Abstract

Weak interactions, particularly hydrogen bonding interactions, play an important role in many biological and chemical systems. Most of the bio-molecular conformations are maintained by the hydrogen bonding. There are many experimental techniques, which have been used to study weak interactions. One such technique is matrix isolation infrared spectroscopy, which serves as a powerful tool to explore weak interactions and conformations. The sharp spectral feature obtained in matrix isolation technique permits the resolution of features due to weak complexes and different conformations. Hydrogen bonding has been extensively studied in last two decades. In recent times, weak hydrogen bonding such as O-H…π and C-H…π has drawn considerable attention. Another interesting aspect is the investigation of competitive hydrogen bonding in a molecule with multiple bonding sites. Formic acid and phenylacetylene are two ideal examples having multiple hydrogen bonding sites. Both can act as proton donor and proton acceptors, which eventually gives rise to a number of hydrogen bonded systems for these two precursor molecules. In this thesis, the hydrogen bonded complexes of formic acid and phenylacetylene have been studied. The main aim of this work is to elucidate the structures of the various hydrogen bonded complexes between the two precursor molecules. The computational work has been performed at M06-2X, MP2 and B3LYP level of theory using 6-311++G (d, p) basis set. Fourteen different geometries at the M06-2X, twelve at MP2 and thirteen at B3LYP level were obtained. Most of the structures at the different levels are similar at all three levels. The O-H…π interaction has been observed as a dominating interaction computationally in the ground state optimized at all three levels. To study these complexes experimentally, the matrix isolation experimental facility has been set up.