

## Inter-IISER Chemistry Meet (IICM 2017)

### **Borazine and its rich spectrum of $\pi$ complexes: A matrix isolation infrared and *ab initio* study**

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#### **Abstract:**

Borazine, also referred to as inorganic benzene presents an interesting case study of non-covalent interactions involving the N-H group as well as the  $\pi$ -system. The interaction of borazine with various other  $\pi$  systems, such as acetylene, benzene and phenylacetylene was studied experimentally, using matrix isolation IR spectroscopy and *ab initio* computations. Borazine itself is a multifunctional molecule with N-H serving as a proton donor and the partially delocalized  $\pi$  electron cloud as a proton acceptor. Its interaction with various other multifunctional molecules provides interesting scenarios, as to which of the molecules acts as a proton donor and which as the proton acceptor.

In the case of all the  $\pi$  systems studied in our work, the global minimum was found to be the N-H group of borazine serving as the proton donor. Computations were carried out at the MP2 level of theory using both 6-311++G\*\* and aug-cc-pVDZ basis sets. In the case of both borazine-acetylene and borazine-phenylacetylene, a bent NH...C structure, where the N-H of borazine was the proton donor to the carbon of the acetylenic group was found to be the global minimum. However, in the case of borazine-benzene, a parallel displaced structure was found to be the global minimum at the MP2/aug-cc-pVDZ level of theory. Details of the experimental data and computational results will be presented.