Abstract

This thesis provides a computational and experimental study of interactions between borazine and water. The motivation of the present work was to study the complexes of borazine and water and compare them with those of the benzene-water system, benzene being the organic chemistry analogue of borazine. It has already been established that the benzene-water system manifests an H-π interaction. The computations on the borazine-water system were performed using the GAUSSIAN 09 suit of programs. The computations, which involved, arriving at the optimized structures, calculations of the stabilization energies of the complexes and vibrational frequencies were carried out at B3LYP, M06 and MP2 levels of theory using 6-311++G(d,p) as the basis set.AIM calculations were also done to determine the nature of bonding in these complexes by examining the bond critical point for the complexes. Three complexes were obtained computationally out of which one was clearly observed in the matrix, which involved an N-H..O interaction. In this complex, complex 1, the borazine was the proton donor through its N-H group and water was the proton acceptor. This complex was also indicated to represent the global minima on the borazine-water potential surface. At this time, it is not clear if we were also observing complex 3, which showed an interesting B..O interaction. This bond, which we refer to as the boron bond, was indicated to be a local minima and to manifest a blue shifted N-H stretch. More work will be required to establish the presence of this complex in thematrix. Complex 2, was a structure in which O-H of water served as aproton donor and N of borazine is the proton acceptor.This complex was the closest in structure to the H-π interaction in benzene-water system. However, no evidence was found for the formation of this complex.It is therefore clear that the borazine-water system has little in common to the benzene-water system. This work clearly indicates that the boron containing systems have surprises to show in the study of the hydrogen bonding systems. Exploring the hydrogen bonded interactions in such systems is therefore an area of work that clearly begs to be performed.