ionization cross sections. Among them, the Binary Encounter model [12] and the Bethe theory underpin many modern formulations. The Binary Encounter approach is effective at low and intermediate energies, where direct electron-electron collisions dominate, whereas Bethe theory provides an accurate description at high incident electron energies, where dipole interactions are significant [20]. Semi-empirical models combine these two approaches to achieve reasonable accuracy over a broad energy range. Such models require molecular parameters like ionization potentials, orbital energies, and electron occupation numbers as input. Well-known semi-empirical models include the Binary Encounter Bethe (BEB) model and the Jain–Khare formalism, both of which have been successfully applied to a variety of atomic and molecular targets. In the present work, the electron impact ionization cross section of the BCl molecule has been calculated using the Jain–Khare formalism. This model was developed to provide a unified description of ionization processes over a wide range of incident electron energies by incorporating both binary collision and dipole interaction effects. The Jain–Khare model expresses the total ionization cross section as a sum of contributions from individual molecular orbitals. Each orbital contribution depends on its ionization energy, electron occupation number, and kinetic energy of the bound electrons. By summing over all occupied molecular orbitals, the total ionization cross section of the molecule is obtained. This orbital-based approach allows the model to capture essential molecular structure effects in a simplified yet effective manner. At low and intermediate electron energies, the ionization process is primarily governed by direct binary collisions between the incident electron and the target electrons. The Jain–Khare model accounts for this mechanism using binary encounter theory, which treats the collision as an interaction between two electrons. This approach successfully describes the rapid rise of the ionization cross section just above the ionization threshold [13].

At higher energies, long-range dipole interactions become increasingly important. To account for this, the Jain–Khare formalism incorporates Bethe-type terms, ensuring the correct asymptotic behavior of the ionization cross section at high incident electron energies. The inclusion of both mechanisms allows the model to reproduce the characteristic peak and high-energy falloff observed in experimental and theoretical ionization cross-section curves [13].

According to the Jain–Khare formalism, the total ionization cross section  $Q_i(E)$  is expressed as the sum of two components: the Bethe term and the Mott term, given by

$$Q_i(E) = Q_i^B(E) + Q_i^M(E) \quad \text{..... (1)}$$

where  $Q_i^B(E)$  represents the Bethe contribution dominant at higher incident energies, and  $Q_i^M(E)$  represents the Mott contribution important near the ionization threshold. This combination allows the model to remain valid across a broad energy range.

At higher incident energies, the ionization process is dominated by direct collisions between the fast incident electron and the bound electrons of the target molecule. This interaction is well described by Bethe's theory, which predicts a logarithmic dependence of the ionization cross section on the incident energy. The Jain–Khare model modifies this expression to include molecular parameters and empirical corrections [4].

The Bethe term is given by:

$$Q_i^B(E) = \frac{4\pi a_0^2 R}{E-I} \left[ M_i^2 - \frac{R}{E} S_i \right] \ln [1 + C_i(E-I)] \quad \text{..... (2)}$$

Here,  $a_0$  is the Bohr radius,  $R$  is the Rydberg energy,  $E$  is the incident electron energy,  $I$  is the ionization potential of the target molecule, and  $C_i$  is the collision constant. The quantities  $S_i$  and  $M_i^2$  represent oscillator strength integrals that account for the energy distribution of the ionized electrons

The oscillator strength distribution plays a central role in describing how energy is transferred from the incident electron to the molecule's bound electrons. In the Jain–Khare formalism, the differential oscillator strength  $df/dW$  is approximated by a simple analytical form, enabling efficient numerical evaluation. It is a very difficult task to evaluate the continuum generalised oscillator strength theoretically. In the present investigation, we employ the semi-phenomenological expression of CGOS, derived from a statistical model of Weizsacker-Williams (from Eq. (38) of Ref. [21]) and which is given by

$$\left[ \frac{df(W,Q)}{dW} \right]_{WW} = h(Q)\delta(W-Q) + \frac{df(W,0)}{dW} \theta(I-Q) \quad \text{..... (3)}$$

