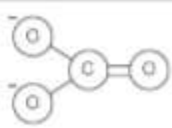
Edexcel AS Chemistry

(Code: WCH11)

Topic 01
Formulae, Equations and Amount of substance

1A Atoms, Elements and Molecules

TERM	DIAGRAM	NAME	SYMBOL OR FORMULA	NOTE
element		copper	Cu	This is an element. All the atoms are the same.
atom		helium	He	This is an atom of an element.
molecule		bromine	Br_2	This is a molecule of an element. The atoms are the same.
compound		hydrogen bromide	HBr	This is a molecule of a compound. The atoms are different.
ion		carbonate	CO_3^{2-}	This is an ion. There are two negative charges shown.

<u>Monatomic</u>
Elements that are made up of single atoms

<u>Diatomic</u>
Elements and compounds made up of two atoms joined together

<u>Polyatomic</u>
Elements and compounds with molecules made up of several atoms joined together

1B Equations and Reaction Types

1B.1 Writing chemical equations

Writing equations: What to remember

Writing formulae for names

You need to remember that:

- Oxygen is O_2, and not O
- Hydrogen is H_2 and not H
- Nitrogen is N_2 and not N
- water is H_2O
- sodium hydroxide is NaOH
- Nitric acid is HNO_3

You should be able to work out that:

- Iron(II) sulfate is FeSO
- Iron(III) oxide is Fe_2O_3
- Calcium carbonate is $CaCO_3$

Writing an equation from description

When carbon dioxide reacts with calcium hydroxide, calcium carbonate and water are formed. The wording of the description makes it clear that carbon dioxide and calcium hydroxide are the reactants, and that calcium carbonate and water are the products.

- $CO_2 + Ca(OH)_2 \rightarrow CaCO_3 + H_2O$

Hydrogen peroxide decomposes to water and oxygen.

- $H_2O_2 \rightarrow H_2O + O_2$

This is already balanced for hydrogen, but not for oxygen. In this case,

- $2H_2O_2 \rightarrow 2H_2O + O_2$

Consider this unbalanced equation for the complete combustion of butane:

- $C_4H_{10} + O_2 \rightarrow CO_2 + H_2O$

The balanced equation can be either.

- $2C_4H_{10} + 13O_2 \rightarrow 8CO_2 + 10H_2O$

or

- $C_4H_{10} + 6\frac{1}{2}O_2 \rightarrow 4CO_2 + 5H_2O$

Using 6.5 instead of $6\frac{1}{2}$ is also acceptable.

Using state symbol

- (s) = solid
- (l) = liquid
- (g) = gas
- (aq)= aqueous (dissolved in water)

After writing the correct formulae, balancing the equation and including state symbols, the equation is:

$$2AgNO_3(aq) + CaCl_2(aq) \rightarrow 2AgCl(s) + Ca(NO_3)_2(aq)$$

Arrows in equation

Most equations are shown with a conventional (left to right) arrow →. However, some important reactions are reversible. This means that the reaction can go both in the forward and backward (reverse) directions. The symbol "⇌" is used in equations for these reactions.

Ionic equations

Simplifying full equations

WORKED EXAMPLE 1

What is the simplest ionic equation for the neutralisation of sodium hydroxide solution by dilute nitric acid?

The full equation is:

$$NaOH(aq) + HNO_3(aq) \rightarrow NaNO_3(aq) + H_2O(l)$$

You should now consider which of these species are ionic and replace them with ions. In this example, the first three compounds are ionic:

$$Na^+(aq) + OH^-(aq) + H^+(aq) + NO_3^-(aq) \rightarrow Na^+(aq) + NO_3^-(aq) + H_2O(l)$$

After deleting the identical ions, the equation becomes:

$$H^+(aq) + OH^-(aq) \rightarrow H_2O(l)$$

WORKED EXAMPLE 2

What is the simplest ionic equation for the reaction that occurs when solutions of lead(II) nitrate and sodium sulfate react together to form a precipitate of lead(II) sulfate and a solution of sodium nitrate?

The full equation is:

$$Pb(NO_3)_2(aq) + Na_2SO_4(aq) \rightarrow PbSO_4(s) + 2NaNO_3(aq)$$

Replacing the appropriate species by ions gives:

$$Pb^{2+}(aq) + 2NO_3^-(aq) + 2Na^+(aq) + SO_4^{2-}(aq) \rightarrow PbSO_4(s) + 2Na^+(aq) + 2NO_3^-(aq)$$

After deleting the identical ions, the equation becomes:

$$Pb^{2+}(aq) + SO_4^{2-}(aq) \rightarrow PbSO_4(s)$$

These remaining ions are not deleted because they are not shown identically. Before the reaction they were free-moving ions in two separate solutions (Pb^{2+} and SO_4^{2-}). After the reaction they are joined together in a solid precipitate ($PbSO_4$).

WORKED EXAMPLE 3

Carbon dioxide reacts with calcium hydroxide solution to form water and a precipitate of calcium carbonate.

The full equation is:

$$CO_2(g) + Ca(OH)_2(aq) \rightarrow CaCO_3(s) + H_2O(l)$$

Replacing the appropriate species by ions gives:

$$CO_2(g) + Ca^{2+}(aq) + 2OH^-(aq) \rightarrow CaCO_3(s) + H_2O(l)$$

Note that carbon dioxide and water are molecules, so their formulae are not changed. In this example, no ions are shown identically on both sides, so this is the simplest ionic equation.

1B.2 Typical reactions of acids

Acids with Metals

Metal + Acid → Salt + Hydrogen

Acids with metal oxides and insoluble metal hydroxides

Metal oxide + Acid → Salt + Water

Metal hydroxide + Acid → Salt + Water

Acids with Alkalis

Alkali + Acid → Salts + Water

There are three replaceable hydrogens in phosphoric acid. The salt formed depends on the relative amounts of acid and alkali used. The ionic equation for all these reactions is:

$$H^+(aq) + OH^- (aq) \rightarrow H_2O(l)$$

These reactions can be classified as neutralisation reactions because the H+ ions react with OH- ions. They are not redox reactions because there is no change in the oxidation number of any of the species.

