

Table of Contents

Chapter 1 Introduction of electron collision processes	12
1.1 Introduction	12
1.2 Electron collisions	13
1.2.1 Electron: A superior probe for collision mechanisms	13
1.2.2 Electron induced molecular processes	14
1.3 Previous studies on electron collisions	16
1.3.1 Theoretical methods	16
1.3.2 Experimental techniques	17
1.4 Applications of electron scattering study	19
1.4.1 Planetary sciences	19
1.4.2 Biomedical research field	21
1.4.3 Industrial fields	22
1.5 Outline of the problem	23
1.6 Bibliography	26
Chapter 2 Theoretical Framework	33
2.1 Introduction	33
2.1.1 Physical interpretation of cross-sections	34
2.1.2 Optical Theorem	35
2.2 Spherical Complex Optical Potential approach (SCOP)	37
2.2.1 Interaction potentials	37
2.2.2 Partial wave analysis	40
2.2.3 Numerov Method	44
2.2.4 Condensed/Aqueous phase computation	45
2.2.5 Two-parameter semi-empirical method (2p-SEM)	46

2.3	Complex Scattering Potential-ionisation contribution method (CSP-ic)	49
2.3.1	Ionisation contribution	49
2.3.2	Evaluation of Q_{ion}	50
2.3.3	Summed total electronic excitation cross-sections (ΣQ_{exc})	51
2.4	Correlation study: Prediction of polarisability (α) and dielectric constant (ϵ) ..	51
2.4.1	Polarisability (α)	51
2.4.2	Dielectric constant (ϵ)	52
2.5	Low-energy computation: R-matrix approach	52
2.5.1	Methodology	53
2.5.2	Polar molecular targets	58
2.5.3	Scattering models used in the calculations	58
2.5.4	Various modules of QUANTEMOL-N code	60
2.6	Bibliography	64
Chapter 3 Electron collisions with D-molecules and H_2SO_4		68
3.1	D-molecules	68
3.1.1	Literature survey	69
3.1.2	Theoretical Methodology	70
3.1.3	Results and Discussion	71
3.2	H_2SO_4 (sulfuric acid)	86
3.2.1	Theoretical Methodology	87
3.2.2	Results and Discussion	88
3.3	Bibliography	91
Chapter 4 Interactions processes for biomolecules		97
4.1	Nucleosides	97
4.1.1	Theoretical Methodology	99
4.1.2	Results and Discussion	100

4.2	Furfural (C ₅ H ₄ O ₂) and para-Benzoquinone (C ₆ H ₄ O ₂)	106
4.2.1	Literature survey and Target properties	109
4.2.2	Results and Discussion.....	110
4.3	Fluoronitriles (C ₃ F ₅ N and C ₄ F ₇ N)	116
4.3.1	Literature survey and Target properties	118
4.3.2	Results and Discussion.....	119
4.4	Correlations study	123
4.4.1	Computation of dielectric constant (ϵ)	129
4.5	Bibliography	133
Chapter 5 Electron intercatons for radiation damage modeling of aqua DNA constituents		141
5.1	Introduction	141
5.2	Various cross-sections	143
5.2.1	Literature survey and Molecular properties	143
5.2.2	Results and discussion	144
5.3	Inelastic Mean Free Path (IMFP)	153
5.3.1	Molecular properties and Literature study	153
5.3.2	Results and Discussion.....	155
5.4	Mass Stopping Power (MSP).....	164
5.4.1	Literature survey and Molecular properties	164
5.4.2	Results and Discussion.....	165
5.5	Absorbed Dose (D)	172
5.5.1	Results and Discussion.....	173
5.6	Bibliography	177
Chapter 6 Molecular processes of Fluoromethanes for wide energy range.....		183
6.1	Introduction	183

6.2	Difluoromethane (CH₂F₂)	184
6.2.1	Literature study	185
6.2.2	Target model.....	187
6.2.3	Results and Discussion.....	189
6.3	Methyl fluoride (CH₃F).....	198
6.3.1	Literature study	199
6.3.2	Target model.....	200
6.3.3	Results and Discussion.....	202
6.4	Bibliography	207
Chapter 7 Summary and future prospects		212
7.1	Summary of the present investigation	212
7.1.1	Advantages and Limitations of the present methodologies.....	215
7.2	Future prospects	215