Executive Summary of the Ph.D. thesis entitled

STUDY OF ELECTRON INDUCED IONIZATION AND OTHER PROCESSES FOR MOLECULES

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By

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Definition of the problem

Deep research into the dynamics of scattering event is necessary given the potential applications of atomic or molecular scattering data in numerous scientific and technological sectors, such as plasma sciences, astro sciences, semiconductor industries, biomedical fields, etc [1–5]. In this thesis, we describe the various interaction processes for electron collision with atoms and molecules, using several modern theories. The detailed outline of the problem has been mentioned in **chapter 1** of the thesis. We have endeavoured to study the electron scattering over a broad energy range, spanning from 0.1 eV to 5000 eV, for gaining a better understanding of the various collision processes that take place at different energy regimes. To account for the fact that no one theory can account for such a wide range of incidence energies, we have made use of two different formalisms: the R-matrix and the Spherical Complex Optical Potential (SCOP). These two formalisms have been used in the present work of exploring a variety of induced interaction processes for the gaseous and aqueous phase molecular compounds and give graphical data on the molecular attributes as well as total cross sections, through which the quantification of probability of occurrence of a variety of events can be accomplished. Other than cross-sections data, three major applied quantities in the DNA damage assessment, viz. Inelastic mean free path, Mass stopping power and Absorbed dose have been also computed for the aqueous phase DNA compounds through modified SCOP formalism.

Brief Research Methodology

The quantification of various molecular interaction processes occurring during the electron-molecules interaction is done through various elastic and inelastic cross-sections, which are calculated for the electron collision with target systems for an extensive impact energy range 0.1-5000 eV [6,7]. For low energy calculations (i.e., 0.1-15 eV) R-matrix approach [6,8–10] and for intermediate to high energy calculations (i.e., ionisation threshold to 5000 eV) spherical complex optical potential (SCOP) formalism [11–14] is employed. Complex scattering potential-ionisation contribution (CSP-ic) technique [15–18] is used to extract out the ionisation cross-sections from the total inelastic cross-sections. Various correlations between the cross-sections and target properties have also been analysed and discussed, leading to the prediction of polarizability and dielectric constant of the targets [12,19]. The computation methodology in case of condensed or solid phase target systems is also described [19,20]. The theoretical methodology is discussed in **chapter 2** of the thesis.

Key findings

The key findings of this investigation are the electron collision cross sections for various applied molecules. The results of the computations of various cross-section data for various applied molecules has been discussed in the **chapter 3** and **chapter 4**. In addition to cross sections, the inelastic mean free path (IMFP), mass stopping power (MSP), and absorbed dose (D) calculations for aqueous target systems are investigated during this research work. The results of these applied quantities (IMFP, MSP, D) has been given in **chapter 5**. Various correlations between the cross-section data and molecular properties have been also analysed, leading to the prediction of polarizability and dielectric constant of the molecules. The findings from the low to high energy calculations (0.1 to 5000 eV) are reported in **chapter 6**.

Conclusion

By employing two theoretical methodologies, viz., (i) SCOP in conjunction with CSP-ic and (ii) R-matrix formalism, we have quantified the various molecular interaction processes induced by the projectile electron through computing the respective cross-sections for an extensive energy range, 0.1 eV to 5000 eV. Other applied quantities in the field of biomedical research, viz., inelastic mean free path, mass stopping power, and absorbed dose has been calculated for the aqueous phase DNA compounds. With this, by producing good reliable data, we are able to publish our work into reputed journals.

Recommendations

The importance of the present research work is underscored by the fact that large amounts of data are needed to create the "virtual laboratories" that are essential for studying atmospheric science, radiation physics, technical plasmas, and astrophysics. Experiments on particular target systems, such as those that are not available in the gas phase, or any radioactive or toxic molecular compounds, can be challenging or perhaps impossible to carry out. If it is conceivable, then the experimental errors can be anywhere from 15% to 25% or even higher. In circumstances like these, the approach that we have developed is of great significance to the field of applied physics. Our goal is to expand the scope of our calculation to include larger

and complex molecular systems such as dimers, bio compounds, clusters, and so on. We plan to focus in the future on other interaction processes as well, such as neutral and ionic dissociation. In this regard, some of the unsolved difficulties and unexplored potential are connected to the following aspects:

- Quantification of the dissociative ionisation, partial ionisation, dissociative electron attachment (DEA) for electron collisions with the molecules.
- Modifying the theoretical models to study the condensed or solid phase molecular systems.
- Apart from electron interactions, positron and positronium collision study can be investigated.
- Apart from cross-sections, other essential quantities applicable in various research and applied fields can also be into the focus for the future work.
- To account for larger and complex molecules, R-matrix calculations can be expanded.
- To compute the rotational and vibrational excitation cross-sections, modification in the model potentials can be aimed.

Detailed description on this can be find in **chapter 7** of this thesis.

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