Mr SGs Introductory Stoichiometry Notes

-In chemistry, we are often required to make measurements regarding the composition of chemicals we are studying, or the rate and/or yield of chemical reactions we are performing

-This often requires performing calculations involving the composition and amounts of various chemicals

-To study chemical reactions in detail, we need a way of counting the particles involved

-If we know the relative masses of different particles, we can count them by weighing

Relative masses

-Atoms, molecules and formula units are assigned a relative atomic mass (A_r), or a molecular/formula mass (M_r) based on 1/12 of the mass of carbon-12 atom (roughly the mass of a proton)

-As it is a relative measure, it is not thought of as having a unit, but is designated as atomic mass units, or u

-While relative masses tell us about the mass of individual particles relative to one another, they don't allow us to calculate the absolute mass of a substance or to calculate the number of particles in a given mass

-The relative molecular/formula mass of a compound/element is equal to the sum of the atomic masses of the atoms in its formula

e.g. $M_r(Na_2CO_3) = 2 \times A_r(Na) + A_r(C) + 3 \times A_r(O)$
$= 2 \times 22.99 + 12.01 + 3 \times 16$
$= 105.99$

The mole

-As the mass of individual atoms is so small (1 ^{12}C atom = 1.99×10^{-23} g), it is not practical to talk about individual particles as we will be handling a very large number of particles whenever we handle a substance

-In chemistry, when we need to think about the number of particles in a substance, we talk about it in terms of moles (mol) of particles

-1 mole = number of particles in 12g of ^{12}C = 6.022×10^{23} (The Avogadro constant (N_A))

-When we talk about the amount of substance in a mole, we need to identify the substance as atoms, molecules, formula units or ions
-we can calculate the number of moles in a substance by using the formula:

$$n = \frac{N}{N_A}$$

where n is number of moles (mol), N is number of particles and N_A is the Avogadro constant (6.022×10^{23})

Molar mass

-The mole can be used to relate the mass of a substance to the number of particles it contains

e.g. 12g ^{12}C contains 6.022×10^{23} particles (1 mole of ^{12}C), so 6g ^{12}C must contain
3.011×10^{23} particles (0.5 moles of ^{12}C)

-This can also be done for other substances with other relative atomic masses

-Because of the way that the mole is defined, we know that 1 mole of a substance is equal to its relative atomic mass (or molecular/formula mass) expressed in grams

e.g. 1 mole of ^{12}C weighs 12 g
1 mole of H weighs 1.008 g
1 mole of CO_2 weighs 12.01g + (2 x 16g) = 44.01g

-The mass of one mole of a substance is known as its molar mass (M)

-This differs from its A_r/M_r as it is expressed in units of grams per mole (g mol^{-1})

-The formula relating the amount of a substance (in moles) to the mass of the substance and the substances molar mass is:

$$n = \frac{m}{M}$$

where n is number of moles (mol), m is mass (g) and M is molar mass (g mol^{-1})

Example 1: In a 1.00 L bottle of methylated spirits there is 780g ethanol (C_2H_5O), how many moles of ethanol molecules are there in the bottle?

Example 2: A sample of seawater contains 0.0392 mol sodium chloride. Find the mass of NaCl.

Relating moles to the number of particles present

-As well as relating the number of moles to mass and molar mass, you can also relate the mass and molar mass to number of particles by combining the formulae:

$$n = \frac{m}{M} \quad \& \quad N = n \times N_a$$

Example 3: How many methanol molecules in 800.0 g of methanol (CH_4O)?

Stoichiometry

-Once you are able to relate masses of materials to the number of particles or moles present, it becomes possible to quantify the amounts of reactants and products that are consumed or produced in a chemical reaction

Stoichiometry: *Calculations involving relative amounts of reactants and products in a chemical reaction*

Using coefficients to relate reactants to products

-The coefficients in a chemical reaction tell us the ratio in which atoms, molecules and ions react and are produced

-They also show the mole ratio in which substances react and are formed, for example:

$$2H_{2(g)} + O_{2(g)} \rightarrow 2H_2O_{(l)}$$

means 2 H_2 molecules will react with 1 O_2 molecule to produce 2 H_2O molecules

OR 2 moles of H_2 react with 1 mole of O_2 to form 2 moles of H_2O

OR 10 moles of H_2 react with 5 moles of O_2 to form 10 moles of H_2O

-You can use these coefficients to relate the number of moles of any substance involved in a reaction to the number of moles of any other substance involved

e.g. How many moles of oxygen gas will react with 5 mol of hydrogen?

-From the coefficients, 1 mol of oxygen will react with 2 mol hydrogen
so, 0.5 mol oxygen react with every mol of hydrogen
so, 0.5 x 5 = 2.5 mol oxygen will react with 5 mol hydrogen

-This calculation can be expressed as:

$$n_2 = \frac{coefficient_2}{coefficient_1} \times n_1$$

e.g. $$n(O_2) = \frac{coefficient(O_2)}{coefficient(H_2)} \times n(H_2) = ½ \times n(H_2) = ½ \times 5 = 2.50 \text{ mol}$$

