ChE 471

Quiz No 1

Closed Book, Closed Notes

1. What is a chemical reaction?
   When there is change in atomic/atomic configuration of a molecule of a particular chemical species bought by interaction/input of energy

2. What is reaction stoichiometry?
   The ratio in which the reactants react to form how much product.
   Conservation of mass is more than one stoichiometric equation.

3. What is (molar) extent of reaction?
   \[ \chi = \frac{n_f - n_{i,0}}{n_{j}} \]

4. What is fractional conversion (of the limiting reactant)? How are molar extent of reaction and conversion related?
   \[ \chi_r = \frac{\text{mass reacted}}{\text{mass fed}} = \frac{n_{f,0} - n_{f}}{n_{i,0}} \]
   \[ n_{f,0} = (1 - \chi_r) \chi \]

5. In multiple reactions how many molar extents of reaction do we need to describe the reaction system?
   \[ \# \text{ of independent reactions} \]
6. What are the conditions for physical equilibrium between chemical species A in the gas and in the liquid phase (in solution).

\[ \text{minimum Gibbs Free Energy} \quad (\min \bar{G}_i) \]

(Henry's law) \quad Henry's constant used to obtain A in liquid (and vice versa.)

7. What are the conditions for chemical equilibrium? How would you express these for a simple isomerization reaction A\( \rightleftharpoons \)B?

\[ \text{minimum Gibbs Free Energy} \quad (\min \bar{G}_i) \]

\[ \min \left( \bar{G}_B - \bar{G}_A \right) \]

8. How is the thermodynamic equilibrium constant \( K \) for a single reaction (say of stoichiometry \( aA + bB = cC + dD \)) calculated at standard conditions? Does this constant have units? Is this constant a function of pressure?

\[ K = \exp \left( -\frac{\Delta G}{RT} \right) = \frac{x_B}{x_A} = \frac{y_i}{y_i} \]

\[ \frac{P_B}{P_A} \frac{P_C}{P_D} \]

9. Write the heat of reaction for reaction \( aA + bB = cC + dD \) at temperature \( T \) if you know the heats of formation of \( A, B, C, D \).

\[ \Delta H_{\text{rxn}} = \sum_j v_{i,j} \Delta H_f^{0,i} \]

10. How do we correct the value of the thermodynamic equilibrium constant \( K \) for temperature?

We use Helfert's equation \( \left( \frac{d \ln K}{dT} = \frac{\Delta H}{RT^2} \right) \).
11. Express the equilibrium constant $K_p$ for the relationship between mole fractions at equilibrium and equilibrium extent or conversion for the reaction stoichiometry listed in 8 and 9 above. What is the effect of pressure on $K_p$.

\[ K = \left( \frac{P}{(RT)^a} \right) \tilde{w}_i \tilde{w}_j = K_p \left( \frac{1}{c_{i}^{a} c_{j}^{b}} \right) \quad \text{assume} \quad \{c, a, b, \ldots \} \]

\[ K_P = \frac{e^{-D}}{\tilde{a} \tilde{b}} \quad \text{and} \quad K = \frac{\tilde{c} \tilde{d}}{(c_{a}^{n} c_{b}^{m})^{k+b}} \quad \text{assume} \quad \text{stoichiometric factors} \]

12. How is the rate of reaction defined? What is it a function of?

The rate of reaction is defined as the number of moles of $j$-th species oxidized per unit area per time.

\[ \text{Rate} = \text{(Temp., Pressure, Composition, Catalyst activity)} \]

13. Write down the representation of an n-th order reaction rate for an irreversible reaction and show what the Arrhenius representation of the rate constant looks like. What is the meaning of activation energy?

* For $\text{A} + \text{B} \rightarrow \text{C} + \text{D}$, $\text{rate} = k_{\text{A}} e^{-E/RT} c_{\text{A}}^{a} c_{\text{B}}^{b}$.

activation energy: energy required for the reaction to take a leap of the energy barrier.

14. What is an elementary reaction? Can we infer its order from its molecularity?

* Single step and one to one.

* Correspondence exists (n) order and molecularity of ran.

15. What does a reaction mechanism represent?

* Represents sequence of elementary reaction in which reactants are made to products.