Acids with Carbonates

metal carbonate + acid → salt + water + carbon dioxide

Acids with hydrogencarbonates

Hydrogencarbonates are compounds containing the hydrogencarbonate ion (HCO_3), and they react with acids in the same way as carbonates.
A word equation for the reaction between baking soda and the acid in lemon juice is:

sodium hydrogencarbonate + citric acid → sodium citrate + water + carbon dioxide

1A.3 Displacement reaction

Displacement reactions involving metals

Here are the equations for two displacement reactions of metals:

Reaction 1 $Mg(s) + CuSO_4(aq) \rightarrow Cu(s) + MgSO_4(aq)$
Reaction 2 $2Al(s) + Fe_2O_3(s) \rightarrow 2Fe(s) + Al_2O_3(s)$

What do these reactions have in common?

- Both involve one metal reacting with the compound of a different metal.
- Both produce a metal and a different metal compound.
- Both are redox reactions.
- You can see that the metal element on the reactants side has taken the place of the metal in the metal compound on the reactants side.

What are the differences between the reactions?

- Reaction 1 takes place in aqueous solution, but Reaction 2 involves only solids.
- Reaction 1 occurs without the need for energy to be supplied, but Reaction 2 requires a very high temperature to start it.
- Reaction 1 is likely to be done in the laboratory, but Reaction 2 is done for a specific purpose in industry.

Metal displacement reaction in aqueous solution

When magnesium metal is added to copper(II) sulfate solution, the blue colour of the solution becomes paler. If an excess of magnesium is added, the solution becomes colourless, as magnesium sulfate forms. The magnesium changes in appearance from silvery to brown as copper forms on it.

The equation can be rewritten as an ionic equation:
$Mg(s) + Cu^{2+}(aq) + SO_2\ (aq) \rightarrow Cu(s) + Mg^{2+}(aq) + SO_4^{2-}\ (aq)$

Cancelling the ions that appear identically on both sides gives:
$Mg(s) + Cu^{2+}(aq) \rightarrow Cu(s) + Mg^{2+}(aq)$

Metal displacement reactions in the solid state

A mixture of aluminium and iron(III) oxide is positioned just above the place where the two rails are to be joined. It is so exothermic that the iron is formed as a molten metal, which flows into the gap between the two rails. The molten iron cools, joining the rails together.

$$2Al(l) + 2Fe^{3+}(l) + 3O^{2-}(l) \rightarrow 2Fe(l) + 2Al^{3+}(l) + 3O^{2-}(1)$$

then:

$$2Al(l) + 2Fe^{3}(l) \rightarrow 2Fe(l) + 2A^{3+}(l)$$

Electrons are transferred from aluminium atoms to iron(III) ions, so aluminium atoms are oxidised (loss of electrons) and iron(III) ions are reduced (gain of electrons).

Displacement reactions involving halogens

- $Cl_2(aq) + 2KBr(aq) \rightarrow Br_2(aq) + 2KCl(aq)$
- $Cl_2(aq) + 2K^+(aq) + 2Br^-(aq) \rightarrow Br_2(aq) + 2K^+(aq) + 2Cl^-(aq)$
- $Cl_2(aq) + 2Br^-(aq) \rightarrow Br_2(aq) + 2Cl^-(aq)$

1B.4 Precipitation reactions

Chemical tests

Carbon dioxide

When carbon dioxide gas is bubbled through calcium hydroxide solution (often called limewater), a white precipitate of calcium carbonate forms. The relevant equation is:

$$Ca(OH)_2(aq) + CO_2(g) \rightarrow CaCO_3(s) + H_2O(l)$$

The formation of the white precipitate was probably described as the limewater going milky or cloudy.

Sulfates

The presence of sulfate ions in solution can be shown by the addition of barium ions (usually from solutions of barium chloride or barium nitrate). The white precipitate that forms is barium sulfate. For example, when barium chloride solution is added to sodium sulfate solution, the relevant equations are:

- $Na_2SO_4(aq) + BaCl_2(aq) \rightarrow BaSO_4(s) + 2NaCl(aq)$
- $SO_4^{2-}(aq) + Ba^{2+}(aq) \rightarrow BaSO_4(s)$

Halides

The presence of halide ions in solution can be shown by the addition of silver ions (from silver nitrate solution). The precipitates that form are silver halides.
For example, when silver nitrate solution is added to sodium chloride solution, the relevant equations are:

- $NaCl(aq) + AgNO_3(aq) \rightarrow AgCl(s) + NaNO_3(aq)$
- $Cl(aq) + Ag^+(aq) \rightarrow AgCl(s)$

1C Energy

1C.1 comparing masses of substances

Relative atomic mass (A_r)

A suitable definition of relative atomic mass is:

The weighted mean (average) mass of an atom compared to $\frac{1}{12}$ of the mass of an atom of ^{12}C

It is often useful to remember this expression:

$$A_r = \frac{mean\ mass\ of\ an\ atom\ of\ an\ element}{\frac{1}{12} of\ mass\ of\ an\ atom\ of\ ^{12}C}$$

Relative molecular mass (M_r)

WORKED EXAMPLE 1

What is the relative molecular mass of carbon dioxide, CO_2?

$M_r = 12.0 + (2 \times 16.0) = 44.0$

WORKED EXAMPLE 2

What is the relative molecular mass of sulfuric acid, H_2SO_4?

$M_r = (2 \times 1.0) + 32.1 + (4 \times 16.0) = 98.1$

ELEMENT	RELATIVE ATOMIC MASS
hydrogen	1.0
carbon	12.0
oxygen	16.0
sulfur	32.1
copper	63.5

Relative formula mass

WORKED EXAMPLE 3

What is the relative formula mass of hydrated copper(II) sulfate, $CuSO_4.5H_2O$?

$M_r = 63.5 + 32.1 + (4 \times 16.0) + 5[(2 \times 1.0) + 16.0] = 249.6$

Molar mass (M)

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

The Avogadro constant

The value of the Avogadro constant is approximately 602 000 000 000 000 000 000 000 mol. It is easier to write this number using standard form: 6.02×10^{23} mol^{-1}.

