Synopsis of the thesis entitled

STUDY OF ELECTRON INDUCED IONIZATION AND OTHER PROCESSES FOR MOLECULES

To be submitted to
The Maharaja Sayajirao University of Baroda, Vadodara

For the degree of

DOCTOR OF PHILOSOPHY

In

PHYSICS

By

Smruti H. Parikh

Under the supervision of

Dr. C. G. Limbachiya

Department of Applied Physics
Faculty of Technology and Engineering
The Maharaja Sayajirao University of Baroda
Vadodara-390 001

February 2023

Synopsis of the thesis for Ph.D. degree in Physics

Title: **Study of electron induced ionization and other processes for molecules**

Submitted to: The Maharaja Sayajirao University of Baroda,
Vadodara – 390001

Submitted by: Smruti H. Parikh
Research Scholar,
Department of Applied Physics,
Faculty of Technology and Engineering,
The Maharaja Sayajirao University of Baroda, Vadodara

Registration No: FOTE/999

Registration Date: 17/07/2019

Ph.D. Supervisor: Dr. C. G. Limbachiya
Head of the Department,
Department of Applied Physics,
Faculty of Technology and Engineering,
The Maharaja Sayajirao University of Baroda, Vadodara

Smruti H. Parikh
(Research scholar)

Dr. C. G. Limbachiya
(Research supervisor)

INTRODUCTION

The present work examines the interactions of electrons with the molecular targets over the wide energy range 0.1 to 5000 eV. The growing significance of electron assisted processes in the advancement of modern technology is what triggers the present interest in the study of electron-molecule collisions [1]. Since the beginning of the 20th century, both theoretical and experimental molecular physics communities have studied electron molecule collisions. This field is sufficiently developed to have direct applicability to processes involving plasma, astrochemistry, the environment, interstellar space, chemistry, and biology.

The rapidly growing technical importance of low-temperature plasmas in fields such as plasma-assisted etching of microstructures and the deposition of high-quality thin films has produced an immediate need for a wide range of electron-impact cross-sections (excitation, ionization, dissociation, etc.). 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].

Radiation damage in bio-molecular systems provides essential insight into cellular DNA damage mechanisms. Owing to ozone layer destruction caused by pollution and technological advancements, we are constantly exposed to radiations. These radiations promote water radiolysis in living human cells, producing OH radicals and many secondary electrons. Most reactive electrons react with the cell molecules to create negative ions. Negative ions can modify base and sugar, break DNA, and destroy living cells. Mutation of DNA causes cancer. Radiation therapy with high-energy photons, electrons, and ions is a common cancer treatment. Hence, estimation of DNA radiation damage in terms of absolute cross sections is crucial. These cross-sections offer the physical foundation for the simulation of the dose distribution in patient before radiation treatment [4,5].

Modern satellite telescopes like Hubble and massive ground-based arrays like ALMA have revealed a rich chemical inventory in the interstellar medium, star and planet formation regions, and cometary and planetary environments [6]. Electron interactions with these

astromolecules result in the chemistry of the synthesis of other compounds, including amino acids, which are thought to be the building blocks of life.

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. We report elastic cross-sections that include symmetry decomposition, differential scattering cross-sections, and inelastic cross-sections that comprise electronic excitations and ionization for the wide energy range 0.1 to 5000 eV. For the low energy calculations (0.1 to 15 eV), we have used R-matrix formalism and 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 of electron collision processes
Chapter II	Theoretical Methodology
Chapter III	Electron collisions with the D-molecules and H_2SO_4
Chapter IV	Interaction processes for biomolecules
Chapter V	Electron interactions for radiation damage modeling of aqua DNA constituents
Chapter VI	Molecular processes of fluoromethanes for wide energy range
Chapter VII	Summary and future prospects

Chapter I: Introduction of electron collision processes

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. [7]. 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] R-matrix formalism:

To compute the electron scattering cross-sections in low energy regime (i.e., 0.1 to 20 eV), the ab-initio R-matrix theory is used. These calculations include the total elastic cross-sections along with their symmetric components, differential and momentum transfer cross-sections. UK molecular R-matrix code is employed for the calculations. The basic idea of the R-matrix is the division of configuration space into inner and outer region. The boundary line of these two regions is decided with the sphere of radius ~$10a_o$ and whose center lies at the center of mass of the target molecule [8].

