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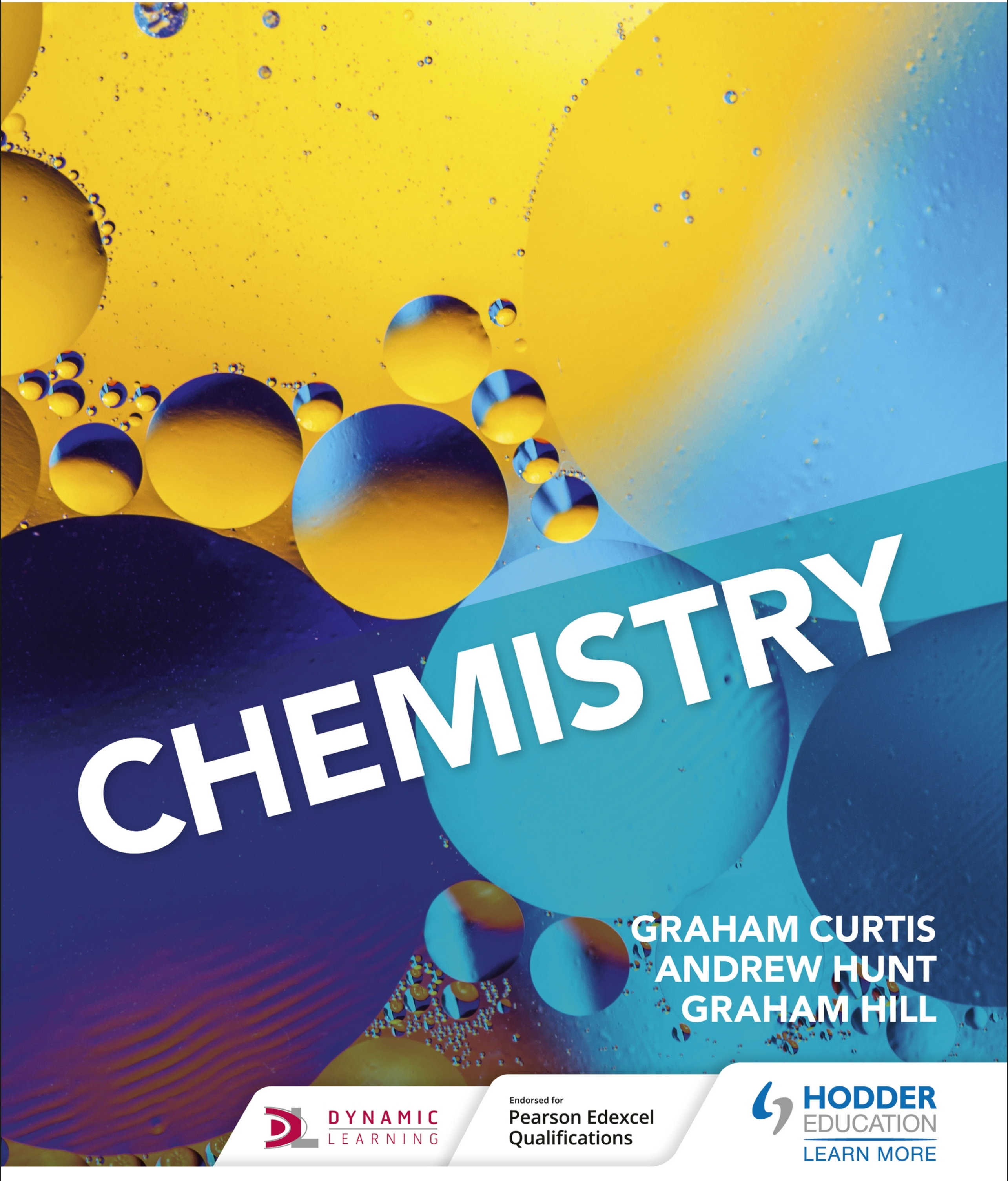

CHEMISTRY

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DYNAMIC LEARNING

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Contents

Appendix

Answers for the 'Test yourself' questions and activities found in this book are available online at www.hoddereducation.co.uk/EdexcelChemistry

Get the most from this book

Welcome to the **Pearson Edexcel A level Chemistry Student's Book**! This book covers Year 1 and Year 2 of the Pearson Edexcel A level Chemistry specification.

The following features have been included to help you get the most from this book.

5 Formulae, equations and amounts of substance

5.1 Understanding chemical quantities

Chemists often need to measure how much of a particular chemical there is in a sample. Analysts in pharmaceutical companies, for example, test samples of tablets and medicines to check that they contain the right amount of a drug. Industrial chemists measure the amounts of substances they need for chemical processes. Laboratory chemists calculate the yield of product they expect when they mix measured quantities of the reactants for a synthesis. In these, and many other contexts, chemists have to be able to measure amounts of substances accurately.

Chemical amounts

In chemistry, the **amount of a substance** is measured in moles. Chemists use the unit 'mole' to measure an amount of substance containing a standard number of atoms, molecules or ions. The word 'mole' entered the language of chemistry at the end of the nineteenth century. It is based on the Latin word for a heap or a pile.

When chemists are determining formulae or working with equations, they need to measure amounts in moles. Chemists have balances to measure masses and graduated containers to measure volumes, but there is no instrument for measuring chemical amounts directly. Instead, chemists must first measure the masses or volumes of substances and then calculate the chemical amounts.

Key terms

Amount of substance is a physical quantity (symbol *n*) which is measured in the unit mole (symbol mol).

Molar masses

The key to working with chemical amounts in moles is to know the relative masses of different atoms. The accurate method for determining **relative atomic masses** involves the use of a mass spectrometer (Section 1.3).

One mole of an element has a mass that is equal to its relative atomic mass in grams. So, the mass of one mole of carbon is 12.0 g and the mass of one mole of copper is 63.5 g. These masses of one mole are called **molar masses** (symbol *M*). So, the molar mass of carbon, $M(C) = 12.0\ g\ mol^{-1}$ and the molar mass of copper, $M(Cu) = 63.5\ g\ mol^{-1}$ (Figure 5.1).

Similarly the molar mass of the molecules of an element or a compound is numerically equal to its relative molecular mass. So, the molar mass of oxygen molecules, $M(O_2) = 32.0\ g\ mol^{-1}$ and the molar mass of sulfuric acid, $M(H_2SO_4) = 98.1\ g\ mol^{-1}$. Likewise, the molar mass of an ionic compound is numerically equal to its relative formula mass. The molar mass of magnesium nitrate, $Mg(NO_3)_2$, is therefore $148.3\ g\ mol^{-1}$ (Figure 5.2).

Key terms

Relative atomic mass, A_r, is the average mass of an element reletive to 1/12th of the mass of an atom of the isotope carbon-12. The values are relative so they do not have units.

Key terms

Molar mass is the mass of one mole of a chemical – the unit is $g\ mol^{-1}$. As always with molar amounts, the symbol or formula of the chemical must be specified.

Figure 5.1 One mole amounts of copper, carbon, iron, aluminium, mercury and sulfur

Figure 5.2 One mole amounts of some ionic compounds

Amount in moles

The mole is the SI unit for amount of substance. The name of the quantity is 'mole'. Its unit is 'mol'. So,

12 g of carbon contains 1 mol of carbon atoms

24 g of carbon contains 2 mol of carbon atoms

240 g of carbon contains 20 mol of carbon atoms.

Notice that:

$$\text{amount of substance/mol} = \frac{\text{mass of substance/g}}{\text{molar mass/g mol}^{-1}}$$

It is important to be precise about the chemical **species** involved when measuring amounts in moles. In calcium chloride, $CaCl_2$, for example, there are two chloride ions, Cl^-, combined with each calcium ion, Ca^{2+}. So in one mole of calcium chloride there is one mole of calcium ions and two moles of chloride ions.

The Avogadro constant

Relative atomic masses show that one atom of carbon is 12 times heavier than one atom of hydrogen. This means that 12 g of carbon contains the same number of atoms as 1 g of hydrogen. Similarly, one atom of oxygen is 16 times as heavy as one atom of hydrogen, so 16 g of oxygen also contains the same number of atoms as 1 g of hydrogen.

In fact, the molar mass of every element (1 g of hydrogen, 12 g carbon, 16 g oxygen, and so on) contains the same number of atoms. This number is called the **Avogadro constant**, after the Italian scientist Amedeo Avogadro. Experiments show that the Avogadro constant, *L*, is $6.02 \times 10^{23}\ mol^{-1}$. Written out in full this is 602000000000000000000000 atoms, molecules or ions per mole.

The Avogadro constant is the number of atoms, molecules or formula units in one mole of any substance. So, one mole of oxygen (O_2) contains 6.02×10^{23} O_2 molecules and two moles of oxygen (O_2) contains $2 \times 6.02 \times 10^{23}$ O_2 molecules.

The number of atoms, molecules or formula units = amount of chemical/mol × the Avogadro constant/mol^{-1}

Tip

Section M[illegible] of the maths chapter on page xx gives advice on how to work out the value of maths equations with brackets and combinations of multiplication and addition.

