PEARSON EDEXCEL INTERNATIONAL AS/A LEVEL

# CHEMISTRY

## Student Book 1

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# UNIT 1: STRUCTURE, BONDING AND INTRODUCTION TO ORGANIC CHEMISTRY

# UNIT 2: ENERGETICS, GROUP CHEMISTRY, HALOGENOALKANES AND ALCOHOLS

# ABOUT THIS BOOK

This book is written for students following the Pearson Edexcel International Advanced Subsidiary (IAS) Chemistry specification. This book covers the full IAS course and the first year of the International A Level (IAL) course.

The book contains full coverage of IAS units (or exam papers) 1 and 2. Students can prepare for the written Practical Paper by using the IAL Chemistry Lab Book (see page x of this book). Each unit has five Topic areas that match the titles and order of those in the specification. You can refer to the Assessment Overview on page xii for further information.

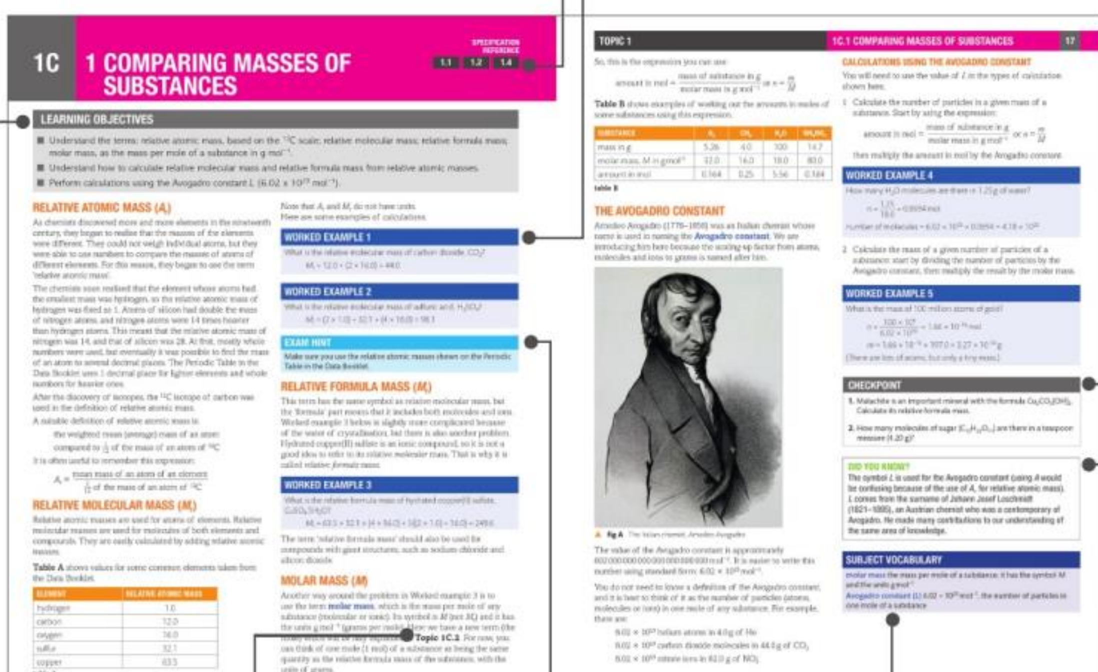
Each Topic is divided into chapters and sections to break the content down into manageable chunks. Each section features a mix of learning and activities.

**Learning objectives**
Each chapter starts with a list of key assessment objectives.

**Specification reference**
The exact specification points covered in the section are provided.

**Worked examples**
show you how to work through questions, and set out calculations.

**Checkpoint**
Questions at the end of each section check understanding of the key learning points in each chapter.




**Cross references**
These help you reference past and future learning.

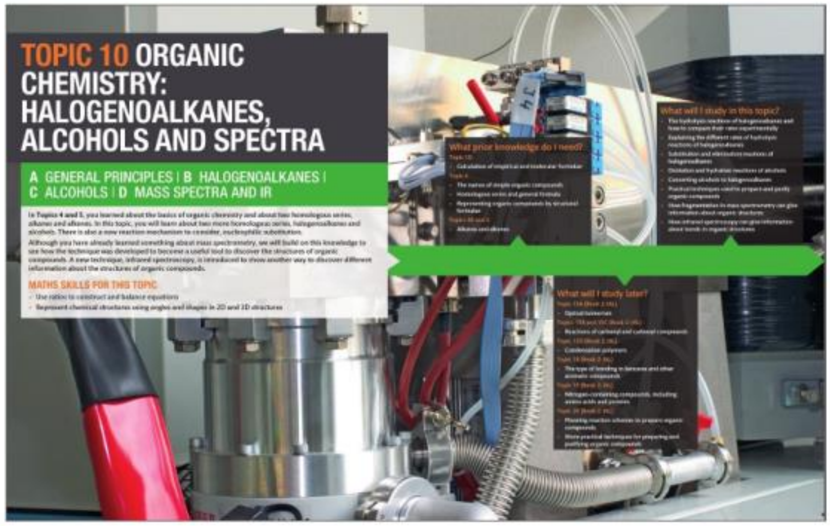
**Exam hints**
Tips on how to answer exam-style questions and guidance for exam preparation.

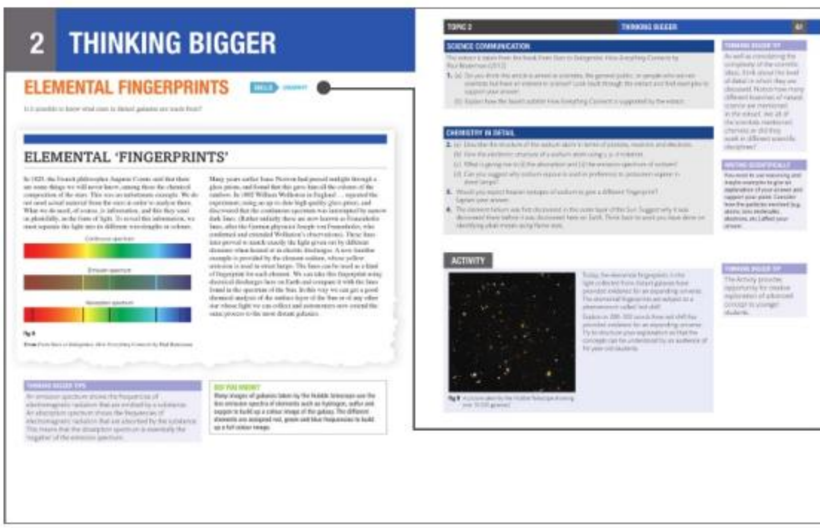
**Subject Vocabulary**
Key terms are highlighted in blue in the text. Clear definitions are provided at the end of each section for easy reference, and are also collated in a glossary at the back of the book.

**Did you know?**
Interesting facts help you remember the key concepts.

Your learning, Topic by Topic, is always put in context:

- Links to other areas of Chemistry include previous knowledge that is built on in the topic, and future learning that you will cover later in your course.
- A checklist details maths knowledge required. If you need to practise these skills, you can use the **Maths Skills** reference at the back of the book as a starting point.

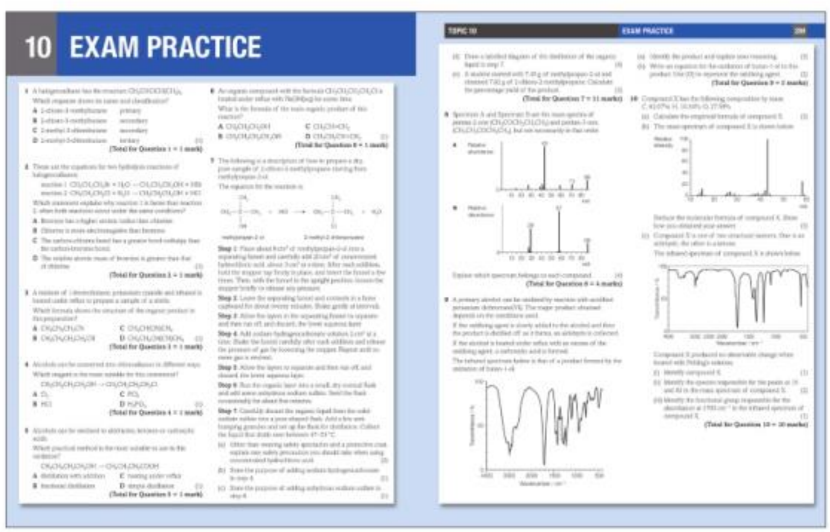



**Thinking Bigger**
At the end of each topic there is an opportunity to read and work with real-life research and writing about science. The activities help you to read real-life material that's relevant to your course, analyse how scientists write, think critically and consider how different aspects of your learning piece together.

**Skills**
These sections will help you develop transferable skills, which are highly valued in further study and the workplace.

**Exam Practice**
Exam-style questions at the end of each chapter are tailored to the Pearson Edexcel specification to allow for practice and development of exam writing technique. They also allow for practice responding to the command words used in the exams (see the **command words glossary** at the back of this book).
You can also refer to the **Preparing for Your Exams** section in the back of the book, for sample exam answers with commentary.



# PRACTICAL SKILLS

Practical work is central to the study of chemistry. The International Advanced Subsidiary (IAS) Chemistry specification includes eight Core Practicals that link theoretical knowledge and understanding to practical scenarios.

Your knowledge and understanding of practical skills and activities will be assessed in all examination papers for the IAS Level Chemistry qualification.

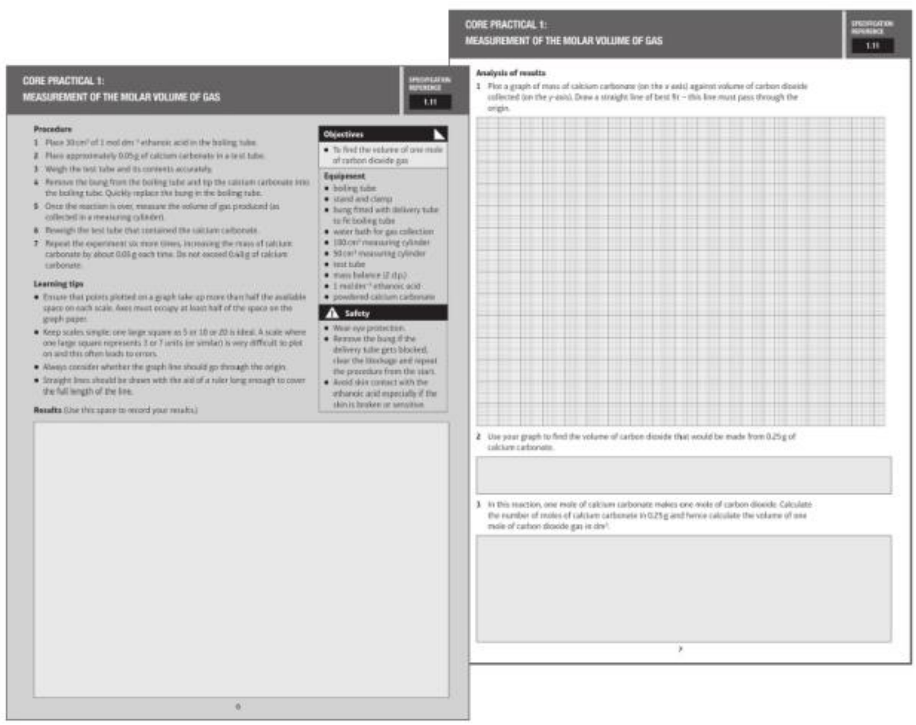
- Papers 1 and 2 will include questions based on practical activities, including novel scenarios.
- Paper 3 will test your ability to plan practical work, including risk management and selection of apparatus.

In order to develop practical skills, you should carry out a range of practical experiments related to the topics covered in your course. Further suggestions in addition to the Core Practicals are included in the specification which is available online.

| STUDENT BOOK TOPIC | IAS CORE PRACTICALS | |
|---|---|---|
| **TOPIC 1**<br>**FORMULAE, EQUATIONS AND AMOUNT OF SUBSTANCE** | **CP1** | Measurement of the molar volume of a gas |
| **TOPIC 6**<br>**ENERGETICS** | **CP2** | Determination of the enthalpy change of a reaction using Hess's Law |
| **TOPIC 8**<br>**REDOX CHEMISTRY AND GROUPS 1, 2 AND 7** | **CP3** | Finding the concentration of a solution of hydrochloric acid |
| | **CP4** | Preparation of a standard solution from a solid acid and use it to find the concentration of a solution of sodium hydroxide |
| **TOPIC 10**<br>**ORGANIC CHEMISTRY: HALOGENOALKANES, ALCOHOLS AND SPECTRA** | **CP5** | Investigation of the rates of hydrolysis of some halogenoalkanes |
| | **CP6** | Chlorination of 2-methylpropan-2-ol with concentrated hydrochloric acid |
| | **CP7** | The oxidation of propan-1-ol to produce propanal and propanoic acid |
| | **CP8** | Analysis of some inorganic and organic unknowns |


1E 1 MOLAR VOLUME CALCULATIONS

In the **Student Book**, the Core Practical specifications are supplied in the relevant sections.


