Chapter 3: Calculations with Chemical Formuals and Equations

These Notes are to SUPPLIMENT the Text, They do NOT Replace reading the Text Material. Additional material that is in the Text will be on your tests!

To get the most information, READ THE CHAPTER prior to the Lecture, bring in these lecture notes and make comments on these notes. These notes alone are NOT enough to pass any test!

Molecular Weight = sum of the atomic weights of all of the atoms in a molecule of the substance
Iron III Sulfate $Fe_2 (SO4)_3$

Formulae weight = sum of the atomic weights of all atoms in a formula unit of the compound.
Usually the same as Molecular Weight

1 Mole = a quantity of a substance that contains as many molecules as the number of atoms in exactly 12 g of Carbon-12.
1 Mole also equals: 6.023×10^{23} atoms = Avogadro's Number
1 Mole of marbles covers the earth to a depth of 50 miles

We use moles in Chemistry so we can work with a give quantity or number of atoms or molecules.

Example 3.1 Formula Mass [Molecular Weight

Chloroform – $CHCL_3$			Iron (III) Sulfate – $Fe_2(SO_4)_3$		
C	1 * 12.01	12.01	Fe	2 * 55.85	111.70
H	1 * 1.008	1.008	S	3 * 32.07	96.21
Cl	3 * 35.45	103.35	O	12 * 16.00	192.00
		116.359			399.91 g/mole
		116.36 g/mole			

Mole Calculations: $H_3C\text{-}CH_2\text{-}OH + 3\ O_2 \rightarrow 2\ CO_2 + 3\ H_2O$
Ethanol Oxygen Carbon Dioxide Water

So **1 molecule of Ethanol** reacts with **3 molecules** [6 atoms] of **Oxygen** to give **2 molecules of Carbon Dioxide** and **3 molecules of Water**

Or we can replace molecules with Moles. The use the molecular weight of each

	$H_3C\text{-}CH_2\text{-}OH$ + C_2H_6O	**$3\ O_2$ ->**	**$2\ CO_2$ +**	**$3\ H_2O$**
C	2 x 12.01		2 x 12.01	
H	6 x 1.01			6 x 1.01
O	1 x 16.00	6 x 16.00	4 x 16.00	3 x 16.00
Mw =	**46.08**	**96.00**	**64.00**	**54.06**

So **46.08 g** of ethanol reacts with **96.00 g** of oxygen to form **64.00 g** of carbon dioxide and **54.06 g** of water!

Percentage Composition: Mass % A = Mass of A in the molecule / mass of the whole molecule * 100%

Example 3.7 Formaldehyde = CH_2O

Mw:	C	1 x 12.00 =	12.00 g/mol
	H	2 x 1.008 =	2.00 g/mol
	O	1 x 16.00 =	16.00 g/mol
Mw =			30.00 g/mol

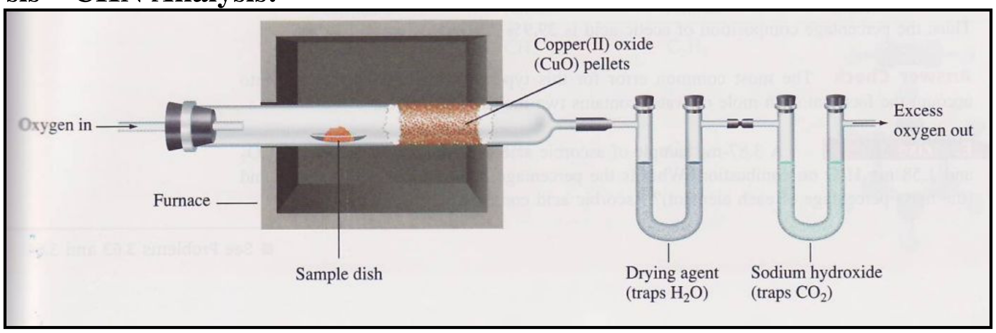
%C = (12.00 g/mol / 30.00 g/mol) * 100% = 40.00% C

%H = (2.00 g/mol / 30.00 g/mol) * 100% = 6.73% H

%O = (16.00 g/mol / 30.00 g/mol) * 100% = 53.3% O, or you can subtract the others from 100%

Acetaldehyde $(CH_2O)_2$ Mw = 60.00, what are the % of C, H and O?

Elemental Analysis – CHN Analysis:



Organic compounds are heated hot in a stream of oxygen.