Key terms

The term **species** is a useful collective noun used by chemists to refer generally to atoms, molecules or ions.

Tip

Section MiC.4 of the maths chapter on page xx gives help with substituting values into mathematical formulae.

Key terms

The **Avogadro constant** is the number of atoms, molecules or ions in one mole of a substance. The constant has the unit mol^{-1}.

Tips

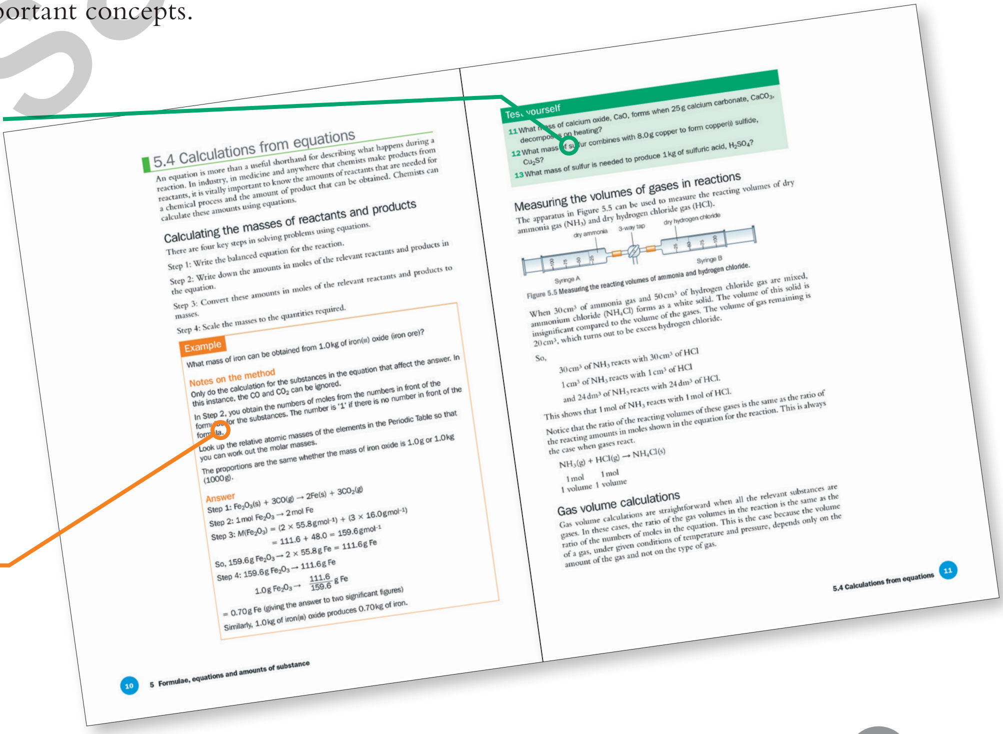
These highlight important facts, common misconceptions and signpost you towards other relevant topics.

Key terms and formulae

These are highlighted in the text and definitions are given in the margin to help you pick out and learn these important concepts.

Test yourself questions

These short questions, found throughout each chapter, are useful for checking your understanding as you progress through a topic.



5.4 Calculations from equations

An equation is more than a useful shorthand for describing what happens during a reaction. In industry, in medicine and anywhere that chemists make products from reactants, it is vitally important to know the amounts of reactants that are needed for a chemical process and the amount of product that can be obtained. Chemists can calculate these amounts using equations.

Calculating the masses of reactants and products

There are four key steps in solving problems using equations.

Step 1: Write the balanced equation for the reaction.

Step 2: Write down the amounts in moles of the relevant reactants and products in the equation.

Step 3: Convert these amounts in moles of the relevant reactants and products to masses.

Step 4: Scale the masses to the quantities required.

Example

What mass of iron can be obtained from 1.0 kg of iron(III) oxide (iron ore)?

Notes on the method

Only do the calculation for the substances in the equation that affect the answer. In this instance, the CO and CO_2 can be ignored.

In Step 2, you obtain the numbers of moles from the numbers in front of the formulae for the substances. The number is '1' if there is no number in front of the formula.

Look up the relative atomic masses of the elements in the Periodic Table so that you can work out the molar masses.

The proportions are the same whether the mass of iron oxide is 1.0 g or 1.0 kg (1000 g).

Answer

Step 1: $Fe_2O_3(s) + 3CO(g) \rightarrow 2Fe(s) + 3CO_2(g)$

Step 2: $1\ mol\ Fe_2O_3 \rightarrow 2\ mol\ Fe$

Step 3: $M(Fe_2O_3) = (2 \times 55.8\ g\ mol^{-1}) + (3 \times 16.0\ g\ mol^{-1})$
$= 111.6 + 48.0 = 159.6\ g\ mol^{-1}$

So, $159.6\ g\ Fe_2O_3 \rightarrow 2 \times 55.8\ g\ Fe = 111.6\ g\ Fe$

Step 4: $159.6\ g\ Fe_2O_3 \rightarrow 111.6\ g\ Fe$

$1.0\ g\ Fe_2O_3 \rightarrow \frac{111.6}{159.6}\ g\ Fe$

$= 0.70\ g$ Fe (giving the answer to two significant figures)

Similarly, 1.0 kg of iron(III) oxide produces 0.70 kg of iron.

Test yourself

11 What mass of calcium oxide, CaO, forms when 25 g calcium carbonate, $CaCO_3$, decomposes on heating?

12 What mass of sulfur combines with 8.0 g copper to form copper(I) sulfide, Cu_2S?

13 What mass of sulfur is needed to produce 1 kg of sulfuric acid, H_2SO_4?

Measuring the volumes of gases in reactions

The apparatus in Figure 5.5 can be used to measure the reacting volumes of dry ammonia gas (NH_3) and dry hydrogen chloride gas (HCl).

Figure 5.5 Measuring the reacting volumes of ammonia and hydrogen chloride.

When $30\ cm^3$ of ammonia gas and $50\ cm^3$ of hydrogen chloride gas are mixed, ammonium chloride (NH_4Cl) forms as a white solid. The volume of this solid is insignificant compared to the volume of the gases. The volume of gas remaining is $20\ cm^3$, which turns out to be excess hydrogen chloride.

So,

$30\ cm^3$ of NH_3 reacts with $30\ cm^3$ of HCl

$1\ cm^3$ of NH_3 reacts with $1\ cm^3$ of HCl

and $24\ dm^3$ of NH_3 reacts with $24\ dm^3$ of HCl.

This shows that 1 mol of NH_3 reacts with 1 mol of HCl.

Notice that the ratio of the reacting volumes of these gases is the same as the ratio of the reacting amounts in moles shown in the equation for the reaction. This is always the case when gases react.

$NH_3(g) + HCl(g) \rightarrow NH_4Cl(s)$

1 mol 1 mol
1 volume 1 volume

Gas volume calculations

Gas volume calculations are straightforward when all the relevant substances are gases. In these cases, the ratio of the gas volumes in the reaction is the same as the ratio of the numbers of moles in the equation. This is the case because the volume of a gas, under given conditions of temperature and pressure, depends only on the amount of the gas and not on the type of gas.

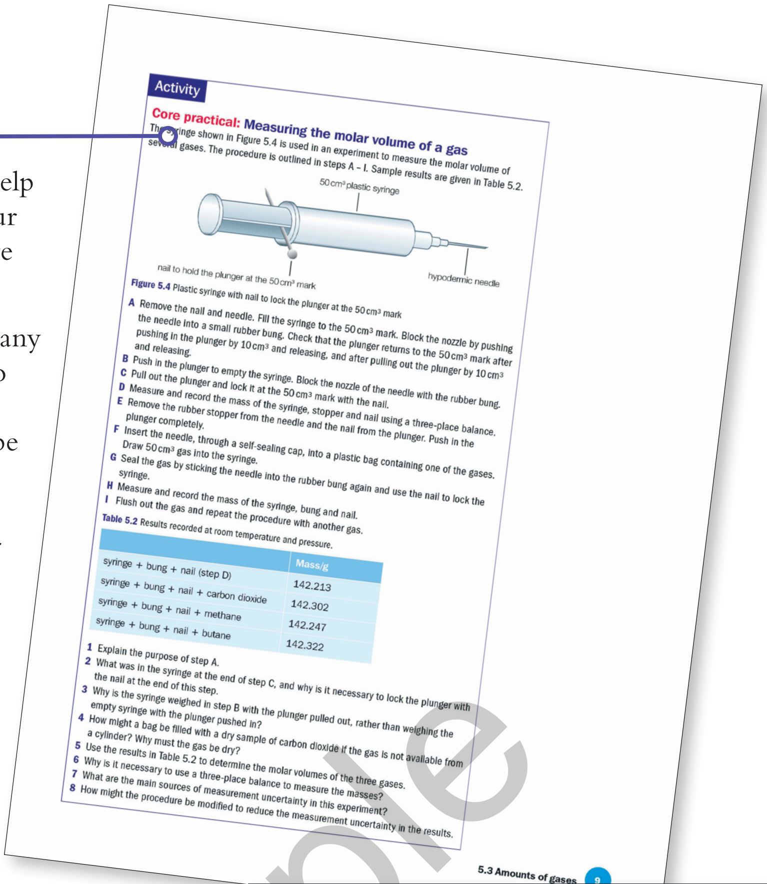
Examples

Examples of questions and calculations feature full workings and sample answers.