Calculating using the Avogadro Constant

WORKED EXAMPLE 4

How many H_2O molecules are there in 1.25 g of water?

$$n = \frac{1.25}{18.0} = 0.0694\,\text{mol}$$

number of molecules $= 6.02 \times 10^{23} \times 0.0694 = 4.18 \times 10^{22}$

WORKED EXAMPLE 5

What is the mass of 100 million atoms of gold?

$$n = \frac{100 \times 10^{6}}{6.02 \times 10^{23}} = 1.66 \times 10^{-16}\,\text{mol}$$

$$m = 1.66 \times 10^{-16} \times 197.0 = 3.27 \times 10^{-14}\,\text{g}$$

(There are lots of atoms, but only a tiny mass.)

1C.2 Calculations involving mole

Definition of a mole

A mole is the amount of substance that contains the same number of particles as the number of carbon atoms in exactly 12g of the ^{12}C isotope.

Calculations using moles

WORKED EXAMPLE 1

What is the amount of substance in 6.51 g of sodium chloride?

$$n = \frac{m}{M} = \frac{6.51}{58.5} = 0.111\,\text{mol}$$

WORKED EXAMPLE 2

What is the mass of 0.263 mol of hydrogen iodide?

$$m = n \times M = 0.263 \times 127.9 = 33.6\,\text{g}$$

WORKED EXAMPLE 3

A sample of 0.284 mol of a substance has a mass of 17.8 g. What is the molar mass of the substance?

$$M = \frac{m}{n} = \frac{17.8}{0.284} = 62.7\,\text{g mol}^{-1}$$

1C.3 Calculations using reaction masses

Calculating reacting masses from equations

WORKED EXAMPLE 1

The equation for a reaction is:

$SO_3 + H_2O \rightarrow H_2SO_4$

What mass of sulfur trioxide is needed to form 75.0 g of sulfuric acid?

Step 1: calculate the molar masses of all substances you are told about and asked about, in this case, sulfur trioxide and sulfuric acid

$M(SO_3) = 80.1\ g\,mol^{-1}$ and $M(H_2SO_4) = 98.1\ g\,mol^{-1}$

Step 2: calculate the amount of sulfuric acid

$n = \frac{m}{M} = \frac{75.0}{98.1} = 0.765\ mol$

Step 3: use the reaction ratio in the equation to work out the amount of sulfur trioxide needed

As the ratio is 1 : 1, the amount is the same, so $n(SO_3) = 0.765\ mol$

Step 4: calculate the mass of sulfur trioxide

$m = n \times M = 0.765 \times 80.1 = 61.2\ g$

WORKED EXAMPLE 2

The equation for a reaction is:

$2NH_3 + H_2SO_4 \rightarrow (NH_4)_2SO_4$

What mass of ammonia is needed to form 100 g of ammonium sulfate?

Step 1:

$M(NH_3) = 17.0\ g\,mol^{-1}$ and $M((NH_4)_2SO_4) = 132.1\ g\,mol^{-1}$

Step 2:

$n((NH_4)_2SO_4) = \frac{100}{132} = 0.757\ mol$

Step 3:

$n(NH_3) = 2 \times 0.757 = 1.51\ mol$

(note the 2:1 ratio in the equation)

Step 4:

$m(NH_3) = n \times M = 1.51 \times 17.0 = 25.7\ g$

Working out formulae and equations from reacting masses

WORKED EXAMPLE 3

Sodium carbonate exists as the pure (anhydrous) compound but also as three **hydrates**. Careful heating can decompose these hydrates to one of the other hydrates or to the anhydrous compound. The measurement of reacting masses can allow you to determine the correct equation for the decomposition.

Question

A 16.7 g sample of a hydrate of sodium carbonate ($Na_2CO_3.10H_2O$) is heated at a constant temperature for a specified time until the reaction is complete. A mass of 3.15 g of water is obtained. What is the equation for the reaction occurring?

Method

Step 1: calculate the molar masses of the relevant substances

$M(Na_2CO_3.10H_2O) = 286.1\ g\ mol^{-1}$
and $M(H_2O) = 18.0\ g\ mol^{-1}$

Step 2: calculate the amounts of these substances

$Na_2CO_3.10H_2O$: $n = \frac{m}{M} = \frac{16.7}{286.1} = 0.0584\ mol$

water: $n = \frac{m}{M} = \frac{3.15}{18.0} = 0.175\ mol$

Step 3: use these amounts to calculate the simplest whole-number ratio for these substances

$Na_2CO_3.10H_2O$ and H_2O are in the ratio 0.0584 : 0.175 or 1 : 3

Step 4: use this ratio to work out the equation for the reaction

$Na_2CO_3.10H_2O \rightarrow Na_2CO_3.7H_2O + 3H_2O$

We have worked out the $Na_2CO_3.7H_2O$ formula by considering the ratio of the other two formulae.

WORKED EXAMPLE 4

Copper forms two oxides. Both oxides can be converted to copper by heating with hydrogen.

Question

An oxide of copper is heated in a stream of hydrogen to constant mass. The masses of copper and water formed are Cu = 17.6 g and H_2O = 2.56 g. What is the equation for the reaction occurring?

Method

Step 1: $M(Cu) = 63.5\ g\ mol^{-1}$ and $M(H_2O) = 18.0\ g\ mol^{-1}$

Step 2: $n(Cu) = \frac{17.6}{63.5} = 0.277\ mol$ and $n(H_2O) = \frac{2.56}{18.0} = 0.142\ mol$

Step 3: ratio is 0.277 : 0.142 = 2 : 1

Step 4: the equation has 2 mol of Cu and 1 mol of H_2O, so the products must be $2Cu + H_2O$

So the equation is:

$Cu_2O + H_2 \rightarrow 2Cu + H_2O$ and not $CuO + H_2 \rightarrow Cu + H_2O$

1C.4 The yield of reaction

Terminology relating to 'yield'

1. Theoretical yield
2. Actual yield
3. Percentage yield

Theoretical yield

WORKED EXAMPLE 1

Copper(II) carbonate is decomposed to obtain copper(II) oxide. The equation for the reaction is:

$$CuCO_3 \rightarrow CuO + CO_2$$

What is the theoretical yield of copper(II) oxide obtainable from 5.78 g of copper(II) carbonate?

