Chapter 1

Electron-atom-molecule scattering processes: relevance in planetary and outer space environments

“This chapter contains our introductory remarks on the fundamental electron-atom-molecule processes in relation to their applications in the planetary and outer space environments. Importance of electron as a potential projectile for the collision studies is also discussed. Further we aim to provide revealing glimpse of a variety of electron impact processes occurring in the atmospheres of our solar system bodies including planets, comets, asteroids also in the interstellar medium (ISM). A brief discussion on all possible collision processes, depending on the incident electron energy, along with its quantifying factor ‘collision cross section’, is made. The chapter concludes with a concise note on wide spread applications of the electron interaction processes ranging from plasma processes to the planetary ionospheres.”
1.1 Prologue

As the world celebrates the 100th year of the Bohr atom model [1], the research field of electron interactions with atoms and molecules, which has grown with atomic structure knowledge, is about equally old and still growing. Bohr's atomic model has had an immense impact on the history of atomic molecular physics and is an icon of the scientific revolutions of the 20th century. Quantization of atomic energy levels proposed in his model was demonstrated in the famous experiment on inelastic scattering of electrons by mercury atoms, performed by Frank and Hertz in 1914 [2]. Scattering interactions of electrons and other charged particles became important with the growth of interest in their passage through gases, in the context of particle detectors in nuclear physics. In this regard, Neils Bohr's 1948 book 'The Penetration of atomic particles through matter' was a masterpiece in itself [3]. One of the earliest treatises on the theory of atomic collisions was given by Mott and Massey [4]. Theoretical and experimental research on electron scattering from atoms and molecules is thus a century old but active field of scientific endeavour and it continues to find a wide variety of applications in natural and man-made systems.

Electron collisional processes have received a great attention due to applications in fields like gaseous electronics, gas discharges and lighting devices, dielectric applications, semiconductor etching, Mass-spectrometry, lasers, plasma and so on. Basically elastic scattering of electrons by atoms/molecules results into deflections of the incident particles. Ionization induced by electrons results into energy loss of the incident projectiles while
a variety of ionic (and neutral) species is produced from the target, and this is quite relevant in many of the environments of planets, satellites, comets and other astrophysical objects. In the ionospheres of the Earth and other planets the photoelectrons of sufficient energy can produce ions and also neutral species and give rise to ion as well as neutral chemistries [5]. On planet Mars the production of ions in its ionospheric E layer is mostly due to photoelectrons, which are produced by primary photo-ionization process [6].

Different experimental and theoretical methods are used to determine various cross sections. Factors such as types of targets and relevant instrumentation, reliability (errors) of the results and speed of the output have restricted the observational study of some targets. The theoretical methods are needed to ponder data that experiments cannot determine (e.g. radical species, and compounds not easily prepared in the gas phase, biomolecules). In theory also, for example, the electron ionization of atoms/molecules poses a difficult quantum mechanical problem, as it involves at least three charged species in the exit channel. Therefore the need for approximation methods is imperative. A semi-empirical approach in this direction was developed over three decades ago in the form of Khare-Jain formula [7]. The two theoretical methods used extensively for calculating electron ionization cross sections are Binary Encounter Bethe (BEB) method of Kim et al. [8] and the Deutch - Märk (DM) formula [9].

It is well known that electron is the most suitable projectile for scattering experiments and hence, electron impact collisions with atoms and molecules have been extensively studied by both experimentalists and theorists since
the early years of the last century [10-11]. We have seen a remarkable renaissance in both experimental and theoretical activities in the study of electron collision processes with molecules in the past ten years or so [12]. In the present thesis we have reported electron impact collision calculations on atomic and molecular targets relevant to atmospheric, planetary and astrophysical systems and employed them to study various macro-parameters such as ionization mean free path, collision frequencies and ion production rates. The targets studied in this thesis are listed in Table 1.1.