where  $WW$  stands for Weizsacker-Williams and  $\delta$ ,  $\theta$  are the delta and step functions, respectively, and

$$h(Q) = \int_I^Q \frac{df(W,0)}{dW} dW \quad \text{..... (4)}$$

The COOS may be experimentally known or computed. The experimental values of COOS are limited to the molecules. The theoretical generation of COOS is a challenging task. Hence,

we use the approximated analytic form of COOS given by Kim and Rudd [22], and it is given by

$$\frac{df(W,0)}{dW} = \frac{b}{(W+I)^2} \quad \text{..... (5)}$$

where  $b=2NI$ , where  $N$  is the occupation number of molecular orbitals. To evaluate the value of  $b$ , we replace  $N_i$  by  $N$  in Eq. (47) of Ref. [22]. Now putting the expression of CGOS given by Eq. (3) with COOS given by Eq. (5) and following Khare et al. [23],

The integrals used in the Bethe term are defined as:

$$S_i = \int_I^E \frac{df}{dW} dW \quad \text{..... (6)}$$

$$3. \quad M_i^2 = \int_I^E \frac{R}{W} \frac{df}{dW} dW \quad \text{..... (7)}$$

Near the ionization threshold, secondary electron emission becomes significant and cannot be neglected. The Mott term in the Jain–Khare model accounts for these low-energy effects by incorporating a secondary-electron integral that describes energy sharing among outgoing electrons [4].

The Mott contribution is expressed as:

$$Q_i^M(E) = \frac{4\pi a_0^2 R^2 (E-I)}{E^2} S_i \int_I^E \frac{1}{(\epsilon^3 + \epsilon_0^3)} \left[ \epsilon - \frac{\epsilon^2}{E-\epsilon} + \frac{\epsilon^3}{(E-\epsilon)^2} \right] d\epsilon \quad \text{..... (8)}$$

The parameter  $\epsilon_0$  is an energy mixing parameter introduced to ensure smooth behavior of the cross section near the threshold energy [20-21]. Equations (2) and (8) jointly make an expression for total ionization cross-sections, i.e.

$$Q_i(E) = \frac{4\pi a_0^2 R}{E} \left[ \frac{E}{(E-I)(1+\frac{I}{E})} \left( M_i^2 - \frac{R}{W} S_i \right) \ln [1 + C_i(E-I)] + \int_I^E \frac{R}{E} S_i \frac{(E-I)}{(\epsilon_0^3 + \epsilon^3)} \left[ \epsilon - \frac{\epsilon^2}{(E-\epsilon)} + \frac{\epsilon^3}{(E-\epsilon)^2} \right] dW \right] \quad \text{..... (9)}$$

For plasma applications, the ionization rate coefficient is an important quantity derived from the ionization cross section using the Maxwell-Boltzmann distribution. The ionization rate coefficient is given by [18-19]:

$$R(T) = \int_{-\infty}^{\infty} 4\pi \left( \frac{1}{2\pi m k T} \right)^{3/2} m E Q_i(E) e^{-E/kT} dE \quad \text{..... (10)}$$

where  $T$  is the electron temperature,  $m$  is the electron mass, and  $k$  is the Boltzmann constant.

