Basic Chemistry Concepts I

Great medical advances in modern age

1. Sanitation (clean water and sewage disposal) – 15.8%
2. Antibiotics – 15%
3. Anaesthesia – 14%
4. Introduction to vaccines – 12%
5. Discovery of the structure of DNA – 9%

(British Medical Journal, 2007)

Today's lecture

- Chemistry – basics of the basics
- Chemical reactions
- Equilibrium chemistry

Mole & molarity

- Mole = Avogadro's number (6.02×10^{23}) of molecules
- Molarity (M) = number of moles per liter of solution (mole/L)

  cf) molality (m) = number of moles per kg of solvent

Activity

- Related to chemical potential of a substance or a component in a mixture

  * chemical potential determines the tendency for a reaction to occur

- Represented by { } (cf. molarity by [ ])

Activity

- In dilute aqueous solutions, the ions do not significantly interact with one another:

  $\{i\} \approx [i]$

- As concentration increases, the ion-ion interaction becomes more significant:

  $\{i\} = \gamma_i \cdot [i]$ where γ_i = activity coefficient

Balancing chemical reactions

$Ca(HCO_3)_2 + NaOH = Ca(OH)_2 + NaHCO_3$

Types of chemical reactions

- Precipitation-dissolution reactions

ex) $CaCl_2 + Na_2CO_3 \underset{\text{dissolution}}{\overset{\text{precipitation}}{\rightleftarrows}} CaCO_3(s) + 2Na^+ + 2Cl^-$

Usage: softening, phosphorous removal, heavy metal removal

Acid-base reactions

- Brønsted-Lowry acid: any substance that can donate a proton (i.e., proton donor)

$$HA + H_2O \rightleftharpoons H_3O^+ + A^-$$

acid base conjugate acid conjugate base

- Brønsted-Lowry base: any substance that can accept a proton (i.e., proton acceptor)

$$B^- + H_3O^+ \rightleftharpoons HB + H_2O$$

base acid conjugate base conjugate acid

Acid-base reactions

- Water is amphoteric – can be either an acid or a base

$$H_2O + H_2O \rightleftharpoons H_3O^+ + OH^-$$

acid base conjugate acid conjugate base

- pH = -log{H^+} ("p" denotes "-log")

Complexation reactions

- Coordination of two or more atoms, molecules, or ions resulting in the formation of a more stable product

ex) $Fe^{2+} + 6H_2O = Fe(H_2O)_6^{2+}$

$Cu^{+} + 4CN^{-} = Cu(CN)_4^{3-}$

- Complex ion = a metal ion with Lewis bases (electron pair donor)
- Ligand = Lewis bases attached to a metal ion

Complexation reactions

- Many metal ions exist as complex ions in water (metal aquo complex)

  ex) $[Cr(H_2O)_6]^{2+}$, $[Cr(H_2O)_6]^{3+}$, $[Fe(H_2O)_6]^{2+}$, $[Fe(H_2O)_6]^{3+}$, $[Co(H_2O)_6]^{2+}$, $[Cu(H_2O)_6]^{2+}$

- Environmental significance: complexation of metals affects the uptake, biodegradability, toxicity, and mobility of the metal

Oxidation-reduction (redox) reactions

- Involves changes in the oxidation state
- Essential for life: photosynthesis and respiration are redox reactions!

ex) respiration: $C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$

Oxidation-reduction (redox) reactions

- Balancing redox reactions

  1) list all elements

  2) identify number of e^- transferred

  3) balance electrons

  4) check atom balance

ex) $SO_2 + O_2 + H_2O \rightarrow H_2SO_4$

Chemical equilibrium

- For a reversible reaction

  $aA + bB \rightleftharpoons cC + dD$

  at chemical equilibrium,

  rate(forward rxn) = rate(reverse rxn)

- Equilibrium constant, K

$$K = \frac{\{C\}^c \{D\}^d}{\{A\}^a \{B\}^b}$$

For pure solid, activity = 1
For gases, activity = partial pressure

Chemical equilibrium: solubility

- For a precipitation-dissolution reaction

$A_aB_b(s) \rightleftharpoons aA^{x+} + bB^{y-}$

$$K = \frac{\{A^{x+}\}^a\{B^{y-}\}^b}{\{A_aB_b\}}$$

as $\{A_aB_b\} = 1$ (pure solid), $K = \{A^{x+}\}^a\{B^{y-}\}^b$

- Solubility product, $K_s = \{A^{x+}\}^a\{B^{y-}\}^b$

Ionic strength

- Recall that {i} = γ[i]:

  $K_s = \{A^{x+}\}^a\{B^{y-}\}^b = (\gamma_A[A^{x+}])^a(\gamma_B[B^{y-}])^b$

- Ionic strength, *I*: measure of interaction among ions in a solution

$$I = \frac{1}{2}\sum C_i z_i^{\,2}$$

C_i = molarity of the i[th] ion

z_i = charge of the i[th] ion

Calculating activity coefficients

- Davies equation (for *I* < 0.5 M):

$$log\,\gamma = -Az^2\left(\frac{\sqrt{I}}{1+\sqrt{I}} - 0.2I\right)$$

A ≈ 0.5 for water at 25°C

z = charge of the ion

Selected solubility products (@ 25ºC)

Substance	Equilibrium Reaction	pK_s	Application
Aluminum hydroxide	$Al(OH)_3 (s) \rightleftharpoons Al^{3+} + 3OH^-$	32.9	Coagulation
Aluminum phosphate	$AlPO_4 (s) \rightleftharpoons Al^{3+} + PO_4^{3-}$	22.0	Phosphate removal
Calcium carbonate (aragonite)	$CaCO_3 (s) \rightleftharpoons Ca^{2+} + CO_3^{2-}$	8.34	Softening, corrosion control
Ferric hydroxide	$Fe(OH)_3 (s) \rightleftharpoons Fe^{3+} + 3OH^-$	38.57	Coagulation, iron removal
Ferric phosphate	$FePO_4 (s) \rightleftharpoons Fe^{3+} + PO_4^{3-}$	21.9	Phosphate removal
Magnesium hydroxide	$Mg(OH)_2 (s) \rightleftharpoons Mg^{2+} + 2OH^-$	11.25	Removal of calcium and magnesium
Dolomite ($CaMg(CO_3)_2$) (ordered)	$CaMg(CO_3)_2 \rightleftharpoons Ca^{2+} + Mg^{2+} + 2CO_3^{2-}$	17.09	Weathering of dolomitic minerals
Kaolinite	$Al_2Si_2O_5(OH)_4 + 6H^+ \rightleftharpoons 2Al^{3+} + 2Si(OH)_4 + H_2O$	7.44	Weathering of kaolinite clays
Gypsum	$CaSO_4 \cdot 2H_2O \rightleftharpoons Ca^{2+} + SO_4^{2-} + 2H_2O$	4.58	Weathering of gypsum minerals

Selected solubility products (@ 25°C)

- Q: Added 30g of $CaCO_3$ in water of make 1.00 L solution containing 0.01 M NaCl. Assuming Ca^{2+} in solution is at equilibrium with $CaCO_3(s)$, what would be the Ca^{2+} concentration?

  (T =25°C, p*Ks* for $CaCO_3$ = 8.48)

Caveat!

- The equilibrium/solubility product constants do not tell anything about the reaction rate!
- Differentiate equilibrium and kinetics

Reading assignment

- Textbook Ch2 p. 32-51