Activities and Core practicals

These practical-based activities will help consolidate your learning and test your practical skills. Pearson Edexcel's Core practicals are clearly highlighted.

In this edition the authors describe many important experimental procedures to conform to recent changes in the A level curriculum. Teachers should be aware that, although there is enough information to inform students of techniques and many observations for exam purposes, there is not enough information for teachers to replicate the experiments themselves, or with students, without recourse to CLEAPSS Hazcards or Laboratory worksheets which have undergone a risk assessment procedure.



Activity

Core practical: Measuring the molar volume of a gas

The syringe shown in Figure 5.4 is used in an experiment to measure the molar volume of several gases. The procedure is outlined in steps A – I. Sample results are given in Table 5.2.

Figure 5.4 Plastic syringe with nail to lock the plunger at the 50 cm³ mark

A Remove the nail and needle. Fill the syringe to the 50 cm³ mark. Block the nozzle by pushing the needle into a small rubber bung. Check that the plunger returns to the 50 cm³ mark after pushing in the plunger by 10 cm³ and releasing, and after pulling out the plunger by 10 cm³ and releasing.
B Push in the plunger to empty the syringe. Block the nozzle of the needle with the rubber bung.
C Pull out the plunger and lock it at the 50 cm³ mark with the nail.
D Measure and record the mass of the syringe, stopper and nail using a three-place balance.
E Remove the rubber stopper from the needle and the nail from the plunger. Push in the plunger completely.
F Insert the needle, through a self-sealing cap, into a plastic bag containing one of the gases. Draw 50 cm³ gas into the syringe.
G Seal the gas by sticking the needle into the rubber bung again and use the nail to lock the syringe.
H Measure and record the mass of the syringe, bung and nail.
I Flush out the gas and repeat the procedure with another gas.

Table 5.2 Results recorded at room temperature and pressure.

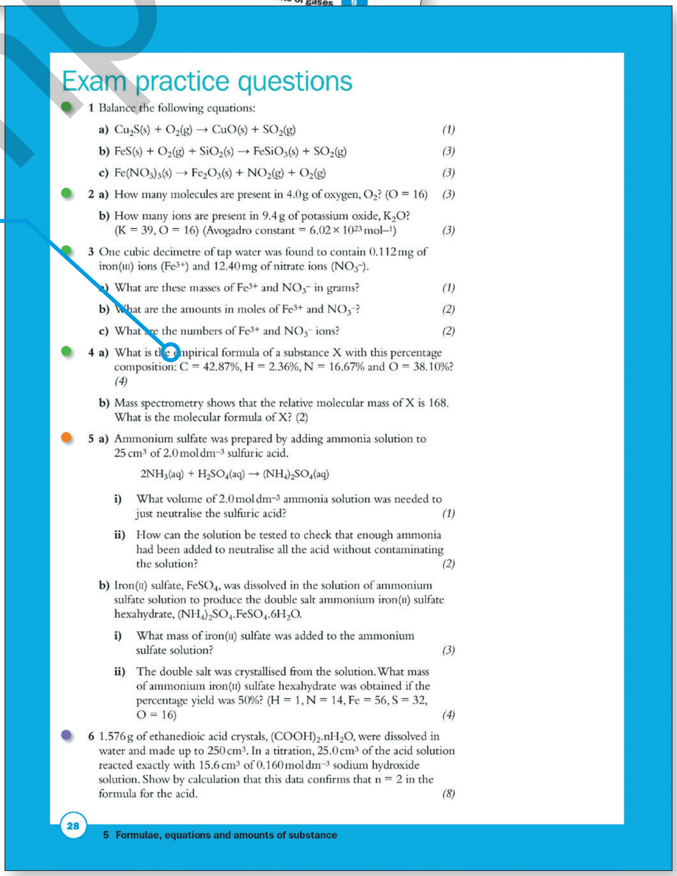
	Mass/g
syringe + bung + nail (step D)	142.213
syringe + bung + nail + carbon dioxide	142.302
syringe + bung + nail + methane	142.247
syringe + bung + nail + butane	142.322

1 Explain the purpose of step A.
2 What was in the syringe at the end of step C, and why is it necessary to lock the plunger with the nail at the end of this step.
3 Why is the syringe weighed in step B with the plunger pulled out, rather than weighing the empty syringe with the plunger pushed in?
4 How might a bag be filled with a dry sample of carbon dioxide if the gas is not available from a cylinder? Why must the gas be dry?
5 Use the results in Table 5.2 to determine the molar volumes of the three gases.
6 Why is it necessary to use a three-place balance to measure the masses?
7 What are the main sources of measurement uncertainty in this experiment?
8 How might the procedure be modified to reduce the measurement uncertainty in the results.

5.3 Amounts of gases 9

Exam practice questions

You will find Exam practice questions at the end of every chapter. These follow the style of the different types of questions you might see in your examination and are colour coded to highlight the level of difficulty. Quality of extended response questions are marked with an asterisk (★).



Exam practice questions

● 1 Balance the following equations:

a) $Cu_2S(s) + O_2(g) \rightarrow CuO(s) + SO_2(g)$ *(1)*

b) $FeS(s) + O_2(g) + SiO_2(s) \rightarrow FeSiO_3(s) + SO_2(g)$ *(3)*

c) $Fe(NO_3)_3(s) \rightarrow Fe_2O_3(s) + NO_2(g) + O_2(g)$ *(3)*

● 2 **a)** How many molecules are present in 4.0 g of oxygen, O_2? (O = 16) *(3)*

b) How many ions are present in 9.4 g of potassium oxide, K_2O? (K = 39, O = 16) (Avogadro constant = 6.02×10^{23} mol–¹) *(3)*

● 3 One cubic decimetre of tap water was found to contain 0.112 mg of iron(III) ions (Fe^{3+}) and 12.40 mg of nitrate ions (NO_3^-).

a) What are these masses of Fe^{3+} and NO_3^- in grams? *(1)*

b) What are the amounts in moles of Fe^{3+} and NO_3^-? *(2)*

c) What are the numbers of Fe^{3+} and NO_3^- ions? *(2)*

● 4 **a)** What is the empirical formula of a substance X with this percentage composition: C = 42.87%, H = 2.36%, N = 16.67% and O = 38.10%? *(4)*

b) Mass spectrometry shows that the relative molecular mass of X is 168. What is the molecular formula of X? (2)

● 5 **a)** Ammonium sulfate was prepared by adding ammonia solution to 25 cm³ of 2.0 mol dm⁻³ sulfuric acid.

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

i) What volume of 2.0 mol dm⁻³ ammonia solution was needed to just neutralise the sulfuric acid? *(1)*

ii) How can the solution be tested to check that enough ammonia had been added to neutralise all the acid without contaminating the solution? *(2)*

b) Iron(II) sulfate, $FeSO_4$, was dissolved in the solution of ammonium sulfate solution to produce the double salt ammonium iron(II) sulfate hexahydrate, $(NH_4)_2SO_4.FeSO_4.6H_2O$.

i) What mass of iron(II) sulfate was added to the ammonium sulfate solution? *(3)*

ii) The double salt was crystallised from the solution. What mass of ammonium iron(II) sulfate hexahydrate was obtained if the percentage yield was 50%? (H = 1, N = 14, Fe = 56, S = 32, O = 16) *(4)*

● 6 1.576 g of ethanedioic acid crystals, $(COOH)_2.nH_2O$, were dissolved in water and made up to 250 cm³. In a titration, 25.0 cm³ of the acid solution reacted exactly with 15.6 cm³ of 0.160 mol dm⁻³ sodium hydroxide solution. Show by calculation that this data confirms that n = 2 in the formula for the acid. *(8)*

28 5 Formulae, equations and amounts of substance

Dedicated chapters for developing your **Maths** and **Preparing for your exam** are also included in this book.

Introduction

This book is an extensively revised, restructured, updated and combined version of *Pearson Edexcel Chemistry for AS* and *Pearson Edexcel Chemistry for A2* by Graham Hill and Andrew Hunt. We have relied heavily on the contributions that Graham Hill made to the original books and are most grateful that he has encouraged us to build on his work. The team at Hodder Education, led initially by Hanneke Remsing and then by Emma Braithwaite, has made an extremely valuable contribution to the development of the book and the website resources. In particular, we would like to thank Abigail Woodman, the project manager, for her expert advice and encouragement. We are also grateful for the skilful work on the print and electronic resources by Anne Trevillion.

At the end of each chapter we have added a 'Chapter Summary'. This contains a brief bulleted list of the main points covered in the Chapter to help with your revision.

