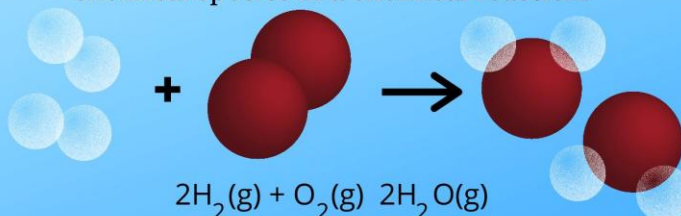


Cambridge
AS level
Chemistry
CODE: (9701)
Chapter 01
Moles and equations

Mole Ratio

The mole ratio is a conversion factor between any two chemical species in a chemical reaction.



Find the mole ratio from the coefficients of the balanced equation.

2 : 1 : 2

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Masses of atoms and molecules

Relative atomic mass, A_r

Atoms of different elements have different masses, making it impossible to weigh a single atom directly. To calculate atom masses, scientists weigh many atoms and compare them with the mass of 'standard' atoms, such as carbon-12. This is called the **relative atomic mass, A_r** .

From this it follows that:
 A_r [element Y]

The average mass of an element's atom is used because most elements are mixtures of isotopes, with values like A_r of hydrogen often not being whole numbers.

Relative isotopic mass

The nucleon number, representing the total number of neutrons and protons in an atom, is the number of protons with the same number of neutrons.

We use the term **relative isotopic mass** for the mass of a particular isotope of an element on a scale where an atom of carbon-12 has a mass of exactly 12 units.

Relative molecular mass, M_r

The **relative molecular mass of a compound (M_r)** is the relative mass of one molecule of the compound on a scale where the carbon-12 isotope has a mass of exactly 12 units. We find the relative molecular mass by adding up the relative atomic masses of all the atoms present in the molecule.

Relative formula mass

For compounds containing ions, we use the term relative formula mass. This is calculated in the same way as for **relative molecular mass**. It is also given the same symbol, M_r .

Determination of A_r from mass spectra

We can use the data obtained from a mass spectrometer to calculate the relative atomic mass of an element very accurately. To calculate the relative atomic mass, we follow this method:

- Multiply each isotopic mass by its percentage abundance
- Add the figures together
- Divide by 100.

We can use this method to calculate the relative atomic mass of neon from its mass spectrum, shown in Figure 1.5.

The mass spectrum of neon has three peaks: ^{20}Ne (90.9%), ^{21}Ne (0.3%) and ^{22}Ne (8.8%).

$$A_r \text{ of neon} = \frac{(20 \times 90.9) + (21.0 \times 0.3) + (22 \times 8.8)}{100} = 20.2$$

The relative atomic mass is the weighted average mass of naturally occurring atoms of an element on a scale where an atom of carbon-12 has a mass of exactly 12 units.

$$= \frac{\text{average mass of one atom of element Y} \times 12}{\text{mass of one atom of carbon-12}}$$

Accurate relative atomic masses

MASS SPECTROMETRY

A **mass spectrometer** (Figure 1.2) can be used to measure the mass of each isotope present in an element. It also compares how much of each isotope is present – the relative abundance (isotopic abundance). A simplified diagram of a mass spectrometer is shown in Figure 1.3. You will not be expected to know the details of how a mass spectrometer works, but it is useful to understand how the results are obtained.

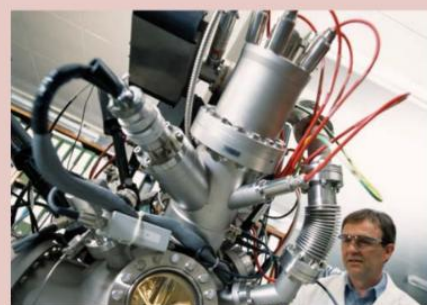


Figure 1.2 A mass spectrometer is a large and complex instrument.

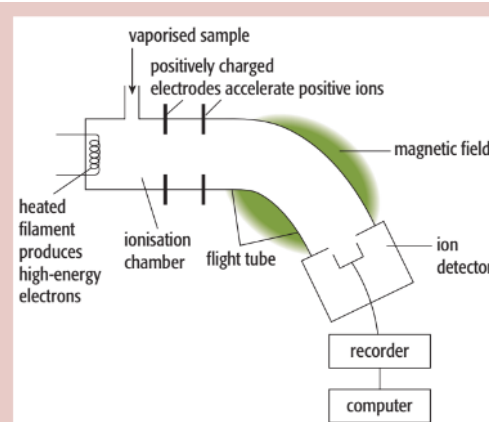


Figure 1.3 Simplified diagram of a mass spectrometer.

