Preface

The field of atomic and molecular physics permeates nearly every aspect of modern scientific and technological endeavours. It serves as the cornerstone for many of the technologies in use today and has been instrumental in driving significant advancements across a range of scientific disciplines. Beyond its direct applications, the intrinsic pursuit of knowledge and discovery continues to grant this field a distinguished status. The scope of atomic and molecular physics is vast, encompassing diverse research areas, and in recent years, the field has experienced a remarkable wave of advancements. Within this broad domain, electron scattering has emerged as a well-established area of research with critical applications spanning both science and technology. The development of new experimental and computational techniques has renewed interest in exploring electron interactions with atomic and molecular targets in both gaseous and condensed phases. The study of atomic-molecular collisions now occupies a central role in contemporary multidisciplinary research, offering valuable insights and models for emerging scientific fields. These interactions, often employed as investigative tools, are fundamental to a wide array of natural processes.

This thesis presents detailed calculations of electron impacts and collisions with molecular targets, focusing on applications in industrial processes, plasma research, biomedical studies, and atmospheric sciences. The theoretical study covers electron collisions with molecular targets across an energy range of 10 eV to 5000 eV, where various elastic and inelastic interaction processes are induced. Due to the growing need for accurate cross section data in both fundamental and applied research fields, interest in collision computations has recently been revitalized. This thesis introduces a method that is both efficient and simple while still delivering reliable results. The primary objective is to estimate a range of cross sections associated with electron scattering from molecules in gaseous and condensed (or aqueous) phases, including total elastic cross sections (Q_{el}), total inelastic cross sections (Q_{inel}), ionization cross sections (Q_{ion}), excitation cross sections (Q_{exc}), and total cross sections (Q_T). The calculated results are then compared with available experimental or theoretical data to validate the approach.

This thesis is organized into seven chapters, each contributing to the overall understanding of electron scattering phenomena, computational methods and present results.

Chapter I provides an introduction to the general phenomenology of electron scattering events, emphasizing the importance of studying electron collisions. It also describes various electron interaction processes that occur when electrons collide with molecular targets.

Chapter II focuses on the theoretical frameworks used in the calculations presented in the thesis. It outlines the Spherical Complex Optical Potential (SCOP) and Complex Scattering Potential-ionization contribution (CSP-ic) formalisms employed for intermediate to high-energy calculations. Also, we have discussed 2 parameter Semi Empirical Method (2p-SEM) for larger and complex molecules.

Chapter III presents theoretical calculations of various cross sections for electron interactions with analogous bio-molecules of DNA/RNA, 3-hydroxy-tetrahydrofuran ($C_4H_8O_2$) and α-tetrahydrofurfuryl alcohol ($C_5H_{10}O_2$), which are similar in structure and functional group to backbone of DNA and RNA. In addition to calculating cross sections, the chapter discusses correlations between target parameters and cross sections.

Chapter IV quantifies both total inelastic and elastic processes for electron collisions with industrial relevance furfural, para-benzoquinone, and fluoronitriles over an energy range from the ionization threshold to 5000 eV. The results of these computations are discussed in detail in this chapter.

Chapter V focuses on electron interactions with aqueous-phase DNA molecules. This chapter evaluates important applied quantities, such as dipole polarizability, dielectric constant and various cross sections which are critical for assessing DNA damage in biological systems.

The ionization of N_2 is presented in **Chapter VI**, where various cross-sections have been calculated, including ionization, excitation, elastic, and inelastic cross sections. These calculations cover a broad energy range from threshold to 5000 eV, providing comprehensive insights into the electron interactions with molecular targets. Experimentally, measurements were done in the laboratory of molecular physics at Tata institute of fundamental research (TIFR), Mumbai, as a part of our collaboration with Prof. Lokesh Tribedi, TIFR- Mumbai.

The thesis concludes with **Chapter VII**, which offers a summary of the thesis, highlighting key conclusions, and discussing the strengths and limitations of the work. A review of the current research and its future prospects is also presented. Notably, the significant results of this study have been published in respected national and international journals and have been presented at various conferences .