The hydrogen reacts with oxygen to form water that is absorbed by drying agent.

The carbon reacts with oxygen to form CO_2 which is passed through sodium hydroxide where it reacts to form sodium carbonate.

Nitrogen can be determined by a complex organic reaction and a GC.

The amount of **Oxygen** cannot easily be determined by normal methods and is usually determined by subtraction of the above from 100%.

CHN analysis gives: 4.24 mg of a sample -> 6.21 mg of CO_2 and 2.54 mg of H_2O. What is the mass % of each element?

$$\frac{6.21 \text{ mg } CO_2}{1} \times \frac{1 \text{ mole } CO_2}{44.0 \text{ g } CO_2} \times \frac{1 \text{ mole C}}{1 \text{ mole } CO_2} \times \frac{12.0 \text{ g C}}{1 \text{ mole C}} = 1.69 \times 10^{-3} \text{ g C}$$

$$\frac{2.54 \text{ mg } H_2O}{1} \times \frac{1 \text{ mole } H_2O}{18.0 \text{ g } H_2O} \times \frac{2 \text{ mole H}}{1 \text{ mole } H_2O} \times \frac{1.01 \text{ g H}}{1 \text{ mole H}} = 2.85 \times 10^{-3} \text{ g H}$$

Mass % of Carbon = (1.69 mg C / 4.24 mg sample) * 100% = 39.9% Carbon in the sample

Mass % of Hydrogen = (0.285 mg H / 4.24 mg sample) * 100% = 6.72% Hydrogen in the sample

Determine Formulae **SEE EXAMPLES IN BOOK**

CHN Calculations Procedure:

1. If the values are given in grams or milligrams, change the those units to %.
2. Add up all of the percentages. If it does not equal 100%, then the remaining is assumed to be Oxygen.
3. Divide each of the percentages by the elemental weight for that element
4. Divide all of those numbers by the smallest number
5. These numbers represent the relative ratio of each of the elements.

    If at least one number ends in 0.9, 0.0 or 0.1 go with those numbers

    If at least one number ends in 0.2, 0.3 or 0.7 or 0.8 then multiply all of the numbers by 3

    If at least one number ends in 0.4, 0.5 or 0.6, then multiply all of the numbers by 2

Empirical Formulae – simplest formula. Shows the simplest ratios of numbers of the atoms

Determine the Empirical Formulae:

P 118 3.61 Potassium Manganate = 39.6% K, 27.9% Mn, 32.5% O

P 118 3.63 Acrylic Acid = 50.0% C, 5.6% H

Molecular Formulae from Empirical Formulae Need molecular weight

P 120, 3.95 MothBalls – para-dichlorobenzene has the composition: C 49.1%, H 2.7%, Cl 48.2% and a molecular weight of 147. What is the molecular formulae?

SPECIAL PROBLEM An organic compound was found to have the following composition: C 92.15 %, H 7.84 %. Two separate determinations of the molecular weight found it to be approximately 25 g/mole and a second trail gave 79 g/mole. What Molecular Formula would support these two molecular weights?

Table 3.1

Acetylene has an empirical formula of CH and a molecular formula of C_2H_2.

Benzene has an empirical formula of CH and a molecular formula of C_6H_6.

1. Calculate the % of C and H in each?
2. If you were given this %C and %H, how would you differentiate between acetylene and benzene?

Exercise 3.11 A sample of Benzoic Acid gave the following analysis: C 68.8% and H 5.0%. What is the empirical formula?

The % add up to 68.8 + 5.0 = 73.8. Therefore it is assumed that O is 100% - 73.8% = 26.2%.

C	68.8 / 12.01	= 5.73	5.73 / 1.64 = 3.49	3.49 * 2 = 6.98 or @ 7
H	5.0 / 1.008	= 4.96	4.96 / 1.64 = 3.02	3.02 * 2 = 6.04 or @ 6
O	26.2 / 16.00	= 1.64	1.64 / 1.64 = 1	1 * 2 = 2

Therefore the empirical formula is $C_7H_6O_2$

Example 3.12 An acetic acid sample has C 39.9%, H 6.7% and a molecular weight of approximately 60.0 g/mol. What is the molecular formula?

