CALCULATION OF EQUILIBRIUM PROPERTIES OF WEAKLY BOUND COMPLEXES

K.A. PETERSON, Department of Chemistry, Washington State University, Richland, WA 99352; D.E. WOON, T. VAN MOURIK, and T.H. DUNNING, JR., Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA 99352.

Using correlation consistent basis sets and advanced methods for treating electron correlation, it is possible to compute the equilibrium properties ($D_e$, $r_e$, etc.) of weakly bound complexes to accuracies of a few wavenumbers and a few milliÅngstroms. We discuss the application of these techniques to selected prototypical systems, namely Ar-HX (X=F, Cl) and N$_2$-HF. Calculation of an extended potential energy surface should allow the detailed prediction of the vibrational states of these complexes.