Table 1.1: Targets studied in this thesis

<table>
<thead>
<tr>
<th>Atoms</th>
<th>Atmospheric molecules</th>
<th>Exotic Molecular Targets</th>
<th>Atom/Molecules In condensed/Solid phase</th>
<th>Atoms in Metastable excited states</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>C</td>
<td>H$_2$, CN</td>
<td>Si</td>
<td>N$^*$</td>
</tr>
<tr>
<td></td>
<td>N</td>
<td>O$_2$, HCN</td>
<td>SiO</td>
<td>O$^*$</td>
</tr>
<tr>
<td></td>
<td>O</td>
<td>N$_2$, HNC</td>
<td>SiO$_2$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CO</td>
<td>C$_2$N$_2$, Al$_2$O$_3$</td>
<td>CO$_2$(Dry Ice)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>CO$_2$</td>
<td>BF</td>
<td>OCS</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>SiCl$_x$ (x=1-4)</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**1.2 Electron: a potential projectile for collision studies**

*Why electron impact studies?* Probably this is the first question that must arise in anyone’s mind. Electron atom/molecule scattering provides a prototype in theoretical as well as experimental studies. The electron interactions with the atoms and molecules have provided basic knowledge on the atomic-molecular properties also the dynamics of the electronic structure and
molecular interactions. They have added the understanding of photo-physical processes, the fates of electron excitation energy and other complex processes. Hence the answer lies within its vast occurrence/appearance in natural as well as man-made systems and subsystems. This ranges from our solar system objects, which are continuously immersed in the solar-wind electrons along with other charged particles, to the small scale laboratory experiments i.e. plasma etching etc. Briefly, in nature electrons are always available to interact with various neutral atoms-molecules and hence interest in electron impact studies is obvious.

In nature, various physical processes are the ultimate result of the electron impact processes. Also, in the laboratory experiments, electrons hold their importance as a versatile probe in the collision processes, since their impact energy can be varied easily from meV to MeV. Collisions of electrons from atoms and molecules provide a unique diagnostic probe of various fundamental interactions, which are the basic physical processes that determine the behavior of ionized gases.

Since in this thesis we are mostly concerned about the electron interactions with the neutral species in various planetary atmospheres, the next question should be; *why electron impact studies in relation to planetary atmospheres?!!*

Let us justify this by a simple example of our own planet, Earth. Our Earth is continuously exposed to the solar radiation, solar-wind, solar flares, and coronal mass ejections from the Sun, as shown in Figure 1.1, and also galactic cosmic rays.
These are the major sources of photons, electrons and other energetic particles to the Earth's atmosphere. The solar-wind electron energy distribution has a peak (~ 12 eV) close to the threshold of ionization for many atomic and molecular targets. In the course of their passage through the atmosphere these primary (precipitated) or secondary electrons (generated via Photo-ionization) can undergo elastic and inelastic collisions and this results into various atmospheric processes like, excitation, ionization, dissociation, recombination etc in these atmospheres.

Electrons may be scattered elastically, in which case there is effectively no energy change in colliding with the more massive atoms, molecules and ions but only angular deflection. Electrons may also be scattered inelastically which involves a change of energy as well as of direction of the incident electrons. Inelastic scattering involves a change in the internal energy of the atmospheric collision partner; this could be excitation of electronic, vibrational and rotational states accompanied by a discrete energy loss and
ionization and molecular dissociation accompanied by continuous energy loss above a threshold, which are responsible for physical and chemical changes in the atmosphere. The Earth's magnetic field guides these solar-wind particles to the poles, and hence the auroras are seen in the polar regions. Thus the solar radiations, and precipitated/secondary generated charged particles, ionize the planet’s atmospheric constituents to produce ionosphere. Similar electron impact processes can occur over other planets such as Mars, Jupiter, Saturn and their satellites; also over other solar system bodies like asteroids, comets and even in the interstellar/interplanetary medium. Apart from solar wind, other ionization sources and their ionization rate variation with altitude in the Earth’s atmosphere is highlighted in Figure 1.2.

Figure 1.2: Sources of ionization in the Earth’s atmosphere [14]
From Figure 1.2 we briefly describe the sources of ionization as under:

- **Solar Extreme Ultra-Violet and X-rays**: They ionize the Earth’s upper atmosphere resulting into ionosphere. X-rays can penetrate further below.

- **Auroral electrons**: They are mainly produced by strong geomagnetic storms. Auroras are created by the collision of charge particles, mostly electrons but also protons and heavier particles with atoms and molecules of Earth’s upper atmosphere in the polar region. These particles have energies of 1 - 100 keV. They can penetrate to about 60 - 80 kms above Earth’s surface causing excess excitation and ionization.

