Chapter 3

Electron Impact Total Ionization Cross-sections of Some Simple Atoms and Molecules

In this chapter a detailed study on the electron scattering with metallic and transition atoms and with some simple molecules and radicals are presented. We begin with the study of simpler targets. Atoms are simpler in view of their well-studied structure and spherical shapes. We have employed the Complex Optical Potential – ionization contribution (CSP-ic) method to extract total ionization cross sections from total inelastic cross sections. It is further applied in the case of selected simple molecular targets of atmospheric and industrial importance.
3.1 Introduction

Study on electron impact scattering and ionization of atoms and molecules is of fundamental interest, since they play vital role in determining the chemistry of any environment during and after a collision process. The applications of electron impact total ionization cross section \( Q_{\text{ion}} \) data in the fields of atmospheric sciences, astrophysical context and technological plasmas, radiation physics, mass spectroscopy and semiconductor industry [1] have already been realized. However, the compilation of all the required data in a single database is still a distant reality. One of the reasons for this is the scarcity of cross section data for many targets like heavy atoms and exotic molecules and radicals. Also, the reliability of the available data has been a major concern.

The Spherical Complex Optical Potential (SCOP) [2, 3] and Complex Optical Potential – ionization contribution (CSP-ic) method [4, 5] discussed in Chapter 2 is used to extract total ionization cross sections from total inelastic cross sections.

Many research groups have determined the electron impact total and ionization cross sections for molecules [6, 7]. Kim and co-workers [8, 9], Deutsch and Märk [11] and Huo et al. [13] are engaged in calculating total ionization cross sections. Many groups began by using the additivity rule (AR) [14] to investigate ionization cross section data for molecules. The AR is a crude high energy approximation in which the total ionization cross sections of molecules are a simple sum of the Total Ionization Cross Sections (TICS) of its constituent atoms. This has led to different variants called modified additivity rules (MAR) [12]. MAR could produce much better results than AR, but still lacks reliability. This reasons motivated us to pursue a better method, which is more reliable and easy to handle. This led to the ‘Single Centre Approach’ which is already discussed in chapter 2.
3.2 Total Ionization cross sections of atoms

Atomic collision phenomena are of fundamental importance in atomic and molecular physics and play an important role in other fields such as astrophysics, chemistry, plasma physics and laser physics. Here we compute the total ionization cross sections of transition metals like Fe, Co, Ni, Cu, Zn and other industrially important metals such as Al and Ga. We present total ionization cross sections ($Q_{\text{ion}}$) of these atomic targets from their ionization potential (IP) to 2 keV incident electron energies.

**Aluminium (Al)** is a silvery white metal belongs to the boron group element. It has an atomic number 13 and is the third most abundant metal in the earth’s crust after oxygen and silicon. It makes up about 8% by weight of the earth’s solid surface [10].

**Iron (Fe)** is a metal in the first transition series having atomic number 26 and is the most common element forming the planet earth’s outer and inner core. It is the fourth most common element in the earth’s crust. Iron plays an important role in biology, forming complexes with molecular oxygen in hemoglobin and myoglobin. Iron is also the metal used at the active site of many important redox enzymes dealing with cellular respiration and oxidation and reduction in plants and animals [10].

**Cobalt (Co)** is a chemical element with atomic number 27 and is found naturally only in chemically combined form [10].

**Nickel (Ni)** is a chemical element with atomic number 28. It is silvery white transition metal and is hard and ductile. Nickel is reactive enough with oxygen so that native nickel is rarely found on earth’s surface, being mostly confined to the interiors of larger nickel–iron meteorites that were protected from oxidation during their time in space. An iron–nickel mixture is thought to compose earth’s inner core [10].
Copper (Cu) is a ductile metal with atomic number 29. It has very high thermal and electrical conductivity. Approximately 65% of copper produced is used for electrical applications [10].

Zinc (Zn) is a metallic chemical element with atomic number 30. It is the first element of group 12 of the periodic table. Zinc is the 24th most abundant element in the Earth’s crust and has five stable isotopes [10].

