Preface

Atomic - molecular collision study has a history of more than 100 years now and has found important place in the exploration of basic processes like excitation, ionization and dissociation or fragmentation at the subatomic level. While the problem of electron scattering with atoms and molecules has been extensively addressed by many theoretical and experimental scientists in recent past, here the main intention is to find theoretically, various cross-sections which are the measures of the probabilities of different processes to occur in the regime of electron - atom / molecule interactions. These processes have gained much importance in environmental sciences, study of aurora, ionosphere of the earth and other astrophysical environments and low-temperature plasmas.

In this thesis we have made an attempt to discuss in detail the theory of electron scattering from atoms and molecules along with the introduction of various approximations, and present calculations to obtain various total cross sections. The results of the present research work have been presented in national and international conferences and published in reputed international and national journals.

The calculations, results and discussion for the targets studied here, are described in seven chapters.

Chapter 1 highlights the present scenario of Atomic and Molecular physics in general and the frontiers of recent research work being done within the field of electron collisions in particular. Current thrust areas are listed to underline the importance of present work and its context. We also present various collision processes and give a survey of previous experimental and theoretical study. Reported are several applications of the present work.

Chapter 2 presents the theoretical methodologies which are employed for the calculations. Basically, we have employed three different formalisms. One the R- Matrix method which is an ab-initio method. This method is used for the Low impact energy calculation from 0.1 eV- 20eV. The other methods which we have employed are Spherical Complex Optical Potential (SCOP) and Complex Scattering Potential – ionization contribution (CSP-ic). These methods are employed for the calculation of various total cross sections from ionization threshold of the target to very incident energy up to 2 keV. Using these methods we calculate various total cross sections. Our main goal is to compute total cross sections from very low energy 0.1 eV to high energy 2 keV by combining the R- Matrix formalism and SCOP formalism. Such hybrid approach is used for the first time by our group. The details are included in this chapter.
Chapter 3 deals with the calculation of total ionization cross sections \( (Q_{\text{ion}}) \) using the CSP-ic method for some atoms and some light molecules from their ionization threshold to 2000 eV energy. The theoretically calculated results are compared with experimental and other theoretical results. Important conclusions of the present calculations are drawn.

In recent times, electron scattering experiments with complex biomolecules in the gas phase are challenging because of the difficulties in the preparation of well-characterized pure gas targets of these molecules and the subsequent quantitative determination of the target densities. Hence theoretical studies are important. In chapter 4 we present total (complete), total elastic, total inelastic and total ionization cross sections for DNA and RNA based biomolecules (Adenine, Guanine, Thymine, Cytosine, Uracil, Phosphoric acid and sugar phosphate backbone) using theoretical methods (Spherical Complex Optical Potential (SCOP), Complex Scattering Potential – ionization contribution (CSP-ic) and compare our results with available other results to draw important conclusions.

Chapter 5 deals with the total cross sections for atmospherically important molecules such as \( \text{N}_2, \text{N}_2\text{O}, \text{O}_3 \) on electron impact from 0.1 eV to 2000 eV. We have combined results from the UK molecular R-Matrix code to determine \( Q_T \) for incident energies from 0.1 eV to 20 eV with calculations based on the spherical complex optical potential formalism for calculation from ionization threshold of the target to the higher energies up to 2 keV. The results are promising with good matching at the transition energy (between 15-20 eV) between the two methodologies and fairly good agreement with available data throughout the energy range. These calculations are compared with experimental and theoretical results wherever available.

In chapter 6 we presents the total cross sections with available comparisons for atmospherically important molecules such as \( \text{HCl}, \text{HBr}, \text{CF}_2 \) and \( \text{SiF}_2 \) on electron impact from 0.1 eV to 2000 eV using the same methodology as per chapter 5. We also discuss about the differential cross section for \( \text{CF}_2 \) and \( \text{SiF}_2 \) in this chapter.

Finally the thesis ends up with chapter 7 containing discussions, conclusions and future prospects of the present work. A significant feature of the hybrid theoretical approach is its applicability to determine different cross sections over a wide energy range.