- **Relativistic electrons**: They are mainly produced from the pair-production of high energy (≈ GeV range) gamma rays. They are highly energetic particles which cause ionization in the lower atmosphere (20 - 30 km above ground level), however their flux is very small.

- **Solar proton events**: Solar winds are the major source of protons. A solar proton event occurs when high energy protons, ejected from Sun during a solar flare, get caught by Earth’s magnetic field and cause ionization in the Earth’s ionosphere, producing secondary electrons.

- **Galactic cosmic rays**: They are high energy particles that flow into our solar system from far away in the Galaxy. They are mostly protons, electrons and bare nuclei. Cosmic rays provide one of our few direct samples of matter from outside the Solar System. The magnetic fields of the Galaxy, the Solar System and the Earth have scrambled the flight paths of these particles so much that we can no longer point back to
their sources in the Galaxy. Many galactic cosmic rays are of extremely high energy, so they must have been originated in very massive explosions.

Figure 1.3 shows normal daytime photoelectron flux \( \text{cm}^{-2}\text{s}^{-1}\text{ev}^{-1}\text{ster}^{-1} \) [15] in Earth's ionosphere. The data plotted were measured by the Atmospheric Explorer Satellite at 195 km [16].

![Figure 1.3: Normal daytime photoelectron flux as a function of electron energy](image)

The two curves in the lower portion of the Figure 1.3 (right hand ordinate) denote the integral cross sections for electron impact excitation of 337.1 nm radiation [17] in \( \text{N}_2 \) and the total (direct plus cascade) integral cross section for excitation of \( \text{N}_2(\text{A}) \) state and have been included to illustrate those portions of the photoelectric spectrum that excite these states in \( \text{N}_2 \). The
vibrational excitation cross section of N\textsubscript{2} at the 2.3 eV resonance energy region is also indicated and it is responsible for the dip in the electron energy distribution curve at that energy.

Studying the electron-molecular impact process is important to understanding the complex relationships among our planet's atmosphere, the sun, and the magnetosphere. The scattering theory underlying this is an essential part of the quantum mechanics. Electron-atom scattering is perhaps a well investigated quantum mechanical processes in physics but not known exactly. Understanding the Earth's upper atmosphere remains a primary motivation for studying electron-molecular impact processes. Thus our main aim is to know, investigate and to study all various atmospheric processes occurring in planetary and other astrophysical systems and this can help to develop theoretical models for understanding these processes, in an approximate way.

1.3 **Electron induced processes in our solar system**

Planets in our solar system possess a gaseous atmosphere of one kind or another. Since these atmospheres are exposed to solar radiation and because they have a magnetosphere, they also have an ionosphere and possibly aurora, in visible as well as other wavelength region [18], analogous to that on the Earth. The solar radiation and precipitating charged particles including electrons, ionize the planet's atmospheric constituents to produce this ionosphere. Therefore the properties of the ionosphere will be directly related to the incident solar and particle (electron) spectra, and associated
planetary magnetic field along with the particular atmospheric constituents and kinetic processes in which they participate [15]. Although tremendous progress has been made in the past 40 years in understanding the intricacies of the solar-terrestrial relationship from the judicious use of rockets and satellites, many major questions still remain to be answered and this is where the theoretical investigations come in the picture. Interest in understanding Earth’s upper atmosphere remains a primary motivation for studying electron-atom-molecule impact processes. Understanding the complex relationship among planets’ atmosphere, the sun, and the magnetosphere has fascinated and intrigued the world’s scientific minds for more than 100 years [19]. Here we have made our efforts to summarize various electron interaction processes occurring in our solar system bodies, with special attention to the Earth’s and Martian atmospheres.

