CHAPTER 3

CHEMICAL COMPOUNDS

There are two fundamental kinds of chemical bonds that holds together the atoms in a compound.

1) Covalent Bond: Covalent bond involves sharing of e^-s betwen atoms, gives rise to a molecular compound.

2) Ionic Bond: Ionin bonds, which involve a transfer of electrons from one atom to another, give rise to formation of ionic compounds.

Molecular Compounds: A molecular compound is made up of discrete units called molecules. Molecules typically consist of a small number of nonmetal atoms held together by covalent bonds.

Molecular compounds are represented by chemical formulas and these formulas indicate

a) The element present.
b) The relative number of atoms of each element.

Two elements present

H_2O

Two H atoms per molecule

One O element per molecule

CCl_4 : One C atom, Four Cl atoms } per molecule

Emprical Formula: Emprical formula is the simplest formula for a compund. It shows;

a) Types of atoms

b) Their relative numbers

Generally, the emprical formula does not tell us a great deal about a compound.

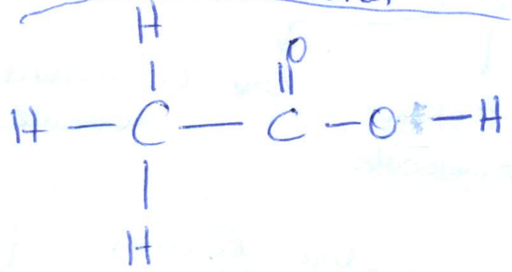
Molecular Formula: Molecular formula is based on an actual molecule of a compound.

→ In some cases, the emprical and molecular formulas are identical.

	Emp. Formula	Molecular Formula
Acedic acid	CH_2O	$C_2H_4O_2$
Formaldehyde	CH_2O	CH_2O
Glucose	CH_2O	$C_6H_{12}O_6$

→ Generally, the molecular formula is a multiple of the emprical formula.

Structural Formula: A structural formula shows the order of atoms that are bonded together in a molecule. It also shows the types of bonds between individual atoms.

Emprical	Structural	Molecular formula
CH_2O		$C_2H_4O_2$

3 H atoms bonded to one of the C atoms

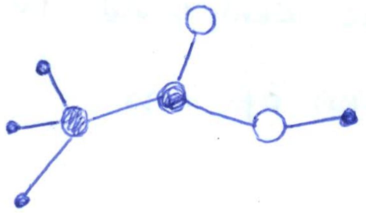
1 H atom bonded to an O atom.

→ The covalent bonds in a structural formula are represented by lines or dashes (—).

— Single covalent bond
= Double " "
≡ Triple " "

↓ Stronger tighter

→ Ball and stick model



$CH_3-\overset{\overset{O}{\|}}{C}-OH$.

IONIC COMPOUNDS: An ionic compound is made up of positive and negative ions joined together by electrostatic forces of attraction.

The atoms of metallic elements tend to loose e⁻s when they combine with nonmetal atoms. They becomes (+)

The nonmetal atoms, vise versa, tend to gain e⁻s when they combine with metal atoms. They become (−)

→ As a result of this e⁻ transfer, the metal atom becomes postive ion (cation), and the nonmetal atom become negative ion (anion).

$Na^+ Cl^-$

looses e⁻
cation

gains e⁻
anion

Na^+Cl^-

gives up $1e^-$ — cation

gains $1e^-$ — anion

Neutral $\Rightarrow$ $+1 - 1 = 0$

Ratio of $\frac{Na^+}{Cl^-} = \frac{1}{1} = 1$

The <u>formula unit</u> of an ionic compound is the smallest electrically neutral collection of ions.

Na^+, Mg^{2+}, Cl^- $\rightarrow$ Monoatomic ions (single atom)

NO_3^-, PO_4^{3-} $\rightarrow$ Polyatomic ions (two or more atoms)

THE MOLE CONCEPT AND CHEMICAL COMPOUNS

→ Formula mass: Mass of <u>formula unit</u> in atomic mass units.

→ Molecular mass: Mass of a <u>Molecule</u> in " " "

We can speak of molecular mass. Because for a molecular compound, the formula unit is an actual molecule.

→ For molecular compound

molecular mass H_2O $= 2\,(\text{atomic mass H}) + 1\,(\text{atomic mass O})$

$= 2\,(1.00794\ u) + 15.9994\ u$

$= 18.0153\ u$

→ For ionic compound

formula mass $MgCl_2$ = 1 (atomic mass Mg) + 2 (atomic mass Cl)

= 24.3050 u + 2(35.453 u)

= 95.211 u

Mole of a Compound

The molar mass is the mass of one mole of compound. A mole of compound is an amount of compound containing Avogadro's number (6.02214×10^{23}) of formula units or molecules.

1 mol H_2O : 18.0153 g H_2O = 6.02×10^{23} H_2O mole.

1 mol $MgCl_2$: 95.211 g $MgCl_2$ = 6.02×10^{23} $MgCl_2$ formula units

1 mol $Mg(NO_3)_2$: 148.3148 g $Mg(NO_3)_2$ = 6.02×10^{23} $Mg(NO_3)_2$ formula units.

