

# Basic Chemistry Concepts I

# Great medical advances in modern age

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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

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

# Mole & molarity

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- Mole = Avogadro's number ( $6.02 \times 10^{23}$ ) of molecules
- Molarity (M) = number of moles per liter of solution (mole/L)  
cf) molality (m) = number of moles per kg of solvent

# Activity

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- 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

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

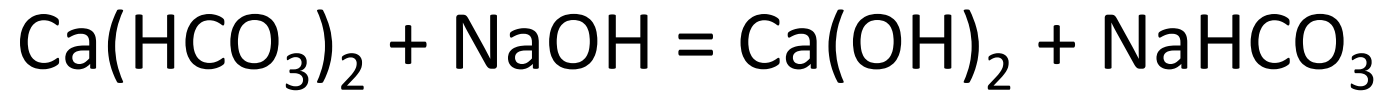
$$\{i\} \approx [i]$$

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

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

# Balancing chemical reactions

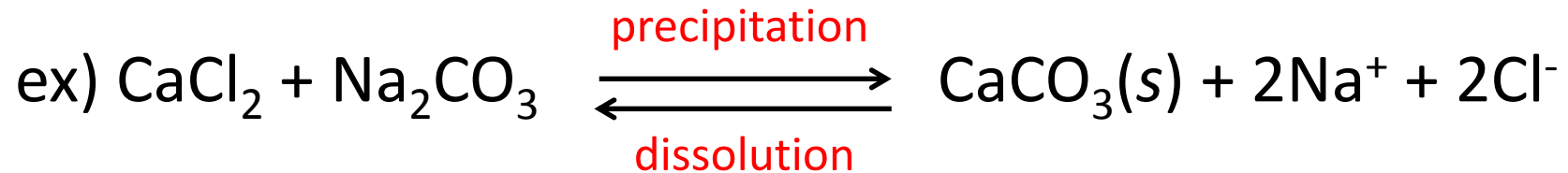
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# Types of chemical reactions

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- Precipitation-dissolution reactions



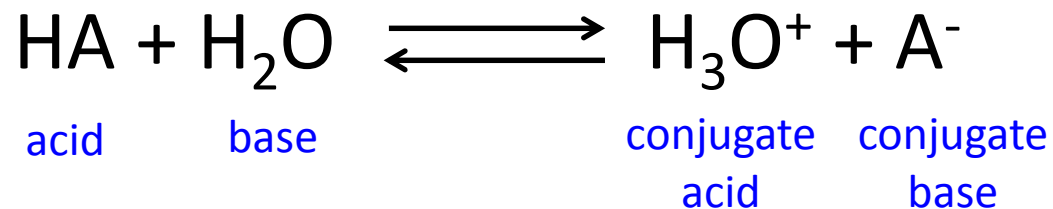
Usage: softening, phosphorous removal, heavy metal removal



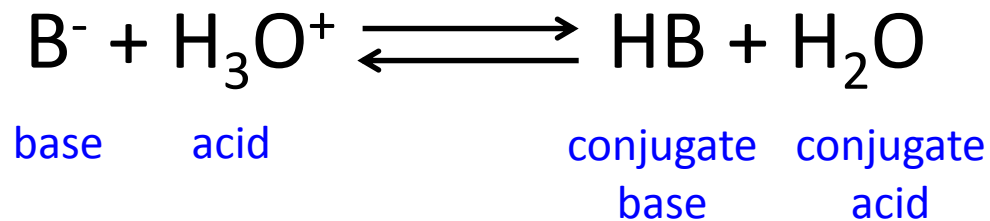
# Acid-base reactions

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



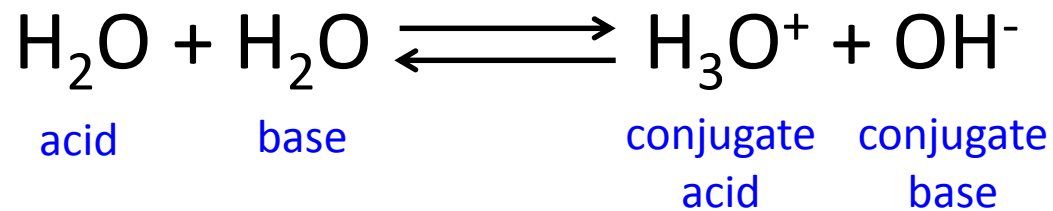
- Brønsted-Lowry base: any substance that can accept a proton (i.e., proton acceptor)



# Acid-base reactions

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

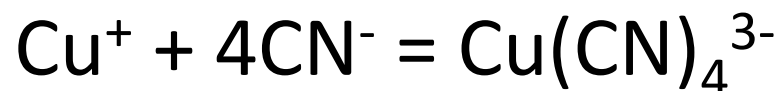


- $\text{pH} = -\log\{\text{H}^+\}$  (“p” denotes “-log”)

