Homework: Lennard Jones Interactions and Hydrogen Bonds

1) Draw a graph of the energy as a function of distance to bring 2 atoms together if they are acting only under the a force

$$van.der.waals.force = \frac{A}{r^{12}} - \frac{B}{r^{6}}$$

A is 2.9×10^{6} kcal/mol•A^{12} and B is 1418 kcal/mol•A^{6}.

What happens if you make the distance too small? Please pick a realistic energy and stop your calculations when the energy goes out of this range. A good range might be 0.1 to 10 kcal/mol.

What's the distance in Å where the energy is most favorable? What is that energy at this distance?

What's the distance where the energy is zero?

2) For a start consider a hydrogen bond as a dipole - dipole interaction.
You have an C=O with a bond distance of 1.5 A between the atoms and a partial charge of +0.6 on the C and -0.6 on the O interacting with a hydroxyl (H-O) with a bond distance of 1 A and partial charges of +0.4 and -0.4. The dipoles lie on a straight line with a distance between hydrogen bond donor and acceptor of 2 A.

- Draw out the alignment of the dipoles.
- Calculate the energy of interaction between these dipoles in vacuum (ε=1) and in water (ε=80) (in kcal/mol). The force connecting them is the Coulomb interaction.

To get this in kcal/mol C=335 kcal/mol/charge^2/Å

$$electrostatic.interaction = \frac{Cq_i q_j}{\varepsilon r_{ij}}$$

Let the dielectric constant (ε=1).

3) TIBS (2001) 26 521. More hydrogen bonds for the (structural) biologist
Give their definition of a classical hydrogen bond? Look at Table 1. Give me 2 amino acids that can form each of the 6 types of hydrogen bonds.

4) Angew. Chem. Int. Ed. 2002, 41, 48-76. The hydrogen bond in the solid state
- List the constituent interactions that contribute to a hydrogen bond and give their distance dependence.
- What is the range of energies for a hydrogen bond?
- What's the most important type of interaction in strong, medium, and weak hydrogen bonds.
- Describe what is plotted in Fig 9. What does this figure say for S and O about the 'angular dependence of the hydrogen bond' and what does it say about the distribution of electron density around S and O.