We have grouped each set of 'Exam practice' questions broadly by difficulty. In general, a question with 🟢 is straightforward and based directly on the information, ideas and methods described in the chapter. Each problem-solving part of the question typically only involves one step in the argument or calculation. A question with 🟠 is a more demanding, but still structured, question involving the application of ideas and methods to solve a problem with the help of data or information from this chapter or elsewhere. Arguments and calculations typically involve more than one step. The questions marked by 🟣 are hard and they may well expect you to bring together ideas from different areas of the subject. In these harder questions, you may have to structure an argument or work out the steps required to solve a problem. In the earlier chapters, you may well decide not to attempt the questions with 🟣 until you have gained wider experience and knowledge of the subject.

Practical work is of particular importance in A Level chemistry. Each of the Core Practicals in the specification features in the main chapters of this book, with an outline of the procedure and data for you to analyse and interpret. Throughout the text there are references to Practical skills sheets, which can be accessed via www.hoddereducation.co.uk/EdexcelChemistry. Sheets 1 to 3 provide general guidance for the first year of your course, and sheets 11 to 15 for the second year of your course, and the remainder provide more detailed guidance for the Core Practicals.

1. Practical skills for advanced chemistry
2. Assessing hazards and risks
3. Researching and referencing
4. Making measurements
5. Identifying errors and estimating uncertainties
6. Measuring chemical amounts by titration
7. Analysing inorganic unknowns
8. Synthesising organic liquids
9. Analysing organic unknowns
10. Measuring enthalpy changes
11. Assessment of practical work
12. Overview of practical skills
13. Assessing hazards and risks
14. Researching and referencing
15. Identifying errors and estimating uncertainties
16. Finding the K_a value for a weak acid
17. Measuring chemical amounts by titration
18. Investigating reaction orders and activation energies
19. Analysing inorganic unknowns
20. Analysing organic unknowns
21. Synthesis of an organic solid

Prior knowledge

1 Working like a chemist

Chemistry is about understanding the material world. Chemists develop their explanations by observing the properties of substances and looking at patterns of behaviour (Figure 1). They devise theories and models that can be used in chemical analysis and synthesis.

Figure 1 Aspirin is probably the commonest medicine in use. The bark of willow trees was used to ease pain for more than 2000 years. Early in the twentieth century, chemists extracted the active ingredient from willow bark. Their understanding of patterns in the behaviour of similar compounds enabled them to synthesise aspirin.

Tip

This first chapter surveys the main themes of chemistry and indicates how you will be learning more about chemistry during your A Level course. The chapters in this book build on what you already know about chemistry. The text and 'Test yourself' questions in the early part of each chapter can help you to check on what you have learned before and what you need to understand at the start of each topic.

Looking for patterns in chemical behaviour

Part of being a chemist involves getting a feel for the way in which chemicals behave. Chemists get to know chemicals just as people get to know their friends and family. They look for patterns in behaviour and recognise that some of the patterns are familiar. For example, the elements sodium and potassium are both soft and stored under oil because they react so readily with air and water; copper sulfate is blue, like other copper compounds. By understanding patterns, chemists can design and make plastics like polythene and medicines like aspirin.

Tip

The Periodic Table links together many of the key patterns of behaviour of elements. You will extend your knowledge of the Periodic Table in Chapter 1. You will also make a detailed study of patterns in the properties of the elements and compounds in some of the Periodic Table groups in Chapter 4.

Test yourself

Remind yourself of some patterns in the ways that chemicals behave.

1. What happens when a more reactive metal (such as zinc) is added to a solution in water of a compound of a less reactive metal (such as copper sulfate)?
2. What forms at the negative electrode (cathode) during the electrolysis of a solution of a salt?
3. What happens on adding an acid (such as hydrochloric acid) to a carbonate (such as calcium carbonate)?
4. What do sodium chloride, sodium bromide and sodium iodide look like?

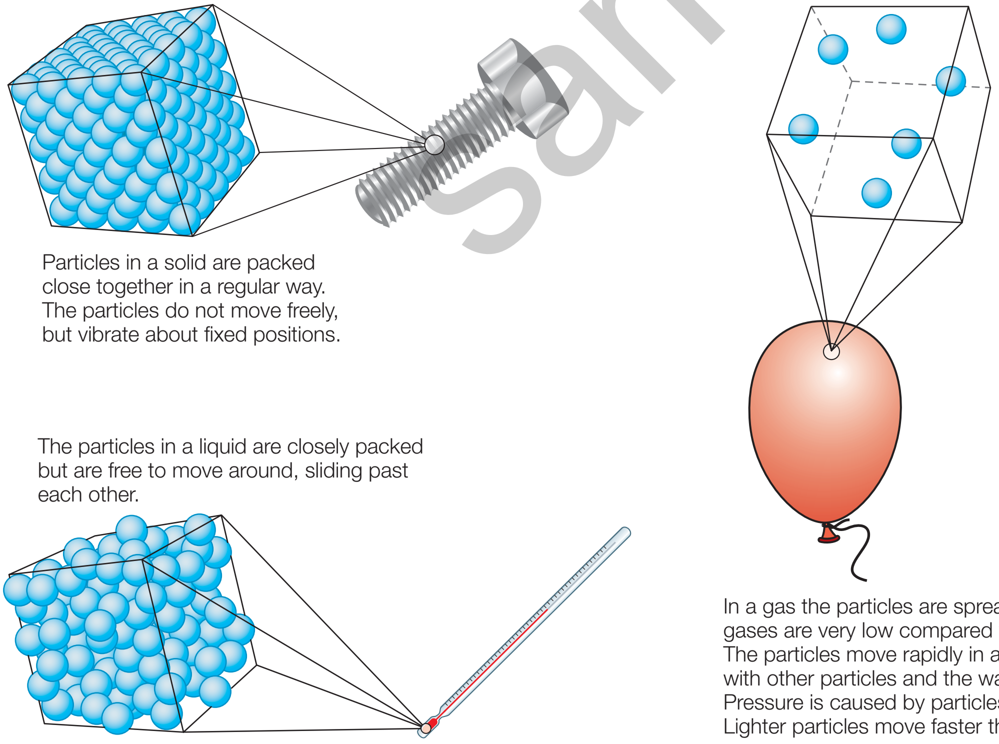
Tip

Theories of structure and bonding are key to understanding the properties of materials. You will extend your knowledge of these ideas when you study Chapter 2. Chapter 8 shows how measuring energy changes can provide evidence of the nature and strength of chemical bonds.

Discovering the composition and structure of materials

New materials exist only because chemists understand how atoms, ions and molecules are arranged in different materials, and about the forces which hold these particles together. Thanks to this knowledge, people can enjoy fibres that breathe but are waterproof, plastic ropes that are 20 times stronger than similar ropes of steel and metal alloys which can remember their shape.

Understanding the structure and bonding of materials is a central theme in modern chemistry. Fundamental to this is an understanding of how the atoms, molecules or ions are arranged in different states of matter (Figure 2).



Particles in a solid are packed close together in a regular way. The particles do not move freely, but vibrate about fixed positions.

The particles in a liquid are closely packed but are free to move around, sliding past each other.

In a gas the particles are spread out, so the densities of gases are very low compared with solids and liquids. The particles move rapidly in a random manner, colliding with other particles and the walls of the container. Pressure is caused by particles hitting the walls. Lighter particles move faster than heavier ones.

Figure 2 The arrangements of particles in solids, liquids and gases.

Explaining and controlling chemical changes

Four key questions are at the heart of many chemical investigations.

- **How much?** – How much of the reactants is needed to make a product, how much of the product is produced, and how much energy is needed?
- **How fast?** – How can a reaction be controlled so that it goes at the right speed: not too fast and not too slow?
- **How far?** – Do the chemicals react completely, or does the reaction stop before all the reactants have turned into products? If it does, what can be done to get as big a yield as possible?
- **How do reactions occur?** – Which bonds between atoms break and which new bonds form during a reaction?

Tip

Chapters 5 and 8 show you how chemists answer the question 'How much?'. The questions 'How fast?' and 'How far?' are the focus of Chapters 9 and 10. Understanding how reactions occur is a feature of organic chemistry and so the study of reaction mechanisms is explored in the three parts of Chapter 6.

Developing new techniques and skills

Chemistry involves *doing* things as well as gaining knowledge and understanding about materials. Chemists use their thinking skills and practical skills to solve problems. One of the frontiers of today's chemistry involves nanotechnology, in which chemists work with particles as small as individual atoms (Figure 3).

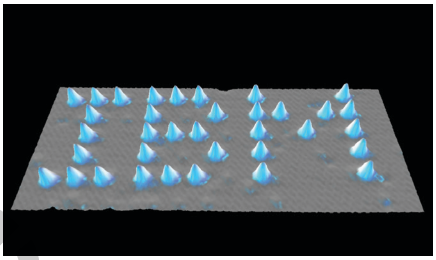


Figure 3 In the 1990s, two scientists working for IBM cooled a nickel surface to −269 °C in a vacuum chamber. Then they introduced a tiny amount of xenon so that some of the xenon atoms stuck to the nickel surface. Using a special instrument called a scanning tunnelling microscope, the scientists were able to move individual xenon atoms around on the nickel surface and construct the IBM logo. Each blue blob is the image of a single xenon atom.

