

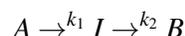
Homework assignment #5 for CCB 422/522, Spring 2021

Please show your work for all problems!

1. Consider a protein sphere with a radius of 18 \AA , and charge $Q = -10e$, in an aqueous solution of 0.05 M NaCl at 25°C . 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 $e\psi/kT$ 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 \AA 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:



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: $A \xrightarrow{k_1} B$, $A \xrightarrow{k_2} B$. 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 $k_0 = 10^3 \text{ M}^{-1} \text{ s}^{-1}$ at $T = 300 \text{ K}$. A catalyst C binds to the transition state with free energy $\Delta G = -5 \text{ kcal/mol}$. What is the rate k_c of the catalyzed reaction at $T = 300 \text{ K}$?
 4. A rule of thumb used to be that chemical reaction rates would roughly double for a 10-degree increase in temperature, say from $T_1 = 300 \text{ K}$ to $T_2 = 310 \text{ K}$. For what activation energy E_a would this be exactly correct?