Note that this answer is given to 3 significant figures, which is consistent with the data given.

Amount of substance

The mole and the Avogadro constant

The formula of a compound indicates the number of atoms in one molecule. In water, the ratio of hydrogen to oxygen atoms is 2:16. This ratio remains constant regardless of the number of molecules. To weigh a substance, more than 1000 atoms are needed.

The relative atomic mass or relative molecular mass of a substance in grams is called a **mole** of the substance. So, a mole of sodium ($A_r = 23.0$) weighs 23.0 g. The abbreviation for a mole is mol. We define the mole in terms of the standard carbon-12 isotope.

We often refer to the mass of a mole of substance as its **molar mass** (abbreviation M). The units of molar mass are g mol^{-1} .

The number of atoms in a mole of atoms is very large: 6.02×10^{23} atoms. This number is called the **Avogadro constant (or Avogadro number)**.

The Avogadro constant, symbol L , refers to the number of atoms, molecules, ions, and electrons in a substance. In 1 mole of sodium, there are 6.02×10^{23} atoms, while in 1 mole of sodium chloride, there are 6.02×10^{23} sodium ions and 6.02×10^{23} chloride ions.

Moles and mass

The SI base unit for mass is the kilogram, but chemists prefer the relative molecular mass or formula mass in grams for general laboratory work in chemistry.

$$\text{number of moles (mol)} = \frac{\text{mass of substance in grams (g)}}{\text{molar mass (g mol}^{-1}\text{)}}$$

To find the mass of a substance present in each number of moles, you need to rearrange the equation.

$$\text{number of moles (mol)} = \frac{\text{mass of substance in grams (g)}}{\text{molar mass (g mol}^{-1}\text{)}}$$

$$\text{mass of substance (g)} = \text{number of moles (mol)} \times \text{molar mass (g mol}^{-1}\text{)}$$

Mole calculations

Reacting masses

Stoichiometry is a crucial concept in chemical reactions, determining the ratio of moles of reactants and products, which is determined through the balanced equation.

To find the mass of products formed in the chemical reaction we use:

- The mass of the reactants
- The molar mass of the reactants
- The balanced equation.

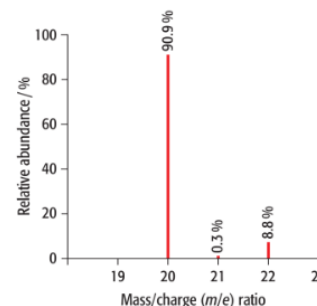


Figure 1.5 The mass spectrum of neon, Ne.

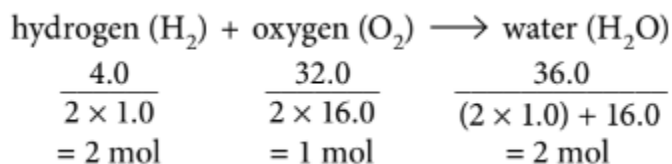
A high-resolution mass spectrometer can give very accurate relative isotopic masses. For example $^{16}\text{O} = 15.995$ and $^{32}\text{S} = 31.972$. Because of this, chemists can distinguish between molecules such as SO_2 and S_2 , which appear to have the same relative molecular mass.

One mole of a substance is the amount of that substance that has the same number of specific particles (atoms, molecules or ions) as there are atoms in exactly 12 g of the carbon-12 isotope.

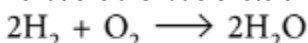
The stoichiometry of a reaction

We can find the stoichiometry of a reaction if we know the amounts of each reactant that exactly react together, and the amounts of each product formed.

For example, if we react 4.0 g of hydrogen with 32.0 g of oxygen we get 36.0 g of water. (A_r values: H = 1.0, O = 16.0)



This ratio is the ratio of stoichiometric numbers in the equation. So, the equation is:



Stoichiometry is a crucial concept in chemistry, allowing us to determine the mole ratio of a reaction, even without knowing the mass of oxygen involved.

Significant figures

When we perform chemical calculations, we must answer the number of significant figures that fit with the data provided.