Gallium (Ga) is a chemical element with atomic number 31. Elemental gallium does not occur in pure form in nature, but as gallium (III) compounds are in trace amounts in zinc ores and in bauxite. Roughly 90-95% of gallium consumption is in the electronics industry. Gallium arsenide (GaAs) can convert light directly into electricity. Further, gallium arsenide is also used in LEDs and transistors. Scientists employ an alloy with Gallium for the plutonium pits of nuclear weapons to stabilize the allotropes of plutonium [10].

The Ionization Potential (IP) [15] for these atoms are listed in Table 3.1

<table>
<thead>
<tr>
<th>ATOMS</th>
<th>Al</th>
<th>Fe</th>
<th>Co</th>
<th>Ni</th>
<th>Cu</th>
<th>Zn</th>
<th>Ga</th>
</tr>
</thead>
<tbody>
<tr>
<td>IP (eV)</td>
<td>5.98</td>
<td>7.90</td>
<td>7.88</td>
<td>7.63</td>
<td>7.72</td>
<td>9.39</td>
<td>5.99</td>
</tr>
</tbody>
</table>

3.2.1 Results and Discussion

Figure 3.1 shows comparison of total ionization cross section for e – Al scattering with other available data. There is only one measurement performed by Freund et al. [16] while theoretical data are provided by Bartlett and Stelbovics [17], Kim and Stone [18] Talukdar et al. [19] and Joshipura et al. [20].
Below 30 eV our results are in good agreement with the Kim and Stone [18] and Talukdar et al. [19]. After 40 eV our theory falls between other theories [17-19] but in good agreement with Joshipura et al. [20]. We get the peak of 8.77 Å² at 24 eV same as Freund et al. [16] and Talukdar et al. [19] but the cross section of Freund et al. [16] at peak is 9.87 Å² which is around 1 Å² higher compared to present result.
Figure 3.2 Total ionization cross section for Fe atom

Solid line: Present Results, Dashed Line: Talukdar et al. [19], Dash dot dot: McGuire et al. [21], Square with cross: Freund et al. [16].

Figure 3.2 shows comparison of total ionization cross section for e – Fe scattering with available comparisons. There is single measurement available for the comparison by Freund et al. [16] while theoretical data is provided by Talukdar et al. [19] and McGuire et al. [21]. McGuire et al. [21] has employed generalized Oscillator-Strength formulation of the Born approximation for the calculation of total ionization cross sections. Talukdar et al. [19] have calculated ionization cross sections using empirical method. Present data is in very good agreement with measurements of Freund et al. [16] and Talukdar et al. [19] beyond 30 eV, below which there is little deviation with present data. Theoretical data of
McGuire et al. [21] are in very good agreement with present data below 10 eV above which they are lower compared to all other data. The cross section at peak is 5.87 Å² at 24 eV incident energies which matches with Talukdar et al. [19] as well as Freund et al. [16].

**Figure 3.3 Total ionization cross section for Co and Ni atoms**

*Solid line: Present Results, Dashed line: McGuire et al. [21]. Dash dotted line: present Co*

Figure 3.3 shows the present result of total ionization cross sections for Co and Ni atoms. There are no theoretical or experimental results available for Co atom to the best of our knowledge. The peak of ionization cross sections for Co is 5.52 Å² at 27 eV. For Ni, there is lone theoretical data by McGuire et al. [21]. The peak of ionization cross sections for Ni is 5.34 Å² at 28 eV while peak obtained by McGuire et al. [21] is 4.43 Å² at 26 eV. The
peak of McGuire et al. [21] is lower compared to the present results for all the atoms studied here.

Figure 3.4  Total ionization cross section for Cu atom

Solid line: Present Results, Short dashed Line: Talukdar et al. [19], Dash dot dot: Kim and Stone [18], short dotted line: Joshipura et al. [20], Circle: Bolorizadeh et al. [22], Square with cross: Freund et al. [16].

