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Title:	COMPETITION BETWEEN HYDROGEN BONDING AND HALOGEN BONDING INTERACTIONS: ICN-H ₂ S SYSTEM
Authors:	Singh, Dipali (/jspui/browse?type=author&value=Singh%2C+Dipali)
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Abstract:	Iodine attached to strongly electron withdrawing group can manifest halogen bonding interaction. In this study, we have examined the ICN molecule for its ability to show halogen bonding; the strong electron withdrawing CN group leads to the formation of σ -hole. Interestingly, ICN can also show hydrogen bonding interactions through nitrogen atom and therefore present the possibility of competitive bonding between the two types of non-covalent interactions – hydrogen and halogen bonding. We have studied this competitive binding with H ₂ S as the partner molecule. The studies have been done on two systems; one is H ₂ S-ICN and CH ₃ SH-ICN. Three types of interactions were seen computationally; halogen bonding, hydrogen bonding and the interaction of S of H ₂ S with pi-cloud of the CN triple bond. Experimentally however we observed evidence only for the hydrogen bonding, even though the halogen bonding was found to be more strongly bound. A comparison of these results have also been made with the corresponding oxygen counterpart; i.e., ICN-H ₂ O system.
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