CORE PRACTICAL 1:
MEASUREMENT OF THE MOLAR VOLUME OF GAS

This Student Book is accompanied by a **Lab Book**, which includes instructions and writing frames for the Core Practicals for you to record your results and reflect on your work. Practical skills practice questions and answers are also provided. The Lab Book records can be used as preparation for the Practical Skills Paper.

# ASSESSMENT OVERVIEW

The following tables give an overview of the assessment for Pearson Edexcel International Advanced Subsidiary (IAS) Level course in Chemistry. You should study this information closely to help ensure that you are fully prepared for this course and know exactly what to expect in each part of the examinations. More information about this qualification, and about the question types in the different papers, can be found in *Preparing for your exams* on page 296 of this book.

| PAPER / UNIT 1 | PERCENTAGE OF IAS | PERCENTAGE OF IAL | MARK | TIME | AVAILABILITY |
|---|---|---|---|---|---|
| **STRUCTURE, BONDING AND INTRODUCTION TO ORGANIC CHEMISTRY**<br>Written exam paper<br>Paper code WCH11/01<br>Externally set and marked by Pearson Edexcel<br>Single tier of entry | 40% | 20% | 80 | 1 hour 30 minutes | January, June and October<br>First assessment: January 2019 |

| PAPER / UNIT 2 | PERCENTAGE OF IAS | PERCENTAGE OF IAL | MARK | TIME | AVAILABILITY |
|---|---|---|---|---|---|
| **ENERGETICS, GROUP CHEMISTRY, HALOGENOALKANES AND ALCOHOLS**<br>Written exam paper<br>Paper code WCH12/01<br>Externally set and marked by Pearson Edexcel<br>Single tier of entry | 40% | 20% | 80 | 1 hour 30 minutes | January, June and October<br>First assessment: June 2019 |

| PAPER / UNIT 3 | PERCENTAGE OF IAS | PERCENTAGE OF IAL | MARK | TIME | AVAILABILITY |
|---|---|---|---|---|---|
| **PRACTICAL SKILLS IN CHEMISTRY 1**<br>Written exam paper<br>Paper / Unit code WCH13/01<br>Externally set and marked by<br>Pearson Edexcel<br>Single tier of entry | 20% | 10% | 50 | 1 hour 20 minutes | January, June and October<br>First assessment: June 2019 |

## ASSESSMENT OBJECTIVES AND WEIGHTINGS

| | | % IN IAS | % IN IA2 | % IN IAL |
|---|---|---|---|---|
| A01 | Demonstrate knowledge and understanding of science. | 34–36 | 29–31 | 32–34 |
| A02 | (a) Application of knowledge and understanding of science in familiar and unfamiliar contexts. | 34–36 | 33–36 | 33–36 |
| | (b) Analysis and evaluation of scientific information to make judgements and reach conclusions. | 9–11 | 14–16 | 11–14 |
| A03 | Experimental skills in science, including analysis and evaluation of data and methods. | 20 | 20 | 20 |

## RELATIONSHIP OF ASSESSMENT OBJECTIVES TO UNITS

| UNIT NUMBER | ASSESSMENT OBJECTIVE | | | |
|---|---|---|---|---|
| | A01 | A02 (a) | A02 (b) | A04 |
| UNIT 1 | 17–18 | 17–18 | 4.5–5.5 | 0.0 |
| UNIT 2 | 17–18 | 17–18 | 4.5–5.5 | 0.0 |
| UNIT 3 | 0.0 | 0.0 | 0.0 | 20 |
| **TOTAL FOR INTERNATIONAL ADVANCED SUBSIDIARY** | **34–36** | **34–36** | **9–11** | **20** |

# TOPIC 1 FORMULAE, EQUATIONS AND AMOUNT OF SUBSTANCE

## A ATOMS, ELEMENTS AND MOLECULES | B EQUATIONS AND REACTION TYPES | C ENERGY | D EMPIRICAL AND MOLECULAR FORMULAE | E CALCULATIONS WITH SOLUTIONS AND GASES

Studying chemistry at this level involves many skills. These skills include describing observations, giving explanations, planning and interpreting experiments. Although all of these skills are discussed in this topic, the most important feature of this part of the course involves using numbers. Some students have a natural ability for numbers, while others find them less attractive. Whatever your mathematical ability, it is important to spend as much time as possible focusing on this topic in order to improve.

Using numbers accurately is an important skill in so many occupations – here are just a few examples:

- in medicine, calculating the dosage of a drug to maximise benefit to the patient and minimise unwanted side-effects
- in business, predicting whether capital investment will produce a sufficient income to justify the investment
- in industry, considering whether the costs and polluting effects of a new method of making a molecule justify making the change
- in shipping operations (for example, the Costa Concordia in 2012), working out the volume of air needed to float a ship after an accident.

As far as your chemistry course is concerned, this topic is the foundation of success in other topics, such as energetics and kinetics.

### MATHS SKILLS FOR THIS TOPIC

- Use appropriate units and conversions, including for masses, gas and solution volumes
- Use standard and ordinary form, decimal places, and significant figures
- Use ratios, fractions and percentages, including in yield and atom economy calculations
- Rearrange expressions and substitute values

## What prior knowledge do I need?

- Using appropriate apparatus to measure masses and volumes, and recording values to the appropriate precision
- Knowing how to convert between different units of mass and volume
- Writing and balancing chemical equations, including the use of state symbols
- Using the mole as the unit for amount of substance
- Calculating the relative formula mass of a compound from relative atomic masses of elements

## What will I study in this topic?

- Using the mole in new situations, to calculate masses, volumes, concentrations and formulae
- Using experiments to obtain evidence for chemical formulae and equations
- Calculating percentage yields and atom economies from equations
- Interpreting observations from test-tube reactions, including displacement, neutralisation and precipitation

## What will I study later?

Topic 11 (Book 2: IAL)

- Kinetics calculations, including those based on measurements of mass and volume changes in experiments

Topic 12B (Book 2: IAL)

- Further calculations of enthalpy changes, including those relating to lattice energies

Topic 13 (Book 2: IAL)

- Calculation of equilibrium constants from concentrations

Topic 14 (Book 2: IAL)

- Calculations of pH, $K_a$, $K_w$ and other terms related to acids and bases

# 1A ATOMS, ELEMENTS AND MOLECULES

SPECIFICATION REFERENCE 1.1

## LEARNING OBJECTIVES

- Know the terms atom, element, ion, molecule, compound.

## THE PURPOSE OF THIS SECTION

In your previous study of chemistry, you have learned about several terms at an introductory level. In this book, you will study them in greater depth.

This topic is designed to revise some of the terms that you have met before, and will meet again in more detail.

## WHAT IS AN ELEMENT?

We can start by looking at a simplified version of the Periodic Table of Elements. You have already learned something about the Periodic Table and will learn more about it in **Topic 2**.

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| | | | H | | | | |
| | | | | | | | He |
| Li | Be | B | C | N | O | F | Ne |
| Na | Mg | Al | Si | P | S | Cl | Ar |

Each box in the Periodic Table contains a capital letter, or more often a pair of letters. The first one is always a capital letter and the second one is never a capital letter. Each letter or pair of letters represents an element. You will know some of them from your everyday life. For example, oxygen is an element you breathe, and iron is an element used to make bodies of cars and bicycles.

You may have been taught that an element is a substance that contains atoms of only one type. Elements are chemically the simplest substances so they cannot be broken down using chemical reactions. For example, neon is an element because it contains only neon atoms, which have the symbol Ne. It cannot be broken down into atoms of any other element. Water is not an element because it can be broken down into the elements hydrogen and oxygen.

This way of describing an element is sufficient for this stage of your studies, but more details will be required as you progress through this course. For example, some elements contain isotopes. You will learn about isotopes in **Topic 2**. Neon contains three stable isotopes, $^{20}Ne$, $^{21}Ne$, and $^{22}Ne$. All isotopes of the same element have the same number of protons and electrons, but different numbers of neutrons.

## WHAT IS AN ATOM?

You already know what an atom is, because we have used the term to help you understand what an element is. Atoms are far too small to be seen with the human eye. You can see a tiny grain of sand and this contains many billions of atoms of silicon and oxygen. An atom can be described as the smallest part of an element that has the properties of that element. This meaning is fine when you work through **Topic 1**. However, in **Topic 2** you will need to recall that atoms contain even smaller particles (protons, neutrons and electrons).

## WHAT IS A MOLECULE?

This is easier now that we know the meanings of element and atom.

You could describe a molecule as a particle made of two or more atoms bonded together.

If a molecule contains atoms of the same element, then the result is a molecule of an element. For example, a molecule that contains two atoms of hydrogen joined together can be represented by the formula $H_2$. This formula contains only one symbol (H), so it is the formula of an element.

If a molecule contains atoms of two or more different elements, then the result is a molecule of a compound. For example, a molecule that contains two atoms of hydrogen and one atom of oxygen joined together can be represented by the formula $H_2O$. This formula contains two different symbols, so it is the formula of a compound (water).

## WHAT IS A COMPOUND?

Now we can describe a compound. This is a substance containing atoms of different elements combined together.

Note that some compounds contain large numbers of atoms bonded together, but other compounds contain molecules with only two atoms. Some compounds contain oppositely charged ions. We will explore these differences in later sections of this book.

## WHAT IS AN ION?

One way to describe an ion is as a species consisting of one or more atoms joined together and having a positive or negative charge.

Note that this is not a description of how an ion is formed. **Topic 3A.1** will cover the formation of ions.

An ion with a positive charge is called a cation. An ion with a negative charge is called an anion.

**Table A** shows diagrams to illustrate the terms referred to. Each atom is shown as a circle containing the symbol of an element. The lines show bonds between atoms.

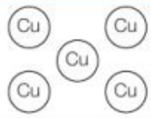
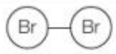
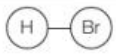
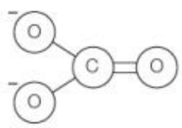
| TERM | DIAGRAM | NAME | SYMBOL OR FORMULA | NOTE |
|---|---|---|---|---|
| element |  | copper | $Cu$ | This is an element. All the atoms are the same. |
| atom |  | helium | $He$ | This is an atom of an element. |
| molecule |  | bromine | $Br_2$ | This is a molecule of an element. The atoms are the 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. |

**table A** Illustrations of terms used in this topic.

## OTHER TERMS

Elements that are made up of single atoms are described as monatomic. One example is helium, the gas used in weather balloons. The symbol for helium is He.

Elements and compounds made up of two atoms joined together are described as diatomic. The two main diatomic gases in the atmosphere are nitrogen ($N_2$) and oxygen ($O_2$).

Elements and compounds with molecules made up of several atoms joined together are described as polyatomic. Examples of polyatomic molecules are phosphorus ($P_4$) and methane ($CH_4$).

The same terms can be used for ions. Chloride ($Cl^-$) is an example of a monatomic ion. Hydroxide ($HO^-$ or $OH^-$) is a diatomic ion. A sulfate ion ($SO_4^{2-}$) is polyatomic as it contains five atoms.

### LEARNING TIP

It is often helpful to refer to a substance by its symbol or formula as well as its name so that your meaning is clear. For example, the word hydrogen could refer to a hydrogen atom (H), a hydrogen molecule ($H_2$) or a hydrogen ion ($H^+$).

### CHECKPOINT

1. Classify each of these symbols and formulae as atoms, molecules or ions.
   $Ne$ $CO_2$ $H^+$ $S_8$ $Al^{3+}$
2. Which of these formulae represent elements, compounds, or neither elements nor compounds? Explain your answer.
   $Br_2$ $H_2O_2$ $NO_3$ $O_3$ $CaO$

### DID YOU KNOW?

The names and symbols of many elements come from the Greek and Latin languages. For example, hydrogen comes from the Greek words for *water* and *producer*. This is because when hydrogen gas is burned, it forms (or 'produces') water. Another example is copper (Cu) – the symbol Cu comes from the Latin word *cuprum*, which means 'metal from Cyprus'. Cyprus is the island where the Romans obtained much of their copper.