Increasingly, chemists rely on modern instruments to explore structures and chemical changes. They also use information technology to store data, search for information and to publish their findings.

Analysis and synthesis

A vital task for chemists is to analyse materials and find out what they are made of. When chemists have analysed a substance, they use symbols and formulae to show the elements it contains. Symbols are used to represent the atoms in elements; formulae are used to represent the ions and molecules in compounds.

Analysis is involved in checking that water is safe to drink and that food has not been contaminated. People may worry about pollution of the environment, but without chemical analysis they would not know about the causes or the scale of any pollution.

Chemists have devised many ingenious methods of analysis. Spectroscopy is especially important. At first spectroscopists just used visible light, but now they have found that they can find out much more by using other kinds of radiation such as ultraviolet and infrared rays, radiowaves and microwaves.

Chemistry is also about making things. Chemists take simple chemicals and join them together to make new substances. This is synthesis. On a large scale, the chemical industry converts raw materials from the earth, sea and air into valuable new products. A well-known example is the Haber process which uses natural gas and air to make ammonia. Ammonia is the chemical needed to make fertilisers, dyes and explosives. On a smaller scale, chemical reactions produce the specialist chemicals used for perfumes, dyes and medicines.

Tip

You will be developing your practical skills and understanding of practical chemistry during your A Level course. Most chapters in this book include activities and core practicals with results and data to analyse. General guidance on practical work can be accessed online at www.hoddereducation.co.uk/EdexcelChemistry.

Tip

Chapter 7 includes an account of some of the modern instrumental techniques used by chemists. Organic reactions that are important in synthesis feature in all parts of Chapter 6. The study of synthesis is a key feature of the organic chemistry in the second half of your A Level course.

Linking theories and experiments

Scientists test their theories by doing experiments. In chemistry, experiments often begin with careful observation of what happens as chemicals react and change. Theories are more likely to be accepted if predictions made from them turn out to be correct when tested by experiment.

One of the reasons why Mendeléev's Periodic Table was so successful was because he left gaps in his table for elements that had not yet been discovered and then made predictions about the properties of missing elements that turned out to be accurate (Table 1).

Table 1 Mendeléev's predictions for germanium in 1871 and the properties it was found to have after its discovery in 1886.

Mendeléev's predictions in 1871	Actual properties in 1886
Grey metal	Pale grey metal
Density 5.5 g cm^{-3}	Density 5.35 g cm^{-3}
Relative atomic mass 73.4	Relative atomic mass 72.6
Melting point 800 °C	Melting point 937 °C
Formula of oxide GeO_2	Ge forms GeO_2

Tip

Chemistry is a quantitative subject which involves a variety of types of calculation. You will find many worked examples in the chapters of this book that will help you to solve quantitative problems. The key mathematical ideas and techniques involved are described in Appendix A1.

Studying chemistry is more than about 'what we know'. It is also about 'how we know'. For example, the study of atomic structure has provided evidence about the nature and properties of electrons, and this has led to an explanation of the properties of elements and the patterns in the Periodic Table in terms of the electron structures of atoms.

2 Elements

Everything is made of elements. Elements are the simplest chemical substances which cannot be decomposed into simpler chemicals by heating or using electricity. There are over 100 elements, but from their studies of the stars, astronomers believe that about 90% of the Universe consists of just one element, hydrogen. Another 9% is accounted for by helium, leaving only 1% for all the other elements.

Metals and non-metals

Most of the elements, nearly 90 of them, are metals. It is usually easy to recognise a metal by its properties. Most metals are shiny, strong, bendable and good conductors of electricity (Figure 4).

There are only 22 non-metal elements: this includes a few which are solid at room temperature, such as carbon and sulfur, several gases, such as hydrogen, oxygen, nitrogen and chlorine, and just one liquid, bromine (Figure 5).

Figure 4 Samples of metals: from left to right, copper, zinc, lead and silver.

Figure 5 Samples of non-metals: sulfur, bromine, phosphorus (behind), carbon and iodine (in front).

Atoms of elements

Each element has its own kind of atom. An atom is the smallest particle of an element. Atoms consist of protons, neutrons and electrons. Every atom has a tiny nucleus surrounded by a cloud of electrons (Figure 6).

The mass of an atom is concentrated in the nucleus which consists of protons and neutrons. The protons are positively charged and the neutrons uncharged. All the atoms of a particular element have the same number of protons in the nucleus.

The electrons are negatively charged. The mass of an electron is so small that it can often be ignored. In an atom the number of electrons equals the number of protons in the nucleus. So the total negative charge equals the total positive charge and overall the atom is uncharged.

Test yourself

5 Give examples of substances which can be split into elements by heating or by using an electric current (electrolysis).

6 Draw up a table to compare metal elements with non-metal elements using the following headings: Property; Metal; Non-metal.

3 Compounds

Compounds form when two or more elements combine. Apart from the atoms of the elements helium and neon, all elements can combine with other elements.

In order to explain the properties of compounds, chemists need to find out how the atoms, molecules or ions are arranged (the structure) and what holds them together (the bonding).

Compounds of non-metals with non-metals

Water, carbon dioxide, methane in natural gas, sugar and ethanol ('alcohol') are examples of compounds of two or more non-metals. These compounds of non-metals have molecular structures.

Tip

You will learn more about the properties of metal and non-metal elements in Chapter 4.

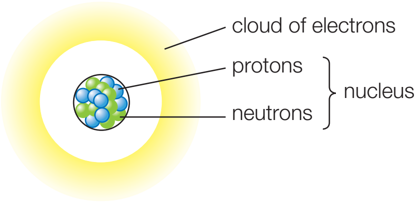


Figure 6 Diagram of an atom showing a nucleus surrounded by a cloud of electrons. This is not to scale. In reality the diameter of an atom is about 100 000 times bigger than the diameter of its nucleus.

Tip

You will learn more about atomic structure in Chapter 1.

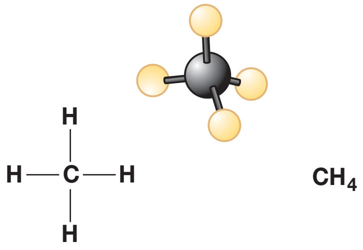


Figure 7 Ways of representing a molecule of methane.

Tip

You will learn more about how chemists determine the formulae of compounds in Sections 5.2 and 5.3.

The covalent bonds between the atoms in molecules are strong but the attractive forces between molecules are weak. This means that molecular compounds melt and vaporise easily. They may be gases, liquids or solids at room temperature and they do not conduct electricity.

Methane contains one carbon atom bonded to four hydrogen atoms. The formula of the molecule is CH_4. Figure 7 shows three ways of representing a methane molecule.

Chemists have to analyse compounds to find their formulae. The results of analysis give an empirical (experimental) formula. This shows the simplest whole number ratio of the atoms of different elements in a compound, for example CH_4 for methane and CH_3 for ethane.

More information is needed to work out the molecular formula of a compound showing the numbers of atoms of the different elements in one molecule of the compound. For example, CH_4 is the molecular formula of methane but C_2H_6 is the molecular formula of ethane.

It is often possible to write the formula of non-metal compounds given how many covalent bonds the atoms normally form (Table 2).

Table 2 Symbols, number of bonds and colour codes of some non-metals.

Element	Symbol	Number of bonds formed	Colour in molecular models
Carbon	C	4	Black
Nitrogen	N	3	Blue
Oxygen	O	2	Red
Sulfur	S	2	Yellow
Hydrogen	H	1	White
Chlorine	Cl	1	Green

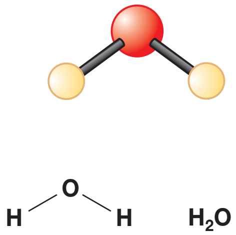


Figure 8 Ways of representing a molecule of water.

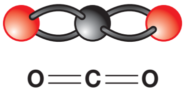


Figure 9 Bonding in carbon dioxide showing the double bonds between atoms.

Water is a compound of oxygen and hydrogen. Oxygen atoms form two bonds and hydrogen atoms form one bond. So two hydrogen atoms can bond to one oxygen atom (Figure 8) and the formula of water is H_2O.

There are double and even triple bonds between the atoms in some non-metal compounds (Figure 9). Notice also that there is a colour code for the atoms of different elements in molecular models – these colours are shown in Table 2.

In practice, it is not possible to predict the formulae of all non-metal compounds. For example, the simplified bonding rules in Table 2 cannot account for the formulae of carbon monoxide, CO, sulfur dioxide, SO_2, or sulfur hexafluoride, SF_6.

Figure 10 Quartz crystal from Sentis, Switzerland. Quartz is one of the commonest minerals of the Earth's crust. It consists of silicon dioxide, SiO_2.