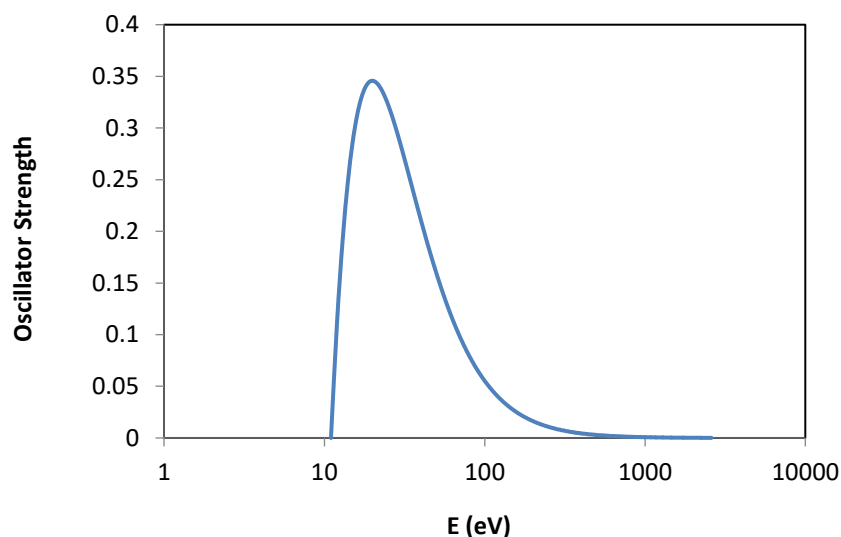
For the BCl molecule, the ionization potential is taken as  $I=10.2$  eV. The collision constant  $C_i = 0.08$  and the mixing parameter  $45$  eV are selected based on previous studies of similar molecular systems [14-17]. The total ionization cross section and ionization rate coefficient are calculated over a wide range of incident electron energies from the ionization

threshold to approximately 5000 eV using Thomas–Reiche–Kuhn (TRK) sum rule [14]

The combined contribution of the Bethe and Mott terms ensures that both high-energy and low-energy ionization mechanisms are accurately represented, making the model suitable for comparison with existing theoretical and experimental results. The computational methodology adopted in the present work is based on the numerical implementation of the Jain–Khare semi-empirical formalism. All calculations were carried out using the MATLAB programming environment, which is well-suited for numerical integration, data handling, and scientific visualization in atomic and molecular collision studies.

### 3. RESULTS AND DISCUSSION

The oscillator strength distribution of the BCl molecule as a function of incident electron energy is shown in **Figure 1**. The curve exhibits a large value at very low energies, followed by a rapid decrease with increasing electron energy. This behaviour is expected on physical grounds, as low-energy electrons interact more strongly with bound molecular electrons via dipole interactions, thereby increasing transition probabilities. As the incident energy increases, the probability of such transitions decreases, resulting in a smooth decay of the oscillator strength distribution.



**Figure 1:** Oscillator strength of the BCl molecule as a function of energy.

The oscillator strength plays a crucial role in determining the dipole (Bethe) contribution to the total ionization cross section in semi-empirical models such as the Jain–Khare formalism. The rapid falloff of oscillator strength at higher energies ensures the correct asymptotic behaviour of the ionization cross section in the high-energy region. The obtained distribution is consistent with previously reported theoretical treatments of molecular oscillator strengths and satisfies the physical requirements imposed by sum rules [20,14].

The calculated total electron impact ionization cross section (TICS) of the BCl molecule using the Jain–Khare formalism is given in **Table-1**, and presented in **Figure 2**. The cross section exhibits the characteristic energy dependence commonly observed in molecular ionization processes. Starting from zero at the ionization threshold, the cross section rises sharply with increasing incident electron energy, indicating an increasing probability of ionization once the threshold energy is exceeded. A well-defined maximum is observed in the intermediate energy region, where both binary collision and dipole interaction mechanisms contribute significantly to the ionization process. Beyond this energy, the cross-section gradually decreases with increasing energy, reflecting the reduced interaction time between the fast incident electron and

