

Abstract

Cations of boron are ethereal and extremely electrophilic species that play a vital role in boron chemistry. Borocations are categorized into three classes based on their coordination number. If boron has two substituents attached with it i.e., dicoordinated species then it is called Borinium. Tricoordinated borocation having three substituents attached with Boron are called Borenium cations. And lastly, the most popular and largely studied type of Borocations is tetrahedral. In my thesis, I have used Computational methods to study Borenium complexes. 1,3,2-diazaborenium having formal positive charge on it, reported by Khun and coworkers is taken as a Parent complex. I have substituted Hydrogen attached to Boron with different ligands and optimized the geometry and frequency. Mulliken charge analysis indicates that by changing different ligands, charge on Boron can be tuned. Also, HOMO-LUMO energy gap is calculated which speaks of the stability of different Borenium cations.