Abstract

The concepts of quantum chemistry/mechanics while putting together with mathematical models and computer algorithms, give rise to computational chemistry. The basic idea behind both the fields of quantum/theoretical chemistry and computational chemistry may be the same, but they differ in the aspects of implementations. Similarly, molecular modelling comprises of all the tools and methods of quantum and computational chemistry, but it is not limited to just the chemistry or small molecules. Herein, the molecular modelling tools such as free energy analysis, molecular graphics, representation of molecules (coordinate system), electrostatic potential and molecular orbital analysis were incorporated to pinpoint the guiding principles and phenomenon. In the coming chapters, we will see how the borane (BH3) and alane (AlH3) react differently with 2,6-diaminopyridine and lead to the formation of different topologies.
On the other hand, the same borane (BH3) when reacts with triazine leads to a completely different type of macromolecule. The triazine units get dearomatized, and after subsequent trimerization, they lead to the formation of a calix like structure. The surprises from boranes continue until the end of this thesis. The various derivatives of boranes showed different reactivity towards bicyclic (alkyl)(amino)carbene (BICAAC). All of these experimental observations were thoroughly examined and well supported by the computational analysis. DFT calculations and their results have proven to be helpful in exploring the properties of macrocycles and adducts. The mechanisms of dearomatization and B-H bond activation were thoroughly examined to show the importance of molecular orbitals and Mulliken charges. The symmetry of molecules, the orientation of molecular orbitals and incorporation of π-character of the bonds have proved to be great factors among all others while determining the shape of the macromolecules.