**Earth**

A number of review articles [20,21] have been written dealing with various aspects of the very complex atomic-molecular processes taking place in Earth’s ionosphere. We draw selectively on their work to identify the role of electron impact processes. As already noted in section 1.2, in Earth’s atmosphere there are several ionization sources and hence plenty of electrons having sufficient energy to perform various elastic as well as inelastic interactions with the available neutrals constituents. The electrons, whose initial energy distributions ranges from a fraction of an electron volt to over 100 eV, lose their energy in atomic-molecular collision as they move through the atmosphere until they recombine or participate in the complex
negative-ion chemistry [22]. In such atmospheres available neutral species plays a crucial role in defining various physico-chemical processes going on. For example there has been so much research done on electron impact and photo-absorption processes in O$_2$ and N$_2$. This is because they and their associated atomic-ionic fragments are dominant constituents throughout the ionospheric D and E regions [23]. Electrons with sufficiently high energy will first ionize the neutral constituent. Upon losing the energy the major mechanisms for electron thermalization in the Earth's ionosphere are electron-electron collisions, excitation of O-atom fine-structure levels, rotational excitation of O$_2$ and N$_2$, vibrational excitation of O$_2$ and N$_2$ and at last the elastic collision with the ions and neutrals [22,23]. Hence almost the entire ionospheric system is governed by the electron-atom-molecule processes.

Any discussion of electron-atom-molecule collision processes in the Earth's atmosphere would be incomplete without at least a glimpse of auroral phenomena. The energy receipts from the solar wind to the magnetosphere are accompanied by geomagnetic disturbances and by electron and proton flows toward the polar regions of the Earth, into the auroral ovals. This gives rise to a glow in the upper atmosphere, ‘auroras’ in a wide spectral region [24]. The physics of these processes is considered in numerous publications [25]. Most of the emissions are excited in the thermosphere and belong to nitrogen and oxygen atoms-molecules. The energetically significant emissions are the 557.7- and 630-nm emissions of atomic oxygen.
Species in the metastable states also significantly contribute to the auroral phenomenon and in this regard electron interaction with the metastable atomic \( \text{N}^* \) and \( \text{O}^* \) are also studied in this thesis. A typical view of aurora as observed from the space is depicted in Figure 1.4(a). Figure 1.4(b) shows the formation of auroral oval at the polar region.

![Aurora and Auroral Oval](image)

**Figure 1.4**: Aurora (a) as observed from the space and (b) auroral oval

Airglow, dayglow and nightglow are other atomic-molecular processes of similar nature but associated with geomagnetically quiet conditions.

**Mars**

The red planet-Mars has always been a center of attraction and fascination to the scientific community, having \( \text{CO}_2 (~95\%) \) as the most dominant neutral constituent. Similar to the Earth, photoionization through solar EUV is the major source for the production of dayside ionosphere where as the photoelectron impact ionization is the secondary source. But unlike the Earth, Mars does not possess any intrinsic internal magnetic field [26] and hence its atmosphere is suffering from continuous bombardment of radiation and
charged particle of solar origin. Electron impact ionization, excitation, charge exchange and dissociative recombination are the dominant atomic-molecular processes occurring in this atmosphere. In the context of this thesis we will focus only on the electron impact ionization processes taking place in Mars. Electron impact ionization is the dominant source of ionization in the ionospheric E region of Mars [6]. Also there are evidences for the electron ionization in the magnetic pileup boundary of Mars [27]. Sustainability of the night-side ionosphere over Mars is one of the possible consequences of the electron impact ionization [28] which may be attributed to the presence of localized crustal magnetic fields observed by MGS as shown in Figure 1.5.

Figure 1.5: Graphical representation of MAG measurements during the sixth orbit after Mars Orbit Insertion. The arrows point in the direction of the measured magnetic field and their length represents the field magnitude. It is clear that the source of this magnetic field is not in the core of the planet, but in its shallow solid crust [29].
**Jupiter**

