CALCULATION OF EQUILIBRIUM PROPERTIES OF HYDROGEN HALIDE DIMERS

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Using correlation consistent basis sets and advanced methods for treating electron correlation, it is possible to compute the equilibrium binding energy and structure of hydrogen bonded species to accuracies of tenths of a kcal/mol and a few milliÅngstroms. We discuss the application of these techniques to the HF and HCl dimers. Comparisons to recent experimentally-derived potentials will be made.