Evaluation of Core-Polarization vs. Molecular Orbital Descriptions of Bending Anomalies in Small Molecules

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Abstract: This summer we will focus on working out the bonding preferences in two simple but intriguing classes of molecules: the group 1 and 13 dihalides. This effort will build on work that has been ongoing in our group on the bonding preferences in the related groups 2 and 12 dihalide systems. In that series of molecules, it is now well known, the bonding preferences evolve from a strong preference for linearity to the extremely floppy bent structures of $SrBr_2$ and BaI_2. The rationalization of this tendency is fascinating, and has allowed us to understand better the bonding preferences in not only the molecules, but also the oligomers and solids of the dihalides. Our job will be to extend this work to the halides of the groups 1 and 13, which have so far never been examined in this context, even though they show a similar variation in the bonding as a function of the position of the metal in the periodic table. Our work is just starting on these systems, but we are confident that by the end of the next several weeks leading up to the meeting we will have significant news to share on the outcome of our studies. That will constitute the bulk of our poster presentation at the MERCURY meeting.