Stoichiometry

Relationship between the moles of the reactants and the moles of the products in a chemical equation is indicated by *Coefficients* in the Chemical Equation

C_3H_8 (g) + $5O_2$ (g) --> $3CO_2$ (g) + $4H_2O$ (l)

Balanced Equations

Mass Balance

Charge Balance

NH_4^+ (aq) + NaOH (aq) -->
NH_3 (aq) + Na^+ (aq) + H_2O (aq)

Avogadro's Number

6.022137×10^{23} = 1 Mole

1 g = 6.02×10^{23} amu

Amedeo Avogadro (1776-1856) Turin, Italy - Avogadro's hypothesis 1811- equal volumes of gas contain equal numbers of particles

Atomic Weight and Molecular Weight

Grams/Mole

(Daltons)

weight is inaccurate these are actually masses

Conversion of Mass to Moles (Moles are the Currency of Exchange for chemists)

Example:

20 g of Glucose ($C_6H_{12}O_6$ - Mwt =180 g/mol)

20.0 g ÷ 180 g/mol = 0.111 mol

$$\boxed{\text{GRAMS}} \underset{\times\ \mathbf{Mwt}}{\overset{\div\text{Mwt}}{\rightleftarrows}} \boxed{\text{MOLES}}$$

Moles to Grams (& volume)

Example:

0.500 moles of Ethanol (C_2H_6O - Mwt =46 g/mol)

0.500 g X 46 g/mol = 23.0 g

D_{EtOH} = 0.90 g/mL

23.0 g ÷ 0.900 g/mL = 20.7 mL EtOH

Problem

How many atoms of Oxygen are present in 4.9 g of H_2SO_4?

4.9 g ÷ 98 g/mol = 0.05 mol H_2SO_4

4 mol of O atoms per H_2SO_4 x 0.05 = 0.20 moles O

6.02×10^{23} atoms/mole X 0.20 moles =
1.2×10^{23}atoms

Percent Composition

The composition of chemical compounds is expressed in percentage by mass

CO2

27.3% C

76.7% O

Calculating Percent Composition

Since percent composition is determined on a mass basis we must calculate the mass of each element in a chemical formula and the mass of the total chemical formula

Example: What is the % composition of aniline (C_6H_7N)?

	C	H	N
Mol wt of aniline =	(6 x 12.01) +	(7 x 1.008) +	14.007
	72.06 g	7.056g	14. 007g
÷ Total molecular weight (93.12 g/mol) x 100%			
percentage =	77.38%	7.58%	15.04%

Calculating Empirical Formulas

The Empirical formula of a compound is the simplest whole number ratio which conforms to the percentage composition.

The Molecular Formula may be equal to the Empirical formula or a whole number multiple of the Empirical formula.

Example: Glucose $C_6H_{12}O_6$ Molecular Weight = 180 g/mol

The simplest whole number ratio of the elements is $C_1H_2O_1$ and this is the result that will be obtained from a calculation from the percent composition.

The Glucose Empirical Formula

The percentage composition must be converted to number of moles for each element.

	C	H	O
Percentage	40.03%	6.667%	53.33%

To do this assume you have 100g of the substance having the composition given. Then you will have masses corresponding to the percentage of each element.

Mass	40.03g	6.667g	53.33g

convert to moles by dividing each by the *<u>correct</u>* atomic weight.

Moles	3.333 mole	6.614 mole	3.333 mole

The Glucose Empirical Formula

	C	H	O
Moles	3.333 mole	6.614 mole	3.333 mole

We always express the composition in terms of whole numbers. To convert to whole numbers divide by the smallest of the values obtained (3.333) often (but not always) this is the *largest common factor* of the numbers

	C	H	O
Whole Number Ratio	1	1.98	1
After Rounding	1	2	1

The Empirical Formula is $C_1H_2O_1$

Converting Empirical Formulas to Molecular Formulas

Glucose Empirical Formula = $C_1H_2O_1$

the Empirical Formula weight = 30.025 g/formula weight

the Molecular Weight (determined by a separate experiment, see Chapter 11) = 180 g/mole

an Integer factor of n = (180 ÷ 30.025) = 6 relates the Empirical formula to the Molecular formula

$$6 \times (C_1H_2O_1) = C_6H_{12}O_6$$

A Tricky Example

A 20.882 g sample is found to have 6.072 g Na, 8.474 g S, & 6.336 g of O.

element (at wt)	Na (22.99)	S (32.07)	O (15.999)
Mass (g)	6.072	8.474	6.336
moles	0.2641	0.2642	0.3960
ratio (÷ 0.2641)	1	1	1.5

for O we <u>do not</u> have an integer **(0.2641 is not the largest common factor)**

note the decimal 0.5 x 2 = the integer 1

multiply all values by 2 ==> $Na_2S_2O_3$

Combustion analysis

A 2.00 g sample of a compound produced 4.86 g of CO_2 and 2.03 g of H_2O upon combustion. What is the Empirical Formula?

4.86÷44.01g/mol = 0.1104 mol CO_2 ==> 0.1104 mol C ==> 1.326 g C

2.03 ÷18.02 g/mol = 11.27 mol H_2O ==> 0.2254 mol H ==>0.2272 g H

determine O by difference

mass of H + C = 1.553 g therefore 2.0 - 1.553 = 0.4468 g O

0.02792 mol O

Combustion cont'd

	C	H	O
Moles	**0.1104**	**0.2254**	**0.02792**
Ratio	**3.95**	**8.07**	**1**

Empirical Formula = C_4H_8O

Empirical formula weight = 72.143 g/mol