FACTFILE:
GCE CHEMISTRY

2.1 FORMULAE, PERCENTAGE YIELD, ATOM ECONOMY

Rewarding Learning

Formulae and amounts of a substance

Students should be able to:

2.1.1 define the terms empirical and molecular formula and explain the relationship between them;

2.1.2 calculate empirical and molecular formulae using data, given composition by mass or percentage composition;

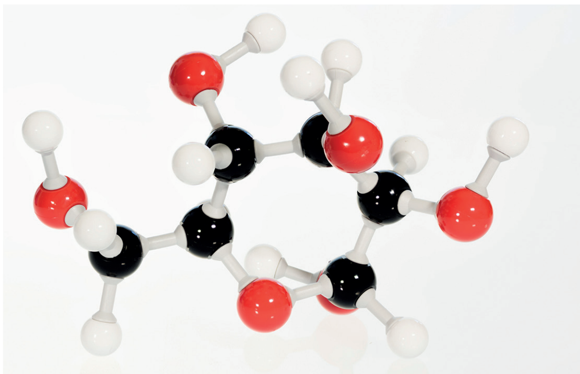
2.1.3 define molar gas volume and calculate reacting gas volumes from chemical equations;

2.1.4 define percentage yield and calculate percentage yields using chemical equations and experimental data;

2.1.5 use a percentage yield to determine the amount of reagent(s) needed for a reaction;

2.1 6 define atom economy and calculate atom economies using chemical equations;

Empirical and molecular formula



The empirical formula is the formula which shows the simplest whole number ratio of atoms of each element in a compound. The molecular formula is a formula which shows the actual number of atoms of each element in a molecule. For example, the molecular formula of phosphorus(V) oxide is P_4O_{10}, whereas its empirical formula is P_2O_5.

To determine the empirical formula of a compound, you must first calculate the amount in moles of each element present in a sample and then calculate the simplest whole number ratio of the moles. For example:

A compound contains 4.6 g of sodium, 2.8 g of nitrogen and 9.6 g of oxygen. Find the empirical formula of the compound.

	Na	N	O
mass (g)	4.6	2.8	9.6
molar mass (mol^{-1})	23	14	16
moles (mol)	$\frac{4.6}{23} = 0.2$	$\frac{2.8}{14} = 0.2$	$\frac{9.6}{16} = 0.6$
divide by smallest number of moles	$\frac{0.2}{0.2} = 1$	$\frac{0.2}{0.2} = 1$	$\frac{0.6}{0.2} = 3$
ratio	1	1	3
formula	$NaNO_3$		

To deduce a molecular formula, first calculate the empirical formula. Then use the RFM, which will be given in the question, to determine the molecular formula. For example, Deduce the molecular formula of a compound with empirical formula be CH_2O. The RMM of the compound is 180g mol^{-1}.

Empirical formula mass
= 12 + 2(1) + 16 = 30 g mol^{-1}

$\frac{180}{30}$ = 6, therefore the molecular formula is 6 times the empirical formula and is $C_6H_{12}O_6$.

The molar gas volume

When gases react, the volumes consumed and produced, measured at the same temperature and pressure, are in ratios of small whole numbers.

The Italian chemist Amedeo Avogadro gave an explanation of this behaviour, proposing what we now know as Avogadro's Law. This states that equal volumes of gases at the same temperature and pressure contain the same number of molecules. It follows from Avogadro's Law that whenever we see an equation for a reaction between gases we can substitute volumes of gases as the same ratio as numbers of molecules. Consider the equation:

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$

Since 1 mole of nitrogen reacts with 3 moles of hydrogen to form 2 moles of ammonia then 1 dm^3 of nitrogen reacts with 3 dm^3 of hydrogen to form 2 dm^3 of ammonia.

The volume of 1 mole of gas for conditions of (293 K) temperature and pressure under specified is called the molar gas volume. For example at 20 °C and 1atmosphere, 1 mole of any gas occupies a volume of 24 dm^3 (1 dm^3 = 1000 cm^3).

Percentage yield

Many chemical reactions do not go to completion. Some of the starting reactants may remain (not matter how long you leave the reaction) or else some product may be lost as it is isolated. The actual amount of product is compared with the amount calculated from the molar masses of the reactants. The ratio of these amounts is expressed as a percentage yield.

$$\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

For example, 23 g of ethanol, C_2H_5OH, is used to form the ester ethyl ethanoate, $CH_3CO_2C_2H_5$, according to the equation:

$$CH_3COOH(l) + C_2H_5OH(l) \rightarrow CH_3COOC_2H_5(l) + H_2O(l)$$

36 g of $CH_3COOC_2H_5$ were obtained. Calculate the percentage yield.

Moles ethanol = $\frac{23}{46}$ = 0.5 moles.

Ratio $C_2H_5OH : CH_3COOC_2H_5$ is 1 : 1 so moles of ethyl ethanoate = 0.5 moles
Theoretical mass (yield) of ethyl ethanoate
= 0.5 x 88 = 44 g

$$\% \text{ Yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$$

$$\% \text{ Yield} = \frac{36}{44} \times 100 = 82\ \%$$

Atom economy

In any reaction, chemists strive for the highest possible percentage yield in order to ensure processes are cost effective and efficient. The percentage yield tells you, after the reaction is completed and the products are purified, how much you made compared to how much you could possibly have made. However, the percentage yield tells you nothing about the amount of waste material you produced. To ensure processes are environmentally friendly, atom economy must also be considered.

$$\text{atom economy} = \frac{\text{mass of desired products}}{\text{total mass of products}} \times 100$$

This is particularly important in industrial processes which often use multi-tonne quantities of reagents.

For example, in the reaction below, ethanol CH_3CH_2OH is the desired product.

$$CH_3CH_2Cl + NaOH \rightarrow CH_3CH_2OH + NaCl$$

The atom economy to produce ethanol:

$$\frac{\text{mass of desired products}}{\text{total mass of products}} \times 100$$

$$= \frac{46}{104.5} \times 100 = 44\%$$

Atom economy can be expressed as a percentage, in this case 44%. Values can be increased by finding a use for the waste product.

Credits

Revision Questions

1 5.0 g of butan-1-ol (RMM 74) reacted with an excess of hydrogen bromide and 6.4 g of 1-bromobutane (RMM 137) were obtained after purification. Calculate the percentage yield of 1-bromobutane.

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2 Analysis of a compound, which contains carbon, hydrogen and bromine only, showed that 22.2% of its mass is carbon and 3.7% is hydrogen. The relative molecular mass of the compound is 216. Calculate the molecular formula of the compound.

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3 Calculate the volume of oxygen gas (measured at 20 °C and 1 atmosphere of pressure) which would be produced when a 50.0 cm^3 sample of 2 mol dm^{-3} hydrogen peroxide solution undergoes complete decomposition.

$$2H_2O_2 \rightarrow 2H_2O + O_2$$

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4 Copper can be extracted by heating copper(II) oxide with carbon. Calculate the atom economy of the reaction.

$$2CuO(s) + C(s) \rightarrow 2Cu(s) + CO_2(g)$$

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