Step 1: calculate the amount of starting material

$$n(CuCO_3) = \frac{5.78}{123.5} = 0.0468 \text{ mol}$$

Step 2: use the reacting ratio to calculate the amount of desired product

$$n(CuO) = 0.0468 \text{ mol}$$

Step 3: calculate the mass of desired product

$$m = 0.0468 \times 79.5 = 3.72 \text{ g}$$

WORKED EXAMPLE 2

Magnesium phosphate can be prepared from magnesium by reacting it with phosphoric acid. The equation for the reaction is:

$$3Mg + 2H_3PO_4 \rightarrow Mg_3(PO_4)_2 + 3H_2$$

What is the theoretical yield of magnesium phosphate obtainable from 5.62 g of magnesium?

Step 1: $n(Mg) = \frac{5.62}{24.3} = 0.231 \text{ mol}$

Step 2: $n(Mg_3(PO_4)_2) = \frac{0.231}{3} = 0.0770 \text{ mol}$

Step 3: $m = 0.0770 \times 262.9 = 20.2 \text{ g}$

Actual yield

This is the actual mass obtained by weighing the product obtained, not by calculation.

Percentage yield

$$\boxed{\frac{actual\ yield\ \times 100}{teoretical\ yield} = percentage\ yield}$$

WORKED EXAMPLE 3

The theoretical yield in a reaction is 26.7 tonnes. The actual yield is 18.5 tonnes. What is the percentage yield?

$$\text{percentage yield} = \frac{18.5 \times 100}{26.7} = 69.3\%$$

WORKED EXAMPLE 4

A manufacturer uses this reaction to obtain methanol from carbon monoxide and hydrogen:

$$CO + 2H_2 \rightarrow CH_3OH$$

The manufacturer obtains 4.07 tonnes of methanol starting from 4.32 tonnes of carbon monoxide. What is the percentage yield?

First, calculate the theoretical yield.

Step 1: $n(CO) = \frac{4.32 \times 10^6}{28.0} = 1.54 \times 10^5$ mol

Step 2: $n(CH_3OH) = 1.54 \times 10^5$ mol (because of 1:1 ratio)

Step 3: $m = 1.54 \times 10^5 \times 32.0 = 4.94 \times 10^6$ mol

Then use that answer to calculate the percentage yield.

$$\text{Percentage yield} = \frac{4.07 \times 10^6 \times 100}{4.94 \times 10^6} = 82.4\%$$

1C.5 Atom economy

$$\boxed{atom\ economy = \frac{molar\ mass\ of\ the\ desired\ product}{sum\ of\ the\ molar\ masses\ of\ all\ products} \times 100}$$

We can make some generalisations about certain types of reaction.

- Addition reactions have 100% atom economy.
- Elimination and substitution reactions have lower atom economies.
- Multistep reactions may have even lower atom economies.

Examples of calculations

WORKED EXAMPLE 1

Sodium carbonate is an important industrial chemical manufactured by the Solvay process. The overall equation for the process is:

$$CaCO_3 + 2NaCl \rightarrow Na_2CO_3 + CaCl_2$$

A manufacturer starts with 75.0 kg of calcium carbonate and obtains 76.5 kg of sodium carbonate. Calculate the percentage yield and atom economy for this reaction.

M_r values are 100.1 for $CaCO_3$ and 106.0 for Na_2CO_3.

$$\text{Theoretical yield} = \frac{75.0 \times 106.0}{100.1} = 79.4\,\text{kg}$$

$$\text{Percentage yield} = \frac{76.5 \times 100}{79.4} = 96.3\%$$

$$\text{Atom economy} = \frac{106.0 \times 100}{106.0 + 111.1} = 48.8\%$$

WORKED EXAMPLE 2

Hydrazine (N_2H_4) can be used as a rocket fuel and is manufactured using this reaction:

$$2NH_3 + NaOCl \rightarrow N_2H_4 + NaCl + H_2O$$

What is the atom economy for this reaction?

You first need to work out the molar masses of the products. These are 32.0, 58.5 and 18.0.

$$\text{Atom economy} = \frac{32.0 \times 100}{32.0 + 58.5 + 18.0} = 29.5\%$$

WORKED EXAMPLE 3

A manufacturer of ethene wants to convert some ethene into 1,2-dichloroethane. He considers two possible reactions:

Reaction 1 $H_2C{=}CH_2 + Cl_2 \rightarrow ClCH_2CH_2Cl$

Reaction 2 $2H_2C{=}CH_2 + 4HCl + O_2 \rightarrow 2ClCH_2CH_2Cl + 2H_2O$

Explain, without doing a calculation, which reaction would be a good choice on the basis of atom economy.

The answer is Reaction 1, because there is only one product, so all the atoms in the reactants end up in the desired product and the atom economy is 100%.

Reaction 2 has a lower atom economy because some of the atoms in the reactants form water, which has no value as a product.

1D Empirical and molecular formula

1D.1 Empirical formula

Calculating empirical formula

The calculation method involves these steps.

- Divide the mass, or percentage composition by mass, of each element by its relative atomic mass.
- If necessary, divide the answers from this step by the smallest of the numbers.
- This gives numbers that should be in an obvious whole number ratio, such as 1 : 2 or 3 : 2.
- These whole numbers are used to write the empirical formula.

1D.2 Molecular formula

Calculating molecular formula

WORKED EXAMPLE 1

In this example, the empirical formula is given.
A compound has the empirical formula CH and a relative formula mass of 104.

The 'formula mass' of the empirical formula is 13.0.

104 ÷ 13.0 = 8, so the molecular formula of the compound is C_8H_8.

WORKED EXAMPLE 2

In this example, you first have to work out the empirical formula. A compound contains the percentage composition by mass Na = 34.3%, C = 17.9%, O = 47.8%, and has a **molar mass** of 134 g mol^{-1}.
The calculations are shown below.

