Homework Assignment H1
(Due: Friday, 2009/10/02, 4:00 PM)

H1.1. Polyalanine Chain. Consider a 16 amino acids long peptide sequence comprised of alanines (a polyalanine chain). Backbone hydrogen bonding occurs between the H-atom of the amino group of the amino acid i and the O-atom of the carbonyl group of the amino acid j. Note that each amino acid can form up to two backbone hydrogen bonds. The potential energy of one hydrogen bond is 5 kcal/mol.

(a) Which secondary structure will the polyalanine chain adopt at very low temperatures if the only interaction between the amino acids is the backbone hydrogen bonding. Sketch the possible secondary structure conformations.

(b) Calculate the potential energy of the polyalanine conformation at very low temperates obtained in (a).

(c) At intermediate temperature the polyalanine chain adopts a β-hairpin conformation (two antiparallel β-strands connected by a turn). Calculate the lowest potential energy of the β-hairpin conformation. Assume that two amino acids that comprise the turn region are not involved in hydrogen bonding.

(d) At high temperatures the polyalanine conformation will unfold and the peptide chain will adopt a random coil conformation. Use the concepts of free energy and entropy to explain why.

H1.2. Van der Waals Interactions (*For Honors Undergraduate & Graduate Students*). Van der Waals attractive interactions between atoms result in non-ideal behavior of gases. For gaseous and liquid phases, we can thus apply the Van der Waals equation of state:

$$\left(p + \frac{a}{V^2}\right)(V - b) = RT ,$$

where $R = N_A k_B$ is the gas constant; p pressure, V volume, T temperature; and the parameters a & b are corrections (to the ideal gas equation) due to attractive interactions between particles (atoms or molecules) & excluded volume effect, respectively. For simplicity, the above equation is normalized to one mole of matter ($n = 1$).

(a) Draw a schematic picture of Van der Waals isotherms in the (p, V) diagram.

(b) Graphically define the critical point (p_C, V_C on the critical isotherm of the liquid–gas transition.

(c) Derive mathematical expressions, by which the critical point (p_C, V_C, T_C) is defined.

(d) Calculate p_C, V_C, and T_C and express each one of them in terms of the parameters a and b.