# Complexation reactions

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



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

# Complexation reactions

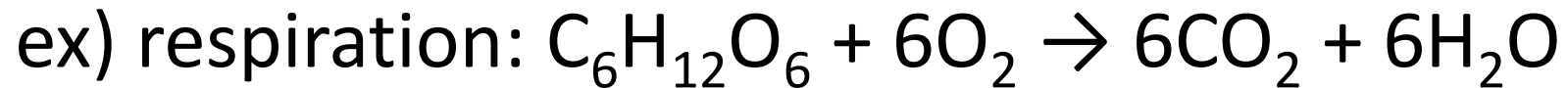
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- Many metal ions exist as complex ions in water (metal aquo complex)  
ex)  $[\text{Cr}(\text{H}_2\text{O})_6]^{2+}$ ,  $[\text{Cr}(\text{H}_2\text{O})_6]^{3+}$ ,  $[\text{Fe}(\text{H}_2\text{O})_6]^{2+}$ ,  
 $[\text{Fe}(\text{H}_2\text{O})_6]^{3+}$ ,  $[\text{Co}(\text{H}_2\text{O})_6]^{2+}$ ,  $[\text{Cu}(\text{H}_2\text{O})_6]^{2+}$
- Environmental significance: complexation of metals affects the uptake, biodegradability, toxicity, and mobility of the metal

# Oxidation-reduction (redox) reactions

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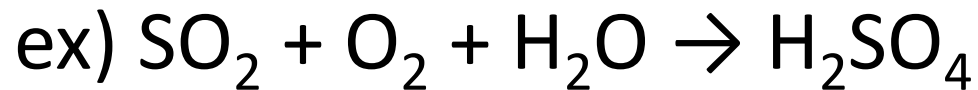
- Involves changes in the oxidation state
- Essential for life: photosynthesis and respiration are redox reactions!



# Oxidation-reduction (redox) reactions

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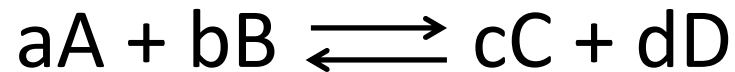
- Balancing redox reactions
  - 1) list all elements
  - 2) identify number of e<sup>-</sup> transferred
  - 3) balance electrons
  - 4) check atom balance



# Chemical equilibrium

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- For a reversible reaction



at chemical equilibrium,

$$\text{rate}(\text{forward rxn}) = \text{rate}(\text{reverse rxn})$$

- Equilibrium constant,  $K$

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

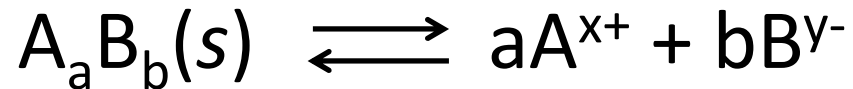
For pure solid, activity = 1

For gases, activity = partial pressure

# Chemical equilibrium: solubility

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- For a precipitation-dissolution reaction



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

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

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



# Ionic strength

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- Recall that  $\{i\} = \gamma[i]$ :

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

- 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  $i^{\text{th}}$  ion

$z_i$  = charge of the  $i^{\text{th}}$  ion

# Calculating activity coefficients

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

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

$A \approx 0.5$  for water at  $25^\circ\text{C}$

$z$  = charge of the ion

# Selected solubility products (@ 25°C)

Substance	Equilibrium Reaction	pK <sub>s</sub>	Application
Aluminum hydroxide	$\text{Al(OH)}_3 (s) \rightleftharpoons \text{Al}^{3+} + 3\text{OH}^-$	32.9	Coagulation
Aluminum phosphate	$\text{AlPO}_4 (s) \rightleftharpoons \text{Al}^{3+} + \text{PO}_4^{3-}$	22.0	Phosphate removal
Calcium carbonate (aragonite)	$\text{CaCO}_3 (s) \rightleftharpoons \text{Ca}^{2+} + \text{CO}_3^{2-}$	8.34	Softening, corrosion control
Ferric hydroxide	$\text{Fe(OH)}_3 (s) \rightleftharpoons \text{Fe}^{3+} + 3\text{OH}^-$	38.57	Coagulation, iron removal
Ferric phosphate	$\text{FePO}_4 (s) \rightleftharpoons \text{Fe}^{3+} + \text{PO}_4^{3-}$	21.9	Phosphate removal
Magnesium hydroxide	$\text{Mg(OH)}_2 (s) \rightleftharpoons \text{Mg}^{2+} + 2\text{OH}^-$	11.25	Removal of calcium and magnesium
Dolomite (CaMg(CO <sub>3</sub> ) <sub>2</sub> ) (ordered)	$\text{CaMg(CO}_3)_2 \rightleftharpoons \text{Ca}^{2+} + \text{Mg}^{2+} + 2\text{CO}_3^{2-}$	17.09	Weathering of dolomitic minerals
Kaolinite	$\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4 + 6\text{H}^+ \rightleftharpoons 2\text{Al}^{3+} + 2\text{Si(OH)}_4 + \text{H}_2\text{O}$	7.44	Weathering of kaolinite clays
Gypsum	$\text{CaSO}_4 \cdot 2\text{H}_2\text{O} \rightleftharpoons \text{Ca}^{2+} + \text{SO}_4^{2-} + 2\text{H}_2\text{O}$	4.58	Weathering of gypsum minerals

# Selected solubility products (@ 25°C)

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- Q: Added 30g of  $\text{CaCO}_3$  in water of make 1.00 L solution containing 0.01 M NaCl. Assuming  $\text{Ca}^{2+}$  in solution is at equilibrium with  $\text{CaCO}_3(s)$ , what would be the  $\text{Ca}^{2+}$  concentration?  
( $T = 25^\circ\text{C}$ ,  $pK_s$  for  $\text{CaCO}_3 = 8.48$ )

# Caveat!

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

# Reading assignment

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- Textbook Ch2 p. 32-51