There are some compounds made up of non-metal elements in which the covalent bonding links all the atoms in a crystal together in a giant lattice. Silicon dioxide, SiO_2, is an important example which is found in many igneous rocks (Figure 10). Compounds with covalent giant structures are hard and melt at high temperatures.

Test yourself

7 Draw the various ways of representing the following molecular compounds in the style of Figure 7:

a) hydrogen chloride **b)** carbon disulfide.

8 Name the elements present and work out the formula of the following molecular compounds:

a) hydrogen sulfide **b)** dichlorine oxide

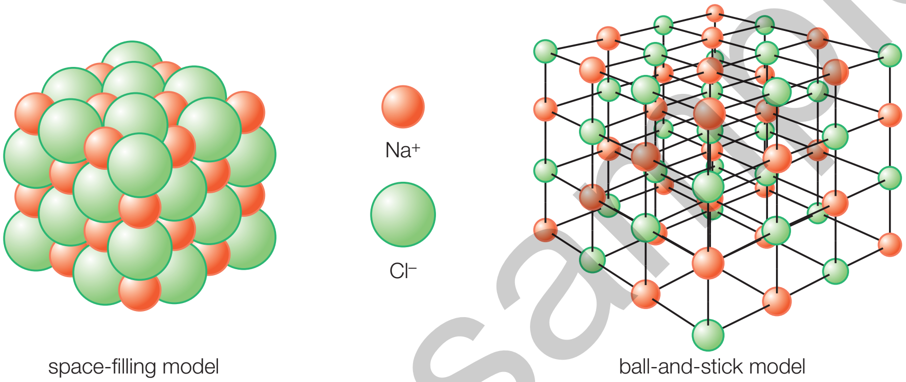
c) ammonia (hydrogen nitride).

Tip

You will learn more about the bonding in compounds of non-metals with non-metals in Chapter 2.

Compounds of metals with non-metals

Common salt (sodium chloride), limestone (calcium carbonate) and copper sulfate are all examples of compounds of metals with non-metals. These metal/non-metal compounds consist of a giant structure of ions. An ion is an atom, or a group of atoms, which has become electrically charged by the loss or gain of one or more electrons. Generally metal atoms form positive ions by losing electrons while non-metal atoms form negative ions by gaining electrons. For example, sodium chloride consists of positive sodium ions, Na^+, and negative chloride ions, Cl^- (Figure 11).



space-filling model

ball-and-stick model

Figure 11 A space-filling model and a ball-and-stick model showing the giant structure of sodium chloride.

The strong ionic bonding between the ions means that such compounds melt at much higher temperatures than the molecular compounds of non-metals. They are solids at room temperature. They conduct electricity as molten liquids but not as solids. Metal/non-metal compounds conduct electricity when heated above their melting points because the ions are free to move in the liquid state.

The formula of sodium chloride is NaCl because the positive charge on one Na^+ ion is balanced by the negative charge on one Cl^- ion. In a crystal of sodium chloride there are equal numbers of sodium ions and chloride ions.

The formulae of all metal/non-metal (ionic) compounds can be worked out by balancing the charges on positive and negative ions. For example, the formula of potassium oxide is K_2O. Here, two K^+ ions balance the charge on one O^{2-} ion.

Elements such as iron, which have two different ions (Fe^{2+} and Fe^{3+}), have two sets of compounds – iron(II) compounds such as iron(II) chloride, $FeCl_2$, and iron(III) compounds such as iron(III) chloride, $FeCl_3$.

Table 3 The names and formulae of some ionic compounds.

Name of compound	Ions present	Formula
Magnesium nitrate	Mg^{2+} and NO_3^-	$Mg(NO_3)_2$
Aluminium hydroxide	Al^{3+} and OH^-	$Al(OH)_3$
Zinc bromide	Zn^{2+} and Br^-	$ZnBr_2$
Lead(II) nitrate	Pb^{2+} and NO_3^-	$Pb(NO_3)_2$
Calcium iodide	Ca^{2+} and I^-	CaI_2
Copper(II) carbonate	Cu^{2+} and CO_3^{2-}	$CuCO_3$
Silver sulfate	Ag^+ and SO_4^{2-}	Ag_2SO_4

Table 3 shows the names and formulae of some ionic compounds. Notice that the formula of magnesium nitrate is $Mg(NO_3)_2$. The brackets round NO_3^- show that it is a single unit containing one nitrogen and three oxygen atoms bonded together with a 1− charge. Other ions, such as OH^-, SO_4^{2-} and CO_3^{2-}, must also be treated as single units and put in brackets when there are two or three of them in a formula.

Tip

You will learn more about ionic crystals and ionic bonding in Chapter 2.

Test yourself

9 This question concerns the substances ice, salt, sugar, copper, steel and limestone.

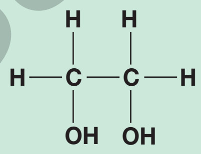
Which of these substances contain:

a) uncombined atoms

b) ions

c) molecules?

10 The structure of the main constituent in antifreeze is:



$$\begin{array}{ccccccc} & & H & & H & & \\ & & | & & | & & \\ H & - & C & - & C & - & H \\ & & | & & | & & \\ & & OH & & OH & & \end{array}$$

What is:

a) its molecular formula

b) its empirical formula?

11 The formula of aluminium hydroxide must be written as $Al(OH)_3$. Why is $AlOH_3$ wrong?

12 Write the formulae of the following ionic compounds given these charges on ions: Al^{3+}, Fe^{2+}, Fe^{3+}, K^+, Pb^{2+}, Zn^{2+}, CO_3^{2-}, O^{2-}, OH^-, SO_4^{2-}:

a) potassium sulfate

b) aluminium oxide

c) lead carbonate

d) zinc hydroxide

e) iron(III) sulfate.

13 Which of the following compounds consist of molecules and which consist of ions?

- **a)** octane (C_8H_{18}) in petrol
- **b)** copper(I) oxide
- **c)** concentrated sulfuric acid
- **d)** lithium fluoride
- **e)** phosphorus trichloride

14 Compare non-metal (molecular) compounds with metal/non-metal (ionic) compounds in:

- **a)** melting temperatures and boiling temperatures
- **b)** conduction of electricity as liquids.

4 Chemical changes

Burning, rusting and fermentation are all examples of chemical reactions. Under the right conditions, chemical bonds break and new ones form. This is what happens during a chemical reaction to create new chemicals.

Figure 12 shows a simple way of demonstrating that when hydrogen burns the product is water. Hydrogen and oxygen (in the air) are both gases at room temperature. When the gases react the changes give out so much energy that there is a flame. Water condenses on cooling the steam that forms in the flame.

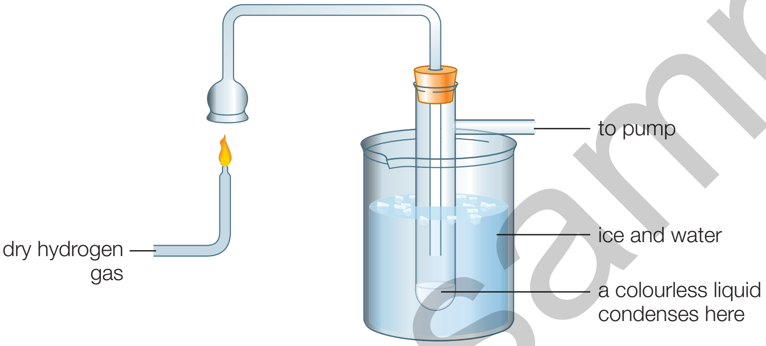


Figure 12 Demonstration that burning hydrogen produces water.

One way of describing what happens during a reaction is to write a word equation. Writing word equations identifies the reactants (on the left) and products (on the right), so it is a useful first step towards a balanced equation with symbols.

When hydrogen burns:

$$\underbrace{\text{hydrogen(g)} + \text{oxygen(g)}}_{\text{reactants}} \rightarrow \underbrace{\text{water(l)}}_{\text{product}}$$

When they are looking at this change, chemists imagine what is happening to the molecules. The trick is to interpret the visible changes in terms of theories about atoms and bonding. Models help to make the connection.

The hydrogen molecules and oxygen molecules consist of pairs of atoms. They are diatomic molecules. Figure 13 shows how molecular models give a picture of the reaction at an atomic level.

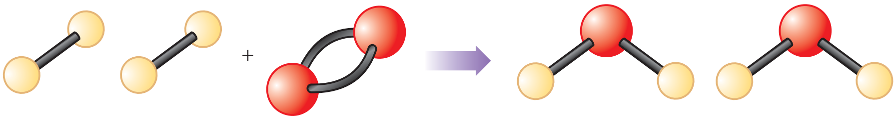


Figure 13 Model equation to show hydrogen reacting with oxygen.

The formula of water is H_2O. Each water molecule contains only one oxygen atom. So one oxygen molecule can give rise to two water molecules, provided that there are two hydrogen molecules available to supply all the hydrogen atoms necessary.

There is the same number of atoms on both sides of the equation. The atoms have simply been rearranged.