# 1B 1 WRITING CHEMICAL EQUATIONS

SPECIFICATION REFERENCE 1.3

## LEARNING OBJECTIVES

- Write balanced full and ionic equations, including state symbols, for chemical reactions.

## WRITING EQUATIONS: WHAT TO REMEMBER

This topic is a useful summary of what you are expected to do when you write equations.

### WRITING FORMULAE FOR NAMES

You may be given the formulae of unfamiliar compounds in a question. You need to work out the formulae of many familiar compounds from their names, and to remember other formulae. You also need to show elements with the correct formulae. It is not possible to provide a complete list, but here are some examples.

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 $FeSO_4$
- iron(III) oxide is $Fe_2O_3$
- calcium carbonate is $CaCO_3$.

### EXAM HINT

Remember to use your Periodic Table in the exam. If you know the formula of *magnesium* sulfate then you can assume *strontium* sulfate has the same formula because Mg and Sr are in the same group.

### WRITING AN EQUATION FROM A DESCRIPTION

You will need to convert words into formulae and decide which ones are reactants and which ones are products.

Consider this 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.

Now you have to write the formulae in the correct places:

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

The next step is balancing the equation. You need to add up the numbers of all the atoms to make sure that, for each element, the totals are the same on both the left and the right side of the equation. In this example, there is one carbon, one calcium, two hydrogen and four oxygen atoms on each side, so the equation is already balanced.

Here is an example where the first equation you write is not balanced.

The description is:

hydrogen peroxide decomposes to water and oxygen.

The formulae are:

$$H_2O_2 \rightarrow H_2O + O_2$$

This is already balanced for hydrogen, but not for oxygen. With careful practice, which sometimes involves guessing until you get it right, you should be able to write the **coefficients** needed to balance the equation. In this case, the balanced equation is:

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

Most equations are balanced using whole-number coefficients, but using fractions or decimals is usually acceptable. This is especially the case in organic chemistry.

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

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

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

### USING STATE SYMBOLS

Many chemical equations include state symbols. The symbols are:
- (s) = solid
- (l) = liquid
- (g) = gas
- (aq) = aqueous (dissolved in water).

It is important to distinguish between (l) and (aq). A common error is to write $H_2O(aq)$ instead of $H_2O(l)$.

Although it is good practice to include state symbols in all equations, in some cases they are essential, while in other cases they are often omitted. For example, when writing equations to represent ionisation energies in **Topic 2A.4**, it is important to include (g) after each atom and ion. However, in **Topics 4 and 5** you will write equations for organic reactions, where state symbols are often not included.

Here is another description:
when aqueous solutions of silver nitrate and calcium chloride are mixed, a white precipitate of silver chloride forms. As this precipitate settles, a solution of calcium nitrate becomes visible.

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 EQUATIONS

Most equations are shown with a conventional (left to right) arrow $\rightarrow$. However, some important reactions are reversible. This means that the reaction can go both in the forward and backward (reverse) directions. The symbol $\rightleftharpoons$ is used in equations for these reactions. You can find guidance later in this book (**Topic 9B**) about when this reversible arrow should be used.

Sometimes a conventional arrow is made longer to allow information about the reaction to be shown above the arrow (and sometimes below it). This information might be about reaction conditions, such as temperature, pressure and the use of a catalyst. In organic chemistry, where reaction schemes are important, a label indicating, for example, Step 1, may be placed on the arrow in a sequence of reactions.

## IONIC EQUATIONS

### SIMPLIFYING FULL EQUATIONS

Ionic equations show any atoms and molecules involved, but only the ions that react together, and not the **spectator ions**.

This is the easiest method to follow for simplifying equations:

1 Start with the full equation for the reaction.

2 Replace the formulae of ionic compounds by their separate ions.

3 Delete any ions that appear identically on both sides.

### 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.

### LEARNING TIP

Consider carefully what the correct state symbol for a species should be. It may be different in different reactions. For example, water is never $H_2O(aq)$, but it may be $H_2O(s)$, $H_2O(l)$ or $H_2O(g)$, depending on the temperature.

### IONIC HALF-EQUATIONS

We write ionic half-equations for reactions involving oxidation and reduction, and they usually show what happens to only one reactant. A simple example is the reaction that occurs at the negative electrode during the electrolysis of aqueous sulfuric acid:

$$2H^+(aq) + 2e^- \rightarrow H_2(g)$$

You will learn much more about ionic half-equations in **Topic 8**.

## CHECKPOINT

1. Sodium thiosulfate ($Na_2S_2O_3$) solution reacts with dilute hydrochloric acid to form a precipitate of sulfur, gaseous sulfur dioxide and a solution of sodium chloride. Write an equation, including state symbols, for this reaction.
2. Solutions of ammonium sulfate and sodium hydroxide are warmed together to form sodium sulfate solution, water and ammonia gas. Write the simplest ionic equation for this reaction.

## SUBJECT VOCABULARY

**coefficient** the technical term for the number written in front of species when balancing an equation
**spectator ion** an ion that is there both before and after the reaction but is not involved in the reaction

# 1B 2 TYPICAL REACTIONS OF ACIDS

SPECIFICATION REFERENCE 1.12(ii)

## LEARNING OBJECTIVES

- Relate ionic and full equations, with state symbols, to observations from simple test-tube reactions, for reactions of acids.

## INTRODUCTION

Acids are common reagents in chemistry. In this topic, we summarise some of their typical reactions, using hydrochloric, nitric, sulfuric and phosphoric acids.

In each of these reactions, a salt is formed. The reactions can be used to prepare samples of salts.

## ACIDS WITH METALS

A general equation for these reactions is:

metal + acid → salt + hydrogen

Bubbles of hydrogen gas form, and if the salt formed is soluble, then a solution forms.

The metal must be sufficiently reactive to react in this way. For example, magnesium reacts but copper does not.

Typical equations for magnesium and hydrochloric acid are:

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

$$Mg(s) + 2H^+(aq) \rightarrow Mg^{2+}(aq) + H_2(g)$$

These reactions may appear to be examples of neutralisation reactions because the $H^+$ ions are removed from the solution when they react with the metal. However, as the $H^+$ ions gain electrons from the metal and are converted to $H_2(g)$, it means that the $H^+$ ions are reduced, not neutralised.

## ACIDS WITH METAL OXIDES AND INSOLUBLE METAL HYDROXIDES

A general equation for these reactions is:

metal oxide + acid → salt + water

metal hydroxide + acid → salt + water

The reactivity of the metal does not matter in these reactions because in the reactant it is present as metal ions, not metal atoms. The only observation is likely to be the formation of a solution.

Typical equations for copper(II) oxide and zinc hydroxide reacting with sulfuric acid are:

$$CuO + H_2SO_4 \rightarrow CuSO_4 + H_2O$$

$$CuO(s) + 2H^+(aq) \rightarrow Cu^{2+}(aq) + H_2O(l)$$

$$Zn(OH)_2 + H_2SO_4 \rightarrow ZnSO_4 + 2H_2O$$

$$Zn(OH)_2(s) + 2H^+(aq) \rightarrow Zn^{2+}(aq) + 2H_2O(l)$$

These reactions can be classified as neutralisation reactions because the $H^+$ ions react with $O^{2-}$ or $OH^-$ ions. They are not redox reactions because there is no change in the oxidation number of any of the species.

## ACIDS WITH ALKALIS

Metal hydroxides that dissolve in water are called alkalis. A general equation for these reactions is:

alkali + acid → salt + water

There are no visible changes during these reactions, although if a thermometer is used, a temperature rise can be noted.

Typical equations for sodium hydroxide reacting with phosphoric acid are:

$$NaOH + H_3PO_4 \rightarrow NaH_2PO_4 + H_2O$$

$$2NaOH + H_3PO_4 \rightarrow Na_2HPO_4 + 2H_2O$$

$$3NaOH + H_3PO_4 \rightarrow Na_3PO_4 + 3H_2O$$

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

A general equation for these reactions is:

metal carbonate + acid → salt + water + carbon dioxide

Bubbles of carbon dioxide gas form. If the salt formed is soluble, then a solution forms.

Typical equations for lithium carbonate reacting with hydrochloric acid are:

$$Li_2CO_3 + 2HCl \rightarrow 2LiCl + H_2O + CO_2$$

$$CO_3^{2-}(aq) + 2H^+(aq) \rightarrow H_2O(l) + CO_2(g)$$

These reactions can be classified as neutralisation reactions because the $H^+$ ions react with $CO_3^{2-}$ ions. They are not redox reactions because there is no change in the oxidation number of any of the species.

▲ **fig A** Many old buildings are made from carbonates such as limestone. Centuries of reaction between limestone and acids in the atmosphere have caused damage to the walls of Kolossi Castle in Cyprus.

## ACIDS WITH HYDROGENCARBONATES

Hydrogencarbonates are compounds containing the hydrogencarbonate ion ($HCO_3^-$), and they react with acids in the same way as carbonates. The best-known example is sodium hydrogencarbonate ($NaHCO_3$), commonly known as bicarbonate of soda or baking soda. Baking soda is used in cooking at home and in the food industry. The 'lightness' of baked food such as cakes is due to the formation of bubbles of carbon dioxide in the cake mixture, which cause the cake to rise.

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

A suitable test for the presence of carbonate or hydrogencarbonate ions in a solid or solution is to add an aqueous acid and to test the gas produced with limewater (see **Topic 8B.4**).

### LEARNING TIP

Practise writing full and ionic equations for different reactions of acids.

### CHECKPOINT

**1.** Write full equations for the reactions between:

(a) zinc and sulfuric acid

(b) aluminium oxide and hydrochloric acid.

**2.** Write the simplest ionic equations for the reactions between:

(a) zinc and hydrochloric acid

(b) magnesium carbonate and nitric acid.

# 1B 3 DISPLACEMENT REACTIONS

SPECIFICATION REFERENCE 1.12(i)

## LEARNING OBJECTIVES

- Relate ionic and full equations, with state symbols, to observations from simple test-tube reactions, for displacement reactions.

## WHAT IS A DISPLACEMENT REACTION?

As you learn about more chemical reactions, you will know that they are often classified into different types of reaction. You will recognise reaction types such as addition, neutralisation, combustion, oxidation and several others.

In this topic, we look at a reaction type called displacement. In simple terms, it is a reaction in which one element replaces another element in a compound.

## 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 REACTIONS IN AQUEOUS SOLUTION

Take a closer look at Reaction 1, shown above. 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:

$$Mg(s) + Cu^{2+}(aq) + SO_4^{2-}(aq) \rightarrow Cu(s) + Mg^{2+}(aq) + SO_4^{2-}(aq)$$

Cancelling the ions that appear identically on both sides gives:

$$Mg(s) + Cu^{2+}(aq) \rightarrow Cu(s) + Mg^{2+}(aq)$$

Now you can see that this is a redox reaction. Electrons are transferred from magnesium atoms to copper(II) ions, so magnesium atoms are oxidised (loss of electrons) and copper(II) ions are reduced (gain of electrons).

This reaction is just one example of many similar reactions in which a more reactive metal displaces a less reactive metal from one of its salts. You may come across this and other similar reactions as examples used in the measurement of temperature changes.

**fig A** The photo shows what happens when a copper wire is placed in silver nitrate solution for some time. You can see the results of the displacement reaction, the 'growth' on the wire is silver metal and the blue solution contains the copper(II) nitrate that is formed.

### METAL DISPLACEMENT REACTIONS IN THE SOLID STATE

Reaction 2 is used in the railway industry to join rails together. You might imagine that a good way to join rails together would be by welding, but the metal rails are good conductors of heat and it is very difficult to get the ends of two rails hot enough for them to melt and join together.

For this reason, the thermite method is used. A mixture of aluminium and iron(III) oxide is positioned just above the place where the two rails are to be joined. A magnesium fuse is lit, and Reaction 2 occurs. 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.

As in Reaction 1, the equation can be rewritten ionically and simplified:

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

then:

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

As with Reaction 1, you can see that this is s a redox reaction. 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).

**fig** B The thermite reaction. The flame comes from the highly exothermic reaction forming molten iron. The molten iron will be used to fill the gap between two rails and form a strong join between them.

## DISPLACEMENT REACTIONS INVOLVING HALOGENS

In **Topic 8C.2**, we will look at how more reactive halogens can displace less reactive halogens from their compounds. For example, chlorine will displace bromine from a potassium bromide solution. The full, ionic and simplified ionic equations for this reaction are:

$$Cl_2(aq) + 2KBr(aq) \rightarrow Br_2(aq) + 2KCl(aq)$$

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

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

As with the metal displacement reactions, this is a redox reaction. Electrons are transferred from bromide ions to chlorine, so bromide ions are oxidised (loss of electrons) and chlorine is reduced (gain of electrons).