The existence of energetic particle precipitation into the upper atmosphere of Jupiter from the magnetosphere is evident from the experiments on the Voyager 1 and 2 spacecraft and observations made by the International Ultraviolet Explorer (IUE) [30]. These auroral precipitations generate large ionization and dissociation rates, to excite auroral emissions, and also to vibrationally excite molecular hydrogen, which is most dominant neutral species on the Jupiter. A variety of processes that can occur on Jupiter over the electron impact on H$_2$ is tabulated in a comprehensive review by Bhardwaj and Gladstone [18] on the auroral emissions of the giant planets. Auroral emissions are also observed on the other gas giants viz. Saturn, Uranus and Neptune [18] at different wave lengths ranging from X-ray to radio wavelengths. We will not go further in detail for electron interactions in other gas giants. Unlike the Earth’s atmosphere-less (so called) satellite-Moon, satellites of Jupiter Io (SO$_2$), Ganymede (O$_2$, O) and Europa (O$_2$) also the Saturnian satellite-Titan (N$_2$) possess atmospheres. Io is an interesting moon of Jupiter. Io is having mostly SO$_2$ [31], S and O [32] as its neutral constituent, where electron impact ionization is possibly an important plasma source [33] in its dense high altitude ionosphere [34]. For the present interest let us visit Titan briefly.

**Titan**

Molecular nitrogen-N$_2$ is a primary and the most dominant (~94%) atmospheric constituent of Saturn’s moon-Titan. Solar EUV – XUV radiation, energetic plasma from Saturn’s magnetosphere, and cosmic rays are the main
sources of the ionization of the neutral gas (N\textsubscript{2}) in Titan's atmosphere. Because of the absence of an intrinsic magnetic field, Titan's atmosphere and ionosphere interact directly with Saturn's magnetospheric plasma [35]. Titan's orbit around Saturn is such that it can be inside or outside of the Saturn's magnetosphere. Hence the particle precipitation and resulting ionization can be highly dynamic depending on the position of the satellite and local plasma conditions [36]. Collisions between these electrons and the atmospheric N\textsubscript{2} result in photon emissions that provide an important diagnostic probe for understanding these environments. De Le Haye et al. [37] have modelled the heat released into Titan's atmosphere through collisions between photo and magnetospheric electrons. They show that N\textsubscript{2} electronic excitation processes dominate the net heating rate throughout the upper atmosphere (~800-2000 km).

Figure 1.6: Titan, Saturn's moon
Further, Cassini observations have shown that, on the nightside, electron impact plays an important role and is the dominant source of ionization [38]. Ionization processes occurring in the atmosphere of Titan is studied in detail in a series of 2 papers by Gronoff et al. [36,38]. Figure 1.6 shows the image taken during the Cassini spacecraft’s closest flyby of Titan on April 16, 2005.

Comets, Asteroids and Interstellar medium

Comets are water-dominated tiny objects in our solar system. The cometary coma, which is generated by sublimation of volatile species from the nucleus, hosts most of the physical, chemical and dynamical processes for comets and this is where the study of electron impact process holds importance [39]. Cravens et al. [40] have assessed quantitatively the importance of electron impact ionization in various regions of the cometary plasma environment and compare this ionization source with the photoionization sources. They [40] have found that the ionization by electrons is of comparable importance to photoionization in the magnetosheaths (coma) of comets.

Now let us imagine the direct impact of radiation and charged particles from the sun to the surface of an asteroid. A different methodology need to be applied to consider for the electron inelastic processes with the solid i.e. the calculation of the inelastic mean free path (IMFP) [41] for the accurate analysis of scattering surfaces.

The space in between the solar system objects is not empty, but filled with the matter called interstellar medium (ISM), mostly H and He along with other atomic molecular species. Isenberg and Feldman [42] have investigated the ionization of interstellar hydrogen and helium due to electron impact by
shock-heated electrons and shown that the electron ionization rates are
matching or exceeding the nominal photoionization or charge-exchange rates
at 1 AU.

1.3.1 Need for electron-atom-molecule collision data

It is very clear from the above discussion that the source for nearly all
atmospheric processes is ultimately the interaction of solar photons and
ergetic particles (electrons/ions) of solar or magnetospheric origin with
the atmosphere. The solar radiation and the photoelectrons that they produce
may interact with thermospheric neutral species producing dissociation,
ionization, excitation, and heating. Energetic particles may precipitate into
the atmosphere, producing auroral emissions.

