Abstract

In this work, a study of weak non-covalent interactions such as C-H---π and πstacking interactions, has been done computationally, employing phenylacetylene and acetylene heterodimer as the system. The experimental facility to study these interactions has also been set up. The prime motivation behind choosing this as a system is that phenylacetylene and acetylene are molecules with multifunctional sites for hydrogen bonding. Therefore it becomes interesting to investigate the hierarchy of hydrogen bonding in such systems. The molecular structure, stabilization energies and vibrational frequencies were computed at MP2(full), M05-2X, M06-2X, and B3LYP levels of theory using 6-311++G(d,p) basis set. Computational studies resulted into four possible types of complexes, with the number and type of the complexes depending mainly on the applied level of theory. In addition to three geometries which involved C-H--- π interactions, a π stacked complex was also obtained. The interaction energy of all the four complexes varied with the level of theory employed in the computation. Matrix isolation infrared spectroscopy, an experimental technique well suited for potentially studying such systems was set up at IISER-Mohali. This technique will be used to investigate the 1:1 adduct of phenyl acetylene and acetylene in Ar or N_2 matrix. The adduct will be generated by depositing acetylene and phenyl acetylene in the Ar or N_2 matrix and the formation of 1:1 complex of these species will be probed using infrared spectroscopy. Formation of these adducts will be evidenced by shifts in the vibrational frequencies of the acetylene and phenylacetylene monomers in the complex.