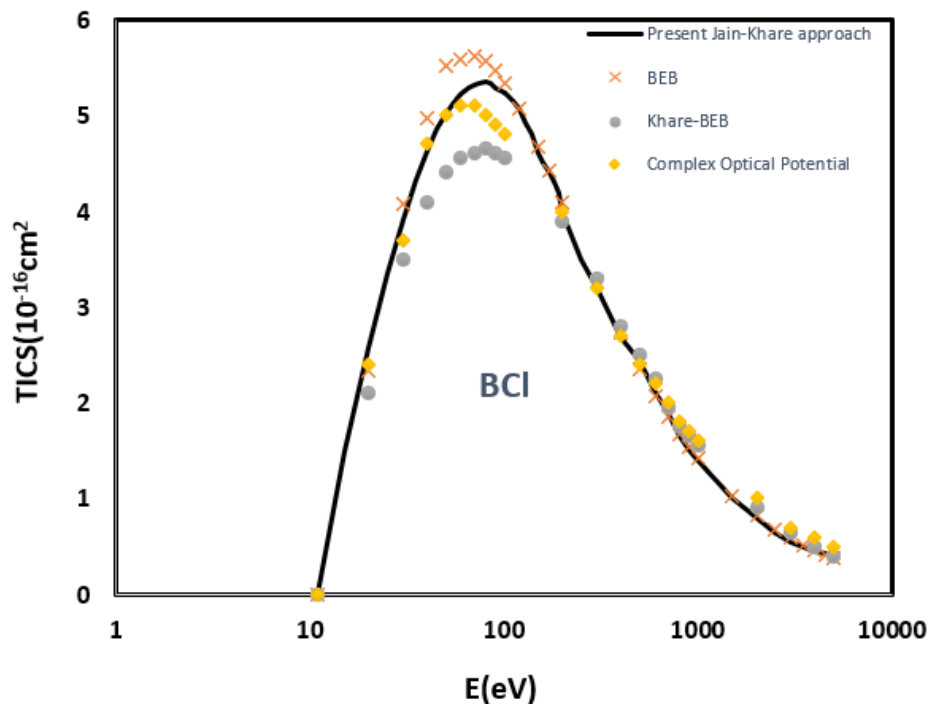
the target molecule. This overall trend agrees well with the general behaviour predicted by semi-empirical and experimental studies of electron impact ionization.

Figure 2 compares the present cross sections evaluated using the Jain–Khare formulation with other available theoretical results, including the BEB model [22], our additional results using the Khare–BEB model [23], and calculations based on complex optical potential methods [24]. The present results show good agreement with these models in terms of the overall shape of the curve and the position of the ionization maximum. Minor variations in the cross-section magnitude, particularly near the peak region, can be attributed to differences in model assumptions, molecular parameters, and the treatment of electron–electron interactions.

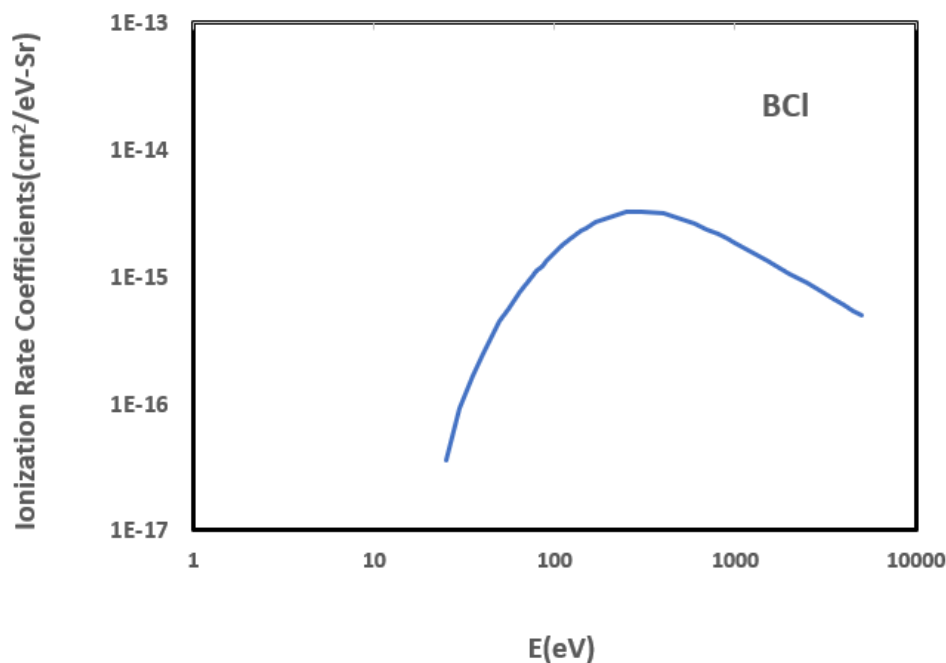
The BEB model generally predicts slightly higher cross-section values near the maximum, whereas the Khare–BEB model predicts lower cross-section values near the maximum; the complex optical potential results lie close to the present calculations over a broad energy range. Such deviations are commonly observed in theoretical ionization studies and reflect the sensitivity of ionization cross sections to the choice of oscillator strengths and collision parameters [12]. Overall, the comparison confirms the reliability of the present Jain–Khare calculations for the BCl molecule.

