Chemical Compounds

1. Classification of Elements and Compounds

**Types of Pure Substances** (Figure 3.4)

- **Elements** -- made up of only one type of atom
  - *atomic* (e.g., He, Cu) or *molecular* (e.g., H\(_2\), N\(_2\), P\(_4\))

- **Compounds** -- made up of atoms of two or more different elements
  - *molecular* (e.g., H\(_2\)O, PF\(_5\)) or *ionic* (e.g., NaCl)

2. Elements combine to form compounds -- two general types

- **Molecular Compounds** -- *Covalent Bonding* -- *electron sharing*
  - atoms linked together by "covalent bonds" in *discrete* electrically neutral particles called *molecules*
  - e.g., H\(_2\)O, CO\(_2\), PCl\(_3\), C\(_{12}\)H\(_{22}\)O\(_{11}\)

- **Ionic Compounds** -- *Ionic Bonding* -- *electron transfer*
  - result from transfer of one or more electrons from one atom to another to yield oppositely-charged particles called *ions*
    - cation = positive ion  anion = negative ion
  - there are not discrete molecules -- the ions are held together by electrostatic forces in a regular, 3-dimensional pattern called a *crystalline lattice*
    - e.g., MgCl\(_2\)  magnesium chloride

\[
\text{Mg} + \text{Cl}^− \rightarrow \text{Mg}^{2+} + 2 \text{Cl}^− \\
\text{MgCl}_2
\]
3. Properties of Ionic and Molecular Compounds

**Ionic compounds:**
- hard, brittle, high-melting crystalline solids
- non-conductors in solid state, but conductors when molten
- electrolytes -- separate into ions in aqueous solution

**Molecular compounds:**
- only weak attractive forces between uncharged molecules
- generally low mp and bp
- non-conductors of electricity
- usually nonelectrolytes

4. Types of Chemical Formulas (e.g., see Table 3.1)

*empirical formula* shows the *simplest ratio* of the elements present

*molecular formula* shows the *actual number* of atoms in one molecule

*structural formula* shows how the atoms are connected

For "hydrogen peroxide" the three formulas are:

empirical: HO  molecular: H₂O₂

structural: \( \text{H—O—O—H} \)

*molecular model* a 3-D rendering of the structure of a molecule
common types are "ball and stick" or "space-filling"
5. Relationship to Periodic Table -- Some General trends

**Molecular compounds** contain only nonmetals and/or metalloids

e.g., PH₃ AsF₅ HBr

some nonmetallic elements actually exist as molecular compounds

e.g., the diatomics (H₂, O₂, N₂, etc. as listed before)
also: P₄, As₄, S₈, Se₈

**Ionic compounds** contain metals and/or polyatomic ions

group IA (1) +1 cations Li⁺, Na⁺, K⁺, ..... 
group IIA (2) +2 cations Mg²⁺, Ca²⁺, ..... 
an important +3 cation Al³⁺ 

other metals may form more than one cation, e.g.:

Fe²⁺ and Fe³⁺ Sn²⁺ and Sn⁴⁺
group VIA (16) -2 anions O²⁻, S²⁻, Se²⁻, ..... 
group VIIA (17) -1 anions F⁻, Cl⁻, Br⁻, ..... 

6. Polyatomic Ions -- two or more atoms combined in a single charged unit

e.g., NH₄⁺ ammonium ion
NO₃⁻ nitrate ion
PO₄³⁻ phosphate ion
HCO₃⁻ hydrogen carbonate (or bicarbonate ion)

**KNOW ALL** of the formulas and names in Table 3.4 plus the following!!!

H₃O⁺ hydronium ion
C₂O₄²⁻ oxalate
PO₃³⁻ phosphite
OCN⁻ cyanate
SCN⁻ thiocyanate
S₂O₃²⁻ thiosulfate

**See the class web site for an organized tabulation of the polyatomic ions!**
Writing Formulas for Ionic Compounds

look for the simplest combination of cations and anions to yield an electrically neutral formula

<table>
<thead>
<tr>
<th>ion combination</th>
<th>compound</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg$^{2+}$ and Cl$^{-}$</td>
<td>MgCl$_2$</td>
</tr>
<tr>
<td>Na$^+$ and O$^{2-}$</td>
<td>Na$_2$O</td>
</tr>
<tr>
<td>Fe$^{3+}$ and SO$_4^{2-}$</td>
<td>Fe$_2$(SO$_4$)$_3$</td>
</tr>
</tbody>
</table>

e.g., What compound should form between sulfur (S) and potassium (K)?