Figure 3.4 shows the comparison of total ionization cross sections of e – Cu scattering with available comparisons. The experimental data are provided by two groups [16, 22]. Theoretical data are provided by Joshipura et al. [20] using CSP-ic method, Kim and Stone [18] by using BEB formalism and Talukdar et al. [19] by employing some empirical formula. Present results are in good agreement with both the measurements. Theoretical data of Kim and Stone [18] is lower compared to all data presented here. Present data is in good agreement with data of Joshipura et al. [20] till 20 eV
beyond which they are higher compared to all other data presented here. Theoretical data of Talukdar et al. [19] is higher compared to the present data till 100 eV, beyond which they are in excellent agreement with present data.

**Figure 3.5 Total ionization cross section for Zn atom**

_Solid line: Present Results, Dashed line: McGuire et al. [21]._

Figure 3.5 shows the present result of total ionization cross sections ($Q_{\text{ion}}$) for Zn atom. As per our knowledge, there is only one theoretical result available by Mc Guire et al. [21] using generalized Oscillator-Strength formulation of the Born approximation for the calculation. Overall range of the energy, good matching obtained between both the theories but slide variation at the peak of the cross sections observed. We get the peak of 4.42 Å$^2$ at 30 eV, while McGuire et al. [21] gets the peak of 4.24 Å$^2$ at 30 eV.
Figure 3.6  Total ionization cross section for Ga atom

Solid line: Present Results, Dashed Line: Bartlett and Stelbovics [17], Dash dot line: Talukdar et al.[19], Circle with cross: Shul et al.[23], Half-filled triangle: Shimon et al. [24].

Figure 3.6 shows the comparison of total ionization cross sections for Ga atom. Present results are going well with the theoretical values of Talukdar et al. [19] and higher compared to Bartlett Stelbovics [17]. The measured results of Shul et al. [23] are in agreement with our present results up to 40 eV. After that the experimental data of Shul et al. [23] goes higher than all the theoretical results. The results of Shimon et al. [24] are lower at intermediate energies but in good agreement with the Shul et al. [23] at high energies. Our results lie between the both available theories [17, 19] throughout the energy range. The peak obtained in present result
Chapter 3

is $8.88 \text{ Å}^2$ at 30 eV. The peak energy of all theories are similar while experimental peak of Shul et al. [23] is $9.11 \text{ Å}^2$ at 30 eV, which is slightly shifted right side from the others [17, 19, 24]. The present computational data of all atoms are given in table 3.2. Cross sections at peak are indicated in bold in table 3.2.

Table 3.2 Total Ionization Cross sections for studied atoms

<table>
<thead>
<tr>
<th>Energy (eV)</th>
<th>Al</th>
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<th>Co</th>
<th>Ni</th>
<th>Cu</th>
<th>Zn</th>
<th>Ga</th>
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<td>0.02</td>
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<tr>
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<td>0.04</td>
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<td>1.58</td>
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<td>0.64</td>
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<tr>
<td>2000</td>
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<td>0.33</td>
<td>0.46</td>
<td>0.37</td>
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</tr>
</tbody>
</table>

3.3 Total Ionization cross sections for molecules

Here we present electron impact total ionization cross sections for some light molecules and radicals for eg. N$_2$, N$_2$O, O$_3$, HCl, HBr, CF$_2$ and SiF$_2$. The molecular properties like IP and Bond length [15] used in our calculations
are listed in table 3.3. The present calculations are carried out using the Spherical Complex Optical Potential (SCOP) and Complex Optical Potential – ionization contribution (CSP-ic) methods.