[2] 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 [9,10].

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

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.

[3] 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 [11-13].

Chapter III: Electron collisions with the D-molecules and H_2SO_4

In this chapter we report the inelastic, ionization and electronic excitation cross-sections data of the twelve D-molecules, viz., HD, D_2, D_2O, ND_x (x=1-3), SiD_x (x=1-3) and CD_x (x=2-4) and H_2SO_4 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. Moreover, from this correlation study, the polarizabilities for ND and SiD_x (x=1-3) molecules have been predicted. For the H_2SO_4, we present the inelastic interaction results for the electron impact [14,15].

Chapter IV: Interaction processes for biomolecules

In this chapter, we present the theoretical investigations of the electron scattering cross-sections of the important complex biomolecules, viz., Nucleosides (Adenosine, Cytosine, Guanosine, Thymidine and Uridine), Furfural and Para benzo quinone 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 [16,17].

Chapter V: Electron interactions for radiation damage modeling of 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 [18], in this chapter we have also reported the inelastic mean free path (IMFP), mass stopping power (MSP) and absorbed dose (D) [19] 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.

Chapter VI: Molecular processes of fluoromethanes for wide energy range

In this chapter, we report an extensive electron scattering cross-sectional data; Elastic cross sections include the symmetry decomposed elastic cross-sections, differential and momentum transfer cross-sections, while inelastic cross-sectional data comprises of discrete electronic excitations and ionization cross-sections for the wide energy range from 0.1 to 5000 eV for fluoromethanes. For the low energy range from 0.1 to 15 eV, the R-matrix method is employed, while for the energy above ionization threshold and up to 5000 eV, SCOP and CSP-iC methods are used [20].

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.

References:

[1] L. Sanche, In: M. Greenberg (Ed.), Radical and Radical Ion Reactivity in Nucleic Acid Chemistry, 239, John Wiley & Sons, Inc., (2009)

[2] R. K. Janev (Ed.), Atomic and Molecular Processes in Fusion Edge Plasmas, Plenum, New York (1995)

[3] S. M. Younger, T. D. Märk, G. H. Dunn (Eds.), Electron Impact Ionization, Springer Verlag, Vienna (1985)

[4] S. Feil *et.al.*, Journal of Physics B: Atomic Molecular and Optical Physics, **37**:3013 496 (2004)

[5] B. Boudaïffa, P. Cloutier, D. Hunting, M. A. Huels, L. Sanche, Science, **287**:1658 (2000)

[6] M. A. Cordiner *et.al.*, Astrophys. J. Lett. **792**: L2 (2014)

[7] Minaxi Vinodkumar, Harshad Bhutadia, Chetan Limbachiya, K. N. Joshipura, International Journal of Mass Spectrometry **308**: 35 - 40 (2011)

[8] Jonathan Tennyson, Physics Reports **491**:29 - 76 (2010)

[9] A. Jain, Physical Review A **34**:3707 (1986)

[10] Jain and K. L. Baluja, Physical Review A **45**:202 (1992)

[11] K. N. Joshipura, M. Vinodkumar, C. G. Limbachiya, and B. Antony, Physical Review A **69**:022705 (2004)

[12] C. Limbachiya, M. Vinodkumar, M. Swadia, and A. Barot, Molecular Physics **112(1)**:101-106 (2014)

[13] M. Vinodkumar, C. Limbachiya, H. Desai, and P. C. Vinodkumar, Physical Review A **89**:062715 (2014)

[14] Smruti Parikh, Chetan Limbachiya, K. N. Joshipura, Calculations of Total Ionization Cross-Sections for Electron Impact on H_2SO_4, In: V. Singh, R. Sharma, M. Mohan, M. S. Mehata, A. K. Razdan, (eds) Proceedings of the International Conference on Atomic, Molecular, Optical & Nano Physics with Applications. Springer Proceedings in Physics, vol 271. Springer, Singapore (2020)