	Na	C	O
% of element	34.3	17.9	47.8
relative atomic mass	23.0	12.0	16.0
division by A_r	1.49	1.49	2.99
ratio	1	1	2

The empirical formula is $NaCO_2$.

The 'formula mass' of the empirical formula is 23.0 + 12.0 + (2 × 16.0) = 67.0.

The molar mass, 134, is 2 × 67.0, so the molecular formula of the compound is $Na_2C_2O_4$.

The ideal gas equation

$$\boxed{pV = nRT}$$

The SI units you should use are:

- p = pressure in pascals (Pa)
- V = volume in cubic metres (m^3)
- T = temperature in kelvin (K)
- n = amount of substance in moles (mol)
- R = the gas constant – this appears in the Data Booklet provided for use in the examinations and has the value 8.31 J $mol^{-1}K^{-1}$.

WORKED EXAMPLE 3

In this example, you will calculate the molar mass of the gas. It may help you (at least until you have had more practice) to write a list of the values with any necessary conversions.

A 0.280 g sample of a gas has a volume of 58.5 cm^3, measured at a pressure of 120 kPa and a temperature of 70 °C. Calculate the molar mass of the gas.

$p = 120\,kPa = 120 \times 10^3\,Pa$

$V = 58.5\,cm^3 = 58.5 \times 10^{-6}\,m^3$

$T = 70\,°C = 343\,K$

$R = 8.31\,J\,mol^{-1}K^{-1}$

So, $$n = \frac{pV}{RT} = \frac{120 \times 10^3 \times 58.5 \times 10^{-6}}{8.31 \times 343} = 0.00246\,mol$$

$$M = \frac{m}{n} = \frac{0.280}{0.00246} = 114\,g\,mol^{-1}$$

CONVERSION	HOW TO DO IT
$kPa \rightarrow Pa$	multiply by 10^3
$cm^3 \rightarrow m^3$	divide by 10^6 or multiply by 10^{-6}
$dm^3 \rightarrow m^3$	divide by 10^3 or multiply by 10^{-3}
$°C \rightarrow K$	add 273

WORKED EXAMPLE 4

In this example, you will calculate the empirical formula, then the amount in moles. After that the molar mass, then the molecular formula.

A compound has the percentage composition by mass C = 52.2%, H = 13.0%, O = 34.8%. A sample containing 0.173 g of the compound had a volume of 95.0 cm^3 when measured at 105 kPa and 45 °C. What is the molecular formula of this compound?

Step 1: calculate the empirical formula

	C	H	O
% by mass of element	52.2	13.0	34.8
relative atomic mass	12.0	1.0	16.0
division by A_r	4.35	13.0	2.175
ratio	2	6	1

The empirical formula is C_2H_6O.

Step 2: calculate the amount in moles

$$n = \frac{pV}{RT} = \frac{105 \times 10^3 \times 95.0 \times 10^{-6}}{8.31 \times 318} = 0.00377\,mol$$

Step 3: calculate the molar mass

$$M = \frac{m}{n} = \frac{0.173}{0.00377} = 45.9\,g\,mol^{-1}$$

Step 4: calculate the molecular formula

The 'formula mass' of the empirical formula is

$(2 \times 12.0) + (6 \times 1.0) + 16.0 = 46.0$

As 46.0 is the same as the molar mass, then the empirical and molecular formulae are the same.

The molecular formula is C_2H_6O.

1E Calculations with Solutions and gases

1E.1 Molar volume calculation

Calculations using molar volume

$$V_m = \frac{volume\ in\ dm^3}{amount\ in\ mol}$$

$V_m = 24dm^3mol^{-1}$ at r.t.p

$V_m = 24\ 000cm^3mol^{-1}$ at r.t.p

EXAMPLE 1

What is the amount, in moles, of CO in $3.8\,dm^3$ of carbon monoxide?

Answer $= \frac{3.8}{24} = 0.16\,mol$

EXAMPLE 2

What is the amount, in moles, of CO_2 in $500\,cm^3$ of carbon dioxide?

Answer $= \frac{500}{24\,000} = 0.021\,mol$

EXAMPLE 3

What is the volume of 0.36 mol of hydrogen?

Answer $= 24 \times 0.36 = 8.64\,dm^3$

EXAMPLE 4

A piece of magnesium with a mass of 1.00 g is added to an excess of dilute hydrochloric acid. What volume of hydrogen gas is formed?

The equation for the reaction is:

$$Mg(s) + 2HCl(aq) \rightarrow MgCl_2(aq) + H_2(g)$$

You are not given any information about the hydrochloric acid, and you are not asked anything about magnesium chloride. You can use the mole expression to calculate the amount of magnesium:

$$n(Mg) = \frac{1.00}{24.3} = 0.0412\,mol$$

You can see that the $Mg : H_2$ ratio in the equation is 1 : 1, which means that 0.0412 mol of hydrogen is formed.

Convert this amount to a volume and you have the answer:

$$volume = 24 \times 0.0412 = 0.99\,dm^3$$

EXAMPLE 5

Calcium carbonate reacts with nitric acid to form calcium nitrate, water and carbon dioxide, as shown in the equation:

$$CaCO_3(s) + 2HNO_3(aq) \rightarrow Ca(NO_3)_2(aq) + H_2O(l) + CO_2(g)$$

In a reaction, 100 cm^3 of carbon dioxide is formed. What mass of calcium carbonate is needed for this?

You are not told anything about nitric acid, or asked anything about calcium nitrate or water. You can use the molar volume expression to calculate the amount of carbon dioxide:

$$\text{amount} = \frac{100}{24000} = 0.00417\ \text{mol}$$

You can see that the $CaCO_3 : CO_2$ ratio in the equation is 1 : 1, which means that 0.00417 mol of calcium carbonate is needed.