Example: How many C_2H_6S (ethyl mercaptan) molecules are contained in a 1.0 μL sample. (d = 0.84 g/mL)

The pathway is: μL → L → mL → g → mol → molecules

$$? \; \cancel{\text{molecules}}\ g\ C_2H_6S = 1.0\ \cancel{\mu L} \times \frac{1 \times 10^{-6}\ \cancel{L}}{1\ \cancel{\mu L}} \times \frac{1000\ \cancel{mL}}{\cancel{L}} \times \frac{0.84\ g\ C_2H_6S}{1\ \cancel{mL}}$$

$$= 8.4 \times 10^{-4}\ g\ C_2H_6S$$

$$? \text{ mol } C_2H_6S = 8.4\times10^{-4}\text{ g } C_2H_6S \times \frac{1 \text{ mol } C_2H_6S}{62.1 \text{ g } C_2H_6S}$$

$$= 1.4\times10^{-5} \text{ mol } C_2H_6S$$

$$? \text{ molecules } C_2H_6S = 1.4\times10^{-5}\ \cancel{\text{mol}}\ C_2H_6S \times \frac{6.02\times10^{23} \text{ molecules } C_2H_6S}{1\ \cancel{\text{mol}}\ C_2H_6S}$$

$$= 8.1\times10^{18} \text{ molecules } C_2H_6S$$

Example: How many moles of F atoms are in a 75.0 mL sample of halothate. ($d = 1.871$ g/mL)

$\boxed{C_2HBrClF_3}$ $M_w = 197.4$ g/mol

3 moles of F in 1 mol of C_2HBrF_3

$$? \text{ mol F} = 75.0\ \cancel{\text{mL}}\ C_2HBrClF_3 \times \frac{1.871 \text{ g } C_2HBrClF_3}{1\ \cancel{\text{mL}}\ C_2HBrClF_3} \times \frac{1\ \cancel{\text{mol}}\ C_2HBrClF_3}{197.4 \text{ g } C_2HBrClF_3} \times \frac{3 \text{ mol F}}{1\ \cancel{\text{mol}}\ C_2HBrClF_3}$$

$$= 2.13 \text{ mol F}$$

Example: what is the mass percentt composition of halothane.

$$\%C = \frac{2\ \cancel{\text{mol}}\ C \times \frac{12.01\text{ g }\cancel{C}}{1\ \cancel{\text{mol}}\ C}}{197.38\ \cancel{g}\ C_2HBrClF_3} \times 100\% = 12.17\%C$$

$$\%H = \frac{1 \text{ mol H} \times \frac{1.01 \text{ g H}}{1 \text{ mol H}}}{197.38 \text{ g } C_2HBrClF_3} \times 100\% = 0.51\%H$$

$$\%Br = \frac{79.90\ \cancel{35.45}}{197.38}\times100\% = 40.48\%Br, \quad \%Cl = \frac{35.45}{197.38}\times100\% = 17.96$$

$$\%F = \frac{3\times19.00}{197.38}\times100\% = 28.88\%F$$

Example:

Dibutylsuccinate

$M_w = 230$ u

	C	H	O
%	62.58	9.63	27.79

Emprical formula?

Molecular formula?

(1) Determine the mass of each element in 100.00 g sample

62.58 g C, 9.63 g H, 27.79 g O

(2) Convert masses to moles

$$? \text{ mol C} = 62.58 \text{ g C} \times \frac{1 \text{ mol C}}{12.011 \text{ g C}} = 5.210 \text{ mol C}$$

$$? \text{ mol H} = 9.63 \text{ g H} \times \frac{1 \text{ mol H}}{1.008 \text{ g H}} = 9.55 \text{ mol H}$$

$$? \text{ mol O} = \frac{27.79}{15.999} = 1.737 \text{ mol O}$$

(3) Write a tentative formula based on mole numbers

$$C_{5.21}H_{9.55}O_{1.74}$$

(4) Devide the subscripts by the smallest one

$$C_{\frac{5.21}{1.74}}H_{\frac{9.55}{1.74}}O_{\frac{1.74}{1.74}} = C_{2.99}H_{5.49}O$$

$$= C_3H_{5.49}O$$

(5) Multiply the subscripts by a small whole number to make them integral to obtain emprical formula

$$C_{2\times 3}H_{2\times 5.49}O_{2\times 1} \qquad (2 \times 5.49 = 10.98 \cong 11)$$

$$\boxed{\text{Emprical formula: } C_6H_{11}O_2}$$

⑥

→ To establish the molecular formula, first find the emprical formula mass

$$C_6H_{11}O_2 = [6 \times 12.0 + 11 \times 1.0 + 2 \times 16.0]\ u$$
$$= 115\ u$$

→ Since the experimentally determined formula mass is 230 u. (230 = 2 × 115)

$$\boxed{\text{The molecular formula is } C_{12}H_{22}O_4}$$

Combustion Analysis

In combustion analysis, a weighed sample of a compound is burned in a stream of oxygen gas. The H_2O vapor and CO_2 gas produced in the combustions are absorbed by appropriate substances. The increases in mass of these absorbers correspond to the mass of H_2O and CO_2.

$$C_xH_yO_z + O_2 \longrightarrow x\,CO_2 + y\,H_2O$$

→ After combustion, all the C atoms in the sample are found in the CO_2.