K is in group IA $\rightarrow$ K$^+$

S is in group VIA $\rightarrow$ S$^{2-}$

therefore, the compound should be K$_2$S

Inorganic Chemical Nomenclature

1. Binary compounds of metals and nonmetals -- ionic compds

cation first, then anion, e.g.:

MgO  magnesium oxide

CaF$_2$  calcium fluoride

FeO  iron(II) oxide  {aka ferrous oxide}

Fe$_2$O$_3$  iron(III) oxide  {aka ferric oxide}

2. Compounds with polyatomic ions -- ionic compds

must first recognize the polyatomic ions, e.g.:

Na$_2$SO$_4$  sodium sulfate

NH$_4$Cl  ammonium chloride

Cr$_3$(PO$_4$)$_2$  chromium(II) phosphate
3. Hydrated ionic compounds

have a specific number of water molecules associated with each formula unit of an ionic substance

e.g.,  \( \text{MgCl}_2 \cdot 6\text{H}_2\text{O} \)  magnesium chloride hexahydrate

\( \text{CuSO}_4 \cdot 5\text{H}_2\text{O} \)  copper(II) sulfate pentahydrate

4. Binary compounds of nonmetals  --  *molecular* compds

use prefixes to indicate numbers of each atom, e.g.:

\( \text{PF}_3 \)  phosphorus trifluoride

\( \text{P}_2\text{F}_4 \)  diphosphorus tetrafluoride

\( \text{N}_2\text{O}_5 \)  dinitrogen pentoxide

exception  --  hydrogen plus one atom of a nonmetal. e.g.:

\( \text{H}_2\text{S} \)  hydrogen sulfide  (not "dihydrogen")

5. Binary acids and their salts

*Acid:*  substance that reacts with water to yield hydronium ions (\( \text{H}_3\text{O}^+ \)) and anions, e.g.:

\[
\text{HBr}\,(\text{g}) + \text{H}_2\text{O} \longrightarrow \text{H}_3\text{O}^+\,(\text{aq}) + \text{Br}^-\,(\text{aq})
\]

\( \text{HBr}\,(\text{aq}) \)  *hydrobromic acid*

\( \text{H}_2\text{Se}\,(\text{aq}) \)  *hydroselenic acid*

**Salt:**  an ionic compound produced by *neutralization* of an acid by a base (a supplier of hydroxide ions, \( \text{OH}^- \)), e.g.:

\[
\text{HBr}\,(\text{aq}) + \text{KOH}\,(\text{aq}) \longrightarrow \text{KBr}\,(\text{aq}) + \text{H}_2\text{O}
\]

\( \text{KBr} \)  potassium bromide  \{a salt of *hydrobromic acid*\}

\( \text{Na}_2\text{S} \)  sodium sulfide  \{a salt of *hydrosulfuric acid*\}
6. Oxoacids and their salts

*oxoacid* (aka *oxyacid*) -- $H_xEO_y$ (where E = nonmetal)

removal of $H^+$ yields polyatomic anions

<table>
<thead>
<tr>
<th>oxoacid</th>
<th>polyatomic ions</th>
<th>salt example</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_2SO_4$</td>
<td>$SO_4^{2-}$</td>
<td>$Na_2SO_4$</td>
</tr>
<tr>
<td>sulfuric acid</td>
<td><em>sulfate</em></td>
<td>sodium <em>sulfate</em></td>
</tr>
<tr>
<td>$H_2SO_3$</td>
<td>$SO_3^{2-}$</td>
<td>$CaSO_3$</td>
</tr>
<tr>
<td>sulfurous acid</td>
<td><em>sulfite</em></td>
<td>calcium <em>sulfite</em></td>
</tr>
<tr>
<td></td>
<td>$HSO_3^-$</td>
<td>$Ca(HSO_3)_2$</td>
</tr>
<tr>
<td></td>
<td><em>hydrogen sulfite</em></td>
<td></td>
</tr>
</tbody>
</table>

review the series of chlorine oxoacids and their salts: $HClO_x$ ($x = 1, 2, 3, 4$)

**Composition of Compounds**

1. Empirical and Molecular Formulas

   *empirical formula* -- shows the *simplest ratio* of the elements present

   *molecular formula* -- shows the *actual number* of atoms in one molecule

2. Percentage Composition -- mass % of elements in a compound

   *theoretical % composition* -- *from given formula*

   **Problem:** What is percentage composition of $H_2CO_3$?

   **mole ratio** = $2 \text{ mol H : 1 mol C : 3 mol O}$

   **molar mass** = $2 (1.0) + 1 (12.0) + 3 (16.0) = 62.0 \text{ g/mole}$

   % composition:

   - $\% \text{ H} = \frac{\text{mass H}}{\text{mass } H_2CO_3} \times 100\%$
     
     $= \frac{2 (1.01)}{62.0} \times 100\% = 3.26\%$

   - $\% \text{ C} = \frac{12.01}{62.0} \times 100\% = 19.36$

   - $\% \text{ O} = \frac{3 (16.00)}{62.0} \times 100\% = 77.38$

   Total: 100.00 %
3. Empirical Formula -- determination from % composition

*Problem:*
A certain fluorocarbon is found to be 36.52% C, 6.08% H, and 57.38% F. What is the empirical formula of this compound?