Thus variety of electron impact processes ranging from elastic scattering;
vibrational, rotational and electronic excitation, parent and multiple
ionization, charge exchange, dissociative attachment and recombination may
occur depending on the energy of the incident electrons. Many atmospheric
processes are understood through the fundamental atomic-molecular
interaction, still plenty to explore. In this regard the electron-atom-molecule
collision data has always been and will always be a fundamental need/input
for a planetary scientist to explain the fundamental physics of any related
atmospheric process. This thesis is our sincere effort to aid a piece of work,
electron impact ionization and its applications, to better serve the
community.
1.4 **Electron impact processes**

After an interesting voyage to our solar system, now it is time to go from macro world to micro (quantum) world and explore some basics of electron impact processes. During a scattering process, where a free electron collides with an atom or molecule (in ground state), various kinetic processes may take place. All these processes fall into two categories: elastic and inelastic processes. In case of elastic scattering of an electron no energy is transferred to the internal motion of the molecule, while in inelastic scattering, the incoming electron loses a portion of its kinetic energy to the excitation of the target.

![Figure 1.7: Schematic diagram of electron scattering experiment](image)

Consider a mono-energetic, non-interacting and well collimated beam of electrons (e\(^{-}\)), incident on a target atom molecule as illustrated in Figure 1.7. The energy of the incident electron will be denoted by \(E_i\). The incident beam flux is just enough so that interactions between the incident electrons are
very weak and hence neglected. The scatterer or the target is an atom or molecule and the source of incident particle is usually kept at a distance quite larger than the de Broglie wave length of the incident particles. The target is very thin and can be considered as a single particle. Hence, our main focus is on the collision of an e\(^{-}\) (A) with target atom/molecule (B). The scattering is a single collision event.

During a collision many processes are possible or channels are open and the outgoing particles resulting from these collisions are collected and registered by the detector. The various processes that can occur are illustrated below.

**Elastic scattering**

\[ A + B \rightarrow A + B \]

In this scattering the total kinetic energy is conserved separately. If \( T_1 \) and \( T_2 \) denote the kinetic energy of reactants and \( T_1' \) and \( T_2' \) those of the products then elastic scattering is defined by,

\[ T_1 + T_2 = T_1' + T_2' \]

For example,

\[ e^- + CO \rightarrow e^- + CO_2 \]

**Inelastic scattering**

\[ A + B \rightarrow A^* + B \]

\[ A + B \rightarrow A + B^* \]

\[ A + B \rightarrow A^* + B^* \]

Here the star (*) indicates the particular excited states.

For example,
\[ e^+ + CO_2 \rightarrow e^+ + CO_2^* \] [Electronic Excitation]
\[ e^+ + CO_2(J) \rightarrow e^+ + CO_2(J') \] [Rotational Excitation]
\[ e^+ + CO_2(v) \rightarrow e^+ + CO_2(v') \] [Vibrational Excitation]
\[ e^+ + CO_2 \rightarrow 2e^+ + CO_2^* \] [Parent ionization]
\[ e^+ + CO_2 \rightarrow 2e^+ + CO^+ + O \] [Dissociative ionization]
\[ e^+ + CO_2 \rightarrow 2e^+ + O^+ + CO \] [Dissociative ionization]
\[ e^+ + CO_2 \rightarrow 2e^+ + C^+ + O_2 \] [Dissociative ionization]
\[ e^+ + CO_2 \rightarrow CO_2^- \] [Electron attachment]
\[ e^+ + CO_2 \rightarrow CO^- + O \] [Dissociative electron attachment]

Reactions

\[ A + B \rightarrow A + B \]
\[ A + B \rightarrow C_1 + C_2 + ... + C_n \]

1.4.1 Scattering cross sections

Before we define various cross sections, let us first introduce the ‘atomic unit system’ which is followed throughout the present calculations in this thesis, unless otherwise stated.

Atomic unit system

Atomic molecular physics deals with quantities much smaller than what we see in normal experiences, e.g. the order of magnitude of length is close to the magnitude of Bohr radius \(a_o\) (most probable radius of hydrogen atom, \(a_o = 0.529 \times 10^{-8}\) cm). So for simplifying the theoretical calculations we use the
atomic unit (a.u.) system in our calculations. Various quantities defined in a.u.
are as follows:

Electron charge, \( e = 1 \); electron rest mass, \( m_e = 1 \); \( h = 1 \) \((h = h/2\pi, \text{Where}
\( h=\text{Plank's constant})\); and \(4\pi\varepsilon_0 = 1 \) \((\varepsilon_0 = \text{permittivity of free space})\); Velocity of
light, \( c = 1 \); Using the a.u. system we can derive the units for other physical
quantities required in our calculations.