Chemists normally use symbols rather than models to describe reactions. Symbols are much easier to write or type. State symbols added to a symbol equation show whether the substances are solid, liquid, gases or dissolved in water.

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l)$$

Tip

You will learn more about writing equations for chemical reactions in Sections 3.2 and 4.1.

Modelling is increasingly important in modern chemistry but now the modelling is usually carried out with computers. In 2013 the Nobel prize for chemistry was awarded to Martin Karplus, Michael Levitt and Arieh Warshel whose work, in the 1970s, laid the foundation for the powerful computer modelling programs that are used to understand and predict chemical processes.

Test yourself

15 a) Write a balanced symbol equation for the reaction of methane, CH_4, with oxygen.

b) Draw a diagram, similar to that shown in Figure 13, to show what happens when methane burns in oxygen.

16 Write balanced equations, with state symbols, for the following word equations:

a) hydrogen + chlorine → hydrogen chloride

b) zinc + hydrochloric acid (HCl) → zinc chloride + hydrogen

c) ethane + oxygen → carbon dioxide + water

d) iron + chlorine → iron(III) chloride.

5 Acids, bases, alkalis and salts

Acids

Figure 14 Crystals of the solid acid citric acid. This acid was first obtained as a pure compound in 1784 when it was crystallised from lemon juice.

Pure acids may be solids (such as citric, Figure 14, and tartaric acids), liquids (such as sulfuric, nitric and ethanoic acids) or gases (such as hydrogen chloride which becomes hydrochloric acid when it dissolves in water). All these acids are compounds with characteristic properties:

- they form solutions in water with a pH below 7
- they change the colour of indicators such as litmus
- they react with metals above hydrogen in the reactivity series forming hydrogen plus an ionic metal compound called a salt

$$Fe(s) + 2HCl(aq) \rightarrow FeCl_2(aq) + H_2(g)$$

- they react with metal oxides and metal hydroxides to form salts and water

$CuO(s) + H_2SO_4(aq) \rightarrow CuSO_4(aq) + H_2O(l)$

- they react with carbonates to form salts, carbon dioxide and water

$ZnCO_3(s) + 2HCl(aq) \rightarrow ZnCl_2(aq) + CO_2(g) + H_2O(l)$

Bases and alkalis

Bases are 'anti-acids'. They are the chemical opposites of acids. Alkalis are bases which dissolve in water. The common laboratory alkalis are sodium hydroxide, potassium hydroxide, calcium hydroxide and ammonia. Alkalis form solutions with a pH above 7, so they change the colours of acid–base indicators. Alkalis are useful because they neutralise acids.

Manufacturers produce powerful oven and drain cleaners containing sodium hydroxide or potassium hydroxide because they can break down and remove greasy dirt. These strong alkalis are highly 'caustic'. They attack skin, producing a chemical burn. Even dilute solutions of these alkalis can be hazardous, especially if they get into your eyes (Section 4.3).

Test yourself

17 Write full balanced equations for the reactions of hydrochloric acid with:

a) zinc
b) calcium oxide
c) potassium hydroxide
d) nickel(II) carbonate.

Salts

Salts are ionic compounds formed when an acid reacts with a base. In the formula of a salt, the hydrogen of an acid is replaced by a metal ion. For example, magnesium sulfate, $MgSO_4$, is a salt of sulfuric acid, H_2SO_4.

Salts can be regarded as having two 'parents'. They are related to a parent acid and to a parent base. Hydrochloric acid, for example, gives rise to the salts called chlorides, such as sodium chloride, calcium chloride and ammonium chloride. The base sodium hydroxide gives rise to sodium salts, such as sodium chloride, sodium sulfate and sodium nitrate.

Neutralisation is not the only way to make a salt. Some metal chlorides, for example, are made by heating metals in a stream of chlorine. This is useful for making anhydrous chlorides, such as aluminium chloride.

Test yourself

18 Name the salts formed from these pairs of acids and bases:

a) nitric acid and potassium hydroxide
b) hydrochloric acid and calcium hydroxide
c) sulfuric acid and copper(II) oxide
d) ethanoic acid and sodium hydroxide.

1

Atomic structure and the Periodic Table

1.1 Models of atomic structure

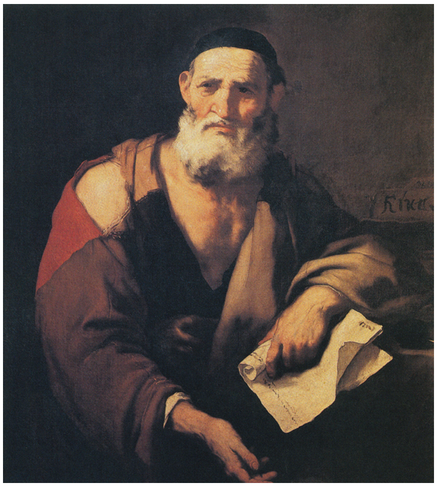


Figure 1.1 The Greek philosopher Democritus, who lived from 460 to 370 BCE.

Early ideas about atoms

The idea that all substances are made of atoms is a very old one. It was suggested by Greek philosophers, including Democritus, more than 2400 years ago (Figure 1.1).

Democritus was a philosopher whose idea was that if a lump of metal, such as iron, was cut into smaller and smaller pieces, the end result would be miniscule and invisible particles that could not be cut any smaller. Democritus called these smallest particles of matter ‘atomos’ meaning ‘indivisible’. He explained the properties of materials such as iron in terms of the shapes of the atoms and the ‘hooks’ that he imagined joined them together.

Democritus was a great thinker but he did not do experiments and he had no way to test his ideas. He, and other atomists of his time, failed to convince everybody that the theory was correct. There were other competing theories and no convincing reasons to accept the idea of atoms in preference to other ideas.

Modern atomic theory grew from work started about 2000 years after Democritus, when scientists in Europe started to purify substances and to carry out experiments with them. They found that many substances could be broken down (decomposed) into simpler substances, which they called elements. These elements could then be combined to make new compounds.

Figure 1.2 John Dalton was born in 1766 in the village of Eaglesfield in Cumbria. His father was a weaver. Dalton was always curious and liked to study. When he was only 12 years old, he started to teach children in the village school. For most of his life, he taught science and carried out experiments at the Presbyterian College in Manchester.

In the eighteenth century, chemists began to make accurate measurements of the quantities of substances involved in reactions. To their surprise, they found that the weights of elements which reacted were always in the same proportions. So, for example, water always contained 1 part by weight of hydrogen to 8 parts by weight of oxygen. And, black copper oxide always contained 1 part by weight of oxygen to 4 parts by weight of copper.

At the start of the nineteenth century, John Dalton puzzled over these results. He concluded that if elements were made of indivisible particles, then everything made sense (Figure 1.2). Compounds, like copper oxide, were made of particles of copper and oxygen with different masses and these always combined in the same ratios. Dalton called the indivisible particles atoms in recognition of the ideas first proposed by Democritus.

Dalton began to publish his atomic theory in 1808. The main points in his theory were that:

- all elements are made up of indivisible particles called atoms
- all the atoms of a given element are identical and have the same mass

- the atoms of different elements have different masses
- atoms can combine to form molecules in compounds
- all the molecules of a given compound are identical.

Although some scientists were reluctant to accept Dalton's ideas, his atomic theory caught on because it could explain the results of many experiments.

Even today, Dalton's atomic theory is still useful and very helpful. However, research has since shown that atoms are not indivisible and that all atoms of the same element are not identical.

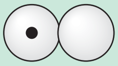
Test yourself

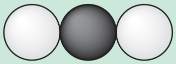
1 Look at the five main points in Dalton's atomic theory. Which of these points:

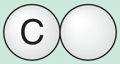
a) are still correct

b) are now incorrect?

2 Look at the formulae below which Dalton used for water, carbon dioxide and black copper oxide.


water


carbon dioxide



black copper oxide

a) Write the formulae that are used today for these compounds.

b) What symbols did Dalton use for carbon, oxygen, hydrogen and copper?

c) Which one of the formulae did Dalton get wrong?

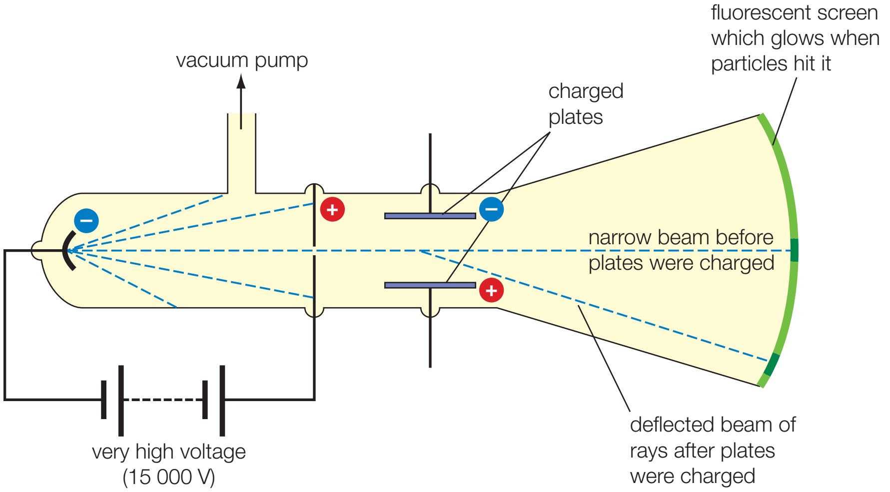
Inside atoms

For much of the nineteenth century, scientists continued with the idea that atoms were just as Dalton had described them: solid, indestructible particles similar to tiny snooker balls. Then, between 1897 and 1932, scientists carried out several series of experiments that revealed that atoms contain three smaller particles: electrons, protons and neutrons.