{we're looking for the *mole ratio* of the elements}

In 100 g of the compound, there are:

\[(36.52 \text{ g C}) \times \left(\frac{1 \text{ mol C}}{12.01 \text{ g C}}\right) = 3.041 \text{ mole C}\]
\[(6.08 \text{ g H}) \times \left(\frac{1 \text{ mol H}}{1.01 \text{ g H}}\right) = 6.020 \text{ mole H}\]
\[(57.38 \text{ g F}) \times \left(\frac{1 \text{ mol F}}{19.00 \text{ g F}}\right) = 3.020 \text{ mole F}\]

So, the mole ratio is:
\[\text{C} 3.041 \quad \text{H} 6.020 \quad \text{F} 3.020\]

Now reduce to simplest ratio (divide by smallest number):
\[\frac{3.041}{3.020} \quad \frac{6.020}{3.020} \quad \frac{3.020}{3.020}\]
\[= \frac{1.007}{1} \quad \frac{1.993}{1} \quad \frac{1}{1}\]
\[\text{C} 1.007 \quad \text{H} 1.993 \quad \text{F}\]

(empirical formula)  

4. Molecular Formula

*empirical formula* combined with *molecular mass = molecular formula*

*Problem:*
The above fluorocarbon is found to have a molecular mass of 66.08 g/mole. What is the molecular formula?

\[n \times \text{mass of empirical formula} = \text{molecular mass}\{ n = ? \}\]

\[\text{empirical formula} = \text{CH}_2\text{F}\]
\[\text{formula mass} = 1 \text{ C} + 2 \text{ H} + 1 \text{ F} = 33.03 \text{ g/mole}\]

\[n \times (33.03 \text{ g/mole}) = 66.08 \text{ g/moles, } n = 2\]
\[\therefore \text{molecular formula is } \text{C}_2\text{H}_4\text{F}_2\]
Chemical Equations

1. Balancing Chemical Equations -- by inspection

*Adjust coefficients to get equal numbers of each kind of element on both sides of arrow.*

*Use smallest, whole number coefficients.*

E.g., start with unbalanced equation (for the *combustion* of butane):

\[
C_4H_{10} + O_2 \rightarrow CO_2 + H_2O
\]

**Reactants**

**Products**

*Hint:* first look for an element that appears only once on each side; e.g., C

\[
C_4H_{10} + 13/2 O_2 \rightarrow 4 CO_2 + 5 H_2O
\]

Multiply through by 2 to remove fractional coefficient:

\[
2 C_4H_{10} + 13 O_2 \rightarrow 8 CO_2 + 10 H_2O
\]

2. Combustion Analysis

See Examples 3.20 and 3.21 in textbook

Based on combustion reactions (like the one above)

\[
C_xH_y \text{ or } C_xH_yO_z \text{ compound} + \text{excess } O_2 \rightarrow CO_2 + H_2O
\]

% C and x determined from amount of CO₂ produced

% H and y determined from amount of H₂O produced

% O (if present) and z must be determined by difference
Organic Compounds -- molecular compounds of carbon
(See Tables 3.6 and 3.7)

<table>
<thead>
<tr>
<th>Family</th>
<th>Main Structural Feature</th>
<th>Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrocarbons:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Alkanes</td>
<td>only single bonds</td>
<td>CH₃CH₃</td>
</tr>
<tr>
<td>Alkenes</td>
<td>C=C</td>
<td>CH₂=CH₂</td>
</tr>
<tr>
<td>Alkynes</td>
<td>C≡C</td>
<td>HCCCC</td>
</tr>
<tr>
<td>Aromatic</td>
<td>benzene ring (e.g., C₆H₆)</td>
<td></td>
</tr>
<tr>
<td>Alcohols</td>
<td>R-OH</td>
<td>CH₃CH₂OH</td>
</tr>
<tr>
<td>Ethers</td>
<td>R-O-R'</td>
<td>CH₃OCH₃</td>
</tr>
<tr>
<td>Aldehydes</td>
<td>R- C-H</td>
<td>CH₃- C-H</td>
</tr>
<tr>
<td>Ketones</td>
<td>R-C-R'</td>
<td>CH₃- C-CH₂CH₃</td>
</tr>
<tr>
<td>Carboxylic Acids</td>
<td>R-C-OH</td>
<td>CH₃-C-OH</td>
</tr>
<tr>
<td>Esters</td>
<td>R-C-OR'</td>
<td>CH₃-C-OCH₂CH₃</td>
</tr>
<tr>
<td>Amines</td>
<td>R NH₂, R₂NH, R₃N</td>
<td>CH₃NH₂</td>
</tr>
</tbody>
</table>

Nomenclature - based on hydrocarbons:

- CH₄ methane
- C₂H₆ ethane
- C₃H₈ propane
- C₄H₁₀ butane
- C₅H₁₂ pentane
- C₆H₁₄ hexane
- C₇H₁₆ heptane
- C₈H₁₈ octane, etc......