A cross section is a measure of the occurrence of a particular event while
scattering between two particles takes place. In this thesis we have used \( \text{Å}^2 \) or
\( 10^{-16}\text{cm}^2 \) as the unit for cross sections unless otherwise specified.

**Differential cross section**

We will now consider the elastic process from Figure 1.7, where \( dN \) number
of particles \((A)\) are scattered elastically per unit time within a solid angle \( d\Omega \).
Then, for a sufficiently thin target, the number of particles scattered per unit
time per unit solid angle is proportional to incident flux \((\Phi_A)\) and the number
of target scatterers \((n_B)\), That is,

\[
dN \propto \Phi_A n_B d\Omega
\]

Thus,

\[
dN = \frac{d\sigma}{d\Omega} (\theta, \phi) \Phi_A n_B d\Omega
\]

where the proportionality factor \( \frac{d\sigma}{d\Omega} (\theta, \phi) \) is called the differential cross
section (DCS) for elastic scattering. DCS at a particular direction \((\theta, \phi)\) is
defined as the number of particles scattered per unit solid angle, per unit
incident flux and per unit time, where the polar angles are defined in Figure
1.7. Thus from equation (1.4.2) we get,
Elastic DCS is related to an important theoretical quantity, scattering amplitude \( f(\theta, \phi) \) as;

\[
\frac{d\sigma}{d\Omega}(\theta, \phi) = |f(\theta, \phi)|^2
\]  

(1.4.4)

**Total elastic cross section**

Total or integrated elastic cross section is obtained by integrating the differential cross section over all the solid angles \((d\Omega)\), which can also be written as,

\[
\sigma_{el} = \int_{\theta}^{\pi} \int_{\phi}^{2\pi} \frac{d\sigma}{d\Omega}(\theta, \phi) \sin\theta \, d\theta \, d\phi
\]  

(1.4.5)

This total elastic cross section is the purely elastic cross section without the presence of any inelastic channels. But realistically we have to consider inelastic channels while finding the total elastic cross section. The total elastic cross section in the presence of inelastic scattering is denoted by \( Q_{el} \), where ‘\( Q \)’ comes from the German word ‘Querschnitt’ meaning cross section. We will use the abbreviation TCS for total cross section.

**Total inelastic cross section**

Besides the elastic process, there can be various inelastic processes that may occur in a scattering event. The total inelastic cross section is denoted by \( Q_{inel} \), which is actually a cumulative inelastic scattering cross section, and is divided into two parts,

\[
Q_{inel} = \sum_{n} Q_{ion}(A^{+n}) + \sum Q_{exc}
\]  

(1.4.6)
The first term in equation (1.4.6) accounts for the total of all total ionization cross sections for all energetically allowed states with $A^{en}$ as the charge state of the ion. The second term indicates the total excitation cross section for all allowed electronic transitions of the target by incident electrons. If $i'$ is the initial (ground) state and $f'$ is final state of electronic transition, and if $Q[i \rightarrow f]$ is the total cross section of this transition then,

\[ \sum Q_{\text{exc}} = \sum_{n} Q[i \rightarrow f] \quad (1.4.7) \]

**Total (complete) cross section**

The sum of both total elastic and total inelastic cross sections will give the total (complete) cross section, $Q_T$. This corresponds to the effect of all the different channels that can be present in any scattering processes. The total cross section indicates the probability that an incident particle interacts with a target particle and has therefore been removed in some way from the incident beam. Thus,

\[ Q_T = Q_{\text{el}} + Q_{\text{inel}} \quad (1.4.8) \]

**Rotational cross section**

The total (complete) cross section we have discussed up to now arises from spherical interactions only. The method we use (discussed in section 2.1.2 in the next chapter) to solve Schrodinger equation is the partial wave analysis with spherical potential. This is satisfactory for atoms as they do not have a permanent dipole moment, but in the case of molecules having a permanent dipole and quadrupole moments, the non-spherical potential and the resulting cross section also need to be considered. These corresponding
rotational (non-spherical) cross sections are appreciable at low energies only and are denoted by $Q_{rot}$.

