10.675 Homework #2

due 10/7/04

(Note: Do not wait until the day before to start these runs.)

1) For the following gas-phase reaction:

$$H_2 + I_2 \rightarrow 2\ HI$$

(a) First optimize each structure using Hartree-Fock, 3-21G, (RHF/3-21G) and calculate thermodynamic data by performing a frequency analysis, including the change in standard-state enthalpy and Gibbs free energy of reaction.

(b) Using the checkpoint file that results from (a), perform a single point calculation using the basis sets assigned to your number (see next page). How does this change the standard-state enthalpy of reaction determined in (a)? (You need not perform another geometry optimization or frequency calculation. Note, in particular, to perform a frequency calculation, you **must** first perform a geometry optimization using the **same method and basis set** as in your frequency calculation. Why?) Also, perform optimizations using your method and report the differences in standard state enthalpies and Gibbs free energy of reaction.

(c) Compare your thermodynamic and structural results with experimental data, for example from the CRC handbook or another source.

2) Compute the hydrogen bond energy of the gas-phase water dimer ($2H_2O \rightarrow H_2O\text{-}H_2O$) using a method and basis set of your choice. Document the approach that you took and report the energy.

Student 1	RHF/3-21G*
Student 2	MP2/3-21G
Student 3	BLYP/3-21G*
Student 4	BLYP/3-21G**
Student 5	BLYP/3-21G+
Student 6	BLYP/3-21G++
Student 7	B3LYP/3-21G
Student 8	BPW91/3-21G
Student 9	SPL/3-21G
Student 10	RHF/6-31G
Student 11	MP2/6-31G
Student 12	BLYP/6-31G
Student 13	BLYP/D95
Student 14	BLYP/6-31G*
Student 15	BLYP/6-31G**
Student 16	B3LYP/6-31G
Student 17	BPW91/6-31G
Student 18	SPL/6-31G
Student 19	BLYP/6-31G+
Student 20	BLYP/6-31G++
Student 21	BLYP/6-31G*+
Student 22	BLYP/6-31G**++
Student 23	MP2/3-21G+

(Image by MIT OCW.)