Molecules, Compounds, and Chemical Equations **(Chapter 3)**

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_2O, 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_2O CO_2 PCl_3 $C_{12}H_{22}O_{11}$

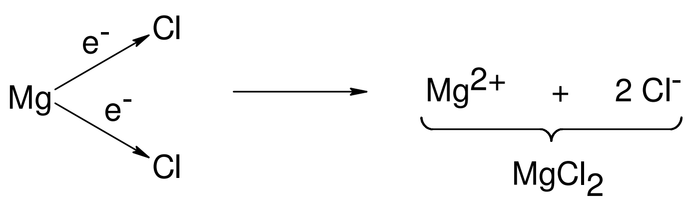
Ionic Compounds -- ***Ionic Bonding*** -- ***electron transfer***

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



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

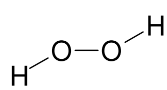
molecular formula shows the *actual number* of atoms in one molecule

structural formula shows how the atoms are connected

e.g., for "hydrogen peroxide" the three formulas are:

empirical: HO molecular: H_2O_2

structural:



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., PH_3 AsF_5 HBr

some nonmetallic elements actually exist as molecular compounds

e.g., the diatomics (H_2, O_2, N_2, etc. as listed before)
also: P_4, As_4, S_8, Se_8

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

group IA (1)	+1 cations	Li^+, Na^+, K^+, ...
group IIA (2)	+2 cations	Mg^{2+}, Ca^{2+}, ...
	an important +3 cation	Al^{3+}

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

Fe^{2+} and Fe^{3+} Sn^{2+} and Sn^{4+}

group VIA (16)	-2 anions	O^{2-}, S^{2-}, Se^{2-}, ...
group VIIA (17)	-1 anions	F^-, Cl^-, Br^-, ...

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

e.g.,	NH_4^+	ammonium ion
	NO_3^-	nitrate ion
	PO_4^{3-}	phosphate ion
	HCO_3^-	hydrogen carbonate (or bicarbonate ion)

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

H_3O^+	hydronium ion
$C_2O_4^{2-}$	oxalate
PO_3^{3-}	phosphite
OCN^-	cyanate
SCN^-	thiocyanate
$S_2O_3^{2-}$	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

e.g.,

ion combination	compound
Mg^{2+} and Cl^{-}	$MgCl_2$
Na^{+} and O^{2-}	Na_2O
Fe^{3+} and SO_4^{2-}	$Fe_2(SO_4)_3$

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_2S

Inorganic Chemical Nomenclature

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

cation first, then anion, e.g.:

MgO	magnesium ox*ide*	
CaF_2	calcium fluor*ide*	
FeO	iron(II) ox*ide*	{aka ferrous oxide}
Fe_2O_3	iron(III) ox*ide*	{aka ferric oxide}

2. Compounds with polyatomic ions -- *ionic* compds

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

Na_2SO_4	sodium sulfate
NH_4Cl	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.,	$MgCl_2 \bullet 6H_2O$	magnesium chloride hexahydrate
	$CuSO_4 \bullet 5H_2O$	copper(II) sulfate pentahydrate

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

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

PF_3	phosphorus trifluoride
P_2F_4	diphosphorus tetrafluoride
N_2O_5	dinitrogen pentoxide

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

H_2S	hydrogen sulfide (not "dihydrogen")

5. Binary acids and their salts

Acid: substance that reacts with water to yield hydronium ions (H_3O^+) and anions, e.g.:

$$HBr_{(g)} + H_2O \longrightarrow H_3O^+{}_{(aq)} + Br^-{}_{(aq)}$$

$HBr_{(aq)}$	*hydro*brom*ic acid*
$H_2Se_{(aq)}$	*hydro*selen*ic acid*

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

$$\underset{\text{acid}}{HBr_{(aq)}} + \underset{\text{base}}{KOH_{(aq)}} \longrightarrow \underset{\text{salt}}{KBr_{(aq)}} + \underset{\text{water}}{H_2O}$$

KBr	potassium bromide	{a salt of *hydro*brom*ic acid*}
Na_2S	sodium sulfide	{a salt of *hydro*sulfur*ic acid*}