**Grand total cross section**

The total cross section $Q_T$ we have defined, is the spherical part of the 'grand' total cross section, denoted by $Q_{TOT}$. For molecules with a permanent dipole moment, rotational excitation cross section is the most important non-spherical contribution. The $Q_{rot}$ can be added to the total cross sections $Q_T$. Here $Q_T$ is the spherical part and $Q_{rot}$ is the non-spherical part of the grand total cross section. Thus grand total cross section ($Q_{TOT}$) is defined as follows.

\[ Q_{TOT} = Q_T(E_i) + Q_{rot}(E_i) \]  

(1.4.9)

**Macro-parameters**

All the above TCSs are microscopic with reference to a single atomic or molecular target. In chapter 5 and 6 we have defined the corresponding macroscopic total cross sections and derived other bulk parameters viz. mean free path, composite mean free path, ionizing collision frequency also ion production rate.

**1.4.2 Other applications and occurrence of electron impact processes**

Relevance and consequences of various electron impact/driven processes in different solar system objects has been discussed significantly so far in this chapter. Now let us briefly discuss the importance of the electron collision data from the application point of view. Electron-atom-molecule collisions initiate and drive almost all the relevant chemical processes associated with
electron-beam transport, gas discharge, radiation chemistry, stability of waste repositories, plasma-enhanced chemical vapor deposition (CVD), plasma processing of materials for microelectronic devices, gas lasers and other applications also novel light sources for research purposes. The life-sciences are a rapidly advancing field where the important role of electron-driven processes is only now begins to be recognized. There are a wide range of applications of electron-initiated processes in gas phase, at surfaces and interfaces, and in condensed matter as also in mass-spectrometry. Few selective applied areas involving the electron driven processes are briefly discussed below.

**Electron beam transport**

There is a considerable interest in the transport properties of, and extraction of energy from, relativistic electron beams passing through atomic and molecular gases. Electron impact cross sections serve as the foundation for all studies involving electrons’ passage through the gases for this purpose.

**Gas lasers**

Elastic electron scattering and rotational excitation of molecules by electrons certainly play an important role in the operation of any molecular gas discharge laser and therefore these processes must be understood for each specific laser system of interest i.e. $\text{H}_2$, $\text{N}_2$, $\text{CO}_2$ or eximer lasers etc.

**Plasma Physics**

Plasma etching, deposition and cleaning are indispensable fabrication techniques in the manufacture of microelectronics components. The plasma equipment for these processes typically use partially ionized, low pressure
plasmas to provide activation energy to dissociate and ionize feedstock gases. The resulting radicals and ions interact with the semiconductor surface, either removing or adding material, to define the desired features or modify the surface. This requires the modeling efforts to simulation for these processes. Essential input for modeling these processes in plasma physics consists of complete cross section data set for all elastic and inelastic interactions.

Life sciences

Role of electron-driven processes is being recognized as crucial to our understanding of radiation damage of cellular material. Radiation therapy is one of the major cancer treatment techniques wherein the secondary electrons produced by radiation can collide with DNA molecules in human cells, causing damage that destroys the cancer cell. In modeling such processes accurate knowledge of electron collision cross sections for relevant biological molecules are needed.

Electron Induced Chemistry

Electron-molecule interactions have contributed substantially in understanding electronic structure of molecules, fast chemical reactions in etc. The interactions are also important for determination of structure and chemical reactivity of species adsorbed on surfaces. In the technological field electron induced reactions underpin most of the multi-billion dollar modern semiconductor industry since it is those reactive fragments produced by electron impact of etchant gases that react directly with the silicon substrate.
1.5 Conclusions

In conclusion, this chapter portrays the field of electron-atom-molecule interactions as an essential and fundamental research area in relation to wide applications ranging from laboratory scale systems to the planetary atmospheres. We have also highlighted electrons as convenient and effective probes for these investigations. An exciting journey to our solar system from the viewpoint of various electron interactions has also been accomplished in this chapter. Developments highlighted in this chapter not only provide motivation but also a challenge for yet another theoretical attempt. Our theoretical attempts are described in the chapters to follow.
Bibliography


