

Executive Summary

of

Thesis Entitled

**“THEORETICAL STUDY OF ELECTRON INDUCED
MOLECULAR PROCESSES”**

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In this thesis, we provide an explanation of electron impact interactions with atoms/molecules using several advanced theories, and we compare our findings to earlier findings whenever possible. Electron scattering difficulties have been extensively investigated by both experimentalists and theorists. The outstanding work in experimental and theoretical activities may be due to developments in experimental apparatus, the availability of powerful computers, and the development of novel theoretical ideas, which enabled the investigation of complicated targets and collision processes.

The current thesis is divided into six chapters.

We offered an introduction and a review of the literature regarding prior investigations in **Chapter 1**. We described scattering phenomenology. We have addressed the fundamental phenomenology of scattering theory, a variety of cross sections expressing the likelihood of occurrence of various phenomena, and their relevance to many domains of current science and industry. We also evaluated prior research on electron-induced processes on atomic/molecular species conducted by various experimental and theoretical groups.

The **chapter 2** presents the theoretical approaches that we have employed to estimate various total cross-sections for various atoms, molecules, and radicals. Total ($Q_{el} + Q_{inel}$) cross sections are calculated using the Spherical Complex Optical Potential (SCOP) technique up to 5 keV in ionization energy. The Complex Scattering Potential-ionization Contribution (CSP-ic) formalism was used to determine the total ionization cross sections and total excitation cross sections. In addition, we developed the 2 Parameters – Semi empirical method (2P-SEM) to determine total and elastic cross sections, and we established a correlation between $Q_{ion}(max)$ and dielectric constant. It will go through several approximations that are employed in this chapter's techniques.

In the **chapter 3**, we examined electron interactions on plasma-relevant molecules such as CF_2O , C_2F_4O , C_3F_6O , C_4F_8O , $C_5F_{10}O$, and $C_6F_{12}O$, among others. These molecules are known as perfluoroketone (PFK) molecules. We present the results of elastic and inelastic (ionisation and excitation) cross section calculations for electron scattering from perfluoroketone (PFK) molecules, $C_xF_{2x}O$ ($x = 1-6$), over a broad energy range, from the ionisation potential (IP) to 5 keV. As described in Chapter 2, when analysing atomic targets, we must make very few approximations when compared to studying molecules.

In the **chapter 4**, we report computed probabilities of various interaction processes taking place during the collision of electrons with DNA molecules, viz., Adenine, Guanine, Cytosine, Thymine and Uracil in their aqueous phase. We have also found various cross sections for furfural and parabezoquinone (pBQ) compounds and Pentafluoropropionic Acid using SCOP, CSP-ic and 2p-SEM formalism. We have also estimated the dielectric constant (ϵ) for these molecules. We have also examined various correlation between total cross section (Q_T), target molecular properties (no. of target electron and dipole polarizability, α) and also observed correlation between Q_{ion} (Max) with dipole polarizability (α) and dielectric constant (ϵ).

In the **chapter 5**, we provide the findings from our studies on electron-driven molecular events for the fluoronitriles C_3F_5N and C_4F_7N over a large energy range, from the ionization potential to 5000 eV. We use SCOP, CSP-ic and 2P-SEM techniques to estimate elastic and inelastic effects. The research encompasses multiple correlations, predicting dipole polarizability, determining the dielectric constant, and calculating the number density N for these fluoronitriles.

Finally, **Chapter 6** is devoted to the thesis summary, conclusion, and benefits and limits of our current study. We have also made an attempt to analyse the current work and its potential for the future.

We theoretically examined electron interaction processes with numerous compounds and radicals based on their applications in this thesis. We investigated ideas for computing electron collision cross sections in high energy regimes (up to 5000 eV).

The purpose of this research was to create reliable theoretical techniques for determining various electron collision total cross sections. In this thesis, we provided estimations for a number of plasma-relevant and environmentally friendly targets. The current theoretical technique has been successfully extended to hydrated DNA and industrially important compounds.

A simple and practical approach was used to compute the total and ionization cross-sections for electron scattering from atoms and molecules.

The key findings of the current study have been published in reputable national and international publications and presented at several national and international conferences.

We picked compounds of pharmaceutical, biological, atmospheric, industrial, and plasma importance for the application's viewpoint of electron-aided processes. We provide in this thesis an innovative and effortless approach developed in recent years by our group to give insight into elastic and inelastic (including ionization) processes for electron scattering from atomic/molecular species. We sought to analyse electron collision for an energy range of ionization threshold to 5000 eV in order to understand diverse physical processes happening at different impact energy regimes. We used the Spherical Complex Optical Potential (SCOP) approach to investigate the probability of occurrence of distinct electron-driven events. Electron-induced atomic and molecule ionization is a crucial component of numerous naturally occurring processes as well as various reactions valuable in scientific and commercial applications. We provide estimates of total ionization cross sections derived from Complex Scattering Potential-ionization Contribution (CSP-ic) approach and compare them to experimental and theoretical data.

Future Prospects

- We wish to use R-matrix computations to investigate low energy electron atoms and molecules scattering.
- Differential cross sections, partial and dissociative ionization of the molecules will be investigated.
- The interactions of electrons with other Bio-molecules, proteins, and pharmaceutical molecules will be investigated.
- We will study diverse phenomena of electron interactions with modern technological compounds and industrially significant chemicals.
- The interactions of positron and photon with atoms and molecules will be investigated.
- To investigate a variety of atmospheric molecules.
- Electron interactions with molecules in condensed phase would be explored, that is, Ices on various planets.
- We would like to explore the electron interactions with newly detected molecules found in various cometary and planetary environments. As a result, application in Astro chemistry field would be explored.

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Chapter 3

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