

Halogen Bonding in Organic and Inorganic Systems – The Halohydrides of Group 14.

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Abstract: Halogen bonding has become a very active area of investigation because of an increasing number of cases of actual and potential applications of this phenomena. Tawfik and Donald have shown that in some cases the halogen bonds formed by halides bonded to inorganic atomic centers (specifically, group 14 atoms below carbon) can be stronger than those formed by their organic analogues. They demonstrated, however, that in $MF_3-I\cdots NH_3$ halogen bonded complexes, for example, where $M = C, Si, Ge, Sn,$ and Pb , the relative strengths of the interactions depend on the extent of the polarization of the M center. So the ordering of the energies will change and the organic compounds may become more (or less) stable depending on the other substituents (if the F atoms are replaced) on the M center. Our ongoing investigation focuses on the halogen bonding achieved by hydrides MH_3I with an array of Lewis bases. We assess the transferability of a set of functions that Tawfik and Donald identified for the dependence of the interaction energies on separations between the Lewis acid and base in the halogen bond.