Convert this amount to a mass and you have the answer:

$$m = n \times M = 0.00417 \times 100.1 = 0.42\ \text{g}$$

EXAMPLE 6

Ammonium sulfate reacts with sodium hydroxide solution to form sodium sulfate, water and ammonia, as shown in the equation:

$$(NH_4)_2SO_4(s) + 2NaOH(aq) \rightarrow Na_2SO_4(aq) + 2H_2O(l) + 2NH_3(g)$$

What volume of ammonia is formed by reacting 2.16 g of ammonium sulfate with excess sodium hydroxide solution?

You are not given any information about the sodium hydroxide, and you are not asked anything about sodium sulfate or water. You can use the mole expression to calculate the amount of ammonium sulfate:

$$n((NH_4)_2SO_4) = \frac{2.16}{132.1} = 0.01635\ \text{mol}$$

You can see that the $(NH_4)_2SO_4 : NH_3$ ratio in the equation is 1 : 2, which means that $0.01635 \times 2 = 0.0327$ mol of ammonia is formed.

Convert this amount to a volume and you have the answer:

$$\text{volume} = 24\,000 \times 0.0327 = 785\ \text{cm}^3$$

1E.2 Concentrations of solutions

Calculations using mass concentrations (g dm^3)

If you know the mass of a solute that you dissolve in a solvent (usually water), and the volume of the solution formed, then it is straightforward to calculate the mass concentration.
You use the expression:

$$\boxed{mass\ concentration = \frac{mass\ of\ solute\ in\ g}{volume\ of\ solution\ in\ dm^3}}$$

EXAMPLE 1

200 cm^3 of a solution contains 5.68 g of sodium bromide. What is its mass concentration?

$$\text{mass concentration} = \frac{m}{V} = \frac{5.68}{0.200} = 28.4\ \text{g dm}^{-3}$$

EXAMPLE 2

The concentration of a solution is 15.7 g dm^{-3}. What mass of solute is there in 750 cm^3 of solution?

$$m = \text{mass concentration} \times V = 15.7 \times 0.750 = 11.8\ \text{g}$$

EXAMPLE 3

A chemist uses 280 g of a solute to make a solution of concentration 28.4 g dm^{-3}. What volume of solution does he make?

$$V = \frac{m}{\text{mass concentration}} = \frac{280}{28.4} = 9.86\ \text{dm}^3$$

Calculations using molar concentrations (mold m^{-3})

$$\boxed{c = \frac{n}{v}}$$

WORKED EXAMPLE 1

A chemist makes 500 cm^3 of a solution of nitric acid of concentration 0.800 mol dm^{-3}. What mass of HNO_3 does she need?

Step 1: You are given values of V and c, so you can use the second expression to calculate a value for n.

$$n = c \times V = 0.800 \times 0.500 = 0.400 \text{ mol}$$

Step 2: You can now use the first expression to calculate the mass of nitric acid.

$$m = n \times M = 0.400 \times 63.0 = 25.2 \text{ g}$$

WORKED EXAMPLE 2

A student has 50.0 g of sodium chloride. What volume of a 0.450 mol dm^{-3} solution can he make?

Step 1: You are given the value of m and can work out M from the Periodic Table, so you can calculate n.

$$n = \frac{m}{M} = \frac{50.0}{58.5} = 0.855 \text{ mol}$$

Step 2: You can now use the second expression to calculate the volume of solution.

$$V = \frac{n}{c} = \frac{0.855}{0.450} = 1.90 \text{ dm}^3$$

WORKED EXAMPLE 3

An excess of magnesium is added to 100 cm^3 of 1.50 mol dm^{-3} hydrochloric acid. The equation for the reaction is:

$$Mg + 2HCl \rightarrow MgCl_2 + H_2$$

What mass of hydrogen is formed?

Step 1: You are given the values of V and c, so you can use the second expression to calculate the value of n for hydrochloric acid.

$$n = 0.100 \times 1.50 = 0.150 \text{ mol}$$

Step 2: The ratio for $HCl : H_2$ is 2 : 1, so $n(H_2) = 0.150 \div 2 = 0.0750$ mol

Step 3: For hydrogen, $m = n \times M = 0.0750 \times 2.0 = 0.15$ g

WORKED EXAMPLE 4

A mass of 47.8 g of magnesium carbonate reacts with 2.50 mol dm^{-3} hydrochloric acid. The equation for the reaction is:

$$MgCO_3 + 2HCl \rightarrow MgCl_2 + H_2O + CO_2$$

What volume of acid is needed?

Step 1: You are given the value of m and can work out M from the Periodic Table, so you can calculate n.

$$n = \frac{47.8}{84.3} = 0.567 \text{ mol}$$

Step 2: The ratio for $MgCO_3 : HCl$ is 1 : 2, so $n(HCl) = 2 \times 0.567 = 1.134$ mol

Step 3: for HCl, $V = \frac{1.134}{2.50} = 0.454 \text{ dm}^3$

1E.3 Concentrations in PPM

Calculations for solutions in PPM

$$concentration\ in\ PPM = \frac{mass\ of\ solute \times 1\,000\,000}{mass\ of\ solvent}$$

WORKED EXAMPLE 1

A solution contains 0.176 g of solute dissolved in 750 g of solvent. What is the concentration in ppm?

As the units of solute and solvent are the same, the values can be directly inserted into the expression.

$$\text{concentration in ppm} = \frac{\text{mass of solute} \times 1\,000\,000}{\text{mass of solvent}}$$

$$= \frac{0.176 \times 1\,000\,000}{750} = 235\ \text{ppm}$$

WORKED EXAMPLE 2

A mass of 23 mg of sodium chloride is dissolved in 900 g of water. What is the concentration of sodium chloride in the solution in ppm?

As the units of solute and solvent are different, either the mass of solute or the mass of solvent must be converted so they are the same. Then the values can be directly inserted into the expression.

First, convert the mass of sodium chloride from mg to g (divide by 1000):

mass of sodium chloride = 23 ÷ 1000 = 0.023 g

$$\text{concentration in ppm} = \frac{\text{mass of solute} \times 1\,000\,000}{\text{mass of solvent}}$$

$$= \frac{0.023 \times 1\,000\,000}{900} = 26\ \text{ppm}$$

WORKED EXAMPLE 3

A sample of river water contains phosphate ions with a concentration of 17 ppm. What is the mass of phosphate ions in 500 g of the river water?

