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Title:	Intermolecular Complexes and Molecular Conformations Directed by Hydrogen Bonds: Matrix Isolation and Ab Initio Studies
Authors:	Saini, J. (/jspui/browse?type=author&value=Saini%2C+J.) Dubey, Pankaj (/jspui/browse?type=author&value=Dubey%2C+Pankaj) Verma, Kanupriya (/jspui/browse?type=author&value=Verma%2C+Kanupriya) Karir, Ginny (/jspui/browse?type=author&value=Karir%2C+Ginny) Viswanathan, K.S. (/jspui/browse?type=author&value=Viswanathan%2C+K.S.)
Keywords:	Ab initio Amino acids Borazine Conformations Hydrogen bonding Matrix isolation Phenylacetylene Propargyl alcohol
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Abstract:	Studies on hydrogen bonding interaction in various systems, involving phenylacetylene (PhAc), propargyl alcohol (PA), borazine (BNH), propargyl amine (PAm) were performed using matrix isolation infrared spectroscopy and supported by ab initio computations. Weak intermolecular interactions of the above mentioned precursors with water, methanol, ether, acetylene and benzene were studied. These systems manifested O–H···π and n–σ ∗ interactions, such as C–H···O, N–H···O, O–H···O and O–H···N. In several cases the complexes were multiply tethered involving two or more of the above mentioned contacts. Many of the weak complexes exhibited a number of isomers, and the relative importance of the multiple non-covalent contacts resulted in a competition between the various isomers for the global minimum. It was found that subtle changes in the structures of the precursors tilted the balance towards one isomer or the other. Our studies also threw up a systematic method of building possible structures for complex systems starting from the known structures of related simple systems. We also studied the homodimers of PA and BNH. The BNH dimer was particularly interesting as one of its isomers was characterized by a bis-dihydrogen bond. We also studied the influence of hydrogen bonding interactions in determining the conformational landscape and preference in amino acids. Here again we were able to draw some generalizations regarding the conformational stability of amino acids. The combination of matrix isolation and ab initio computation is a powerful tool for studies on weak intermolecular interactions and conformations.
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