Abstract

Hydrogen bond is a unique interaction which has important ramifications in chemical and bio-chemical reactions including life processes. It comes under the class of non-covalent interactions. In spite of this concept being about a century old and extensive work being done in this area, the concept of hydrogen bonding is still not completely understood. Starting from the conventional type of hydrogen bonding to the discovery of non- conventional types, the definition of hydrogen bonding is continuously expanding. There are many experimental methods such as infrared spectroscopy, NMR etc. that are available to study hydrogen bonding interactions. In the present work we have combined infrared spectroscopy with the Matrix Isolation technique for hydrogen bonding studies, as this technique serves as a powerful tool to study weak interactions. In this method the molecules are trapped at low temperature which results in sharp spectral feature and hence permits the resolution of features of the complexes formed in the matrix. In this work, we studied the hydrogen bonding interaction between phenylacetylene with methanol and methylamine. Phenylacetylene is an ideal molecule as it contains multiple hydrogen bonding sites; it can act as proton donor or proton acceptor. We have taken methanol and methylamine as we want to study the preferred hydrogen bonding interaction of phenylacetylene when we switch from O-H to N-H group. The computation work have been performed at B3LYP and M06-2x level of theories using 6-311G++(d,p) basis set. For the phenylacetylene-methanol complexe, three different geometries at B3LYP and four at M06-2x were obtained. In the case of phenylacetylene-methylamine complex, three different geometries were obtained at both levels of theory. Computationally, at the B3LYP level, C-H...O and C-H...N interaction has been observed to be dominant. At M06-2x, O-H...π and N-H...π have been observed as dominant interaction. However, experimental studies have shown that C-H...O, O-H...π and C- H...N as the dominant interaction.