

## *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  $\sigma$ -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<sub>2</sub>S as the partner molecule.

The studies have been done on two systems; one is H<sub>2</sub>S-ICN and CH<sub>3</sub>SH-ICN. Three types of interactions were seen computationally; halogen bonding, hydrogen bonding and the interaction of S of H<sub>2</sub>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<sub>2</sub>O system.