## Homework assignment #5 for CCB 422/522, Spring 2021

*Please show your work for all problems!*

1. Consider a protein sphere with a radius of 18 Å, and charge Q = −10e, in an aqueous solution of 0.05 M NaCl at 25C. Consider the small ions as point charges and use the Debye–Huckel linear approximation of the Poisson–Boltzmann equation.
   a) What is the dimensionless surface potential eψ/kT of the protein?
   b) What are the concentrations of Na+ and Cl− ions at the surface of the protein?
   c) What are the concentrations of Na+ and Cl− ions at a distance of 4 Å from the protein surface?

2. Series and parallel reactions:
   a) You have a reaction in which A converts to B through two steps in series:

   $$A \rightarrow^{k_1} I \rightarrow^{k_2} B$$

   where the temperature dependences of the steps are given by the Arrhenius law: $k_1 = Ae^{-E_1/RT}$ and $k_2 = Ae^{-E_2/RT}$. Derive an expression for the total rate $k_{tot}$, from A to B, as a function of $A$, $E_1$ , $E_2$ and $T$. (Hint: the time from A to B is the sum of times from A to I and from I to B).
   b) Now consider instead two steps in parallel: $A \rightarrow^{k_1} B$, $A \rightarrow^{k_2} B$. Using the Arrhenius equations from (a) the individual steps, derive the temperature dependence for $k_{tot}$ in this case. (Hint: now the rates add.)

3. The reaction rate of an uncatalyzed reaction is $k_0 = 10^3$ $M^{-1}$ $s^{-1}$ at T = 300 K. A catalyst C binds to the transition state with free energy ΔG = −5 kcal/mol. What is the rate $k_c$ of the catalyzed reaction at T = 300 K?

4. A rule of thumb used to be that chemical reaction rates would roughly double for a 10-degree increase in temperature, say from $T_1$ = 300 K to $T_2$ = 310 K. For what activation energy $E_a$ would this be exactly correct?