Percentage composition by mass

We can use the formula of a compound and relative atomic mass to calculate the percentage by mass of a particular element in a compound.

% by mass

$$\begin{array}{l}
 \text{atomic mass} \times \text{number of moles of particular} \\
 \text{element in a compound} \\
 = \frac{\quad}{\text{molar mass of compound}} \times 100
 \end{array}$$

Empirical formulae

The **empirical formula** of a compound is the simplest whole number ratio of the elements present in one molecule or formula unit of the compound. The **molecular formula** of a compound shows the total number of atoms of each element present in a molecule.

Table 1.2 shows the empirical and molecular formulae for several compounds.

- The formula for an ionic compound is always its empirical formula.
- The empirical formula and molecular formula for simple inorganic molecules are often the same.
- Organic molecules often have different empirical and molecular formulae.

The empirical formula can be found by determining the mass of each element present in a sample of the compound. For some compounds, this can be done by combustion. An organic compound must be very pure to calculate its empirical formula. Chemists often use gas chromatography to purify compounds before carrying out formula analysis.

An empirical formula can also be deduced from data that give the percentage composition by mass of the elements in a compound.

The molecular formula

The molecular formula, a multiple of the empirical formula, provides a precise representation of the actual number of atoms in a molecule.

To deduce the molecular formula, we need to know:

- The relative formula mass of the compound
- The empirical formula.

Chemical formulae and chemical equations

Deducing the formula

The formula of a compound is determined by the electronic structure of individual elements, with the number of positive and negative charges balanced to achieve zero charges. The Periodic Table, which has 18 groups, is used to determine the formula, with elements like aluminium and chlorine in Group 13.

The positive charge of simple metal ions in Groups 1 and 2 is equal to the group number, while in Group 13, it's 3+, and in Groups 15-17, it's 18 minus the group number.

Ion	Formula
ammonium	NH_4^+
carbonate	CO_3^{2-}
hydrogencarbonate	HCO_3^-
hydroxide	OH^-
nitrate	NO_3^-
phosphate	PO_4^{3-}
sulfate	SO_4^{2-}

Table 1.3 The formulae of some common compound ions.

Ions that contain more than one type of atom are called **compound ions**. Some common compound ions that you should learn are listed in Table 1.3. The formula for an ionic compound is obtained by balancing the charges of the ions.

The formula of a covalent compound is determined by the number of electrons needed for a noble gas to form a stable electronic configuration, with carbon atoms bonding with hydrogen and oxygen.

Compounds containing a simple metal ion and non-metal ions are named by changing the end of the name of the non-metal element to -ide. Compound ions containing oxygen are usually called **-ates**.

sodium + chlorine $\longrightarrow$ sodium chloride

zinc + sulfur $\longrightarrow$ zinc sulfide

Balancing chemical equations

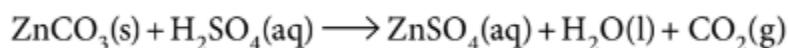
Chemical reactions require equal atom types on both the reactants and product sides. A balanced symbol equation reflects the number and type of atoms in both reactants and products, indicating a chemical reaction.

Using state symbols

We sometimes find it useful to specify the physical states of the reactants and products in a chemical reaction. This is especially important where chemical equilibrium and rates of reaction are being discussed (see Chapter 8 and Chapter 9). We use the following state symbols:

- (s) solid
- (l) liquid
- (g) gas
- (aq) aqueous (a solution in water).

State symbols are written after the formula of each reactant and product. For example:



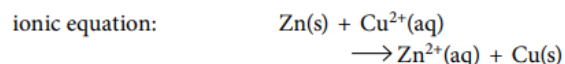
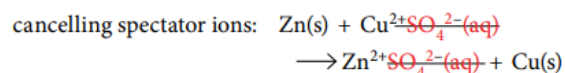
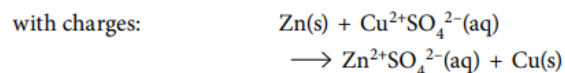
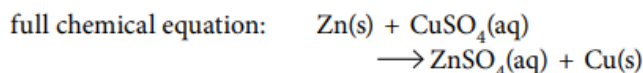
Balancing ionic equations

When ionic compounds dissolve in water, the ions separate from each other. For example.

Ionic compounds include salts such as sodium bromide, magnesium sulfate and ammonium nitrate. Acids and alkalis also contain ions.