The ionization rate coefficient for electron impact ionization of BCl, derived from the calculated ionization cross section, is shown in **Figure 3** with **Table-2**. The rate coefficient increases rapidly at low energies, reaches a maximum, and then decreases

gradually at higher energies. This behavior directly reflects the energy dependence of the ionization cross section and the contribution of the electron energy distribution in the rate coefficient formulation [14].



**Figure 2:** The present total ionization cross-sections of the BCl molecule (solid line) with the comparison of available theoretical results i.e.,  $\times$  by BEB modal [22],  $\bullet$  by Khare-BEB modal evaluated with present results and  $\blacklozenge$  by M. Vinodkumar et.al. using optical complex potential [24]



**Figure 3:** The results of ionization rate coefficients for the BCl molecule corresponding to total ionization cross-sections using M-B distribution law.

**Table 1:** Total ionization cross-sections of BCl molecules

| E (eV) | Cross-Sections ( $10^{-16} \text{ cm}^2$ ) | E (eV) | Cross-Sections ( $10^{-16} \text{ cm}^2$ ) |
|--------|--------------------------------------------|--------|--------------------------------------------|
| 15     | 1.4878                                     | 160    | 4.5                                        |
| 20     | 2.5692                                     | 170    | 4.4                                        |
| 25     | 3.3468                                     | 180    | 4.3014                                     |
| 30     | 3.9105                                     | 190    | 4.2                                        |
| 35     | 4.3225                                     | 200    | 4                                          |
| 40     | 4.6255                                     | 250    | 3.5                                        |
| 45     | 4.8491                                     | 300    | 3.1982                                     |
| 50     | 5.0137                                     | 400    | 2.6848                                     |
| 55     | 5.134                                      | 500    | 2.4401                                     |
| 60     | 5.2203                                     | 600    | 2.1                                        |
| 65     | 5.2802                                     | 700    | 1.8823                                     |
| 70     | 5.3192                                     | 800    | 1.6473                                     |
| 75     | 5.3416                                     | 900    | 1.5                                        |
| 80     | 5.3504                                     | 1000   | 1.3817                                     |
| 85     | 5.337                                      | 1500   | 1                                          |
| 90     | 5.2934                                     | 2000   | 0.7878                                     |
| 100    | 5.2293                                     | 2500   | 0.63502                                    |
| 110    | 5.1512                                     | 3000   | 0.541                                      |
| 120    | 5.0641                                     | 3500   | 0.48992                                    |
| 130    | 4.9214                                     | 4000   | 0.44815                                    |
| 140    | 4.8                                        | 4500   | 0.42539                                    |
| 150    | 4.6                                        | 5000   | 0.41506                                    |

Ionization rate coefficients are particularly important for plasma modeling, as they determine the frequency of ionization events in electron–molecule collisions. The obtained rate coefficient values for BCl indicate efficient ionization in the intermediate energy range, which is relevant for plasma-assisted material

processing and gas discharge environments. The smooth variation of the rate coefficient further confirms the numerical stability and physical consistency of the present calculations [5].

