Contents

CHAPTER 1: Introduction 1
1.1 Preamble 2
1.2 Quantum Chemical Methods 5
   1.2.1 Hartree-Fock method 7
   1.2.2 Post-Hartree-Fock Methods 14
   1.2.3 Configuration Interaction 15
   1.2.4 Perturbation Theory 17
   1.2.5 Density Functional Theory 20
1.2 Molecular properties 26
   1.3.1 Molecular Electron density 27
   1.3.2 Molecular Electrostatic Potential 30
   1.3.3 Population Analysis 32
   1.3.4 Natural Bond Orbital Analysis (NBO) 36
   1.3.5 Vibrations Frequencies 38
   1.3.6 NMR Chemical Shifts 42
   1.3.7 Self consistent reaction field (SCRF) Methods 45
1.4 High Energy Molecules 48
1.5 Biologically Important Molecules 49

CHAPTER 2: Molecular electrostatic potentials and electron densities in aza-, nitroaza- and nitro- tripriprismanes 60
2.1 Introduction 61
2.2 Computational method 63
2.3 Results and Discussion 67
   2.3.1 Azatriprismanes 67
   2.3.2 Nitroazatriprismanes 77
   2.3.3 Nitrotripriprismanes 86
2.4 Conclusions 97
CHAPTER 3: Theoretical investigations on electronic structures and charge distribution in nitronorbornanes

3.1 Introduction 101
3.2 Computational method 102
3.3 Results and Discussion 103
3.4 Conclusions 104

CHAPTER 4: Electronic structure and vibrational analysis of AHA--HX complexes

4.1 Introduction 128
4.2 Computational method 129
4.3 Results and Discussion 130
4.4 Conclusions 130

CHAPTER 5: Theoretical investigations on the structure and vibrational spectra of N-(2-hydroxy-1- naphthylidene)threonine

5.1 Introduction 150
5.2 Computational method 151
5.3 Results and Discussion 152
5.4 Conclusions 152

CHAPTER 6: Charge distributions and vibrational characteristics of Glycine/NMDA receptor antagonists

6.1 Introduction 163
6.2 Computational method 164
6.3 Results and Discussion 165
6.4 Conclusions 166

Appendices 191