→ Similarly, all the H atoms are in the H_2O.

→ Oxygen atoms in H_2O and CO_2 could have come partly from the sample and partly from the O_2 gas.

Example: Combustion of a 0.2000 g sample of vitamin C yields 0.2998 g CO_2 and 0.0819 g H_2O.

What are the percent composition and the emprical formula of vitamin C?

$$\underset{(C_xH_yO_z)}{\text{Vitamin C}} + O_2 \longrightarrow CO_2 + H_2O$$

Percent Composition

$$? \text{ mol C} = 0.2998 \text{ g } CO_2 \times \frac{1 \text{ mol } CO_2}{44.01 \text{ g } CO_2} \times \frac{1 \text{ mol C}}{1 \text{ mol } CO_2} = 0.006812 \text{ mol C}$$

$$? \text{ g C} = 0.006812 \text{ mol C} \times \frac{12.011 \text{ g C}}{1 \text{ mol C}} = \boxed{0.08182 \text{ g C}}$$

$$? \text{ mol H} = 0.0819 \text{ g } \cancel{H_2O} \times \frac{1 \text{ mol } \cancel{H_2O}}{18.02 \cancel{\text{ g } H_2O}} \times \frac{2 \text{ mol H}}{\cancel{1 \text{ mol } H_2O}} = 0.00909 \text{ mol H}$$

$$? \text{ g H} = 0.00909 \text{ mol H} \times \frac{1.008 \text{ g H}}{1 \text{ mol H}} = \boxed{0.00916 \text{ g H}}$$

→ The difference gives the mass of O

$$? \text{ g O} = 0.2000 \text{ g sample} - \underset{\text{g C}}{0.08182} - \underset{\text{g H}}{0.00916} = \boxed{0.1090 \text{ g O}}$$

→ percent compositions

$$\%C = \frac{0.08182 \text{ g C}}{0.2 \text{ g sample}} \times 100\% = 40.91\% \text{ C}$$

$$\%H = \frac{0.00916 \text{ g H}}{0.2000 \text{ g sample}} \times 100\% = 4.58\% \text{ H}$$

$$\%O = \frac{0.1090 \text{ g O}}{0.2000 \text{ g sample}} \times 100\% = 54.50\% \text{ O}$$

Emprical Formula

→ First we need to find the mole of O.

$$? \text{ mol O} = 0.1090 \text{ g O} \times \frac{1 \text{ mol O}}{15.999 \text{ g O}} = 0.006813 \text{ mol O}$$

$$C_{0.006812}O_{0.006813}H_{0.00909}$$

When we divede each subscripts by 0.006812 $\quad CH_{1.33}O \times 3$

$\boxed{C_3H_4O_3}$ Emprical formula

OXIDATION STATES

Oxidation state is related to the number of electrons that an atom loses or gains in in its compounds.

$Na^+ Cl^-$

Na^+	Cl^-
metal	nonmetal
loses 1 e^-	gains 1 e^-
+1 oxidation state	−1 oxidation state

Rules for Assigning Oxidation States

1. The oxidation state (OS) of an individual atom in a free element is 0. (Na, Cu, Al, H_2, Cl_2)
2. The total OS of all the atoms
   a) neutral species, such as isolated atoms, molecules, and formula units, is 0.
   (all the sum of the OS atoms in CH_3OH and all the ions $MgCl_2$ is 0)

   b) an ion is equal to the charge on the ion.
   (Fe in Fe^{3+} = +3 , Sum OSs in MnO_4^- = −1)
3. In their compounds

	OS
Group 1 metals	+1
Group 2 metals	+2

Compound	OS of	
KCl	K	+1
K_2CO_3	K	+1
$MgBr_2$	Mg	+2
$Mg(NO_3)_2$	Mg	+2

4. In its compounds, the OS of F is −1
   (HF, ClF_3, SF_6)
5. In its compounds, the OS of H is usually +1
   (HI, H_2S, NH_3, CH_4)
6. In its compounds, the OS of O is usually −2
   (H_2O, CO_2, $KMnO_4$)
7. In binary (two element) compounds with metals,

Group	OS of element
17	−1
16	−2
15	−3

Binary Compound	OS of	
$MgBr_2$	Br	−1
Li_2S	S	−2
Li_3N	N	−3

Example :

	Rule #	OS
P_4	1	0
Al_2O_3	2, 6	+3
MnO_4^-	2	+7
NaH	3, 5	−1
H_2O_2	5, 6	−1
Fe_3O_4		$+2\frac{2}{3}$