In this example, the expression needs to be rearranged:

$$\text{mass of solute} = \frac{\text{concentration in ppm} \times \text{mass of solvent}}{1\,000\,000}$$

$$= \frac{17 \times 500}{1\,000\,000} = 0.0085\ \text{g}$$

Calculations for gases in PPM

$$concentration\ in\ PPM = \frac{volume\ of\ gas \times 1\,000\,000}{volume\ of\ air}$$

WORKED EXAMPLE 4

Some nitrogen dioxide gas, with a volume of $1.5\,dm^3$, mixes with $10\,000\,dm^3$ of air. What is the concentration of nitrogen dioxide, in ppm, in the air?

As the volume units of both gases are the same, then the values can be directly inserted into the expression.

$$\text{concentration in ppm} = \frac{\text{volume of gas} \times 1\,000\,000}{\text{volume of air}}$$

$$= \frac{1.5 \times 1\,000\,000}{10\,000} = 150\text{ ppm}$$

WORKED EXAMPLE 5

$5000\,dm^3$ of air is found to contain ozone with a concentration of 87 ppm. What volume of ozone is in this sample of air?

In this example, the expression needs to be rearranged:

$$\text{volume of gas} = \frac{\text{concentration in ppm} \times \text{volume of air}}{1\,000\,000}$$

$$= \frac{87 \times 5000}{1\,000\,000} = 0.435\,dm^3$$

WORKED EXAMPLE 6

Two samples of air containing sulfur dioxide were analysed. The results for Sample 1 showed that $500\,dm^3$ of air contained $37\,cm^3$ of sulfur dioxide. The results for Sample 2 showed that there were $1.4\,dm^3$ of sulfur dioxide in $4000\,dm^3$ of air. Show, by calculation, which sample has the higher concentration, in ppm, of sulfur dioxide.

Sample 1

$$\text{concentration in ppm} = \frac{\text{volume of gas} \times 1\,000\,000}{\text{volume of air}}$$

$$= \frac{37 \div 1000 \times 1\,000\,000}{500} = 74\text{ ppm}$$

Sample 2

$$\text{concentration in ppm} = \frac{\text{volume of gas} \times 1\,000\,000}{\text{volume of air}}$$

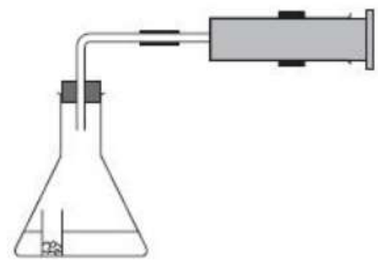
$$= \frac{1.4 \times 1\,000\,000}{4000} = 350\text{ ppm}$$

Sample 2 has the higher concentration.

EXCERSISE

1. A student wanted to measure the volume of a gas and use the results to find the volume occupied by one mole of the gas. The following method was used.
   - A sample of calcium carbonate was weighed out in a small plastic container.
   - 20 cm3 of hydrochloric acid of concentration 2.00 mol dm–3 was added to a conical flask. A small pinch of calcium carbonate was added to the acid.
   - The container was placed in the conical flask and a gas syringe was connected to the top of the conical flask.
   - The flask was carefully shaken so that the small plastic container fell over, allowing the acid and calcium carbonate to mix.

   The apparatus set up is shown.

   The student repeated the experiment five times using different masses of calcium carbonate on each occasion, with the concentration and volume of the hydrochloric acid constant.

Experiment number	Mass / g	Volume of CO_2 / cm^3
1	0.10	23
2	0.20	44
3	0.30	67
4	0.40	96
5	0.50	115

   a.
      i. Write the equation for the reaction between calcium carbonate and hydrochloric acid. Include state symbols.
      ii. Calculate the molar mass of calcium carbonate.
      iii. Show that, in each experiment, the hydrochloric acid is in excess

   b.
      i. Plot a graph of volume of carbon dioxide produced against mass of calcium carbonate on the grid. Include a line of best fit.
      ii. State how your graph supports the idea that the volume of gas produced depends directly on the mass of calcium carbonate added.

   c. Calculate the volume, under these conditions, of one mole of carbon dioxide gas from these data. Give your answer in dm^3 to two significant figures.

   d. Give a reason why the student added a small pinch of calcium carbonate to the acid before starting the reaction.

2. This question is about some reactions of chlorine and hydrogen chloride. When hydrogen gas and chlorine gas are mixed and passed over a hot platinum catalyst, hydrogen chloride gas is formed. The equation for this reaction is

   $H_2(g) + Cl_2(g) \rightarrow 2HCl(g)$

   In an experiment, 20 cm^3 of dry hydrogen gas was reacted with 20 cm^3 of dry chlorine gas. All gas volumes were measured at room temperature and pressure (r.t.p.). Calculate the number of gas molecules in the product at r.t.p.
   [Molar volume of a gas at r.t.p. = 24 000 $cm^3\ mol^{-1}$
   Avogadro constant (L) = $6.02 \times 10^{23}\ mol^{-1}$]

3. This question is about some reactions of chlorine and hydrogen chloride. Chlorine reacts with hot concentrated aqueous sodium hydroxide to produce sodium chlorate(V) as one of the products. The equation for this reaction is

   $3Cl_2 + 6NaOH \rightarrow 5NaCl + NaClO_3 + 3H_2O$

   i. Explain, using oxidation numbers, why this is a disproportionation reaction.
   ii. Calculate the atom economy, by mass, of sodium chlorate(V) in this reaction.

4. Many vehicles are fitted with airbags which provide a gas-filled safety cushion to protect the occupant of the vehicle if there is a crash.
   a. The first reaction in airbags is the thermal decomposition of sodium azide, NaN3, to form sodium and nitrogen gas.
      i. Write the equation for this decomposition of sodium azide. State symbols are not required.
      ii. In the reaction in (i), a typical airbag is inflated by about 67 dm3 of gas. Calculate the minimum mass of sodium azide, in grams, needed to produce this volume of gas. Use the Ideal Gas Equation and give your answer to an appropriate number of significant figures. For the purpose of this calculation, assume that the temperature is 300 °C and the pressure is 140 000 Pa.
   b. The second reaction in the airbag is between the sodium produced in the reaction (a) (i) and potassium nitrate.

