Structural and Electronic properties of heavy analogues of halomethanes ($MH_{4-n}X_n$; M=C, Si, Ge, Sn, Pb; X=F, Cl, Br, I; n=1-4)

Chad Crigger, Bernard Wittmaack and Kelling Donald

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

In this poster we continue our work on the tetracoordinate square planar group 14 compounds: ($MH_{4-n}X_n$) (M = Si, Ge, Sn, Pb; X=H, F, Cl, Br, I). These systems are of large interest for both theoretician and synthetic chemists for different reasons depending on the particular element. Most of the attention has been focused on carbon compounds; and so for good reasons, since they are of relevance to organic systems. We report on work that we have done in the past year in improving our understanding of the variations in the charge distribution in the halomethanes and their heavier group 14 analogues, and the effects on the M—X bond length contractions and elongations we observe in these molecules as a function of *n,* the number of halogen substituents. the stability of the tetrahedral systems compared to the square planar alternatives. For this work, we use the MP2 computational methods to study the energy profiles for linear transits from the preferred of the MX_4 molecules. The dependence of the distortion energies (along the way from the tetrahedral (Td) to square planar (Sq-pl) geometry) on where M and X are in the periodic table is explained by a competition between geometrical and electronic parameters i) the X---X (electrostatic) hard sphere repulsive interactions, and ii) differences in the M—X bond strengths, going from X = F to X = I. Some of the data presented previously on these systems have been update using the more demanding MP2(full)/6-311+G* level for all eighty of the $MH_{4-n}X_n$ (n = 1 to 4) molecules.