-By using these coefficients along with our other stoichiometry knowledge, we can calculate the mass or volume of a substance involved in a reaction when given the mass or volume of another substance involved

$$m_1 \xrightarrow{n = \frac{m}{M}} n_1 \xrightarrow{n_2 = \frac{coefficient_2}{coefficient_1} \times n_1} n_2 \xrightarrow{m = nM} m_2$$

e.g: Calculate the mass of water produced when 3.00 kg of hydrogen is combusted in excess oxygen

$$2H_2 + O_2 \rightarrow 2H_20$$

$n(H_2) = \frac{m}{M}$ $\quad$ $M(H_2) = 2 \times A_r(H)$

$= \frac{3000}{2.016}$ $\quad$ $= 2 \times 1.008$

$= 1488\ mol$ $\quad$ $= 2.016\ gmol^{-1}$

$n(H_2O) = \frac{2}{2} \times n(H_2) = 2/2 \times 1488 = 1488\ mol$

$m(H_2O) = nM$ $\quad$ $M(H_2O) = 2 \times A_r(H) + A_r(O)$

$= 1488 \times 18.016$ $\quad$ $= 2 \times 1.008 + 16$

$= 26809.5g$ $\quad$ $= 18.016\ gmol^{-1}$

$= 26.8\ kg$

Example 4: Calculate the mass of carbon dioxide produced when 254 g of copper (II) carbonate decomposes to produce copper (II) oxide and carbon dioxide

Calculations involving the composition of materials

-In chemistry, we often refer to the elemental, ionic and molecular formulae of substances

-For some substances, it is also useful to consider the hydrated formula (crystalline substances/analytical chemistry), the empirical formula (analytical chemistry) and/or the percentage composition

Hydrated Formulae

-Some crystalline substances contain water of crystallisation within their crystal structure

-Hydrated formulae show the number of molecules of water per formula unit or molecule

e.g. $CuSO_4.5H_20$ contains 5 water molecules per unit of $CuSO_4$

Empirical Formulae

-The simplest whole number ratio of elements present in a compound e.g. the empirical formulae of N_2O_4 is NO_2, the empirical of $C_6H_{12}O_6$ is CH_2O and the empirical formula of H_2O is H_2O

Percentage Composition

-In chemistry we often describe the composition of a compound by giving the percentage of the mass made up of each element

e.g. 100 g of carbon dioxide contains 27.3g C and 72.7 g O

-We can calculate % composition, given the chemical formula of a compound by comparing the relative atomic masses of the elements present in the compound to the relative molecular/formula mass of the compound as a whole

-The general formula for calculating % composition for a compound A_wB_z is:

$$\%(A): \frac{w \times A_r(A)}{M_r(AwBz)} \times 100$$

e.g. Calculate the percentage of potassium in K_2SO_4

$$\%(K) = \frac{2 \times A_r(K)}{M_r(K_2SO_4)} \times 100 = \frac{2 \times 39.1}{2 \times 39.1 + 32.01 + 4 \times 16} \times 100 = 44.89\ \%\ (4\ sf)$$

Example 5: Calculate the percentage of hydrogen in water (H_2O) and ethanol (C_2H_6O)

Solutions to examples

Example 1: *In a 1.00 L bottle of methylated spirits there is 780g ethanol (C_2H_5O), how many moles of ethanol molecules are there in the bottle?*

$M(C_2H_5O) = 2 \times 12.01 + 5 \times 1.008 + 16 = 45.06\ g\ mol^{-1}$

$n(C_2H_5O) = \frac{m}{M} = \frac{780}{45.06} = 17.310253 = 17\ mol\ (2\ sf)$

Example 2: *A sample of seawater contains 0.0392 mol sodium chloride. Find the mass of NaCl.*

$M(NaCl) = 22.99 + 35.45 = 58.44\ g\ mol^{-1}$

$m(NaCl) = nM = 0.0392 \times 58.44 = 2.290848 = 2.29\ g\ (3\ sf)$

Example 3: *How many methanol molecules in 800.0 g of methanol (CH_4O)?*

$M(CH_4O) = 12.01 + 4 \times 1.008 + 16 = 32.042\ g\ mol^{-1}$

$n(CH_4O) = \frac{m}{M} = \frac{800}{32.042} = 24.97\ mol$

$N(CH_4O) = n \times N_A = 24.94 \times 6.02 \times 10^{23} = 1.504 \times 10^{25}$ molecules

Example 4: *Calculate the mass of carbon dioxide produced when 254 g of copper (II) carbonate decomposes to produce copper (II) oxide and carbon dioxide*

$CuCO_3 \rightarrow CuO + CO_2$

$M(CuCO_3) = 63.55 + 12.01 + 3 \times 16 = 123.56\ g\ mol^{-1}$

$n(CuCO_3) = \frac{m}{M} = \frac{254}{123.56} = 2.06\ mol$

$n(CO_2) = n(CuCO_3) = 2.06\ mol$

$M(CO_2) = 12.01 + 2 \times 16 = 44.01\ g\ mol^{-1}$

$m(CO_2) = nM = 2.06 \times 44.01 = 97.5\ g$

Example 5: *Calculate the percentage of hydrogen in water (H_2O) and ethanol (C_2H_6O)*

$$\%(H) = \frac{2 \times A_r(H)}{M_r(H_2O)} \times 100 = \frac{2 \times 1.008}{2 \times 1.008 + 2 \times 16} \times 100 = 11.19\ \%$$

$$\%(H) = \frac{6 \times A_r(H)}{M(C_2H_6O)} \times 100 = \frac{6 \times 1.008}{2 \times 12.01 + 6 \times 1.008 + 2 \times 16} \times 100 = 9.744\ \%$$