### LEARNING TIP

When describing displacement reactions, be careful to refer to the correct species. For example, in the reaction between magnesium and copper(II) sulfate, magnesium *atoms* and copper(II) *ions* are involved.

### CHECKPOINT

1. Iron metal reacts with silver nitrate in a displacement reaction to form silver and iron(II) nitrate. Write a full equation, an ionic equation and a simplified ionic equation for this reaction. Include state symbols in all your equations.
2. A mixture of zinc metal and copper(II) oxide is ignited, causing an exothermic reaction to occur. Write a full equation, an ionic equation and a simplified ionic equation for this reaction. Do not include state symbols in your equations.

### SUBJECT VOCABULARY

**displacement reaction** a reaction in which one element replaces another, less reactive, element in a compound

# 1B 4 PRECIPITATION REACTIONS

SPECIFICATION REFERENCE 1.12(iii)

## LEARNING OBJECTIVES

- Relate ionic and full equations, with state symbols, to observations from simple test-tube reactions, for precipitation reactions.

In this topic, we focus on two aspects of **precipitation reactions**:
- their use in chemical tests
- their use in working out chemical equations.

## CHEMICAL TESTS

### CARBON DIOXIDE

This may be your earliest memory of a precipitation reaction. 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.

▲ **fig A** Limewater is a colourless solution. As more carbon dioxide is bubbled through it, the amount of white precipitate increases.

### 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:

$$Na_2SO_4(aq) + BaCl_2(aq) \rightarrow BaSO_4(s) + 2NaCl(aq)$$

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

This test is covered in more detail in **Topic 8B.4**.

### 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:

$$NaCl(aq) + AgNO_3(aq) \rightarrow AgCl(s) + NaNO_3(aq)$$

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

This test is covered in more detail in **Topic 8C.4**.

## WORKING OUT EQUATIONS

A good example of using a precipitation reaction to work out an equation is the reaction between aqueous solutions of lead nitrate and potassium iodide. Both reactants are colourless solutions. When they are mixed, a yellow precipitate of lead iodide forms.

The word equation for this reaction is:

lead nitrate + potassium iodide → lead iodide + potassium nitrate

Here is an outline of the experiment.

- Place the same volume of a potassium iodide solution in a series of test tubes.
- Add different volumes of a lead nitrate solution to the tubes.
- Place each tube in a centrifuge and spin the tubes for the same length of time.
- Measure the depth of precipitate in each tube.

**Table A** shows the results of one experiment.

The concentration of both solutions is $1.0\,mol\,dm^{-3}$.

The depth of each precipitate indicates the mass of precipitate formed.

| TUBE | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|---|---|---|---|---|---|---|---|
| volume of potassium iodide solution / $cm^3$ | 5.0 | 5.0 | 5.0 | 5.0 | 5.0 | 5.0 | 5.0 |
| volume of lead nitrate solution / $cm^3$ | 0.5 | 1.0 | 1.5 | 2.0 | 2.5 | 3.0 | 3.5 |
| depth of precipitate / cm | 2.5 | 3 | 4 | 5 | 6 | 6 | 6 |

**table A** Results of the reaction between aqueous solutions of lead nitrate and potassium iodide in one experiment.

The diagram shows the tubes at the end of the experiment.

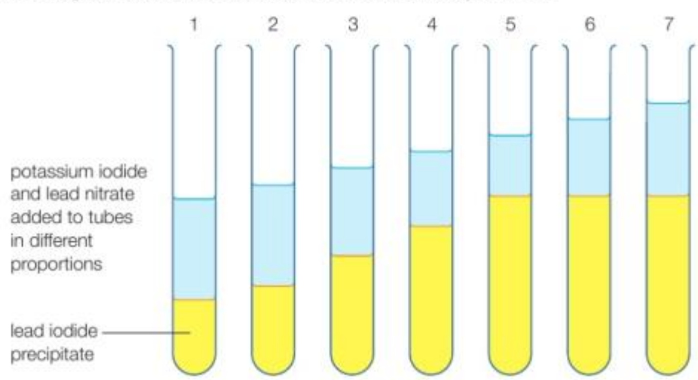



**fig B** As more lead nitrate solution is added, more lead iodide precipitate forms.

You can see that there is no increase in the amount of precipitate from tube 5 to tube 6. This shows that the reaction is incomplete in tubes 1, 2, 3 and 4, but is complete in tube 5. The amounts, in moles, of reactants used in tube 5 are calculated as follows:

$n$(potassium iodide) = 0.005 × 1.0 = 0.005 mol

$n$(lead nitrate) = 0.0025 × 1.0 = 0.0025 mol

This shows that lead nitrate reacts with potassium iodide in the ratio 1 : 2.

The equations for the reaction are:

$$Pb(NO_3)_2(aq) + 2KI(aq) \rightarrow PbI_2(s) + 2KNO_3(aq)$$

$$Pb^{2+}(aq) + 2I^-(aq) \rightarrow PbI_2(s)$$

## LEARNING TIP

Practise calculating the amounts of reactants and products in tubes 1–4.

## CHECKPOINT

1. Write the simplest ionic equation, including state symbols, for:
   (a) the test for a sulfate
   (b) the test for a chloride.
2. Calculate the amounts, in moles, of each reactant and product in tube 7 in **fig B**.

SKILLS PROBLEM SOLVING

## SUBJECT VOCABULARY

**precipitation reaction** reaction in which an insoluble solid is formed when two solutions are mixed

# 1C 1 COMPARING MASSES OF SUBSTANCES

SPECIFICATION REFERENCE 1.1 1.2 1.4

## LEARNING OBJECTIVES

- Understand the terms: relative atomic mass, based on the $^{12}C$ scale; relative molecular mass; relative formula mass; molar mass, as the mass per mole of a substance in g $mol^{-1}$.
- Understand how to calculate relative molecular mass and relative formula mass from relative atomic masses.
- Perform calculations using the Avogadro constant $L$ ($6.02 \times 10^{23}$ $mol^{-1}$).

## RELATIVE ATOMIC MASS ($A_r$)

As chemists discovered more and more elements in the nineteenth century, they began to realise that the masses of the elements were different. They could not weigh individual atoms, but they were able to use numbers to compare the masses of atoms of different elements. For this reason, they began to use the term 'relative atomic mass'.

The chemists soon realised that the element whose atoms had the smallest mass was hydrogen, so the relative atomic mass of hydrogen was fixed as 1. Atoms of silicon had double the mass of nitrogen atoms, and nitrogen atoms were 14 times heavier than hydrogen atoms. This meant that the relative atomic mass of nitrogen was 14, and that of silicon was 28. At first, mostly whole numbers were used, but eventually it was possible to find the mass of an atom to several decimal places. The Periodic Table in the Data Booklet uses 1 decimal place for lighter elements and whole numbers for heavier ones.

After the discovery of isotopes, the $^{12}C$ isotope of carbon was used in the definition of relative atomic mass.

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:

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

## RELATIVE MOLECULAR MASS ($M_r$)

Relative atomic masses are used for atoms of elements. Relative molecular masses are used for molecules of both elements and compounds. They are easily calculated by adding relative atomic masses.

**Table A** shows values for some common elements taken from the Data Booklet.

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

**table A**

Note that $A_r$ and $M_r$ do not have units.
Here are some examples of calculations.

### 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, $H_2SO_4$?

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

### EXAM HINT

Make sure you use the relative atomic masses shown on the Periodic Table in the Data Booklet.

## RELATIVE FORMULA MASS ($M_r$)

This term has the same symbol as relative molecular mass, but the 'formula' part means that it includes both molecules and ions. Worked example 3 below is slightly more complicated because of the water of crystallisation, but there is also another problem. Hydrated copper(II) sulfate is an ionic compound, so it is not a good idea to refer to its relative *molecular* mass. That is why it is called relative *formula* mass.

### WORKED EXAMPLE 3

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

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

The term 'relative formula mass' should also be used for compounds with giant structures, such as sodium chloride and silicon dioxide.

## MOLAR MASS ($M$)

Another way around the problem in Worked example 3 is to use the term **molar mass**, which is the mass per mole of any substance (molecular or ionic). Its symbol is $M$ (not $M_r$) and it has the units g $mol^{-1}$ (grams per mole). Here we have a new term (the mole) which will be fully explained in **Topic 1C.2**. For now, you can think of one mole (1 mol) of a substance as being the same quantity as the relative formula mass of the substance, with the units of grams.

So, this is the expression you can use:

$$\text{amount in mol} = \frac{\text{mass of substance in g}}{\text{molar mass in g mol}^{-1}} \text{ or } n = \frac{m}{M}$$

**Table B** shows examples of working out the amounts in moles of some substances using this expression.

| SUBSTANCE | $O_2$ | $CH_4$ | $H_2O$ | $NH_4NO_3$ |
|---|---|---|---|---|
| mass in g | 5.26 | 4.0 | 100 | 14.7 |
| molar mass, $M$ in g mol$^{-1}$ | 32.0 | 16.0 | 18.0 | 80.0 |
| amount in mol | 0.164 | 0.25 | 5.56 | 0.184 |

table B

## THE AVOGADRO CONSTANT

Amedeo Avogadro (1776–1856) was an Italian chemist whose name is used in naming the **Avogadro constant**. We are introducing him here because the scaling-up factor from atoms, molecules and ions to grams is named after him.

▲ **fig A** The Italian chemist, Amedeo Avogadro

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

You do not need to know a definition of the Avogadro constant, and it is best to think of it as the number of particles (atoms, molecules or ions) in one mole of any substance. For example, there are:

$6.02 \times 10^{23}$ helium atoms in 4.0 g of He

$6.02 \times 10^{23}$ carbon dioxide molecules in 44.0 g of $CO_2$

$6.02 \times 10^{23}$ nitrate ions in 62.0 g of $NO_3^-$

### CALCULATIONS USING THE AVOGADRO CONSTANT

You will need to use the value of $L$ in the types of calculation shown here.

1 Calculate the number of particles in a given mass of a substance. Start by using the expression:

$$\text{amount in mol} = \frac{\text{mass of substance in g}}{\text{molar mass in g mol}^{-1}} \text{ or } n = \frac{m}{M}$$

then multiply the amount in mol by 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 = $6.02 \times 10^{23} \times 0.0694 = 4.18 \times 10^{22}$

2 Calculate the mass of a given number of particles of a substance: start by dividing the number of particles by the Avogadro constant, then multiply the result by the molar mass.

### 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.)

### CHECKPOINT

**1.** Malachite is an important mineral with the formula $Cu_2CO_3(OH)_2$. Calculate its relative formula mass.

**2.** How many molecules of sugar ($C_{12}H_{22}O_{11}$) are there in a teaspoon measure (4.20 g)?

### DID YOU KNOW?

**The symbol $L$ is used for the Avogadro constant (using $A$ would be confusing because of the use of $A_r$ for relative atomic mass). $L$ comes from the surname of Johann Josef Loschmidt (1821–1895), an Austrian chemist who was a contemporary of Avogadro. He made many contributions to our understanding of the same area of knowledge.**

### SUBJECT VOCABULARY

**molar mass** the mass per mole of a substance; it has the symbol $M$ and the units g mol$^{-1}$

**Avogadro constant ($L$)** $6.02 \times 10^{23}$ mol$^{-1}$, the number of particles in one mole of a substance

# 1C 2 CALCULATIONS INVOLVING MOLES

SPECIFICATION REFERENCE 1.2

## LEARNING OBJECTIVES

- Know that the mole (mol) is the unit for the amount of a substance.

## WHAT IS A MOLE?

So far, we have referred to the mole and have used it in a simple form of calculation, but we have not properly explained what it is.

### THE 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 12 g of the $^{12}C$ isotope.

This definition is not easy to understand, but will be explained as you read on.

▲ **fig A** From left to right: tin (Sn), magnesium (Mg), iodine (I) and copper (Cu). Each sample contains $6.02 \times 10^{23}$ atoms.

### COUNTING ATOMS

As you know, atoms are very tiny particles that cannot be seen by the human eye. When we look at the sand on a beach, we are looking at billions and billions of atoms of, mostly, silicon and oxygen in the compound silicon dioxide ($SiO_2$). Quoting the actual numbers of atoms involved in a reaction, whether in a test tube or on an industrial scale, would involve extremely large numbers that would be very difficult to handle.

