Problem Set # 1

Due @ 11:59 pm Tuesday Feb. 19, by electronic submission on BlackBoard

1. Obtain the minimum interaction energy (in kJ/mol) for a Na^+ Cl^- pair in the gas phase. Non-coulombic Na^+– Cl^- interactions can be approximated by the Lennard-Jones 12-6 potential with ε/k_B = 51.2 K, σ = 0.353 nm. What is the ratio of the minimum energy to the thermal energy, k_BT, at 300 K? What is the minimum approach distance? What is the minimum energy if you fail to include non-coulombic interactions?

2. A common molecular model for H_2O is the SPC/E model, which has the following parameters: O–H distance = 0.100 nm; HOH angle = 109.5°, q(O) = –0.8476 e, q(H) = +0.4238 e.

   (a) Obtain the dipole moment of this model, and compare it to the dipole moment of real water molecules in the gas phase. Can you suggest a possible reason for the difference?

   (b) Compute the coulombic interaction energy (in kJ/mol) of two co-planar SPC/E waters with dipoles aligned to the O-O line and pointing in the same direction, for O–O distances of 0.4, 2.0, and 10.0 nm, using their explicit charges.

   (c) Repeat the energy calculation using the molecular dipoles computed in (a), instead of the actual charges, for the interactions. What do you observe?

3. The adsorption spectrum of $^1H^{79}Br$ shows a first vibrational line at 2648 cm^{-1}. Calculate the classical force constant (in N/m) for a harmonic bond potential of $^1H^{79}Br$.

4. Use Hyperchem and the OPLS force field to compute the potential energy versus dihedral angle for 1,2 dichloroethane. Compare to Fig. 5.2.

5. The relationship $\ln x_n = -3.907 - 1.519n$ has been obtained by correlating experimental data for the equilibrium solubility (mole fraction x_n) of normal alkanes with n carbon atoms in water at T = 298 K and P = 1 bar, for n between 5 and 9. Obtain the solvent-accessible surface area for these alkanes in their minimum energy conformations (using MM+) and develop a correlation for water solubility in terms of this parameter.

6. Obtain the minimum energy conformation for cyclohexane (using MM+), and report its energy in kcal/mol. Be careful on how you draw the initial structure, as it is common for minimization to get "stuck" near local minima. What does the correlation obtained in [5] suggest for the solubility of cyclohexane? How does this value compare to the experimentally measured solubility (which you will need to find)?

Please submit your results electronically, as a single **PDF** file. 20% of the grade is assigned to the "aesthetics" of your submission: how easy it is to follow, quality and proper labeling of graphs, good information density, etc.