[15] Smruti Parikh, Minaxi Vinodkumar, Chetan Limbachiya, Electron impact inelastic molecular processes for deuterated compounds, Chemical Physics **565**, 111766 (2023)

[16] Smruti Parikh, Chetan Limbachiya, Electron driven molecular processes for Nucleosides, Radiation Physics and Chemistry (communicated)

[17] Dhaval Chauhan, Smruti Parikh, Chetan Limbachiya, Theoretical investigations of electron interaction processes for Furfural and para-Benzoquinone (to be communicated)

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

[19] Smruti Parikh, Chetan Limbachiya, Electron interactions with DNA constituents in aqueous phase, The Journal of Physical Chemistry B (communicated)

[20] Smruti Parikh, Tejas Jani, Nirali Bhavsar, Minaxi Vinodkumar, and Chetan Limbachiya, Electron interaction study with CH_2F_2 molecule over wide energy range 0.1-5000 eV (to be communicated)

Publications:

[1] **Smruti Parikh**, Chetan Limbachiya, K. N. Joshipura, Calculations of Total Ionization Cross-Sections for Electron Impact on H_2SO_4, In: V. Singh, R. Sharma, M. Mohan, M. S. Mehata, A. K. Razdan, (eds) Proceedings of the International Conference on Atomic, Molecular, Optical & Nano Physics with Applications. Springer Proceedings in Physics, vol 271. Springer, Singapore (2020)

[2] **Smruti Parikh**, Minaxi Vinodkumar, Chetan Limbachiya, Electron impact inelastic molecular processes for deuterated compounds, Chemical Physics **565**, 111766 (2023)

[3] **Smruti Parikh**, Chetan Limbachiya, Electron interactions with DNA constituents in aqueous phase, The Journal of Physical Chemistry B
(Under review)

[4] **Smruti Parikh**, Chetan Limbachiya, Electron driven molecular processes for Nucleosides, Radiation Physics and Chemistry
(Under review)

[5] **Smruti Parikh**, Tejas Jani, Nirali Bhavsar, Minaxi Vinodkumar, and Chetan Limbachiya, Electron interaction study with CH_2F_2 molecule over wide energy range 0.1-5000 eV
(Manuscript to be communicated)

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

[7] Dhaval Chauhan, **Smruti Parikh**, Chetan Limbachiya, Theoretical investigations of electron interaction processes for Furfural and para-Benzoquinone
(Manuscript to be communicated)

Papers presented in the conferences:

[1] Theoretical Calculations of Total Ionization Cross-sections for Electron Impact on H_2SO_4 molecule
Smruti Parikh, Chetan Limbachiya, K. N. Joshipura
International conference on Atomic, Molecular, Optical and Nano Physics with Applications (CAMNP 2019), 18^{th} – 20^{th} December 2019, DTU, Delhi

[2] Electron interactions with Fluorocompounds for application in Plasma sciences
Smruti Parikh, Chetan Limbachiya
Topical conference (TC 2020) on Atomic and Molecular collisions for Plasma Applications, 3^{rd} – 5^{th} March 2020, IIT Roorkee, Uttarakhand

[3] Electron interaction with Deuterated molecules
Smruti Parikh, Chetan Limbachiya (FSQT 2020)
Fundamental science & Quantum technologies using Atomic Systems (FSQT 2020), 28^{th} September – 1^{st} October 2020, Physical Research Laboratory, Ahmedabad (online mode)

[4] Inelastic processes for electron scattering with deuterated compounds
Smruti Parikh, Chetan Limbachiya
XXII International Symposium on Electron-Molecule Collisions and Swarms (POSMOL) Conference, 29^{th} - 30^{th} July 2021, University of Norte Dame, USA (online mode)

[5] Electron Inelastic Mean Free Path and Mass Stopping Power Calculations for DNA Molecules
Smruti Parikh, Chetan Limbachiya
International Seminar on Advanced Materials and Applications (ISAMA 2022), 18^{th} July 2022, The Maharaja Sayajirao University of Baroda, Vadodara