

Homework: Ion association and packing

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/r^{12} repulsion and B/r^6 attractive force. A is 2.9×10^6 and B is 1418 kcal/mol. What happens if you make the distance too small? Please pick a realistic energy to stop your calculations - think about the range of energies of interest (maybe 0.1-10 kcal/mol). What's the distance in Å where the energy is most favorable? What is that energy? What's the distance where the energy is zero?

2) For a start consider a hydrogen bond as a dipole - dipole interaction. If you have an C=O with a bond distance of 1.5 Å 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 Å 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 Å.

- Draw out the alignment of the dipoles.

- Calculate the energy of interactions between these dipoles in vacuum and in water (in kcal/mol).

3) TIBS (2001) 26 521. More hydrogen bonds for the (structural) biologist
In B what is the 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 of 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.