Title: Group 12 Metal Halide Clusters: A Search for the Cause and Location of a Structrual Transition in Mercury Difluoride

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Abstract: Structure prediction remains a challenge for modern computational chemistry. The extraction of data from computationally-accessible, small to medium sized clusters in the gas phase is a practical way to obtain information in order to make predictions for the bonding tendencies and even maximum coordination numbers in extended solids. While making such predictions is easy for compounds such as CO_2, H_2O, and MgF_2, where clusters are held together by van der Waals, hydrogen bonding, and polar/ionic bonds, the situation is not so simple for certain other systems where the bonding in small clusters changes radically on the way to the extended solid. Following up on the work of Donald, Kretz, and Omorodion, we employ the CLUSTER and Gaussian 09 computational chemistry programs to examine this transition in mercury difluoride clusters $(HgF_2)_n$. We confirm that the transition appears to occur before n = 10 at the M062X and B97D3 levels of theory. We have located previously unidentified minima on the potential energy surfaces for both weak van der Waals and polar clusters for several values of n, and examined the progression in the relative energies of the two classes of cluster in search for the transition point from weak to strong bonding as n increases.