You are already familiar with the use of relative atomic masses to compare the relative masses of atoms. In a water molecule, the oxygen atom has a mass that is 16 times greater than the mass of a hydrogen atom. You know this because in the Periodic Table the relative atomic masses are H = 1.0 and O = 16.0. Note the word 'relative'. These values do not tell us the actual mass in grams of an oxygen atom or a hydrogen atom. They only tell us that an oxygen atom has a mass 16 times greater than that of a hydrogen atom.

Now consider using these numbers (16.0 and 1.0) with the familiar unit g (grams). You can more easily visualise 16.0 g of oxygen than a single atom of oxygen. Doing this is effectively scaling up on a very large scale. The number of oxygen atoms in 16.0 g of oxygen is the same as the number of hydrogen atoms in 1.0 g of hydrogen.

## CALCULATIONS USING MOLES

### WHAT TO REMEMBER WHEN DOING CALCULATIONS

You can use the mole to count atoms, molecules, ions, electrons and other species. So, it is important to include an exact description of the species being referred to. Consider the examples of hydrogen, oxygen and water.

One mole of water has a mass of 18.0 g, but what is the mass of one mole of hydrogen or oxygen? It depends on whether you are referring to atoms or molecules, so you need to make this clear.

Remember that the symbol $n$ is used for the amount of substance in mol.

Consider the substances in **table A**. The masses are the same, but the amounts are different.

| | 1g OF OXYGEN ATOMS (O) | 1g OF OXYGEN MOLECULES ($O_2$) | 1g OF OZONE MOLECULES ($O_3$) |
|---|---|---|---|
| $n$ (amount in mol) | 1 ÷ 16.0 = 0.0625 mol | 1 ÷ 32.0 = 0.0313 mol | 1 ÷ 48.0 = 0.0208 mol |

**table A**

You should always clearly identify the species that you are referring to if there is any possibility that there could be more than one meaning. This is not usually necessary for compounds.

It is good practice to refer to both the formula and the name. Examples include:

- the amount, in moles, of O in 9.4 g of oxygen atoms (0.59 mol)
- the amount, in moles, of $O_2$ in 9.4 g of oxygen molecules (0.29 mol)
- the amount, in moles, of $O_3$ in 9.4 g of ozone molecules (0.20 mol)
- the amount, in moles, of $CO_2$ in 9.4 g of carbon dioxide (0.21 mol)
- the amount, in moles, of $SO_4^{2-}$ in 9.4 g of sulfate ions (0.098 mol).

### THE EQUATION FOR CALCULATING MOLES

The equation for calculating moles is:

$$\text{amount of substance in moles} = \frac{\text{mass in grams}}{\text{molar mass}} \text{ or } n = \frac{m}{M}$$

You will use this expression in many calculations during your study of chemistry. It is often rearranged as:

$$M = \frac{m}{n} \text{ or } m = n \times M$$

### 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?

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

## LEARNING TIP

When using moles, always make clear what particles you are referring to: atoms, molecules, ions or electrons. It is also a good idea to state the formula.

## CHECKPOINT

**1.** What is the amount of substance in each of the following?

(a) 8.00 g of sulfur, S

(b) 8.00 g of sulfur dioxide, $SO_2$

(b) 8.00 g of sulfate ions, $SO_4^{2-}$

**2.** How many particles are there of the specified substance?

(a) atoms in 2.00 g of sulfur, S

(b) molecules in 4.00 g of sulfur dioxide, $SO_2$

(b) ions in 8.00 g of sulfate ions, $SO_4^{2-}$

SKILLS ADAPTIVE LEARNING

## SUBJECT VOCABULARY

**mole** the amount of substance that contains the same number of particles as the number of carbon atoms in exactly 12 g of $^{12}C$

# 1C 3 CALCULATIONS USING REACTING MASSES

SPECIFICATION REFERENCE

1.7 1.10

## LEARNING OBJECTIVES

- Use chemical equations to calculate reacting masses and vice versa, using the concepts of amount of substance and molar mass.
- Determine a formula or confirm an equation by experiment, including evaluation of the data.

## INTRODUCTION TO REACTING MASSES

You can use the ideas from previous topics about amounts of substance and equations to do calculations involving the masses of reactants and products in equations.

A balanced equation for a reaction shows the same number of each species (atoms, molecules, ions or electrons) on both sides of the equation. It is also balanced for the masses of each species. This means that we can make predictions about the masses of reactants, which are needed to form a specified mass or amount of a product, or the other way round.

Consider this equation used in the manufacture of ammonia:

$$N_2 + 3H_2 \rightarrow 2NH_3$$

This shows that one molecule of nitrogen reacts with three molecules of hydrogen to form two molecules of ammonia.

This statement can be made about the amounts involved:

1 mol of $N_2$ reacts with 3 mol of $H_2$ to form 2 mol of $NH_3$.

This statement can be made about the masses involved:

28.0 g of $N_2$ reacts with 6.0 g of $H_2$ to form 34.0 g of $NH_3$.

These amounts and masses can have many other values, as long as the ratio does not change.

### CALCULATING REACTING MASSES FROM EQUATIONS

Using a balanced equation, predictions can be made about reacting masses.

#### 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

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

Step 2: calculate the amount of sulfuric acid

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

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

$$m = n \times M = 0.765 \times 80.1 = 61.2\ \text{g}$$

## 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

You might assume that the formulae and equations for all reactions are already known. However, there are sometimes two or more possible formulae for a substance. There can also be more than one reaction for the same reactants. Reacting masses can be used to identify the correct formula, or which of the reactions is occurring.

## 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 $CuO + H_2 \rightarrow Cu + H_2O$

## LEARNING TIP

One important part of both these calculation methods is the use of the relevant ratio from the equation. Practise deciding which substances should be used for the ratio and which way round to use the ratio.

## CHECKPOINT

SKILLS ADAPTIVE LEARNING

1. A fertiliser manufacturer makes a batch of 20 kg of ammonium nitrate. What mass of ammonia, in kg, does the manufacturer need to start with?
2. A sample of an oxide of iron was reduced to iron by heating with hydrogen. The mass of iron obtained was 4.35 g and the mass of water was 1.86 g. Deduce the equation for the reaction that occurred.

▲ **fig A** Chemistry on this scale needs careful calculations so that no reactants are wasted.

## SUBJECT VOCABULARY

**hydrate** compound containing water of crystallisation, represented by formulae such as $CuSO_4.5H_2O$ .

# 1C 4 THE YIELD OF A REACTION

SPECIFICATION REFERENCE 1.9

## LEARNING OBJECTIVES

- Calculate percentage yields in laboratory and industrial processes using chemical equations and experimental results.

**fig A** Pharmaceutical companies are always looking for ways to increase the percentage yield when manufacturing a drug.

## THEORETICAL YIELD, ACTUAL YIELD AND PERCENTAGE YIELD

In the laboratory, when you are making a product, you naturally want to obtain as much of it as possible from the reactants you start with. In industry, where reactions occur on a much larger scale, and there is economic competition between manufacturers, it is even more important to maximise the product of a reaction.

There are some reasons why the mass of a reaction product may be less than the maximum possible.
- The reaction is reversible and so may not be complete.
- There are side-reactions that lead to other products that are not wanted.
- The product may need to be purified, which may result in loss of product.

### TERMINOLOGY RELATING TO 'YIELD'

We normally use the term 'yield' with other words, such as:
- **theoretical yield**
- **actual yield**
- **percentage yield**.

In the laboratory, theoretical yield and actual yield may be measured in grams, but in industry, kilograms and tonnes are more likely to be used. Percentage yield is the term most often used, but you need to understand the other two terms first.

### THEORETICAL YIELD

We calculate theoretical yield using the equation for the reaction, and we use a method you are familiar with from previous topics. It is always assumed that the reaction goes to completion, with no losses.

### 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

Percentage yield is calculated using the equation:

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

This calculation may be done independently or in conjunction with the calculation of theoretical yield.

### EXAM HINT

You may be asked in a question to suggest why you have a low yield. If so, you should give a specific example in the reaction method where you may have lost product such as, 'some solution was left on the filter paper during filtration'.

### 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.

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

### LEARNING TIP

For calculations using kilograms and tonnes, remember that:

$1\text{ kg} = 1 \times 10^3\text{ g}$

$1\text{ tonne} = 1 \times 10^6\text{ g}$

### CHECKPOINT

SKILLS ADAPTIVE LEARNING

1. A student prepares a sample of copper(II) sulfate crystals, $CuSO_4.5H_2O$, weighing 7.85 g. She started with 4.68 g of copper(II) oxide. What is the percentage yield?
2. A manufacturer makes some ethanoic acid using this reaction:

   $$CH_3OH + CO \rightarrow CH_3COOH$$

   Starting with 50.0 kg of methanol, the manufacturer obtains 89.2 kg of ethanoic acid. What is the percentage yield?

### SUBJECT VOCABULARY

**theoretical yield** the maximum possible mass of a product in a reaction, assuming complete reaction and no losses

**actual yield** the actual mass obtained in a reaction

**percentage yield** the actual yield divided by the theoretical yield, expressed as a percentage

# 1C 5 ATOM ECONOMY

SPECIFICATION REFERENCE 1.9

## LEARNING OBJECTIVES

- Calculate percentage atom economies using chemical equations and experimental results.

## BACKGROUND TO ATOM ECONOMY

In **Topic 1C.4**, we looked at the percentage yield of a reaction. The closer the value is to 100%, the better. A higher percentage means that less of the starting materials are lost or end up as unwanted products.

Percentage yield is an important factor to take into consideration when assessing the suitability of an industrial process. However, it is not the only one. Other factors include:

- the availability or scarcity of non-renewable raw materials
- the cost of raw materials
- the quantity of energy needed.

## HOW ATOM ECONOMY WORKS

Here is an example of **atom economy** in action.

There are two main processes in the manufacture of phosphoric acid. To make the comparison easier to follow, a single summary equation is shown for each process.

Process 1 $Ca_3(PO_4)_2 + 3H_2SO_4 \rightarrow 2H_3PO_4 + 3CaSO_4$

Process 2 $P_4 + 5O_2 + 6H_2O \rightarrow 4H_3PO_4$

There are advantages and disadvantages of both processes. However, what you can see from these equations is that all of the atoms in the starting materials for Process 2 end up in the desired product. In Process 1, many of the atoms end up in a second, unwanted product, calcium sulfate. Process 1 has a lower atom economy than Process 2.

### THE CONTRIBUTION OF BARRY TROST

fig A Barry Trost is a pioneer of the concept of atom economy.

A chemist from the USA, Barry Trost, developed the idea of atom economy as an alternative way of assessing chemical reactions, especially in industrial processes. He believed that it was important to consider how many atoms from the reactants end up in the desired product.

The expression we use to calculate atom economy (usually described as percentage atom economy) is:

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

You can see that you do not need a calculator to work out the atom economy of Process 2. There is only one product, so it must be 100%.

$$\text{For Process 1, atom economy} = \frac{(98.0 \times 2) \times 100}{(98.0 \times 2) + (136.2 \times 3)} = 32.4\%$$

So, you can see that less than one-third of the mass of the starting materials ends up in the desired product, which does not look good if the $CaSO_4$ is a waste product that has to be disposed of. If the other product has a use, then the manufacturer can sell it, which would partly balance the low atom economy of the process. Even if the percentage yield of Process 1 was as high as 100%, the atom economy is still only 32.4%.

### REACTION TYPES AND ATOM ECONOMY

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.

### CHECKPOINT

**1.** Ethanol can be manufactured by the hydration of ethene:

$C_2H_4 + H_2O \rightarrow C_2H_5OH$

What is the atom economy of this process?

**2.** Ethene can be manufactured by the dehydration of ethanol:

$C_2H_5OH \rightarrow C_2H_4 + H_2O$

What is the atom economy of this process?

### SUBJECT VOCABULARY

**atom economy** the molar mass of the desired product divided by the sum of the molar masses of all the products, expressed as a percentage

### LEARNING TIP

Remember that percentage yield indicates how efficient a reaction is at converting the reactants to the products. Atom economy indicates the percentage of atoms from the starting materials that end up in the desired product.

### EXAM HINT

Also note that if you have more than one product, you will need time and energy to separate the desired product from the mixture.

# 1D 1 EMPIRICAL FORMULAE

SPECIFICATION REFERENCE 1.1 1.6

## LEARNING OBJECTIVES

- Know the term empirical formula.
- Use experimental data to calculate empirical formulae.

## INTRODUCTION TO EMPIRICAL FORMULAE

The three letters 'mol' appear in several words used in chemistry. You will know some of these from your previous studies, especially 'molecule', which is a group of two or more atoms joined together by covalent bonds. You know that a molecule of water can be represented by the formula $H_2O$, so this is the molecular formula of water. You have already come across the term 'relative molecular mass', which you will probably remember is 18 (or more accurately, 18.0) for water.