      $\_\_\_Na + \_\_\_KNO_3 \rightarrow \_\_\_K_2O + \_\_\_Na_2O + \_\_\_N_2$

      Balance the above equation, justifying your answer in terms of the changes in oxidation numbers.
   c. The third reaction in the airbag is between the metal oxides and silicon dioxide. State the type of reaction taking place and justify why this reaction is necessary.

5. Ammonium cobalt(II) sulfate is made by mixing aqueous solutions of ammonium sulfate and excess cobalt(II) sulfate.
   Dry crystals of ammonium cobalt(II) sulfate, $(NH_4)2SO_4 \cdot CoSO_4 \cdot 6H_2O$, are obtained by the procedure shown.
   Step 1 The reaction mixture is transferred to an evaporating basin, heated gently and then left to crystallise.
   Step 2 The crystals are separated by gravity filtration.
   Step 3 The crystals are then rinsed with a small amount of ice-cold water.
   Step 4 The rinsed crystals are placed in a warm oven for 30 minutes.
   The percentage yield of this reaction is 70.0%.
   Give two possible reasons, other than an incomplete reaction, why the yield is less than 100%.

6. Ethanol, C_2H_5OH, is a member of the homologous series of alcohols. Calculate the number of molecules in 55.2kg of ethanol.
   [Avogadro Constant = 6.02×10^{23} mol^{-1}]

7. Sulfur is a bright yellow crystalline solid at room temperature.
   Sulfur forms rings of 8 sulfur atoms so the formula of the yellow solid is S8.
   Compound X is an oxide of sulfur. A gaseous sample of 0.318 g of X occupied a volume of 132 cm^3 at a temperature of 420 K and pressure of 105 kPa.
   The number of moles of a gas and the volume occupied by it can be found using the ideal gas equation

   $$pV = nRT$$

   Calculate the relative molecular mass of X and hence its molecular formula.
   You must show all your working.
   [R = 8.31 J mol–1 K^{-1}]

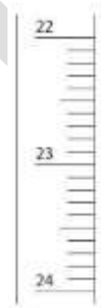
8. In an experiment, 1.000 g of a hydrocarbon, A, was burned completely in oxygen to produce 3.143 g of carbon dioxide and 1.284 g of water. In a different experiment, the molar mass of the hydrocarbon, A, was found to be 84.0 g mol^{-1}. Calculate the empirical formula and the molecular formula of the hydrocarbon, A.

9. Boron and aluminium are in the same group of the Periodic Table. Both form compounds with chlorine and with fluorine.
   Aluminium also reacts directly with chlorine to form a compound, aluminium chloride, containing only aluminium and chlorine.
   A 0.500 g sample of aluminium chloride was analysed and found to contain 0.101 g of aluminium.
   Another 0.500 g sample was heated to 473 K. The gas produced occupied a volume of 73.6cm^3 at a pressure of 1.00×10^2 kPa.
   Determine the molecular formula of the gas.
   You will need to use the equation pV = nRT and R = 8.31 J mol^{-1} K^{-1}

10. A group of students analysed a hydrated salt with the formula $KH_3(C_2O_4)_y.\ zH_2O$ where y and z are whole numbers.
    The students carried out experiments to determine the values of y and z.
    a. Experiment 1 – to determine the value of y
       One student was provided with a 0.0235 mol dm^{-3} solution of the salt.
       25.0 cm^3 portions of the salt solution were acidified with excess dilute sulfuric acid and heated to about 60 °C.
       Each portion was titrated with 0.0203 mol dm^{-3} potassium manganate(VII). The results of four titrations are shown in the table.

Titration number	1	2	3	4
Final burette reading / cm^3	23.85	47.20	24.05	48.10
Initial burette reading / cm^3	0.00	24.00	0.50	25.00
Titre / cm^3	23.85	23.20	23.55	23.10

       i. Complete the diagram to show the final burette reading in Titration 1.



       ii. Explain why this student should use a mean titre of 23.15 cm^3 and not 23.43 cm^3 in the calculation.
       iii. The uncertainty in each burette reading is ±0.05 cm^3. Calculate the percentage uncertainty in the titre volume of potassium manganate(VII) solution used in Titration 2
       iv. The equation for the reaction is
       $$2MnO_4^- + 5C_2O_4^{2-} + 16H^+ \rightarrow 2Mn^{2+} + 10CO_2 + 8H_2O$$
       Deduce, by calculation, the value of y, to the nearest whole number, in the formula $KH_3(C_2O_4)_y.\ zH_2O$.
       Use the mean titre of 23.15 cm3 and other data from Experiment 1.
       You must show your working.

b. Experiment 2 – to determine the value of z

Another student wrote an account of the method for this experiment.

A crucible was weighed.

A sample of the hydrated salt was added to the crucible and it was reweighed.

The crucible and salt were heated to remove the water of crystallisation and then allowed to cool.

The crucible and contents were weighed again.

Results

Mass of crucible	= 19.56 g
Mass of crucible + $KH_3(C_2O_4)_y.zH_2O$	= 22.97 g
Mass of crucible + $KH_3(C_2O_4)_y$	= 22.52 g

i. Deduce, by calculation, the value of z, to the nearest whole number, in the formula $KH_3(C_2O_4)_y.\ zH_2O$.
You must use the data from Experiment 2 and your value of y in (a)(iv).
You must show your working.

ii. A third student carried out Experiment 2 and calculated a value of z that was lower than expected.
This student evaluated the experiment and gave two suggestions for z being lower.

Suggestion 1 "Some of the crystals jumped out of the crucible while it was being heated."

Suggestion 2 "It was difficult to tell when all the water of crystallisation had been lost."

Evaluate these two suggestions to decide whether they could account for the lower value of z obtained from the experimental results. Include an explanation of the effect each suggestion would have on the calculated value of z and how the method could be improved to prevent these errors.