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Title: Matrix Isolation Infrared and ab-initio study of Hydrogen Bonded Complexes Between Phenylacetylene and Chloroform

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Keywords: Chemistry
Hydrogen Bonds
Phenylacetylene-D
Chloroform

Issue Date: 26-Jun-2015

Publisher: IISER-M

Abstract: Non covalent and weak interactions form an important part of various chemical and biological systems among which hydrogen bonding plays the most important role. Over the last few decades, this interaction has been widely studied and well appreciated. Only recently, weak hydrogen bonding such as O-H... π and C-H... π has drawn considerable attention. Several spectroscopic techniques have been employed for the studies of such hydrogen bonded interaction in molecules including IR and NMR studies. One such technique is matrix isolation infrared spectroscopy, which serves as a powerful tool for exploring weak interactions and conformations. This technique has several advantages such sharp spectral features, absence of collisional and Doppler broadening and populating in only a few rovibronic levels. The current study involves the study of weak non-covalent interactions between two molecules of interest namely, phenylacetylene and chloroform both computationally and experimentally. The experimental technique utilized for the study is matrix isolation IR while GAUSSIAN 09 software is employed for the computations. The motivation behind choosing these two molecules is that they possess multiple hydrogen bonding sites and therefore it becomes interesting to investigate the hierarchy of hydrogen bonding in such systems. The main aim of this study is to elucidate the structures of the various hydrogen bonded complexes between the two precursor molecules. The computational work has been performed at B3LYP and M06-2X level of theory using 6-311++G(d,p) basis set. The calculations reveal the formation of four different complexes between the two monomers. The most dominating interaction observed computationally is the C-H... π which is confirmed by the experiments through the shifts observed in the vibrational frequencies of the submolecules in the complexes.


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