UNUSUAL BONDING MECHANISMS IN BERYLLIUM COMPOUNDS

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Metal clusters and small molecules that involve Be exhibit unusual bonding characteristics. For example, the Be_2 dimer exhibits a weak bond, short equilibrium bond length and an atypical potential energy curve. Although the bond is weak, the dissociation energy of Be_2 exceeds that of Mg_2 by a factor of two. Be_2O is more strongly bound than would be expected on the basis of simple molecular orbital theory, and higher level theoretical calculations indicate that it has a highly multi-reference ground state. Indeed, calculations for many Be species indicate multi-reference character. To obtain results that are even qualitatively correct often requires the correlation of all electrons and the use of basis sets that include at least triple excitations. Consequently, spectroscopic data for these molecules provide a valuable set of benchmarks for the evaluation of highly correlated, multi-reference computational techniques.
We are currently exploring the characteristics of Be compounds using electronic spectroscopy and photoionization techniques. The species being investigated include Be_2O, BeC and BeOH. Experimental results and theoretical calculations for these molecules will be presented, along with a progress report for studies of larger Be clusters.