**Table 2:** Ionization rate coefficients ( $\text{cm}^3/\text{eV}\cdot\text{Sr}$ ) of the BCl molecule

| E (eV) | Ionization rate coefficients ( $\text{cm}^3/\text{eV}\cdot\text{Sr}$ ) | E (eV) | Ionization rate coefficients ( $\text{cm}^3/\text{eV}\cdot\text{Sr}$ ) |
|--------|------------------------------------------------------------------------|--------|------------------------------------------------------------------------|
| 15     | 1.24E-17                                                               | 160    | 2.56E-15                                                               |
| 20     | 2.43E-17                                                               | 170    | 2.68E-15                                                               |
| 25     | 3.59E-17                                                               | 180    | 2.78E-15                                                               |
| 30     | 9.20E-17                                                               | 190    | 2.87E-15                                                               |
| 35     | 1.64E-16                                                               | 200    | 2.95E-15                                                               |
| 40     | 2.47E-16                                                               | 250    | 3.20E-15                                                               |
| 45     | 3.41E-16                                                               | 300    | 3.28E-15                                                               |
| 50     | 4.41E-16                                                               | 400    | 3.14E-15                                                               |
| 55     | 5.46E-16                                                               | 500    | 2.88E-15                                                               |
| 60     | 6.55E-16                                                               | 600    | 2.60E-15                                                               |
| 65     | 7.67E-16                                                               | 700    | 2.36E-15                                                               |
| 70     | 8.80E-16                                                               | 800    | 2.15E-15                                                               |
| 75     | 9.93E-16                                                               | 900    | 1.98E-15                                                               |
| 80     | 1.11E-15                                                               | 1000   | 1.83E-15                                                               |
| 85     | 1.22E-15                                                               | 1500   | 1.34E-15                                                               |
| 90     | 1.33E-15                                                               | 2000   | 1.06E-15                                                               |
| 100    | 1.55E-15                                                               | 2500   | 8.88E-16                                                               |
| 110    | 1.75E-15                                                               | 3000   | 7.64E-16                                                               |
| 120    | 1.94E-15                                                               | 3500   | 6.72E-16                                                               |
| 130    | 2.12E-15                                                               | 4000   | 6.01E-16                                                               |
| 140    | 2.28E-15                                                               | 4500   | 5.44E-16                                                               |
| 150    | 2.43E-15                                                               | 5000   | 4.98E-16                                                               |

## CONCLUSION

In the present work, a comprehensive theoretical investigation of electron impact ionization of the boron monochloride (BCl) molecule has been carried out using the semi-empirical Jain–Khare formalism. The study provides a consistent set of ionization-related parameters, including the optical oscillator strength distribution, total ionization cross section, and ionization rate coefficient, which are essential for understanding electron–molecule collision processes and for plasma modeling

applications. The calculated oscillator strength distribution exhibits a physically meaningful energy dependence, with higher values at low incident electron energies followed by a smooth decay at higher energies. This behavior confirms the reliability of the adopted analytical form and its suitability for describing dipole interaction effects within the Jain–Khare framework. The oscillator strength integrals obtained from this distribution play a crucial role in determining the Bethe contribution to the ionization cross section.

The total electron impact ionization cross section of BCl shows the characteristic features of molecular ionization processes, including a sharp rise just above the ionization threshold, a well-defined maximum at intermediate energies, and a gradual decrease at higher energies. Comparisons with other theoretical models, such as the BEB and complex optical potential approaches, indicate reasonable agreement in overall shape and peak position, thereby validating the applicability of the Jain–Khare formalism to the BCl molecule.

The ionization rate coefficient, derived from the calculated cross sections by assuming a Maxwell-Boltzmann electron energy distribution, displays the expected variation with electron energy and highlights the energy range where ionization is most effective. This parameter is particularly important for plasma diagnostics and kinetic modelling, as it directly governs ion production rates in plasma environments.

Overall, the present study confirms that the Jain–Khare formalism provides a reliable and consistent description of electron impact ionization processes for the BCl molecule. The results presented in this work fill an important gap in the available ionization data for boron-containing molecules, for which experimental information is scarce. The calculated ionization cross sections, oscillator strength, and ionization rate coefficient are expected to be useful for plasma modelling, material processing studies, and future theoretical investigations. The methodology adopted here can be readily extended to other molecular systems of technological and scientific interest.

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