

# Contents

Abstract	page
Acknowledgments	i
Contents	iii
List of Figures	v
List of Tables	vii
List of Symbols	xi
List of Abbreviations	xiii
<b>Chapter 1: Introduction</b>	xv
1.1 Reaction Dynamics in Gas-Phase	1
1.2 Electronic Structure Calculations	2
1.3 Classical Trajectory Simulations	2
1.4 Organization of Thesis	5
	7
<b>Chapter 2: Theoretical Methods and Techniques</b>	9
2.1 Potential Energy Surface	9
2.1.1 Dimensionality	9
2.1.2 Geometry Optimization and Stationary Points	10
2.1.3 Normal Mode Analysis	12
2.2 Born-Oppenheimer Molecular Dynamics (BOMD)	13
2.2.1 Integration Methods	14
2.2.2 Integration Time-step	15
2.2.3 Trajectory Initial Conditions	16
2.2.4 Unimolecular Dynamics	16
2.2.5 Non-RRKM behavior	17
2.3 Software	18
<b>Chapter 3: Unimolecular Decomposition of Formamide</b>	19
3.1 Computational Methodology	21
3.2 Results and Discussion	21
3.2.1 Potential Energy Surface	21
3.2.2 Direct Dynamics	25
3.3 Discussion	32
3.4 Summary	34
<b>Chapter 4: Dissociation Chemistry of Formyl Halides</b>	35
4.1 Computational Methodology	37
4.2 Results and Discussion	40
4.2.1 Potential Energy Surface	40
4.2.2 Direct Dynamics	45
4.2.3 Lifetime and RRKM Calculations	49
4.3 Summary	52
<b>Chapter 5: Collision Induced Dissociation of Deprotonated Glycolaldehyde</b>	53
5.1 Computational Methodology	54
5.2 Results and Discussion	57
5.2.1 Dynamics of ${}^1\text{C}$	59
5.2.2 Dynamics of ${}^1\text{O}$	61
5.3 Discussion	62
5.4 Summary	63
<b>Chapter 6: Conclusions and Future Scope</b>	65
A.1 Potential Energy Profile	69
A.2 Trajectory Snapshots	71
A.2.1 HFCO	71
A.2.2 HCICO	72
A.2.3 HBrCO	73
A.2.4 HICO	74

