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STUDY OF MOLECULAR PROCESSES THROUGH CHARGED PARTICLE SCATTERING

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INTRODUCTION

The present work examines and explain the scattering processes of intermediate to high energy electron collision with variety of atomic and molecular targets. It will cover the impact energy range from ionization energy of most atoms and molecules (about 10-15 eV) to energy at or above 5000 eV. Since the response of an atomic and molecular target to the incident electron depends on its impact energy and the structural properties of the target itself [1]. Since the beginning of the 20th century, both theoretical and experimental molecular physics communities have studied electron molecule collisions.

Our interest in the present collision calculations arises in view of the applications of relevant cross section data in both pure and applied sciences. The selected targets find applications in atmospheric science, plasma physics / chemistry and radiation physics. In addition to photo-induced processes in the ionosphere, atmospheric ionization is also produced by high energy particles emitted from the Sun and the cosmic rays. These particles may also play a role in cloud formation and climate change. Therefore, it is important to be able to determine the electron impact total and ionization cross sections of Aeronomy species. Different techniques to characterise, describe, and model various processes in low-temperature plasmas, which are increasingly useful in a variety of quickly evolving high-tech applications (such as the manufacture of microelectronic chips) and semiconductor physics, heavily rely on electron-molecule collisions [2,3].

Recently it has been recognized that electron driven processes also play an important role in life sciences, for example by initiating single and double strand breaking in DNA. DNA double-strand breaks (DSB) and single strand breaks are not formed as a consequence of the direct absorption of UV radiation by DNA. Rather, they occurred as the consequence of the attempted repair of UV radiation-induced base damage in DNA. Radiation therapy is one of the major cancer treatment techniques other than chemical and surgical therapy. During radiation therapy electrons are produced with a wide range of energies from the irradiated areas. The secondary electrons produced can collide with DNA molecules in human cells, causing damage that destroys the cancer cells [4,5].

Electron scattering experiments with complex molecules e.g. bio-molecules (thymine, adenine, guanine, 3-hydroxytetrahydroFuran, α-Tetrahydrofurfuryl alcohol etc.), industrial relevance molecules (Furfural, para-Benzo quinone etc.) and reactive radicals in the gas phase are

challenging because of the practical difficulties involved in the preparation of well-characterized pure gas targets of these molecules and in the subsequent quantitative determination of the target densities. Hence, there is a need for more comprehensive theoretical investigations of electron scattering studies evaluating various quantitative and qualitative cross sections for these molecules/radicals. Therefore, there has been an ever - increasing emphasis on the development of theoretical methods to provide data using simpler approximate theories, capable of delivering cross sections accurately and quickly over a wide range of energy so as to encompass many important phenomena, e.g. ionization of the target.

In modeling such processes there is a need for accurate knowledge of electron collision cross sections for relevant biological molecules. All these fundamental as well as technological reasons motivated us to take up this study. In this work we investigate the molecular processes induced by the electrons and quantify them through various cross sections e.g. ionization, excitation, inelastic, elastic, total cross sections etc. For the intermediate and high energy calculations we have employed the Spherical Complex Optical Potential (SCOP) approach and Complex Scattering Potential-ionization contribution (CSP-ic) method.

CHAPTERS OF THE THESIS

The study of electron-molecule interactions conducted for the thesis is presented in the following chapters:

Chapter I	Introduction
Chapter II	Theoretical Methodology
Chapter III	Electron collisions with analogous of DNA/RNA nucleobases
Chapter IV	Interaction processes for molecules of industrial relevance
Chapter V	Electron driven processes for aqua DNA constituents
Chapter VI	Ionization of N_2
Chapter VII	Summary and future prospects

Chapter I: Introduction

The scattering of particles provides a wealth of information about the structure of matter. Collision techniques have been effectively used to analyze the internal structure of the atoms and even of their constituent particles and also their nature of interactions. The basic scattering phenomena are explained in this chapter, along with the different electron interaction processes that can be observed in daily life. It also seeks to provide a summary of the history of electron-driven processes from different atoms and molecules. The study of electron interactions with biomolecules, astromolecules, plasma molecules or technological applied molecules is essential in the various applied fields, such as plasma sciences, radiation dosimetry, astrophysics and semiconductor industries etc. [6]. This chapter provides a brief summary of the significance of the target molecules chosen for the present investigation.

Chapter II: Theoretical Methodology

In this chapter the details of theoretical formalisms used for the present electron interactions study is given. We have used three different methodologies to study various molecular processes quantitively through the cross-sections.

[1] Spherical Complex Optical Potential (SCOP):

The study of scattering of electrons from the target molecules for the energies from ionization threshold (*IE*) to 5000 eV is done using the SCOP formalism. The spherically symmetric complex optical potential of the following form is employed for the calculations of inelastic and elastic cross-sections through the partial wave analysis method [8,9].

$$V_{opt}(r, E_i) = V_R(r, E_i) + iV_I(E_i, r)$$

Here, V_R includes the static potential, exchange potential and polarization potential. The imaginary part V_I of the optical potential includes the absorption potential.

[2] Complex Scattering Potential-ionization contribution (CSP-iC):

To bifurcate the continuum (Q_{ion}) and discrete (Q_{exc}) contributions of the inelastic cross-sections, this CSP-ic approach is employed. In this method we compute ionization cross section from inelastic cross sections by defining the dynamic ratio,

$$R(E_i) = \frac{Q_{ion}(E_i)}{Q_{inel}(E_i)} = 1 - C_1 \left[\frac{C_2}{U+a} + \frac{\ln U}{U} \right]$$

The dimension less parameters C_1, C_2 and a are obtained by applying the boundary conditions of $R(E_i)$, which is given by,

$$R(E_i) = \begin{cases} 0, & for\ E_i \leq IE \\ R_P, & for\ E_i = E_P \\ 1, & for\ E_i \gg IE \end{cases}$$

where, E_p stands for the peak energy at which the Q_{inel} has its maximum value. From the several results of the experiments and theories the value of R_p at the E_p, is found to be around 0.7 - 0.8 [10-12].

