

Title: Substituent Control of Halogen Bonding Interactions for Inorganic Acceptors

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Abstract: Understanding the nature of sigma hole interactions and halogen bonding in particular has become a very active area of investigation as an increasing number of actual and potential applications of this phenomena are identified in the literature. Previous studies in our group have demonstrated that halogen bonding interactions such as $R_3MX\cdots NH_3$ can be extremely sensitive to changes in the chemical environment of the Lewis acids, for example the identity of R in R_3MX . However, the extent and the progression of the tuning enforced by systematic changes in R have not been investigated for a wide variety of M centers or verified. The ongoing investigation on which we report in this poster focuses on the effects of substitutions on the M center on halogen bonding by halomethanes and their Si, Ge, Sn, and Pb analogues. We assess the interaction energies and halogen bond distances for $R_3MX\cdots NH_3$, where R = H, F, Cl, and Br.

