Tutorial 2

To be discussed during the tutorial on Friday 9 Feb. 2007. You should hand over your home Your contributions toward the discussion are strongly encouraged and will be evaluated.

1. Given the fact that for a multi-component system, \( dE \) can be written

\[
dE = TdS - PdV + \sum \mu_\alpha dN_\alpha
\]

a. what are the expressions of \( dH, dF, dG? \)

b. To show that the chemical potential under constant \( T, V, \) and constant \( T, P, \) can be given by

\[
\mu_\alpha = \left[ \frac{\partial F}{\partial N_\alpha} \right]_{T,V,N_T}, \quad \mu_\alpha = \left[ \frac{\partial G}{\partial N_\alpha} \right]_{T,P,N_T}
\]

respectively.

2. Calculate \( W \) and \( \Delta S \) for the isothermal reversible expansion of 3 moles of an ideal gas from 12 to 80 liters at 25°C.

3. Assuming that a polypeptide chain has only one \( \alpha \)-helical conformation and that there are three possible orientations for each amino acid residue in the random-coil state, calculate \( \Delta S \) for the conformational change

\( \alpha \)-helix \( \rightarrow \) random coil

for a polypeptide of 100 residues. What value of \( \Delta H \) per residue would be required to make the melting point (the temperature at which the equilibrium constant equals 1) be 50°C? Compare this with the hydrogen-bond energy, estimated to be 0 to 12 kJ/mol.

4. Two energy levels of a molecule are separated by \( 1 \times 10^{-15} \) erg. The degeneracy of the higher level is twice that of the lower. Calculate

a. the relative populations of these levels at 0°C

b. the temperature at which they will be equally populated.

5. a. Consider a chemical reaction in which a molecule moves from gas to a water solution. At atmospheric pressure, each gas molecule occupies a volume of about 24 L/mole, whereas in solution, the volume is closer to the volume occupied by a water molecule, or \( 1/(55 \text{ mole/L}) \). Estimate \( (\Delta V)_p \), expressing your answer in units of \( k_B T_r \).

b. Consider a reaction in which two molecules in aqueous solution combine to form one. Compare an estimate of \( (\Delta V)_p \) with what you found in (a) and comment on why we usually don’t need to distinguish between \( F \) and \( G \) for such reactions.

![molecular structures](image.png)