

## Lecture 2: Chemistry and Chemical Reactions

### Oxidation state

- Number of electrons lost (or gained) by an element when forming an ion or chemical bond

Determining the oxidation state of an element in a compound:

1. An element bonded to itself has an oxidation state of zero (supersedes the other rules)
2. Hydrogen (H) is always +1
3. Oxygen (O) is always -2
4. The sum of the oxidation states of all elements in the compound must add up to the total charge on the compound

Examples: O<sub>2</sub> gas, CO<sub>2</sub>, CH<sub>4</sub>, CH<sub>2</sub>O (organic matter), SO<sub>4</sub><sup>2-</sup>

### Charge Balance

- Water contains positively charged (cations) and negatively charged (anions) dissolved ions
- Charge balance – Positive and negative charges must cancel each other out
- Solute charge is represented in terms of equivalents per volume (e.g., eq/L or meq/L for milliequivalents per liter)
- eq/L = mol/L x solute charge

### Unit Conversion

One of the most important skills you will ever learn is how to convert between different units.

Examples:

- (a) What is the molarity (mol L<sup>-1</sup>) of Mg<sup>2+</sup> in a solution prepared as 50 mg L<sup>-1</sup> MgCl<sub>2</sub>·6H<sub>2</sub>O?
- (b) What is the molarity (mol L<sup>-1</sup>) of Cl<sup>-</sup> in a solution prepared as 50 mg L<sup>-1</sup> MgCl<sub>2</sub>·6H<sub>2</sub>O?

First, what is the molecular mass (g/mol) of MgCl<sub>2</sub>·6H<sub>2</sub>O? 203.31 g/mol

$$(c) (50 \text{ mg MgCl}_2 \cdot 6\text{H}_2\text{O} / \text{L})(1 \text{ g} / 1000 \text{ mg})(1 \text{ mol MgCl}_2 \cdot 6\text{H}_2\text{O} / 203.31 \text{ g MgCl}_2 \cdot 6\text{H}_2\text{O})(1 \text{ mol Mg} / 1 \text{ mol MgCl}_2 \cdot 6\text{H}_2\text{O}) = 2.5 \times 10^{-4} \text{ mol/L}$$

$$(d) (50 \text{ mg MgCl}_2 \cdot 6\text{H}_2\text{O} / \text{L})(1 \text{ g} / 1000 \text{ mg})(1 \text{ mol MgCl}_2 \cdot 6\text{H}_2\text{O} / 203.31 \text{ g MgCl}_2 \cdot 6\text{H}_2\text{O})(2 \text{ mol Cl} / 1 \text{ mol MgCl}_2 \cdot 6\text{H}_2\text{O}) = 4.9 \times 10^{-4} \text{ mol/L}$$

Are these charge balanced? Yes! Cl<sup>-</sup> has one equivalent per mol (eq/mol) and Mg<sup>2+</sup> has two equivalents per mol.

$$(e) (4.9 \times 10^{-4} \text{ mol/L Cl}^-) \times (1 \text{ eq/mol}) = 4.9 \times 10^{-4} \text{ eq/L}$$

$$(f) (2.5 \times 10^{-4} \text{ mol/L Mg}^{2+}) \times (2 \text{ eq/mol}) = 4.9 \times 10^{-4} \text{ eq/L}$$

\*note that the 2.5 and 4.9 are rounded, so it's actually like 2.45

### Geochemical Models

Steps to build a model:

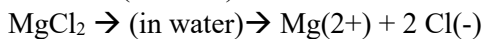
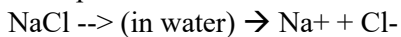
1. Define the system
2. Define the identity and quantity of the constituents (reactants and products) in the system
3. Write a balanced equation for the chemical reaction of interest

1. Define the system
  - a. Closed System – composition is fixed; no mass transfer (box)
  - b. Open System – mass can enter and leave the system via fluxes (box + arrows)
2. Define the constituents
  - a. Example constituents (ensure they are expressed in comparable units)
    - i. Water
    - ii. Minerals
    - iii. Gases (defined by their partial pressure)
    - iv. Solutes (defined by their concentration; e.g., mass/volume)
3. Write a balanced equation for the chemical reaction of interest



- a. Start with an unbalanced equation of reactants and products
- b. Make an element inventory
- c. Adjust the numbers in front of the reactants and products until balanced on either side of the arrow
- d. Assuming the reaction takes place with water as a solvent, add  $H^+$ ,  $OH^-$  and  $H_2O$  as needed to balance the equation (but only if  $H_2O$  participates in the reaction)
- e. Double check for **mass balance** and **charge balance!**

Examples:



## Chemical Reactions

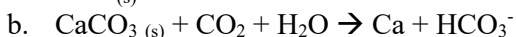
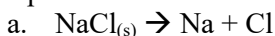
Types of chemical reactions

1. Dissolution/precipitation
2. Acid-base
3. Adsorption/desorption
4. Oxidation-reduction (redox)

\*reactions can be more than one type

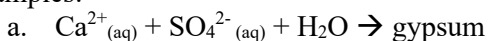
1. Dissolution reaction:  $A_{vA}B_{vB(s)} \rightarrow v_A A^{qA}_{(aq)} + v_B B^{qB}_{(aq)}$ 
  - a. A – element
  - b.  $v_A$  – stoichiometric amount of A
  - c.  $q_A$  – charge on the ion A

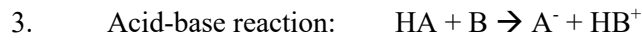
Examples:



2. Precipitation reaction:  $v_A A^{qA}_{(aq)} + v_B B^{qB}_{(aq)} \rightarrow A_{vA}B_{vB(s)}$

Examples:





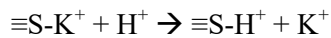
Brønsted-Lowry definition: transfer of a proton from an acid (the proton donor) to a base (the proton acceptor)

Examples (which are the acid, base, conjugate acid, conjugate base?)

- a.  $HCl + H_2O \rightarrow Cl^- + H_3O^+$
- b.  $NH_3 + H_2O \rightarrow NH_4^+ + OH^-$
- c.  $CaCO_3 + H_2SO_4 \rightarrow H_2CO_3 + Ca^{2+} + SO_4^{2-}$

4. Surface complexation reactions

- a. Adsorption – the adhesion of a substance (e.g., solute) onto a surface
- b. Desorption – the release of a substance from a surface into solution



Inner-sphere complex – ion forms a chemical bond with the surface at a specific site

Outer-sphere complex – electrostatic interaction between ion and charged surface; ion remains in hydration shell

5. Redox (oxidation-reduction) reactions

- a. Transfer of electrons from e- donor (reducing agent) to e- acceptor (oxidizing agent)  
OILRIG – oxidation is loss, reduction is gain

