ABSTRACT

We encounter hydrogen bonding interactions in our day to day life. It is important to understand these interactions in the biochemical, astrochemical and atmospheric fields. Hydrogen bonding interaction studies were performed in very simple π systems like benzene to more complex graphene, fullerene etc. with water. These kinds of π rich polycyclic aromatic hydrocarbons are abundant in astrochemical environments, which demand their further study. Naphthalene and anthracene being higher candidates of the ring systems are eligible for the hydrogen bonding studies. Matrix isolation infrared spectroscopy is a powerful tool to study the hydrogen bonding interactions. Rigid matrix cage, sample in excess of matrix gas, negligible intermolecular interactions and elimination of Doppler and collisional broadening give rise to peaks with small line width, which enables us to study features of weakly bound complexes and conformations. In this thesis, hydrogen bonded complexes of naphthalene-water was studied both experimentally and computationally and other PAH-water systems like naphthalene anion-water and anthracene anion-water has been investigated computationally. Computational work was carried out in B3LYP, M06, M06-2X and MP2 levels of theory using 6-311++G(d,p) basis set.