Again, the % add up to 39.9 + 6.7 = 46.6. Therefore it is assumed that O is 100% - 46.6% = 54.5%

C	39.9 / 12.01	= 3.32	3.32 / 3.32 = 1	Empirical Formulae = C_1H_2O
H	6.7 / 1.008	= 6.65	6.65 / 3.32 = 2.00	
O	54.5 / 16.00	= 3.41	3.41 / 3.32 = 1.03	

Empirical Formula Weight =	C	1 * 12.01	12.01
	H	2 * 1.008	2.016
	O	1 * 16.00	16.00
			30.026 = 30.03 g/ mole

The molecular weight is 60.00, the empirical formula weight is 30.03, so
60.00 / 30.03 = 2. Multiply the empirical formula by 2 to get the **molecular formula = $C_2H_4O_2$**

Stoichiometry is the calculation of the quantities of reactants and products involved in a chemical reaction

1. Molar Interpretation of a Chemical Reaction

$$\underset{?}{3\ NO_2} + H_2O \rightarrow \underset{7.50\ g}{2\ HNO_3} + NO$$

P 118, 3.77 $3\ NO_2 + H_2O \rightarrow 2\ HNO_3 + NO$ How many g of NO_2 is needed to make 7.50 g HNO_3

It will take 3 moles of NO_2 reacting with one mole of H_2O to produce 2 moles of HNO_3 and one mole of NO.

2 HNO_3

H	2 * 1.008 =	2.016
N	2 * 14.01 =	28.02
O	6 * 16.00 =	96.00
		126.036
		126.04 g/mole

3 NO_2

N	3 * 14.01 =	42.03
O	6 * 16.00 =	96.00
		138.03 g/mole

$$\frac{7.50\ g\ [\ 2\ HNO_3\ ]}{126.04\ g/mole} = \frac{X\ \ [\ 3\ NO_2\ ]}{138.03\ g/mole} \qquad X = 8.21346\ g = \mathbf{8.21\ g\ NO_2}$$

$$\underset{2.60\ Kg}{CaO} + \underset{2.60\ Kg}{3\ C} \rightarrow \underset{?}{CaC_2} + CO$$

P 121, 3.105 $CaO + 3\ C \rightarrow CaC_2 + CO$ How many grams of CaC2 are made?

2. Amounts of substances in a Chemical Reaction - % Yield

Theoretical Yield is the amount of calculated product you can produce form a given amount of starting material. It is also know as 100% yield.

% Yield = 100 % * Actual Yield / Theoretical Yield

$$\underset{10.6\ g}{2\ C_2H_4} + O_2 \rightarrow \underset{9.91\ g}{2\ C_2H_4O}$$

P 120, 3.101 $2\ C_2H_4 + O_2 \rightarrow 2\ C_2H_4O$ What is the Percent Yield?

3. Limiting Reactant

Example: 10 slices of bread and 2 slices of cheese to make sandwiches
Demo: Walk down the aisle dropping $100 bills!

A. Calculate the number of moles of each compound.
B. Set up the ratio of number of moles of each compound to the Reactant Coefficient

Example: **<u>NOTE I HAVE NOT RECHECKED THESE PROBLEMS 3-Oct-08</u>**

Use 1.0 mole of H_2 and one mole of O_2 and determine which is the limiting reagent.

$\mathbf{2\,H_2 + O_2 \rightarrow 2\,H_2O}$
1 mole 1 mole

Determine the amount of H2O generated using each reactant

$1 \text{ mole } H_2 * \frac{2 \text{ mole } H_2O}{2 \text{ mole } H_2} = \mathbf{1\ Mole\ H_2O}$ **The** Limiting Reagent is the LEAST AMOUNT

$1 \text{ mole } O_2 * \frac{2 \text{ m } H_2O}{1 \text{ mole } O_2} = 2 \text{ mole } H_2O$

$\mathbf{Zn + 2\,HCl \rightarrow ZnCl_2 + H_2}$
0.30 mole 0.52 mole

$0.30 \text{ mole Zn} * \frac{1 \text{ mole } H_2}{1 \text{ mole Zn}} = 0.30 \text{ mole } H_2$

$0.52 \text{ mole HCl} * \frac{1 \text{ mole } H_2}{2 \text{ mole HCl}} = 0.26 \text{ mole } H_2$ Smallest number, Limiting Reagent

$\mathbf{2\,Al + 6\,HCl \rightarrow 2\,AlCl_3 + 3\,H_2 \uparrow}$
0.15 mole 0.35 mole ?

