1 Stoichiometry and reactions

1. Molecules and reactions
2. Stoichiometric coefficients
3. Advancements

2 Chemical thermodynamics and equilibria

1. Chemical reactions
2. Thermodynamic potential differences
   (a) Standard states
   (b) Reaction entropy $\Delta S^\circ(T) = S^\circ_{\mathrm{B}}(T) - S^\circ_{\mathrm{A}}(T)$
   (c) Reaction energy $\Delta U^\circ(T) = U^\circ_{\mathrm{B}}(T) - U^\circ_{\mathrm{A}}(T) + \Delta E(0)$
   (d) Gibbs-Helmholtz
3. Equilibrium-closed system
   (a) Equilibrium constants and algebraic solutions
   (b) Free energy minimization
   (c) Parallel reactions
4. Equilibrium-open system
   (a) Reaction phase diagrams
5. Partition functions and K_{eq}
6. Non-ideal activities
7. Electrochemical reactions

3 Empirical kinetics

1. rates
2. rate expressions
3. rate orders
4. apparent orders, Arrhenius expression
5. integrated rate expressions
6. analyzing reactor data?

Table 1: Equilibrium and Rate Constants

Equilibrium Constants $a\ \mathrm{A} + b\ \mathrm{B} \rightleftharpoons c\ \mathrm{C} + d\ \mathrm{D}$

$$K_{eq}(T) = e^{\Delta S^\circ(T,V)/k_B} e^{-\Delta H^\circ(T,V)/k_B T}$$

$$K_c(T) = \left(\frac{1}{c^\circ}\right)^{\nu_c+\nu_d-\nu_a-\nu_b} \frac{(q_c/V)^{\nu_c}(q_d/V)^{\nu_d}}{(q_a/V)^{\nu_a}(q_b/V)^{\nu_b}} e^{-\Delta E(0)\beta}$$

$$K_p(T) = \left(\frac{k_B T}{P^\circ}\right)^{\nu_c+\nu_d-\nu_a-\nu_b} \frac{(q_c/V)^{\nu_c}(q_d/V)^{\nu_d}}{(q_a/V)^{\nu_a}(q_b/V)^{\nu_b}} e^{-\Delta E(0)\beta}$$

Unimolecular Reaction $[A] \rightleftharpoons [\mathrm{A}]^\ddagger \rightarrow C$

$$k(T) = \nu^\ddagger \bar{K}^\ddagger = \frac{k_B T}{h} \frac{\bar{q}_\ddagger(T)/V}{q_A(T)/V} e^{-\Delta E^\ddagger(0)\beta}$$

$$E_a = \Delta H^{\circ\ddagger} + k_B T \quad A = e^1 \frac{k_B T}{h} e^{\Delta S^{\circ\ddagger}}$$

Bimolecular Reaction $\mathrm{A} + \mathrm{B} \rightleftharpoons [\mathrm{AB}]^\ddagger \rightarrow \mathrm{C}$

$$k(T) = \nu^\ddagger \bar{K}^\ddagger = \frac{k_B T}{h} \frac{q_\ddagger(T)/V}{(q_A(T)/V)(q_B(T)/V)} \left(\frac{1}{c^\circ}\right)^{-1} e^{-\Delta E^\ddagger(0)\beta}$$

$$E_a = \Delta H^{\circ\ddagger} + 2k_B T \quad A = e^2 \frac{k_B T}{h} e^{\Delta S^{\circ\ddagger}}$$

4 Molecular basis

1. reaction pathway, detailed balance
2. bimolecular, collision theory, TST
3. unimolecular reactions

5 Mechanisms

1. QSSA
2. Pre-equilibrium

6 Heterogeneous reactions

1. adsorption, L-H
2. TPD
3. catalysis
4. Sabatier analysis

7 Liquid-phase reactions

