

Halogen Bonding Interactions between Group 14 Halomethane Analogues and Lewis Bases

Tianxiang Liu and Kelling J. Donald,

Department of Chemistry, Gottwald Center for the Sciences, University of Richmond, Richmond, VA 23173.

Abstract

Investigations of halogen bonding continue to improve our understanding of weak intermolecular forces and provide insights into non-covalent interaction in materials and biological systems. The interactions in a extensive series of complexes with Lewis acids of the form MH_3I ($M = C, Si, Ge, Sn, Pb$) are being examined using the MP2(full) level of theory. Calculations show that the strength of the halogen bond decreases monotonously as the size of M increases. Patterns of halogen bond strength for interactions with CH_3X systems are still under investigation. Three indicators -- bond distances, energy differences, and electrostatic potential maps --are provided in our poster to give a thorough understanding of the trends of halogen bond strength, and the viability for several different types of Lewis bases for participation in relatively strong halogen bonds.