**Table 3.3: Molecular properties used for the present calculation**

<table>
<thead>
<tr>
<th>Molecule</th>
<th>HCl</th>
<th>HBr</th>
<th>CF₂</th>
<th>SiF₂</th>
<th>N₂</th>
<th>N₂O</th>
<th>O₃</th>
</tr>
</thead>
<tbody>
<tr>
<td>IP (eV)</td>
<td>12.74</td>
<td>11.68</td>
<td>11.44</td>
<td>13.11</td>
<td>15.58</td>
<td>12.88</td>
<td>12.43</td>
</tr>
<tr>
<td>Bond Length(Å)</td>
<td>H-Cl</td>
<td>H-Br</td>
<td>C-F</td>
<td>Si-F</td>
<td>N-N</td>
<td>N-N</td>
<td>N-O</td>
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<td></td>
<td>1.275</td>
<td>1.445</td>
<td>1.297</td>
<td>1.59</td>
<td>1.097</td>
<td>1.12</td>
<td>1.18</td>
</tr>
</tbody>
</table>

In the case of halogen hydrides (HCl and HBr) there are no measurements available. This may be due to their high volatile nature and hence, difficulty in performing experiments. For Hydrochloric acid (HCl) and Hydrogen Bromide (HBr), theoretical data for limited energy range between 30 and 150 eV is reported by Deutsch et al. [11]. They used modified additivity rule for calculating total ionization cross sections. Deutsch and Schmidt [11] have also employed Additivity Rule (AR) for their computations. For HCl and HBr, sample results were predicted by Bobeldijk et al. [25] using the AR. More recent calculations on halogen hydrides were done by Huo and Kim [26]. They have compared their data using two different methods viz. Binary Encounter Bethe (BEB) method and Effective Core Potentials (ECP) method. Ali and Kim [27] reported theoretical data for Halogen atoms and halogen hydride molecules. In ECP method, the potentials are developed solely on the coordinates of the valence electrons, thereby eliminating the need for the core basis functions which usually require a large set of Gaussians to describe them.
Figure 3.7 Total ionization cross sections for e–HCl scattering in Å²


Present results are computed using Complex Optical Potential – ionization contribution (CSP-ic). For these targets (HCl and HBr) present CSP-ic results are in good agreement with all the available theoretical results. In the case of HCl molecule, we get the peak of 3.75 Å² at 60 eV which is similar to other available results [11, 25-27]. For HBr the peak is observed at 53 eV and corresponding cross section is 4.66 Å². Present results are in good agreement with other results [11, 25-27]. Radjenovic and Petrovic [28] have used BEB method by Quanemol-N. The present cross sectional data is tabulated in table 3.4.
Figure 3.8 Total ionization cross sections for e– HBr scattering in Å²


Figure 3.9 corresponds to the total ionization cross section for Di-fluoromethylene (CF₂). All the previous theoretical results [11, 30, 31] as well as present results for CF₂ radical are found to be on the higher side of the experimental data of Huo et al. [32] except the simplified Binary-Encounter-Dipole (BED), simplified version of the improved BED (siBED) calculations by the same authors [32]. Nevertheless it should be noted that their experimental data [32] involves a higher uncertainty of 25 %. All the theoretical predictions vis a vis the present values, the data of Joshipura et al. [29] and Kim et al. [30] exceed the measurement and calculation of Huo.
et al. [32] by more than 50\%, at the peak energy while DM calculations [11] are lower.

A comparison of the total ionization cross section of the difluoro-silicon radical SiF$_2$ is presented in figure 3.10. There is only one experimental data available [33] best of our knowledge. Binary Encounter Bethe (BEB) formalism is used by Kim et al. [32], Hwang et al. [36], de Souza et al. [34]. Joshipura et al. [35] have employed CSP-ic method using AR rule for the calculations while Deutsch et al [37] have used Deütsch and Märk (DM) formalism [37] for the calculation. As compared to the measurements of Shul et al. [33] and the available theoretical data [32, 34-37] present results of CSP-ic, Kim et al. [32], Hwang et al. [36], Joshipura et al. [35] and

Figure 3.9 Total ionization cross sections for e– CF$_2$ scattering in Å$^2$

*Solid line: Present CSP-ic; Short dash: Joshipura et al. [29]; Short dot: si-BED [32]. Dash-dot dot: DM [11]; Dash Dot: Kim et al. [30]; Circles: Huo et al. [32].*
Deutsch et al. [37] are in good agreement with experiment up to 60 eV but after that all theories show higher values. At high energies, mismatching between the experiment and in all the theories [32, 34-37] are found. Present CSP-ic results are in good agreement with Kim et al. [32] and Joshipura et al. [35]. The cross section peak of present result is 4.97 Å² at 97 eV.

