

Abstract

Among the weak interactions the hydrogen bond is one of the most interesting and abundant interactions that influences a variety of chemical and biochemical processes. The study of hydrogen bonding systems, using both experimental and theoretical methods, is therefore of considerable interest. Hydrogen bonding such as O-H...O, O-H... π , (acetylenic) C-H...O and C-H... π have drawn considerable attention. Another interesting aspect is the investigation of competitive hydrogen bonding in a molecule having multiple bonding sites. Among the several experimental techniques, which have been used to study weak interactions, matrix isolation infrared spectroscopy, together with quantum chemical calculations is a powerful tool. The spectral linewidths of features in a matrix isolated technique being small allows for the identification of weak complexes and conformations. Propargyl alcohol is an example of a molecule with multiple hydrogen bonding sites and thus, can act as proton donor (acetylenic C-H and O-H) as well as proton acceptors (O atom and π electron cloud), which eventually gives rise to a number of possible hydrogen bonded systems. In this thesis, we have explored experimentally and computational the rich potential energy landscape of the propargyl alcohol-water system. The computational work was performed at M06, MP2 and B3LYP levels of theory using 6-311++G (d, p) basis set. Nine different geometries at the M06, nine at MP2 and eight at B3LYP level were obtained. Most of the structures at the different levels (M06, MP2 and B3LYP) were similar at all three levels. The O-H...O interaction has been observed as a dominating interaction followed by weak H... π interaction computationally in the ground state optimized at all three levels. These complexes were studied experimentally using the matrix isolation technique.