GAS PHASE DIHYDROGEN BONDED COMPLEXES OF PHENOL AND BORANE-AMINE ADDUCTS

NARESH PATWARI GANPATHI, TAKAYUKI EBATA, and NAOHIKO MIKAMI, *Department of Chemistry, Graduate School of Science, Tohoku University, Sendai 980-8578, Japan*.

It is well known that a hydrogen atom attached to an electronegative element, such as oxygen or nitrogen or halogen, acquires a partial positive charge, while a hydrogen atom bonded to an electropositive element, such as boron or metal, acquires a partial negative charge. It is therefore possible for these oppositely charged hydrogen atoms to interact favorably. Thus the dihydrogen bond is an electrostatic / dipolar interaction of the type E-H...H-X (where E and X are electropositive and electronegative atoms, respectively, with respect to hydrogen). Though the existence of dihydrogen bond is known for more than a decade, almost all the evidence is crystallographic and theoretical. Recently we have observed dihydrogen bonded complexes between phenol and borane-amine adducts (borane-dimethylamine and borane-trimethylamine) in the gas phase. The characterization of these complexes using infrared spectroscopy together with the ab-initio calculations will be discussed.