The term 'empirical' indicates that some information has been found by experiment. An **empirical formula** shows the smallest whole number ratio of the atoms of each element in a compound.

### ONE EXAMPLE OF AN EXPERIMENTAL METHOD

A simple example involves determining the formula of an oxide of copper. This oxide can be converted to copper by removing the oxygen.

Here are the steps in the experiment.

- Place a known mass of the oxide of copper in the tube.
- Heat the oxide in a stream of hydrogen gas (or natural gas, which is mostly methane).
- The gas reacts with the oxygen in the copper oxide and forms steam.
- The colour of the solid gradually changes to orange-brown, which is the colour of copper.
- The excess gas is burned off at the end of the tube for safety reasons.
- After cooling, remove and weigh the solid copper.
- It is good practice to heat the solid again in the stream of the gas to check whether its mass changes. Heating to a constant mass suggests that the conversion to copper is complete.

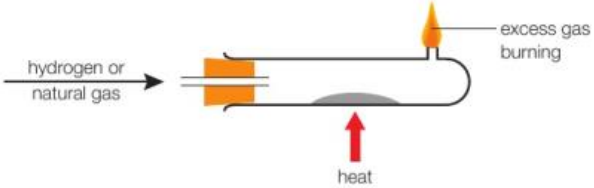



**fig A** This apparatus can be used to convert copper oxide to copper by removing the oxygen.

## CALCULATING EMPIRICAL FORMULAE

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.

The numbers may not be in an exact ratio because of experimental error, but you should be able to decide what the nearest whole-number ratio is.

Use at least two significant figures in the calculation (preferably three), and beware of inappropriate rounding. For example, you cannot convert a 1.2 : 1.2 : 1.9 ratio to 1 : 1 : 2, because that would give you the wrong answers.

It may help you to organise the calculation using a table, although this is not essential.

### CALCULATION USING MASSES

Assume that these are the results of the experiment outlined on the left.

mass of copper oxide = 4.28 g

mass of copper = 3.43 g

mass of oxygen removed is 4.28 − 3.43 = 0.85 g

**Table A** is the calculation table for these results.

| | Cu | O |
|---|---|---|
| mass of element / g | 3.43 | 0.85 |
| relative atomic mass | 63.5 | 16.0 |
| division by $A_r$ | 0.0540 | 0.0531 |
| ratio | 1 | 1 |

**table A**

Here, the ratio is obviously 1 : 1, so the empirical formula is CuO.

### CALCULATION USING PERCENTAGE COMPOSITION BY MASS

You do the calculation in the same way, except that you divide percentages instead of masses by the relative atomic masses.

The calculation table, **table B**, refers to a compound containing three elements. The compound has the percentage composition by mass C = 38.4%, H = 4.8%, Cl = 56.8%.

| | C | H | Cl |
|---|---|---|---|
| % of element | 38.4 | 4.8 | 56.8 |
| relative atomic mass | 12.0 | 1.0 | 35.5 |
| division by $A_r$ | 3.2 | 4.8 | 1.6 |
| ratio | 2 | 3 | 1 |

**table B**

You can see that the empirical formula is $C_2H_3Cl$.

## CALCULATION WHEN THE OXYGEN VALUE IS NOT PROVIDED

The results for some compounds do not include values for oxygen because it is often difficult to obtain an experimental value for the mass of oxygen. Sometimes you will need to remember to calculate the percentage of oxygen by subtraction. Here is an example.

A compound has the percentage composition by mass Na = 29.1%, S = 40.5%, with the remainder being oxygen.

The percentage of oxygen = 100 − (29.1 + 40.5) = 30.4%.

**Table C** is the calculation table.

| | Na | S | O |
|---|---|---|---|
| % of element | 29.1 | 40.5 | 30.4 |
| relative atomic mass | 23.0 | 32.1 | 16.0 |
| division by $A_r$ | 1.27 | 1.26 | 1.90 |
| division by the smallest | 1 | 1 | 1.5 |
| ratio | 2 | 2 | 3 |

**table C**

You can now see that the empirical formula is $Na_2S_2O_3$.

### EXAM HINT

Take care to look out for decimals that indicate obvious fractions, e.g., simplest ratio 1 : 1.33 indicates an empirical formula of 3 : 4. How would a ratio of 1 : 1.25 convert into an empirical formula?

## CALCULATION USING COMBUSTION ANALYSIS

Many organic compounds contain carbon and hydrogen, or carbon, hydrogen and oxygen. When a known mass of an organic compound is completely burned, it is possible to collect and measure the masses of carbon dioxide and water formed. The calculation is more complex because there are extra steps. Here is an example.

A 1.87 g sample of an organic compound was completely burned, forming 2.65 g of carbon dioxide and 1.63 g of water.

In this type of calculation, the first steps are to calculate the masses of carbon and hydrogen in the carbon dioxide and water.

- The relative molecular mass of carbon dioxide is 44.0 but, because the relative atomic mass of carbon is 12.0, the proportion of carbon in carbon dioxide is always 12.0 ÷ 44.0.
- Similarly, the proportion of hydrogen in water is always (2 × 1.0) ÷ 18.0.

All of the carbon in the carbon dioxide comes from the carbon in the organic compound. Similarly, all of the hydrogen in the water comes from the hydrogen in the organic compound. In this example:

$$\text{mass of carbon} = \frac{2.65 \times 12.0}{44.0} = 0.723\,\text{g}$$

$$\text{mass of hydrogen} = \frac{1.63 \times 2.0}{18.0} = 0.181\,\text{g}$$

These two masses add up to 0.904 g.

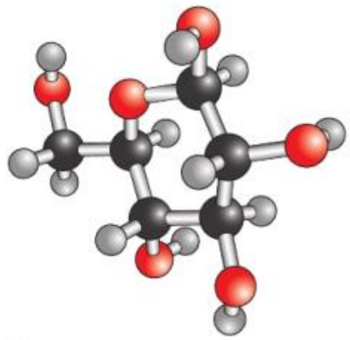
The original mass of the organic compound was 1.87 g, so the difference must be the mass of oxygen present in the organic compound. The mass of oxygen = 1.87 − 0.904 = 0.966 g.

**Table D** is the calculation table. You can see that the empirical formula of the sample compound is $CH_3O$.

| | C | H | O |
|---|---|---|---|
| mass of element / g | 0.723 | 0.181 | 0.966 |
| relative atomic mass | 12.0 | 1.0 | 16.0 |
| division by $A_r$ | 0.0603 | 0.181 | 0.0604 |
| ratio | 1 | 3 | 1 |

**table D**

**Fig B** shows a model of the glucose molecule. You can count the numbers of the three different atoms in the molecule.



▲ **fig B** A ball-and-stick model of glucose.

### LEARNING TIP

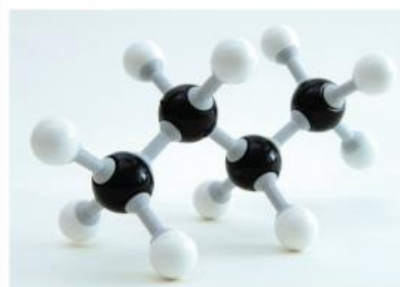
Divide by the relative atomic mass, not the atomic number or the relative molecular mass.

For oxygen, only divide by 16.0, not by 8 or 32.

### CHECKPOINT

**1.** A compound has the percentage composition by mass Ca = 24.4%, N = 17.1% and O = 58.5%.
What is its empirical formula?

**2.** Combustion analysis of 2.16 g of an organic compound produced 4.33 g of carbon dioxide and 1.77 g of water.
What is its empirical formula?



**3.** Can you work out the empirical formula of this molecule? Black represents carbon and white represents hydrogen.

### SUBJECT VOCABULARY

**empirical formula** the smallest whole-number ratio of atoms of each element in a compound

# 1D 2 MOLECULAR FORMULAE

SPECIFICATION REFERENCE 1.1 1.6 1.8(iii)

## LEARNING OBJECTIVES

- Know the term molecular formula.
- Use experimental data to calculate molecular formulae.
- Use the expression $pV = nRT$ for gases and volatile liquids.

## INTRODUCTION TO MOLECULAR FORMULAE

In **Topic 1D.1**, you learned how to calculate empirical formulae. Sometimes the empirical formula of a compound is the same as its molecular formula. Carbon dioxide ($CO_2$) and water ($H_2O$) are common examples you will know. The **molecular formula** of a compound shows the actual numbers of the atoms of each element in the compound.

Examples of compounds with different empirical and molecular formulae are:

| | | |
|---|---|---|
| hydrogen peroxide | empirical formula is HO | molecular formula is $H_2O_2$ |
| butane | empirical formula is $C_2H_5$ | molecular formula is $C_4H_{10}$ |

To determine the molecular formula of a compound, you need to already know or to calculate:

- the empirical formula
- the relative formula mass.

For example, if you had already found that the empirical formula of a compound was HO and you then found that its relative formula mass was 34, you could compare the relative mass of the empirical formula (17) with 34 and work out that the molecular formula was double the empirical formula.

## CALCULATING MOLECULAR FORMULAE

You have already practised calculating an empirical formula from experimental data. Now look at how to calculate a molecular formula from an empirical 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.

$104 \div 13.0 = 8$, 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 $23.0 + 12.0 + (2 \times 16.0) = 67.0$.

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

## THE IDEAL GAS EQUATION $pV = nRT$

$pV = nRT$ is the ideal gas equation, and can be used for gases (or volatile liquids above their boiling temperatures) to find the amount of a substance in moles. If the mass of the substance is also known, then the molar mass of the substance can be calculated. This gives the extra information needed to work out a molecular formula from an empirical formula.

The expression can also be rearranged to calculate a value of $p$, or $V$ or $T$.

### SI UNITS

When using this equation, you need to be careful that the units are the correct ones. It is always safest to work in SI units.

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

Sometimes in a question you may find that the units quoted are not SI units. If this is the case, then you will need to convert them to SI units. **Table A** shows the conversions you are likely to need.

| 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 |

**table A**

### 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, $$n = \frac{pV}{RT} = \frac{120 \times 10^3 \times 58.5 \times 10^{-6}}{8.31 \times 343} = 0.00246\ mol$$
$$M = \frac{m}{n} = \frac{0.280}{0.00246} = 114\ g\,mol^{-1}$$

### 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 $C_2H_6O$.

### LEARNING TIP

Be careful when using the word 'amount'. It should only be used for the amount, in moles, of a substance. For example, 'The amount of magnesium used was 0.150 mol' is correct.

You should not use it instead of quantities with other units. For example, 'The amount of magnesium used was 3.6 g' should be 'The mass of magnesium used was 3.6 g'.

Another example:

'The amount of water used was $25.0\ cm^3$' should be 'The volume of water used was $25.0\ cm^3$'.

### CHECKPOINT

SKILLS PROBLEM SOLVING

**1.** A 2.82 g sample of a gas has a volume of $1.26\ dm^3$, measured at a pressure of 103 kPa and a temperature of 55 °C. Calculate the molar mass of the gas.

**2.** A compound has the percentage composition by mass C = 40.0%, H = 6.7%, O = 53.3%. A sample containing 0.146 g of the compound had a volume of $69.5\ cm^3$ when measured at 98 kPa and 63 °C. What is the molecular formula of this compound?

### SUBJECT VOCABULARY

**molecular formula** the actual number of atoms of each element in a molecule

**molar mass** the mass per mole of a substance; it has the symbol $M$ and the units $g\,mol^{-1}$

# 1E 1 MOLAR VOLUME CALCULATIONS

SPECIFICATION REFERENCE 1.8(ii) CP1

## LEARNING OBJECTIVES

- Use chemical equations to calculate reacting volumes of gases and vice versa using the concept of molar volume of gases.

## MOLAR VOLUME

The work of Avogadro and others led to the idea of **molar volume**, the volume of gas that contains one mole of that gas. The molar volume is approximately the same for all gases, but its value varies with temperature and pressure. The value most often used is for gases at room temperature and pressure (sometimes abbreviated as r.t.p.). Room temperature is 298 K (or 25 °C) and standard pressure varies, but is often quoted as $1.01 \times 10^5$ Pa. The value of molar volume is usually quoted as $24\,\text{dm}^3\,\text{mol}^{-1}$ (equivalent to $24\,000\,\text{cm}^3$). Its symbol is $V_m$.

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

and

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

## CALCULATIONS USING MOLAR VOLUME

### CALCULATIONS INVOLVING A SINGLE GAS

If you are asked about a single gas, the calculation is straight forward. Assume that in these examples, all volumes are measured at r.t.p.