6. Oxoacids and their salts

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

removal of H^+ yields polyatomic anions

oxoacid	polyatomic ions	salt example
H_2SO_4 sulfur***ic*** acid	SO_4^{2-} sulf***ate***	Na_2SO_4 sodium sulf***ate***
	HSO_4^- hydrogen sulf***ate***	$NaHSO_4$ sodium hydrogen sulf***ate***
H_2SO_3 sulfur***ous*** acid	SO_3^{2-} sulf***ite***	$CaSO_3$ calcium sulf***ite***
	HSO_3^- hydrogen sulf***ite***	$Ca(HSO_3)_2$ calcium hydrogen sulf***ite***

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 mol H : 1 mol C : 3 mol O

molar mass = 2 (1.0) + 1 (12.0) + 3 (16.0) = 62.0 g/mole

% composition:

% H = [mass H / mass H_2CO_3] x 100%

= [2 (1.01) / 62.0] x 100 % = 3.26 %

% C = (12.01 / 62.0) x 100 % = 19.36

% O = [3 (16.00) / 62.0] x 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 ~~g C~~) x (1 mol C / 12.01 ~~g C~~) = 3.041 mole C

(6.08 ~~g H~~) x (1 mol H / 1.01 ~~g H~~) = 6.020 mole H

(57.38 ~~g F~~) x (1 mol F / 19.00 ~~g F~~) = 3.020 mole F

so, the mole ratio is:

$C_{3.041}\ H_{6.020}\ F_{3.020}$

now reduce to simplest ratio (divide by smallest number):

$C_{3.041 / 3.020}\ H_{6.020 / 3.020}\ F_{3.020 / 3.020}$

= $C_{1.007}\ H_{1.993}\ F$ = CH_2F (the *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 x (mass of empirical formula) = molecular mass{ n = ? }

empirical formula = CH_2F
formula mass = 1 C + 2 H + 1 F = 33.03 g/mole

n x (33.03 g/mole) = 66.08 g/moleso, n = 2

∴ molecular formula is $C_2H_4F_2$

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):

$$C_4H_{10} + O_2 \longrightarrow CO_2 + H_2O$$

reactants ***products***

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

$$C_4H_{10} + 13/2\ O_2 \longrightarrow 4\ CO_2 + 5\ H_2O$$

multiply through by 2 to remove fractional coefficient:

$$2\ C_4H_{10} + 13\ O_2 \longrightarrow 8\ CO_2 + 10\ H_2O$$

2. Combustion Analysis

see Examples 3.20 and 3.21 in textbook

based on combustion reactions (like the one above)

C_xH_y or $C_xH_yO_z$ compound + excess O_2 $\longrightarrow$ CO_2 + H_2O

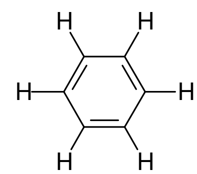
% C and x determined from amount of CO_2 produced

% H and y determined from amount of H_2O produced

% O (if present) and z must be determined by difference

Organic Compounds -- molecular compounds of carbon

(See Tables 3.6 and 3.7)

Family	Main Structural Feature	Examples
Hydrocarbons:		
Alkanes	only single bonds	CH_3CH_3
Alkenes	C=C	$CH_2{=}CH_2$
Alkynes	C≡C	HC≡CH
Aromatic	benzene ring (e.g., C_6H_6)	
Alcohols	R-OH	CH_3CH_2OH
Ethers	R-O-R'	CH_3OCH_3
Aldehydes	$R-\overset{\overset{\Large O}{\|\|}}{C}-H$	$CH_3-\overset{\overset{\Large O}{\|\|}}{C}-H$
Ketones	$R-\overset{\overset{\Large O}{\|\|}}{C}-R'$	$CH_3-\overset{\overset{\Large O}{\|\|}}{C}-CH_2CH_3$
Carboxylic Acids	$R-\overset{\overset{\Large O}{\|\|}}{C}-OH$	$CH_3-\overset{\overset{\Large O}{\|\|}}{C}-OH$
Esters	$R-\overset{\overset{\Large O}{\|\|}}{C}-OR'$	$CH_3-\overset{\overset{\Large O}{\|\|}}{C}-OCH_2CH_3$
Amines	RNH_2, R_2NH, R_3N	CH_3NH_2

Nomenclature - based on hydrocarbons:

CH_4	methane	C_5H_{12}	pentane
C_2H_6	ethane	C_6H_{14}	hexane
C_3H_8	propane	C_7H_{16}	heptane
C_4H_{10}	butane	C_8H_{18}	octane, etc......