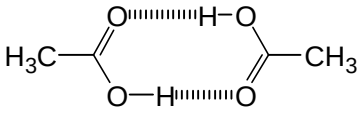
Hydrogen Bonding in Molecular Recognition

Basic problem: One of the key features of modern molecular recognition research is the use of complementary hydrogen bonding to produce specific geometric relationships between molecules or between portions of a larger molecule. While hydrogen bonding is not always treated effectively by some computational methods, it can be very useful to model hydrogen bonds in dimers and other aggregates, in order to get at least some idea of the effects of hydrogen bonding on a system. In this exercise, you will build and optimize some simple hydrogen bonded aggregates and compare their energies to those of the isolated fragments, in order to evaluate the strength of the interactions involved.

Method: AM1 or 6-31G* can be used for these comparisons. Build and geometry optimize the following recognition pairs. Record the enthalpies of formation of each molecule. Next, build appropriate dimers, optimize, and record the enthalpy of formation of the dimer. The energy difference between the sum of the parts and the aggregate gives the net stabilization in the latter due to the hydrogen bonding.

Literature: A variety of books exist describing hydrogen bonding. Look up individual enthalpies of formation and the hydrogen bonding value (dimeric hydrogen bond value for acetic acid) using Beilstein Online, Chemical Abstracts, and/or NIST database programs.



	AM1	6-31G*
Exptl ΔH° monomer		
Computed ΔH° monomer		
Computed ΔH° dimer		
Exptl ΔH° dimerization		
Estimated ΔH° dimerization		