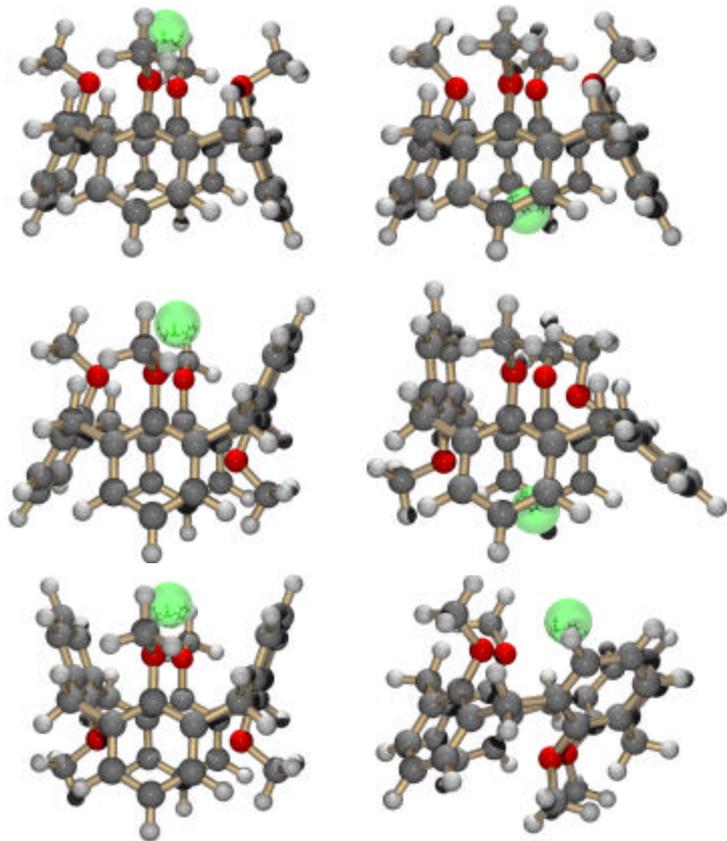


Multiple Binding Modes in Calixarene Hosts



Derivatized calixarenes exhibit unprecedented selectivity for cesium-137, a radionuclide of concern in both tank wastes and groundwater. In collaboration with Dr. B. A. Moyer of Oak Ridge National Laboratory, electronic structure calculations (MP2/aug-cc-pVDZ) have revealed that the coordination chemistry of the calixarene scaffold is unexpectedly complex. Pictured here are the six distinct tetradentate binding modes found for cesium complexes with the prototype tetramethoxycalix[4]arene. The results reveal that a rational approach to the design of a calixarene-based receptor must not only account for the macrocyclic conformation, but also must consider ways that a given conformation can interact with the guest.

Hay, B. P.; Nicholas, J. B.; Feller, D. *J. Am. Chem. Soc.* **2000**, *122*, 10083.