Halogen Bonding Interactions between Group 14 Halomethane Analogues and Lewis Bases

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The halogen bond is a weak non-covalent interaction that has been the subject of much recent interest. Research in this field has led to a deeper understanding of weak interactions and has opened up doors in the fields of supramolecular chemistry and crystal engineering. In this work, the possibility of halogen bonding interactions in 136 systems is explored at the MP2(full) level of theory. The systems explored utilize all the CF_3X (X=F, Cl, Br, I) and MF_3I (M=Si, Ge, Sn, Pb) compounds as Lewis acids, paired with 18 unique Lewis bases. In interactions with CF_3X electrophiles, the strength of the halogen bond has been found to have some dependence on the electron-donating atom of the Lewis base. Preliminary findings indicate that Group 16 elements (O, S, Se) as electron donors in Lewis bases may exhibit stronger halogen bonds as the size of the halogen decreases, while group 15 elements (N, P) display the opposite phenomenon, with stronger halogen bonds as the size of the halogen increases. In the MF_3I systems, it has been observed that regardless of the base used, the strength of the halogen bond increases as the size of M increases. In this poster we report our results to date for these systems, utilizing X-bond distances, interaction energy values, and electrostatic potential maps as indicators for the strengths of the halogen bonds being formed.