Many chemical reactions in aqueous solutions involve ionic compounds. Only some of the ions in the solution take part in these reactions. The ions that play no part in the reaction are called **spectator ions**.

An ionic equation is simpler than a full chemical equation. It shows only the ions or other particles that are reacting. Spectator ions are omitted. Compare the full equation for the reaction of zinc with aqueous copper (II) sulfate with the ionic equation.



In the ionic equation, you will notice that:

- There are no sulfate ions – these are the spectator ions as they have not changed
- Both the charges and the atoms are balanced.

Chemists usually prefer to write ionic equations for precipitation reactions. A precipitation reaction is a reaction where two aqueous solutions react to form a solid – the precipitate. For these reactions, the method of writing the ionic equation can be simplified. All you must do is:

- Write the formula of the precipitate as the product
- Write the ions that make up the precipitate as the reactants

Solutions and concentration

Calculating the concentration of a solution

The concentration of a solution is the amount of solute dissolved in a solvent to make 1dm^3 (one cubic decimetre) of solution. The solvent is usually water. There are 1000 cm^3 in a cubic decimetre. When 1 mole of a compound is dissolved to make 1dm^3 of solution the concentration is 1mol dm^{-3} .

$$\text{concentration (mol dm}^{-3}\text{)} = \frac{\text{number of moles of solute (mol)}}{\text{volume of solution (dm}^3\text{)}}$$

We use the terms ‘concentrated’ and ‘dilute’ to refer to the relative amount of solute in the solution. A solution with a low concentration of solute is a dilute solution. If there is a high concentration of solute, the solution is concentrated. When performing calculations involving concentrations in mol dm^{-3} you need to:

- Change mass in grams to moles
- Change cm^3 to dm^3 (by dividing the number of cm^3 by 1000)

We often need to calculate the mass of a substance present in a solution of known concentration and volume. To do this we:

- Rearrange the concentration equation to number of moles (mol) = concentration (mol dm^{-3}) $\times$ volume (dm^3)
- Multiply the moles of solute by its molar mass of solute (g) = number of moles (mol) $\times$ molar mass (g mol^{-1})

CARRYING OUT A TITRATION

A procedure called a titration is used to determine the amount of substance present in a solution of unknown concentration. There are several different kinds of titration. One of the commonest involves the exact neutralisation of an alkali by an acid (Figure 1.15).

If we want to determine the concentration of a solution of sodium hydroxide we use the following procedure.

- Get some of acid of known concentration.
- Fill a clean burette with the acid (after having washed the burette with a little of the acid).
- Record the initial burette reading.
- Measure a known volume of the alkali into a titration flask using a graduated (volumetric) pipette.
- Add an indicator solution to the alkali in the flask.
- Slowly add the acid from the burette to the flask, swirling the flask all the time until the indicator changes colour (the end-point).

- Record the final burette reading. The final reading minus the initial reading is called the **titre**. This first titre is normally known as a 'rough' value.
- Repeat this process, adding the acid drop by drop near the end-point.
- Repeat again, until you have two titres that are no more than 0.10 cm^3 apart.
- Take the average of these two titre values.

Your results should be recorded in a table, looking like this:

	rough	1	2	3
final burette reading / cm^3	37.60	38.65	36.40	34.75
initial burette reading / cm^3	2.40	4.00	1.40	0.00
titre / cm^3	35.20	34.65	35.00	34.75

Calculating solution concentration by titration

Titration is often used to find the exact concentration of a solution. Worked example 20 shows the steps used to calculate the concentration of a solution of sodium hydroxide when it is neutralized by aqueous sulfuric acid of known concentration and volume.

Deducing stoichiometry by titration

We can use titration results to find the stoichiometry of a reaction. To do this, we need to know the concentrations and the volumes of both reactants. The example below shows how to determine the stoichiometry of the reaction between a metal hydroxide and an acid.

Calculations involving gas volumes

Using the molar gas volume

Amedeo Avogadro's hypothesis, proposed in 1811, suggests that equal volumes of all gases contain the same number of molecules. This is true if the pressure isn't too high, or the temperature isn't too low. Measured at room temperature and pressure, one mole of any gas has a volume of 24.0 dm^3 .

