CALCULATION OF EQUILIBRIUM PROPERTIES OF WEAKLY BOUND COMPLEXES

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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.