You need the expression $V_m = 24\,\text{dm}^3\,\text{mol}^{-1}$ which you might want to consider using in these alternative forms:

$$V_m = 24.0 = \frac{\text{volume in dm}^3}{\text{amount in mol}} \text{ or } V_m = 24\,000 = \frac{\text{volume in cm}^3}{\text{amount in mol}}$$

You will need to rearrange the expression depending on the actual question. Make sure that you use only 24 and $\text{dm}^3$, or only 24 000 and $\text{cm}^3$, in the calculation.

### EXAMPLE 1

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

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

### EXAMPLE 2

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

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

### EXAMPLE 3

What is the volume of 0.36 mol of hydrogen?

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

### CALCULATIONS INVOLVING GASES AND SOLIDS OR LIQUIDS

You may be given a chemical equation that involves one or more gases and a solid or a liquid. If you use information about the amount (in mol) of a solid or liquid, you can combine two of the calculation methods that we have already used.

The basis of this type of calculation is that for gases you can interconvert between amount and volume. For solids and liquids you can interconvert between amount and mass.

Step 1: Calculate the amount in moles from either the mass or the volume, depending on which one is given.

Step 2: Use the relevant reaction ratio in the equation to calculate the amount of the other substance.

Step 3: Convert this amount to a mass or a volume, depending on what the question asks.

### EXAM HINT

When attempting multistep calculations involving different units, it is important to show the units for each step of the reaction. It will force you to think about what you have just calculated rather than leaving a number floating.

### 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:

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

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:

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

### 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, $100\,\text{cm}^3$ 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:

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

## LEARNING TIP

Practise using the three-step method for calculating masses from volumes, and volumes from masses, in some reactions.

## CHECKPOINT

SKILLS PROBLEM SOLVING

In these questions, assume that all volumes are measured at r.t.p.

1. A flask contains 2 $dm^3$ of butane. What is the amount, in moles, of gas in the flask?
2. 10.0 g of copper(II) oxide is heated with hydrogen according to this equation:

$$CuO(s) + H_2(g) \rightarrow Cu(s) + H_2O(l)$$

What volume of hydrogen gas is needed to react with the copper(II) oxide, and what mass of copper is formed?

## SUBJECT VOCABULARY

**molar volume** the volume occupied by 1 mol of any gas; this is normally 24 $dm^3$ or 24 000 $cm^3$ at r.t.p.

# 1E 2 CONCENTRATIONS OF SOLUTIONS

SPECIFICATION REFERENCE 1.5

## LEARNING OBJECTIVES

- Calculate the concentration of a solution, in $g\,dm^{-3}$ and $mol\,dm^{-3}$.

## CALCULATIONS USING MASS CONCENTRATION ($g\ dm^{-3}$)

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:

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

In this topic, we only use values based on g and $dm^3$. You may sometimes see other units, such as $g\,cm^{-3}$ and $kg\,m^{-3}$.

As with other similar expressions, you will need to rearrange it, depending on the wording of the question. You also need to remember to convert $cm^3$ to $dm^3$ (by dividing by 1000).

### EXAMPLE 1

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

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

### 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?

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

### 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?

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

**fig A** These containers indicate increasing relative solute concentrations by increasing colour intensity. Unfortunately, most solutions we use are not coloured, so we cannot rely on different colour intensities to indicate different concentrations.

## CALCULATIONS USING MOLAR CONCENTRATION ($mol\ dm^{-3}$)

**Molar concentration** (it used to be called molarity) is used more often than mass concentration. If only the term 'concentration' is mentioned, then you should assume that it refers to molar concentration.

The units of molar concentration are $mol\,dm^{-3}$, and this is often denoted by using square brackets. If a solution of hydrochloric acid has a concentration of $0.150\,mol\,dm^{-3}$, this can be shown as $[HCl] = 0.150\,mol\,dm^{-3}$. The symbol $c$ is sometimes used to represent molar concentration.

You need to be able to use these two expressions together:

$$\text{amount} = \frac{\text{mass}}{\text{molar mass}} \text{ or } n = \frac{m}{M}$$

and

$$\text{(molar) concentration} = \frac{\text{amount}}{\text{volume}} \text{ or } c = \frac{n}{V}$$

As previously, you may need to rearrange these expressions. Look at the question wording to decide which one to use first.

### 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 $n$.

$$n = c \times V = 0.800 \times 0.500 = 0.400\,mol$$

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

$$m = n \times M = 0.400 \times 63.0 = 25.2\,g$$

### 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 $n$.

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

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

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

## CALCULATIONS FROM EQUATIONS USING CONCENTRATION AND MASS

In this type of calculation, you can use an equation to calculate the mass of a reactant or product if you are given the volume and molar concentration of another substance, and vice versa.

The expressions you need are the same as those you have just used, but you also need the equation for the reaction so that you can see the reacting ratio.

## 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.

$n = 0.100 \times 1.50 = 0.150$ 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 $n$.

$n = \frac{47.8}{84.3} = 0.567$ 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, $V = \frac{1.134}{2.50} = 0.454$ $dm^3$

## LEARNING TIP

Remember that the volumes referred to in this topic are of solutions, not solvents. If you dissolve a solute in 100 $cm^3$ of a solvent, the volume of the solution is not exactly 100 $cm^3$.

## CHECKPOINT

SKILLS PROBLEM SOLVING

1. 50.0 g of sodium hydroxide is dissolved in water to make 1.50 $dm^3$ of solution. What is the molar concentration of the solution?
2. 150 $cm^3$ of 0.125 mol $dm^{-3}$ lead(II) nitrate solution is mixed with an excess of potassium iodide solution. The equation for the reaction that occurs is:

   $Pb(NO_3)_2(aq) + 2KI(aq) \rightarrow PbI_2(s) + 2KNO_3(aq)$

   What mass of lead(II) iodide is formed?

## SUBJECT VOCABULARY

**solute** a substance that is dissolved
**solvent** a substance that dissolves a solute
**solution** a solute dissolved in a solution
**mass concentration** (of a solution) the mass (in g) of the solute divided by the volume of the solution
**molar concentration** (of a solution) the amount (in mol) of the solute divided by the volume of the solution

# 1E 3 CONCENTRATIONS IN PPM

SPECIFICATION REFERENCE 1.4(iv)

## LEARNING OBJECTIVES

- Understand the term parts per million (ppm), e.g. gases in the atmosphere.

## CONCENTRATIONS OF SOLUTIONS

Concentrations of solutions can also be compared using the term **parts per million**, or **ppm**. It is often used for pollutants in water.

Think of the word 'percent' – the 'cent' part refers to 100, so 50% means 50 out of 100, and parts per million means out of a million. 50 ppm means 50 parts out of 1 000 000 parts. The 'parts' usually refer to mass. The parts can be measured in any unit of mass, but grams or milligrams are the most commonly used.

### CALCULATIONS FOR SOLUTIONS IN PPM

A concentration of 1 ppm means 1 g in 1 000 000 g, or 1 mg in 1 000 000 mg.

This expression can be used to calculate concentrations in ppm:

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

The masses can be in any units, but they must be the same units. If different units are given, then one of them must be converted.

### 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:

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

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

## GASES IN THE ATMOSPHERE

Mauna Loa is the name of a volcano in Hawaii. It is also the location of a weather observatory that has recorded the levels of carbon dioxide in the atmosphere over a long period of time.

**Fig A** shows how the levels of carbon dioxide at Mauna Loa have changed over a period of 50 years. There are small variations during each year. In 1960, the level was about 316 ppm. By 2010, the level had reached nearly 390 ppm. Since 2015 it has been over 400 ppm, and many scientists believe that it will always remain above this value.

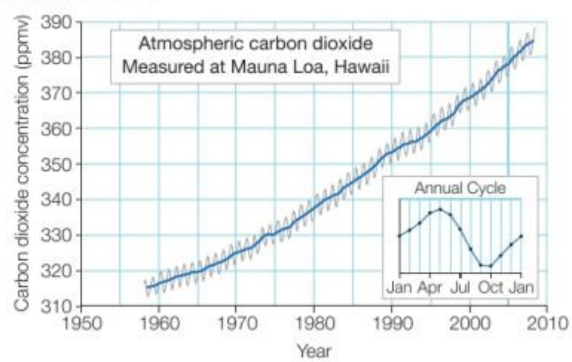



**fig A** This graph shows the steady increase in atmospheric carbon dioxide over five decades.

The concentrations of pollutant gases in the atmosphere are often given as values in ppm. Instead of using masses, the comparison is usually by volume, so calculations are done in a different way. Sometimes the values are quoted in ppmv – the v shows that the value refers to concentration by volume.

A concentration of 1 ppmv means 1 $cm^3$ in 1 000 000 $cm^3$, or 1 $cm^3$ in 1 000 $dm^3$.

Residents of Dhaka, the capital city of Bangladesh, are concerned about air quality. As in many cities, road traffic leads to high levels of carbon monoxide, especially during rush hours, when many people are travelling to and from work. Levels of CO in the air can be as high as 100 ppm. Outside the city there are many factories producing bricks for constructing buildings. These factories are responsible for many pollutants, including sulfur dioxide and particulate matter.

▲ **fig B** This brick factory releases pollutant gases into the atmosphere.

### CALCULATIONS FOR GASES IN PPM

This expression can be used to calculate concentrations in ppm.

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

The volumes can be in any units, but they must be the same units. If different units are given, then one of them must be converted.

### 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.

### LEARNING TIP

For ppm calculations with solutions, use the expression involving masses. For calculations with gases, use the expression involving volumes.

### CHECKPOINT

1. 0.2 g of potassium sulfate is dissolved in water to make 800 g of solution. What is the concentration of the salt in ppm?
2. 200 $dm^3$ of air contains 58 $cm^3$ of chlorine. What is the concentration of chlorine in ppm?

### SUBJECT VOCABULARY

**parts per million (ppm)** the number of parts of one substance in one million parts of another substance; a measure used to describe chemical concentration; usually, 'parts' refers to masses of both substances, or to volumes of both substances

# COINS IN HISTORY

SKILLS PROBLEM SOLVING

The chemical analysis of coinage from earlier periods in history can offer insights into the technology of metal extraction available at the time and give key insights into contemporary geopolitical questions. Note that these Thinking Bigger sections are synoptic and use knowledge from the different parts of the course. In this case, you will need to understand redox reactions (Topic 8) before you attempt the 'Chemistry in detail' section.

## 'ALL THAT GLISTENS IS NOT GOLD

**fig A** Trajan Decius, 249–251 BCE. Denomination: Silver Antoninianus. Mint: Rome.

Over the centuries, the base metals Fe, Cu, Ni, Zn, Al, Sn and Pb have been used as minor alloy constituents or as principal components in coins. Generally, a metal must be reasonably hard-wearing to ensure the economic lifetime of a coin, and must retain an acceptable appearance on exposure to the atmosphere. And it must not be too expensive. As a soft and expensive metal, gold is now usually alloyed with copper to give a hard-wearing alloy. British gold sovereigns, which are still minted, are made from 2 carats of alloy and 22 carats of gold. They comprise 91% Au and, 8.3% Cu. (A carat is a measure of the purity of gold, with pure gold being 24 carat.) Bronze (Cu–Sn alloy) farthings issued between 1897 and 1917 were darkened using $Na_2S_2O_3$, resulting in a surface layer of copper sulfide. This was done to avoid confusion between a newly minted farthing and a gold half-sovereign. The half-sovereign being worth 480 times as much as the farthing. Bronze pennies issued between 1944 and 1946 were similarly treated to deter the hoarding of new pennies at the end of the Second World War.

Platinum made only a brief appearance as a coinage metal. A few high-value coins in Russia were made in the mid-nineteenth century, at a time when platinum had recently been found in the Ural Mountains. For a while, the value of platinum fell below that of gold, and this gave rise to the emergence of counterfeit sovereigns in the 1870s. These were made from platinum and had a thin layer of electrochemically deposited gold.

Silver coinage was the universal medium of trading for centuries. The silver content of the coins made in city mints was a reflection of the status of the city as a trading centre. Traders of good repute only dealt in high quality silver coins, as evidenced by the high silver content of those coins found along the old established trading routes, e.g. from the Mediterranean, through the Middle East and Central Asia, to China.

