Title: Structure and Bonding in Mixed Group 2 Dihalides: An Assessment of the Hard-Bends Soft Criterion for Bending.

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Abstract: The anomalous bending in group 2 dihalides and the absence of this behavior in group 12 is now very well established. The bonding in the mixed dihalide molecules has received little or no attention in the literature, however, despite the unusual behavior in the binary systems. The gas phase structural preferences of the group 2 mixed (ternary) dihalides MXY (M=Be, Mg, Ca, Sr, Ba, Ra and X and Y=F, Cl, Br, I, At) have been determined and analysed. The molecular geometries and harmonic vibrational frequency analyses of all of the systems have been examined at the density functional (B3PW91), MP2(full), and CCSD(T) computational levels. Quintuple zeta quality basis sets have been employed for all elements preceding Br, and small core pseudopotentials for the heavier elements with quintuple zeta basis sets for valence electrons. At the B3PW91, and MP2 levels bent structures have been identified for CaFCl, and all of the Sr, Ba, and Ra molecules, except SrBrAt, and SrIAt. The Be and Mg systems are linear. We are in the process of developing an extension of a criterion based on atomic hardness to asymmetric molecules, and analyzing our structural observations on the basis of ideas proposed for being in the symmetric dihalides.