$0.15 \text{ mole Al} * \frac{2 \text{ mole } AlCl_3}{2 \text{ mole Al}} = 0.15 \text{ mole } AlCl_3$

$0.35 \text{ mole HCl} * \frac{2 \text{ mole } AlCl_3}{6 \text{ mole HCl}} = 0.12 \text{ mole } AlCl_3$ Smallest number, Limiting Reagent

2 CH_3COH + O_2 → 2 CH_3COOH
20.0g 10.0 g ?

CH_3COH		O_2		CH_3COOH	
C 2 * 12.01	24.02			C 2 * 12.01	24.02
O 1 * 16.00	16.00			O 2 * 16.00	32.00
H 4 * 1.008	4.032	O 2 * 16.00	32.00	H 4 * 1.008	4.032
	44.05l2				60.05l2
	44.05 g/mole		32.00 g/mole		60.05 g/mole

20.0g / 44.05 g/mole = 0.454 mole   10.0g / 32.00 g/mole = 0.313 mole

0.454 mole CH_3COH * $\frac{\text{2 mole } CH_3COOH}{\text{2 mole } CH_3COH}$ = 0.454 mole CH_3COOH Smallest number Limiting Reagent

0.313 mole O2 * $\frac{\text{1 mole } O_2}{\text{2 mole } CH_3COH}$ = 0.157 mole CH_3COOH

0.454 mole CH_3COOH * 60.05 g/mole = 27.3 g CH_3COOH

Now Determine the amount of the Xcs O_2:

0.454 mole CH_3COH * $\frac{\text{1 mole } O_2}{\text{2 mole } CH_3COH}$ = 0.227 mole O_2

0.227 mole O_2 * 32.00 g/mole = 7.26 g O_2 are used up.

10.0 g O_2 starting – 7.26 g O_2 used up = 2.74 g O_2 remaining

	0.25 moles		0.15 moles				?	
P 119, 3.85	$4\ KO_2$	+	$2\ H_2O$	->	4 KOH	+	$3\ O_2$	What is the limiting reactant?

$$\frac{0.25\ M}{4\ KO_2} = \frac{X}{2\ H_2O}$$

So, to react 0.25 moles of KO_2 will require
X = 0.125 moles of H_2O.

Since we have 0.15 moles of H_2O, the KO_2 is the limiting reagent and the H_2O is in excess.

	35.4g		10.2g		?	
P 119, 3.87	CO	+	H_2	->	CH_3OH	What reactant is in xcs?
						How much of the non-xcs reactant remains?

P 105	Fe_2O_3	+	3 CO	→	2 Fe	+	$3\ CO_2$ (gas)
	1 Kg				? g of		

P 120, 3.101	$2\ C_2H_4\ +\ O_2 \rightarrow 2\ C_2H_4O$		
	10.6 g	9.91 g	What is the % yield?

Rev 8 Book Example Problems starting on page 114

3.1	3.3	3.4	3.7		3.13	3.14	3.17	
3.21	3.22	3.24	3.31	3.32	3.51	3.55	3.61	3.63
3.77					3.85	3.87		
3.95	3.101	3.105			3.117 – Instructor gets video			

Steps for working a problem

5.01 grams of Iron (III) Carbonate is reacted with xcs [Excess] Sulfurous Acid. What are the products and how much of each is formed?

1. Translate the English to Chemical REACTANTS — $Fe\ CO_3 \quad + \quad H_2SO_3$ ->

2. Balance the ions in each Reactant Compound so the net charge is zero — $Fe^{+3}\ CO_3^{-2} \quad + \quad H_2^{+1\ \mathbf{ea = +2}}\ SO_3^{-2}$ ->

   $Fe_2^{+3}\ (CO_3)_3^{-2} \quad + \quad H_2^{+1\ \mathbf{ea = +2}}\ SO_3^{-2}$ ->

   $Fe_2\ (CO_3)_3 \quad + \quad H_2SO_3$ ->

3. Determine the Products and write down the basic compounds. — AB + CD -> AD + CB
   Use the simple ionic exchange

4. Balance the ions in each Product Compound so the net charge is zero

5. Balance the equation of there are equal number of each element on each side of the reaction arrow

6. With the known amount of starting compound / reactant, determine the molecular weight of that compound

7. Determine the molecular weight of each of the Product Compounds.

8. Set up the simple ratio of known amount of starting material to molecular weight equals x over the mw of each product and calculate the amount of each product. Don't forget to put in all the units!!

9. Write out the answers – the amount of each product in grams [or milligrams] corrected to the proper number of significant digits with the units.