If military expenditure increased, or during times of declining prosperity, a government would put only enough silver in its coins for them to remain acceptable to the public. Sometimes, however, there was a more subtle reason for the decline in silver content. Up to circa 100 BCE, Roman silver coins contained more than 90% Ag. Thereafter, silver supplies grew scarcer, and Roman technology was unable to extract silver from low-grade ores, which by the third century BCE were the only primary sources of silver available. However, at around this time, deposits of AgCl (chlorargynite) were found in Cornwall, Brittany and Alsace. The Romans observed that if copper or bronze coins were dipped in molten AgCl (mp 455 °C), they became coated with silver:

$$Cu + 2AgCl \rightarrow 2Ag + CuCl_2$$

From an article in *Education in Chemistry* magazine, published by the Royal Society of Chemistry

**DID YOU KNOW?**

**In April 1940 during the Nazi occupation of Denmark, the Hungarian-born chemist George de Hevesy decided to hide the Nobel Prize medals of colleagues Max von Laue and James Franck by dissolving them in *aqua regia* (a mixture of concentrated nitric and hydrochloric acid). The resulting solution sat on a shelf for the next 5 years attracting no particular attention. At the end of the war, the gold was recovered from the solution and the two medals recast.**

## SCIENCE COMMUNICATION

1 The article is about the development of a coin-based currency from the earliest times. Answer the following three questions and explain your answers with reasons or examples. In what ways is an article of this type different from a research paper? Which audience is this article aimed at? Is there any bias present in the report?

## CHEMISTRY IN DETAIL

**2.** (a) Modern gold sovereigns weigh 7.99 g (to two decimal places). Using the information in the article, calculate the number of moles of gold in a sovereign.

(b) Calculate the percentage of gold in an 18 carat ring.

**3.** (a) According to the reaction between copper and silver chloride in the article how many moles of silver are produced from 1 mole of copper?

(b) Calculate the number of moles of copper in 2.17 g (Ar Cu = 63.5)

(c) When 2.17 g of copper reacts with excess silver chloride according to the equation a total of 5.40 g of silver is recovered. Assuming that all of the copper reacts calculate the percentage yield of the silver recovered. (Ar Ag = 107.9)

**4.** Reread the third paragraph of the article. Using the information given, write half-equations for

(i) the reduction of thiosulfate ions to sulfide in acidic solution, and

(ii) the oxidation of copper metal to copper(II) ions.

**5.** A gold sovereign is analysed using the following chemical procedure.

1 The sovereign is reacted with excess concentrated nitric acid in a fume cupboard.

2 The resultant mixture is filtered to remove the unreacted gold.

3 The resultant solution is made up in distilled water to a volume of 250 $cm^3$.

4 A volume of 25 $cm^3$ of this solution is pipetted into a conical flask and 50 $cm^3$ of 0.1 mol $dm^{-3}$ KI(aq) is added (this is an excess). The resultant solution immediately turns an orange-brown colour.

5 This solution is then titrated with 0.050 mol $dm^{-3}$ $Na_2S_2O_3$(aq) solution until the solution fades to a straw yellow colour.

6 Starch indicator is then added to give a blue-black colour.

7 Further $Na_2S_2O_3$(aq) solution is added until the solution becomes colourless.

8 The first titration volume is recorded.

9 The titration is repeated 3 times and the results recorded to the nearest 0.05 $cm^3$.

| Titre number | 1 | 2 | 3 | 4 |
|---|---|---|---|---|
| Final volume / $cm^3$ | 26.00 | 26.35 | 25.90 | 25.85 |
| Initial volume / $cm^3$ | 0.00 | 0.55 | 0.00 | 0.00 |
| Titre / $cm^3$ | 26.00 | | | |

**Results table**

(a) Suggest why step 1 must be done in a fume cupboard.

(b) Complete the results table and calculate a suitable mean titre.

(c) Calculate the percentage uncertainty in the reading for titre number 3.

(d) Match the equations below with the reactions taking place in the method described.

$Cu(s) + 4H^+(aq) + 2NO_3^-(aq) \rightarrow Cu^{2+}(aq) + 2NO_2(g) + 2H_2O(l)$

$2Cu^{2+}(aq) + 4I^-(aq) \rightarrow 2CuI(s) + I_2(aq)$

$2S_2O_3^{2-}(aq) + I_2(aq) \rightarrow 2I^-(aq) + S_4O_6^{2-}(aq)$

(e) Using appropriate calculations, decide whether the sovereign is genuine or not.

(f) What assumptions have been made in the procedure?

### THINKING BIGGER TIP

In your previous study of chemistry, you will have covered metals and their methods of extraction. This would be a good chance for you to review some of that work. Consider how metal reactivity relates to methods of extraction.

### INTERPRETATION NOTE

See if you can find a similar article on the development of pigments and dyes over the ages or the development of textiles. Consider how the the chemical ideas are represented.

### ACTIVITY

The history of human technology is closely associated with metals.

Draw a timeline identifying the metals used and the cultures responsible for developing the technology.

- You should consider the following metals: gold, silver, copper, iron, aluminium, titanium and uranium.
- Consider also the methods of extraction and the key usages of the metals.

# 1 EXAM PRACTICE

**1** How many molecules of oxygen are there in a 1.00 g sample of $O_2$?

(Avogadro constant, $L = 6.02 \times 10^{23}$ mol$^{-1}$)

**A** $1.88 \times 10^{22}$
**B** $3.76 \times 10^{22}$
**C** $9.63 \times 10^{24}$
**D** $1.93 \times 10^{25}$ [1]

**(Total for Question 1 = 1 mark)**

**2** What is the concentration, in mol dm$^{-3}$, of a solution of sodium chloride containing 4.27 g of NaCl in 300 cm$^3$ of solution?

**A** 0.0219
**B** 0.243
**C** 4.11
**D** 45.7 [1]

**(Total for Question 2 = 1 mark)**

**3** The overall equation for one method of manufacturing hydrogen from methane is

$CH_4 + 2H_2O \rightarrow 4H_2 + CO_2$

In one batch, 5.12 tonnes of hydrogen were obtained from 13.6 tonnes of methane.

What is the percentage yield of hydrogen for this batch?

**A** 37.6
**B** 42.5
**C** 54.4
**D** 75.3 [1]

**(Total for Question 3 = 1 mark)**

**4** The equation for a reaction that can be used to manufacture lithium carbonate is

$2Li_2O_2 + 2CO_2 \rightarrow 2Li_2CO_3 + O_2$

What is the atom economy for this reaction?

**A** 58.9
**B** 62.1
**C** 69.8
**D** 82.2 [1]

**(Total for Question 4 = 1 mark)**

**5** The equation for a displacement reaction is

$Zn + FeSO_4 \rightarrow Fe + ZnSO_4$

Which species is displaced in this reaction?

**A** zinc
**B** iron
**C** sulfur
**D** oxygen [1]

**(Total for Question 5 = 1 mark)**

**6** The equation for a precipitation reaction is

$AgNO_3(aq) + NaCl(aq) \rightarrow AgCl(s) + NaNO_3(aq)$

A solution containing 0.04 mol silver nitrate is added to a solution containing 0.06 mol sodium chloride.

What mass of precipitate forms?

**A** 5.74 g
**B** 7.17 g
**C** 8.60 g
**D** 14.3 g [1]

**(Total for Question 6 = 1 mark)**

**7** Magnesium chloride may be prepared by reacting magnesium with dilute hydrochloric acid.

A sample of magnesium of mass 1.215 g was added to 60.0 cm$^3$ dilute hydrochloric acid of concentration 2.00 mol dm$^{-3}$.

The equation for the reaction is

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

(a) State two observations that are made when magnesium reacts with dilute hydrochloric acid. [2]

(b) (i) Calculate the amount, in moles, of magnesium used. [1]

(ii) Calculate the amount, in moles, of hydrochloric acid used. [1]

(iii) Use your answers to (b)(i) and (b)(ii) to show that the hydrochloric acid is in excess. [2]

(c) Calculate the volume, measured at r.t.p. of hydrogen produced in this reaction.

(The molar volume of hydrogen at r.t.p. is 24 dm$^3$ mol$^{-1}$) [2]

**(Total for Question 7 = 8 marks)**

**8** Ammonium nitrate ($NH_4NO_3$) can be prepared by the reaction of ammonia with nitric acid.

The equation for the reaction is

$NH_3(aq) + HNO_3(aq) \rightarrow NH_4NO_3(aq)$

(a) (i) Calculate the minimum volume of nitric acid, of concentration 0.500 mol dm$^{-3}$, that is required to react completely with 25.0 cm$^3$ of aqueous ammonia of concentration 2.00 mol dm$^{-3}$. [2]

(ii) How could a solid sample of ammonium nitrate be obtained from the reaction mixture? [1]

(b) When ammonium nitrate is heated, it decomposes according to the following equation:

$NH_4NO_3(s) \rightarrow N_2O(g) + 2H_2O(l)$

A 4.00 g sample of ammonium nitrate was carefully heated to produce only $N_2O$ and water.

(i) Calculate the amount, in moles, of ammonium nitrate used. [2]

(ii) Calculate the volume of $N_2O$ that was formed. [1]

(Assume that the molar volume of $N_2O$ is $24\,dm^3\,mol^{-1}$ under the experimental conditions.)

(iii) $N_2O$ can be decomposed into its elements by further heating. Write an equation for this reaction. Include state symbols. [2]

**(Total for Question 8 = 8 marks)**

**9** Phosphorus forms three chlorides of molecular formulae $PCl_3$, $PCl_5$ and $P_2Cl_4$.

(a) State what is meant by molecular formula. [1]

(b) $PCl_5$ can be prepared by reacting white phosphorus ($P_4$) with chlorine gas.

Write an equation for this reaction. State symbols are not required. [1]

(c) Solid $PCl_5$ reacts vigorously with water to form a solution containing a mixture of two acids, $H_3PO_4$ and HCl.

Write an equation for this reaction. Include state symbols. [2]

(d) A compound was found to have the following percentage composition by mass:

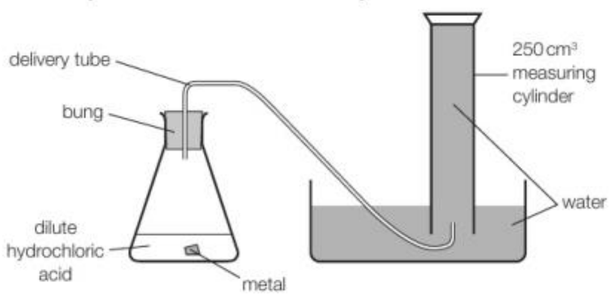
P = 30.39%; Cl = 69.61%

(i) Use this information to identify the chloride. [3]

(ii) Give the systematic name for this chloride. [1]

**(Total for Question 9 = 8 marks)**

**10** The diagram shows the apparatus used to collect and measure the volume of hydrogen given off when a sample of a Group 2 metal reacts with dilute hydrochloric acid.




The equation for the reaction is

$$M(s) + 2HCl(aq) \rightarrow MCl_2(aq) + H_2(g)$$

where M is the symbol for the Group 2 metal.

The apparatus was set up as shown in the diagram.

A sample of the metal was weighed and then placed into the conical flask.

The bung was removed and an excess of acid was then added to the metal. The bung was replaced.

When the reaction was complete, and the gas collected had cooled to room temperature, the volume of gas collected in the measuring cylinder was measured.

The results are shown in the table.

| | |
|---|---|
| Mass of metal | 0.24 g |
| Volume of hydrogen collected | 230 cm³ |

(a) (i) Use the results to calculate the molar mass of the metal.

Assume the molar volume of hydrogen is $24.0\,dm^3\,mol^{-1}$ under the experimental conditions. [3]

(ii) Give the most likely identity of the metal. Justify your answer. [2]

(b) (i) Identity the major procedural error in the experiment. [1]

(ii) State a modification that would reduce this procedural error. [1]

**(Total for Question 10 = 7 marks)**

**11** Azides are compounds of metals with nitrogen. Some azides are used as detonators in explosives. However, sodium azide ($NaN_3$) is used in air bags in cars.

(a) Sodium azide decomposes into its elements when heated.

$$2NaN_3(s) \rightarrow 2Na(l) + 3N_2(g)$$

What is the volume of gas produced, measured at r.t.p., when one mole of sodium azide is decomposed?

**A** $24\,dm^3$

**B** $36\,dm^3$

**C** $48\,dm^3$

**D** $72\,dm^3$

(Assume one mole of gas occupies $24\,dm^3$ at r.t.p.) [1]

(b) (i) A student completely decomposed 3.25 g of sodium azide. Calculate the mass of sodium she obtained. [2]

(ii) She then carefully reacted the sodium obtained with water to form $25.0\,cm^3$ of aqueous sodium hydroxide.

$$2Na(s) + 2H_2O(l) \rightarrow 2NaOH(aq) + H_2(g)$$

Calculate the concentration, in $mol\,dm^{-3}$, of the aqueous sodium hydroxide. [2]

**(Total for Question 11 = 5 marks)**