COMPUTATIONAL AND SPECTROSCOPIC STUDY OF THE B-N DATIVE BOND IN AMMONIA BORANE

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Ammonia borane is the archetypal small molecule employed to study dative bonds (also known as coordinate covalent or dipolar bonds) theoretically. We analyze the sensitivity of the B-N dative bond to method and basis set by computing the B-N bond length and the B-N stretching frequency. Our goal is to find the least computationally demanding method and basis set combination that yields trustworthy results. Previous researchers have demonstrated the inaccuracy of the B3LYP method for describing this type of bond. Here, we compare results using the M06-2X hybrid density functional with ab initio methods including MP2, CCSD, and CCSD(T) with different sized basis sets. We compare these results to experimental solid state and gas phase Raman spectra. Monomer calculations overestimate the B-N bond length and underestimate the B-N stretch in ammonia borane when compared to experimental values. However, calculations performed on clusters of ammonia borane molecules do a better job of reproducing the solid state experimental results. This agreement could be due to dihydrogen bonding between the ammonia borane molecules.