Title:	ICN – A Treasure Mine of Non-Covalent Interactions: A Matrix Isolation FTIR and Ab Initio Study
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Abstract:	Non-covalent interactions are molecular interactions that involve dispersion type interactions between the interacting species. Although the energies of non-covalent interactions are very small compared with that of a covalent bond, the cooperative nature of non-covalent interactions make them significant in determining supramolecular architectures. One of the interesting types of non-covalent interactions is the halogen bond. In order to experimentally observe the halogen bond, cyanogen iodide (ICN) was chosen for the study, as this molecule allows for the manifestation of a strong iodine bond. The electrostatic potential map of ICN shows the presence of halogen bonding, hydrogen bonding and carbon bonding sites in it. The ICN molecule can therefore, manifest an iodine bond, a hydrogen bond and a carbon bond. Matrix isolation infrared spectroscopy is a powerful tool to study non-covalent interactions. Negligible intermolecular interactions and elimination of Doppler and collisional broadening give rise to sharp peaks, which enables us to study features of weakly bound complexes. In this thesis, non-covalent interactions in ICN-water and ICN-methanol complexes were studied both experimentally and computationally. Calculations were carried out in the M06-2X/DGDZVP level of theory.
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