[3] Semi-empirical model:

The semi-empirical model is a relatively quick and computationally cheap method for predicting the Total Cross section (TCS) of complex molecules. In this work, TCS for Furfural and Para Benzoquinone are calculated for the energy rang 500 eV to 10,000 eV. Further it might serve to audit both the theoretical approaches commonly used to estimate the TCS and also the experimental data, in the range above several hundreds of eV.

In, reference of [13] following two parameter analytical equation was proposed:

$$\sigma_T = \frac{0.78(Z) + 0.016(\alpha) - 17.9}{E^{0.77}}$$

Where, σ_T= Total cross section in atomic unit (a_0^2), Z= total no. of electrons in the target molecule, α= molecular polarizability in atomic unit (a_0^3) and E is the energy of incident particles in KeV.

Chapter III: Electron collisions with analogous of DNA/RNA nucleobases

In this chapter we report the inelastic, ionization, electronic excitation, elastic and total cross-sections data of the analogous of DNA/RNA nucleobases: 3-hydroxytetrahydroFuran and α-Tetrahydrofurfuryl alcohol for the energy from ionization threshold to 5000 eV. For the calculations, SCOP and CSP-iC methods have been employed. Also, the correlation analysis between the peak of Q_{ion} and polarizability of the molecule has been done. Also, we used another formalism called complex scattering potential – ionization contribution (CSP-ic), to compute ionization cross sections (Q_{ion}) and summed excitation cross-sections ($\sum Q_{exc}$). These cross-section data which may serve as the input parameters in predicting damage in biomolecular system induced by an electron within the energy range [14].

Chapter IV: Interaction processes for molecules of industrial relevance

In this chapter, we present the theoretical investigations of the electron scattering cross sections of the important complex molecules of industrial relevance, viz., Furfural and p-Benzoquinone for the energy range from molecular ionization energy to 5000 eV. For all of these molecules, the total (Q_T), elastic (Q_{el}), inelastic (Q_{inel}), ionization (Q_{ion}) and excitation (Q_{exc}) cross-sections are reported. Also, TCS for Furfural and Para Benzoquinone are calculated for the energy rang 500 eV to 10,000 eV using Semi- empirical model [15].

Chapter V: Electron driven processes for aqua DNA constituents

Since in the human body DNA is always covered by the water molecules, for the present investigations of electron interactions with DNA bases, we have considered the molecules in their aqueous phase. Apart from the cross-sections [16], in this chapter we have also reported the inelastic mean free path (IMFP), mass stopping power (MSP) and absorbed dose (D) from the cross-sectional data for the aqueous DNA bases upon the impact of the electrons. All of these three quantities are essential input parameters in the modelling of DNA damage assessment. Also, we have calculate, TCS for aqua DNA constituents for energy rang 500 eV to 10,000 eV using Semi- empirical model.

Chapter VI: Ionization of N_2

In this chapter, we report an electron scattering cross-sectional of N_2 molecule viz. Ionization cross sections for the wide energy range, ionization threshold to 10,000 eV, CSP-iC method is used. And present data are compared with CB1 model, and CTMC model. The CTMC calculations also fall below these existing data and the difference increases for higher energy. The CB1 model is closer to the present measurements and has a large deviation from the existing data. The TCS values predicted by the CSP-ic model overestimates the measured data for all the energies, but provides a good qualitative behavior regarding the energy dependence. This discrepancy could be due to the consideration of the spherical charge density of the N_2 molecule and other approximations used in the semi-empirical model. It is to be noted that the TCS calculations obtained using the two *ab initio* models, (CB1 and CTMC), lie below and just above the experimental values, respectively [17].

Chapter VII: Summary and future prospects

In this last chapter of the thesis, we summarize the present results and draw important conclusions of the present work. The future prospects of the present work in terms of latest experimental and theoretical status, will be also discussed in this chapter. We believe that the present comprehensive electron scattering studies will help in understanding of the various electron induced molecular processes for different important applied molecules studied here.

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[4] Smruti Parikh, **Dhaval Chauhan**, Chetan Limbachiya, "Electron induced inelastic processes for aqua DNA compounds" (Manuscript to be communicated)

Papers presented in the conferences:

[1] Investigation of Electron Interaction With FURFURAL(C5H4O2)
Dhaval Chauhan, Chetan Limbachiya
AISAMP-13th (Asian International Seminar on Atomic and Molecular Physics), 3 to 8 December 2018, IIT Bombay and TIFR-mumbai.

[2] Study of Electron Interactions with plasma processing gases like TiClx and CFx (x= 1-4)
Dhaval Chauhan, Rakesh Bhavsar, Chetan Limbachiya
National Conference on Atomic and Molecular Physics (NCAMP), 25th to 28th March 2019, IIT Kanpur

[3] Cross-sectional Study of electron interaction with Bio-Molecules, Furfural($C_5H_4O_2$), α-Tetrahydrofurfuryl alcohol ($C_5H_{10}O_2$) ,3-HydroxytetrahydroFuran($C_4H_8O_2$)
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[4] Electron interaction with Para-Benzoquinone($C_6H_4O_2$) and Naphthoquinone($C_{10}H_6O_2$)
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