CARRYING OUT A TITRATION (CONTINUED)

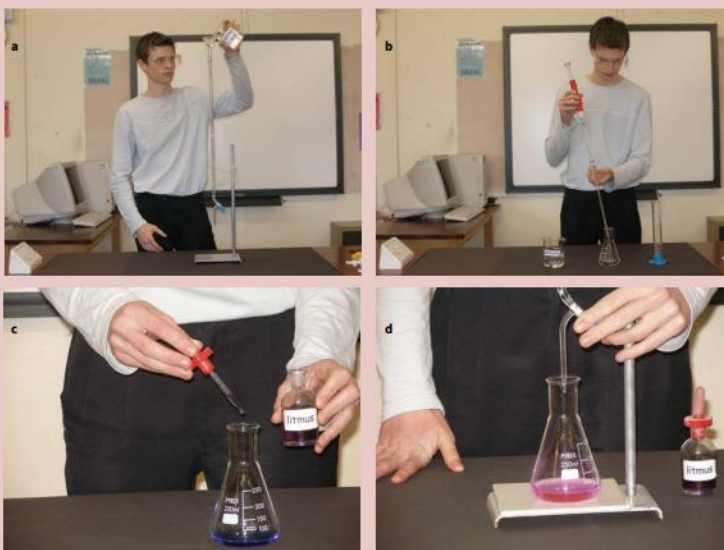


Figure 1.15 a A funnel is used to fill the burette with hydrochloric acid. b A graduated pipette is used to measure 25.0 cm^3 of sodium hydroxide solution into a conical flask. c An indicator called litmus is added to the sodium hydroxide solution, which turns blue. d 12.5 cm^3 of hydrochloric acid from the burette have been added to the 25.0 cm^3 of alkali in the conical flask. The litmus has gone red, showing that this volume of acid was just enough to neutralise the alkali.

You should note:

- all burette readings are given to an accuracy of 0.05 cm^3
- the units are shown like this ' cm^3 '
- the two titres that are no more than 0.10 cm^3 apart are 1 and 3, so they would be averaged
- the average titre is 34.70 cm^3 .

In every titration there are five important pieces of knowledge:

- 1 the balanced equation for the reaction
- 2 the volume of the solution in the burette (in the example above this is hydrochloric acid)

- 3 the concentration of the solution in the burette
- 4 the volume of the solution in the titration flask (in the example above this is sodium hydroxide)
- 5 the concentration of the solution in the titration flask.

If we know four of these five things, we can calculate the fifth. So in order to calculate the concentration of sodium hydroxide in the flask we need to know the first four of these points.

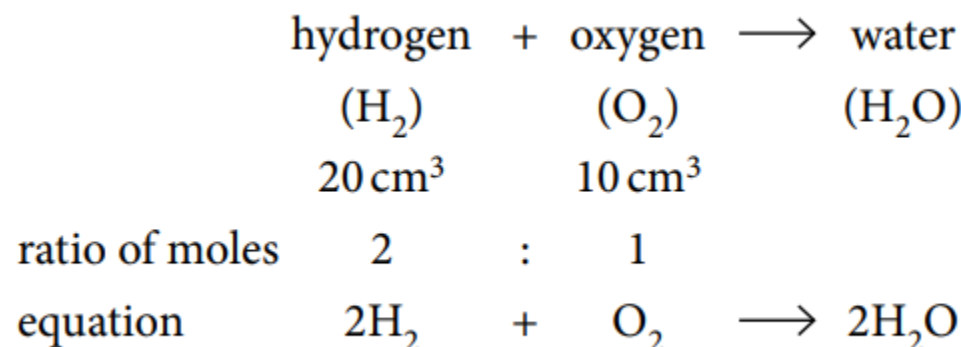
We can use the molar gas volume of 24.0dm³ at r.t.p. to find:

- The volume of a given mass or number of moles of gas
- The mass or number of moles of a given volume of gas

Gas volumes and stoichiometry

The stoichiometry of a reaction can be determined by comparing the reacting volumes of gases. For example, when hydrogen and oxygen are mixed, the reaction is exact, indicating that equal volumes of gases contain equal numbers of molecules.

So, the mole ratio of hydrogen to oxygen is 2: 1. We can summarise this as:



We can extend this idea to experiments involving combustion data of hydrocarbons. The example below shows how the formula of propane and the stoichiometry of the equation can be deduced. Propane is a hydrocarbon – a compound of carbon and hydrogen only.

Revision questions

1) A compound, A, has the following composition by mass.