![Graph](image)

**Figure 3.10** Total ionization cross sections for e– SiF₂ scattering in Å²

_Solid line: Present CSP-ic; Short dash: Joshipura et al. [35]; Dash dot dot: Hwang et al. [36]. Dash-dot: Deutsch et al [37]; Dot: Kim et al. [32]; Short dot: de Souza et al. [34]; Square with plus: Shul et al. [33]._
Figure 3.11 Total ionization cross sections for e– N₂ scattering in Å²

Solid line: Present CSP-ic; Short dash: Deutsch et al. [37]; Dash dot: Hwang et al. [32]. Dash-dot dot: Antony et al. [38]; Square: Saksena et al.[44] Diamond: Schram et al. [40], Triangle: Schram et al. [41], Stars: Krishnakumar[42], Circle: Rapp et al. [39], Square with cross: Lindsay et al. [43].

Figure 3.11 presents comparisons of total ionization cross sections for N₂ molecule. More experimental results [39-44] are available compared to theoretical data [32, 37, 38] for this diatomic molecule. Present results are in excellent agreement with other theoretical [32, 37 38] as well as experimental results [40-43] except Saksena et al. [44] and Rapp et al. [39]. Up to 200 eV these two experiments show underestimated values compared to all other theories [32, 37, 38] including the present results and experiments [40-43] but after 150 eV onwards all results show good match.
In figure 3.12, we present the total ionization cross sections of N₂O along with other theories [32, 38, 49, 50] and experiments [45-48]. Theories employed for the calculations of N₂O are Plane Wave Born Approximation method by Yogeshkumar et al. [49], Binary Encounter Bethe (BEB) [32] and CSP-ic with the modified additivity approach by Joshipura et al. [50] are available. We have also employed CSP-ic for the calculations but using single centre approach. The results obtained by single centre approach should be lower compared to the modified additivity rule which is reflected clearly in figure 3.12. Antony et al. [38] has also employed the
same approach for CSP-ic and hence the present results are in excellent agreement with them. Present results are also in very good agreement with the experimental [45-48] as well as other theoretical results [32, 49] throughout the energy range.

Figure 3.13 Total ionization cross sections for e– O₃ scattering in Å²
Solid line: Present CSP-ic; Short dash: Antony et al. [38]; Dot: DM [32]; Short dot: Kim et al. [30]; Triangle: Siegel [51]; Square with cross: Newson Renormalized [52]; Circle: Newson et al. [52].

Figure 3.13 shows comparative results of O₃. Two experimental data sets are available for O₃. The absolute cross sections measured by Siegel [51] and the relative cross section measurement of Newson et al. [52]. These authors normalized their data to the absolute cross section of Siegel [51]. The calculated BEB [30], DM [32] and the CSP-ic [38] cross sections are
found to overestimate the experimental data of [51, 52] particularly in the region around the peak. Overall, the DM cross section is closer to the experimental data than the BEB cross section but present CSP-ic data are in the range of error bar of renormalized data of Newson et al. [52]. Present data for Total ionization cross section ($Q_{\text{ion}}$) obtained using CSP-ic method for these molecules are listed in table 3.4. The cross section at peak is indicated as Bold in the table 3.4.

Table 3.4 Total ionization cross section for studies molecules

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<th>Energy (eV)</th>
<th>HCl</th>
<th>HBr</th>
<th>CF$_2$</th>
<th>SiF$_2$</th>
<th>N$_2$</th>
<th>N$_2$O</th>
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In this chapter study of electron impact total ionization cross sections for atoms and some simple molecules are presented and discussed. These results are in good agreement with other available experiments as well as theory throughout the energy range and the methodology employed for this calculation is consistent, simple and fast. The success of the present method provided us confidence to extend the method for other atoms as well as complex molecules and radicals for which experiments are difficult.


References

10. From: http://www.explainthatstuff.com
32. NIST database - http://physics.nist.gov/PhysRefData/Ionization