C, 66.7%; H, 11.1%; O, 22.2%.

It has a M_r of 72.

(a) Calculate the molecular formula of A.

2) 1.20 dm³ of ammonia gas was dissolved in water to form 200 cm³ of aqueous alkali at room temperature and pressure.

(i) Use the Data Booklet to calculate how many moles of NH₃(g) were dissolved.

(ii) Write the equation for the neutralization of aqueous ammonia by dilute sulphuric acid.

(iii) Calculate the volume of 0.50 mol dm³ sulphuric acid that is required to neutralize the 200 cm³ of aqueous ammonia.

3) Mohr's salt is a pale green crystalline solid which is soluble in water. Mohr's salt is a 'double salt' which contains

two cations, one of which is Fe²⁺,

one anion which is SO₄²⁻

and water crystallization.

(a) The identity of the second cation was determined by the following test.

Solid Mohr's salt was heated with solid sodium hydroxide and a colorless gas evolved. The gas readily dissolved in water giving an alkaline solution.

(i) What is the gas?

(ii) What is the formula of the second cation identified by this test?

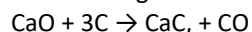
(iii) In this test, a grey/green solid residue was also formed. Suggest a name or formula for this solid.

(4) When CH_2Cl_2 is heated under reflux with an excess of $\text{NaOH}(\text{aq})$, a compound W is formed.

W has the following composition by mass: C, 40.0%; H, 6.7%; O, 53.3%.

Use this information and the Data Booklet to show that the empirical formula of W is CHAO .

(5) In some countries, ethyne is manufactured from calcium carbide, CaC_2 , which is produced by heating quicklime and coke together at 2300 K.



When water is added to the CaC_2 , calcium hydroxide, $\text{Ca}(\text{OH})_2$, and ethyne, C_2H_2 , are produced.

(i) Construct a balanced equation for the formation of ethyne from calcium carbide.

(ii) Use this equation and your answer to part (b) to calculate the mass of CaC_2 which will react with an excess of water to produce enough ethyne to fill 100 cylinders of the gas.

(6) Titanium also reacts with chlorine.

When an excess of chlorine was reacted with 0.72 g of titanium, 2.85 g of chloride A was formed.

(i) Calculate the amount, in moles, of titanium used.

(ii) Calculate the amount, in moles, of chlorine atoms that reacted.

(iii) Hence, determine the empirical formula of A.

(iv) Construct a balanced equation for the reaction between titanium and chlorine.

(7) A third polycarboxylic acid present in unripe fruit is a colourless crystalline solid, W, which has the following composition by mass: C, 35.8%; H, 4.5%; O, 59.7%.

(d) (i) Show by calculation that the empirical formula of W is $\text{C}_2\text{H}_2\text{O}_5$

(ii) The M_r of W is 134. Use this value to determine the molecular formula of W.

(8) In an experiment to determine K a student placed together in a conical flask 0.10 mol of ethanoic acid, 0.10 mol of an alcohol ROH , and 0.005 mol of hydrogen chloride catalyst. The flask was sealed and kept at 25°C for seven days.

After this time, the student titrated all the contents of the flask with 2.00 mol dm^{-3} NaOH using a phenolphthalein indicator.

At the endpoint, 22.5 cm^3 of NaOH had been used.

(b) (i) Calculate the amount, in moles, of NaOH used in the titration.

(ii) What amount, in moles, of this NaOH reacted with the hydrogen chloride?

(iii) Write a balanced equation for the reaction between ethanoic acid and NaOH .

(iv) Hence calculate the amount, in moles, of NaOH that reacted with the ethanoic acid.

(9) Compound R is a weak diprotic (dibasic) acid which is very soluble in water.

(a) A solution of R was prepared which contained 1.25 g of R in 250 cm^3 of solution. When 25.0 cm^3 of this solution was titrated with $0.100 \text{ mol dm}^{-3}$ NaOH , 21.6 cm^3 of the alkali was needed for a complete reaction.

(i) Using the formula HX to represent R, construct a balanced equation for the reaction between H_2X and NaOH .

(ii) Use the data above to calculate the amount, in moles, of OH^- ions used in the titration.

(iii) Use your answers to (i) and (ii) to calculate the amount, in moles, of R present in 25.0 cm^3 of solution.

(iv) Calculate the amount, in moles, of R present in 250 cm^3 of solution.