The discovery of electrons

In 1897, J.J. Thomson was investigating the conduction of electricity by gases in his laboratory at Cambridge. When he connected 15 000 volts across the terminals of a tube containing air, the glass walls glowed bright green. Rays travelling in straight lines from the negative terminal hit the glass and made it glow. Experiments showed that a narrow beam of the rays could be deflected by an electric field (Figure 1.3). When passed between charged plates, the rays always bent towards the positive plate. This showed they were negatively charged.

Figure 1.3 The effect of charged plates on a beam of electrons.



Further study showed that the rays consisted of tiny negative particles about 2000 times lighter than hydrogen atoms. This surprised Thomson. He had discovered particles smaller than atoms. Thomson called the tiny negative particles electrons.

Thomson obtained the same electrons with different gases in the tube and when the terminals were made of different substances. This suggested to him that the atoms of all substances contain electrons. Thomson knew that atoms had no electrical charge overall. So, the rest of the atom must have a positive charge to balance the negative charge of the electrons.

In 1904, Thomson published his model for the structure of atoms. He suggested that atoms were tiny balls of positive material with electrons embedded in it like fruit in a Christmas pudding. As a result, Thomson's idea became known as the 'plum pudding' model of atomic structure (Figure 1.4).

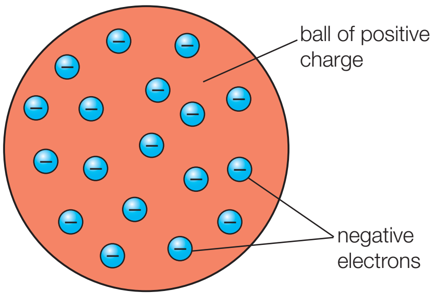


Figure 1.4 Thomson's plum pudding model for the structure of atoms.

Rutherford and the nuclear atom

Radioactivity was discovered by Henri Becquerel in Paris in 1896. Two years later, Ernest Rutherford, in Manchester, showed that there were at least two types of radiation given out by radioactive materials. He called these alpha rays and beta rays.

At the time, Rutherford and his colleagues didn't know exactly what alpha rays were. But they did know that alpha rays contained particles. These alpha particles were small, heavy and positively charged. Rutherford and his colleagues realised that they could use the alpha particles as tiny 'bullets' to fire at atoms.

In 1909, two of Rutherford's colleagues, Hans Geiger and Ernest Marsden, directed narrow beams of positive alpha particles at very thin gold foil only a few atoms thick (Figure 1.5). They expected the particles to pass straight through the foil or to be deflected slightly.

The results showed that:

- most of the alpha particles went straight through the foil
- some of the alpha particles were scattered (deflected) by the foil
- a few alpha particles rebounded from the foil.

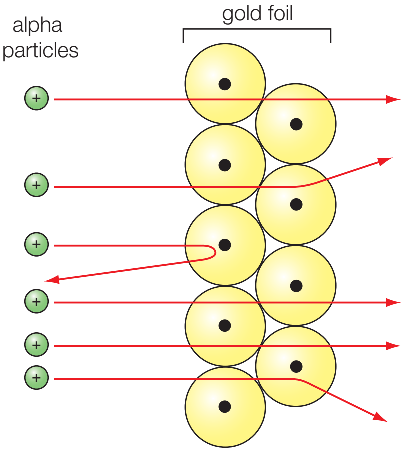


Figure 1.5 When positive alpha particles are directed at a very thin sheet of gold foil, they emerge at different angles. Most pass straight through the foil, some are deflected and a few appear to rebound from the foil.

Test yourself

3 Suggest explanations for these results of the Geiger–Marsden experiment:

- **a)** Most of the alpha particles passed straight through the foil.
- **b)** Some alpha particles were deflected.
- **c)** A few alpha particles rebounded from the foil.

4 a) What did the Geiger–Marsden experiment suggest about the size of any positive and negative particles in the gold atoms.

b) Why did the results cast doubts on Thomson's plum pudding model for atomic structure?

5 Rutherford and his team published a series of papers about their work, including a paper *The Laws of Deflexion of α Particles through Large Angles* in a 1913 edition the *Philosophical Magazine.* Why is it important that scientists publish their experimental results and theories?

Rutherford came up with a new model of the atom to explain the results of Geiger and Marsden's experiment. In this model a very small positive nucleus is surrounded by a much larger region of empty space in which electrons orbit the nucleus like planets orbiting the Sun (Figure 1.6).

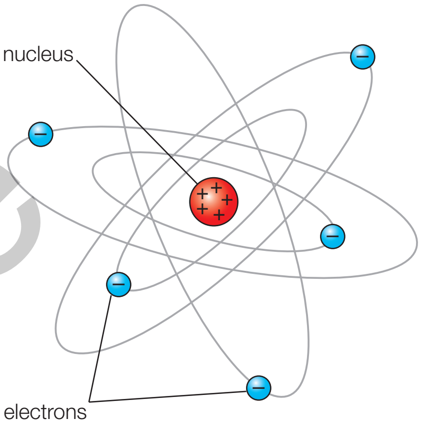


Figure 1.6 Rutherford's nuclear model for the structure of atoms. Rutherford pictured atoms as miniature solar systems with electrons orbiting the nucleus like planets around the Sun.

Rutherford's nuclear model quickly replaced Thomson's plum pudding model and it is still the basis of models of atomic structure used today.

The work of Thomson, Rutherford and their colleagues showed that:

- atoms have a small positive nucleus surrounded by a much larger region of empty space in which there are tiny negative electrons (Figure 1.7)
- the positive charge of the nucleus is due to positive particles which Rutherford called protons
- protons are about 2000 times heavier than electrons
- the positive charge on one proton is equal in size, but opposite in sign, to the negative charge on one electron
- atoms have equal numbers of protons and electrons, so the positive charges on the protons cancel the negative charges on the electrons
- the smallest atoms are those of hydrogen with one proton and one electron. The next smallest atoms are those of helium with two protons and two electrons, then lithium atoms with three protons and three electrons, and so on.

Figure 1.7 If the nucleus of a hydrogen atom were to be enlarged to the size of a marble and put in the centre of the Wembley pitch, the atom's one electron would be whizzing around somewhere in the stands.

Chadwick and the discovery of neutrons

Although Rutherford was successful in explaining many aspects of atomic structure, one big problem remained. If hydrogen atoms contain one proton and helium atoms contain two protons, then the relative masses of hydrogen and helium atoms should be one and two, respectively. But the mass of helium atoms relative to hydrogen atoms is four and not two. It took the discovery of isotopes and much further research before the problem was solved.

In 1932, James Chadwick, in Cambridge, solved the mystery of the extra mass in helium atoms. Chadwick studied the effects of bombarding a beryllium target with alpha particles. This produced a new kind of radiation with no electric charge but with enough energy to release protons when fired at a material such as wax. In time, Chadwick was able to demonstrate that there must be uncharged particles in the nuclei of atoms, as well as positively charged protons. Chadwick called these particles neutrons. It was soon found that neutrons had the same mass as protons.

The discovery of neutrons accounted for the relative masses of hydrogen and helium atoms. Hydrogen atoms have one proton and no neutrons, so a hydrogen atom has a relative mass of one unit, Helium atoms have two protons and two neutrons, so a helium atom has a relative mass of four units. This makes a helium atom four times as heavy as a hydrogen atom.

It is now understood that all atoms are made up from protons, neutrons and electrons. The relative masses, relative charges and positions within atoms of these sub-atomic particles are summarised in Table 1.1.

Tip

For a time, protons, neutrons and electrons were described as 'fundamental' or 'elementary' particles – that is particles not made up of anything smaller or simple. Electrons are still thought to be fundamental particles but protons and neutrons are now known to be made up of quarks.

Table 1.1 Relative masses, relative charges and positions in atoms of protons, neutrons and electrons.

Particle	Mass relative to that of a proton	Charge relative to that on a proton	Position in the atom
Proton	1	+1	Nucleus
Neutron	1	0	Nucleus
Electron	$\frac{1}{1840}$	–1	Shells

Test yourself

6 Draw and label a diagram to show how Chadwick explained that the mass of a helium atom is four times the mass of a hydrogen atom.

7 Summarise the development of atomic models in a table with the models listed in the left-hand column and a brief note on the evidence which gave rise to the models in the right-hand column.

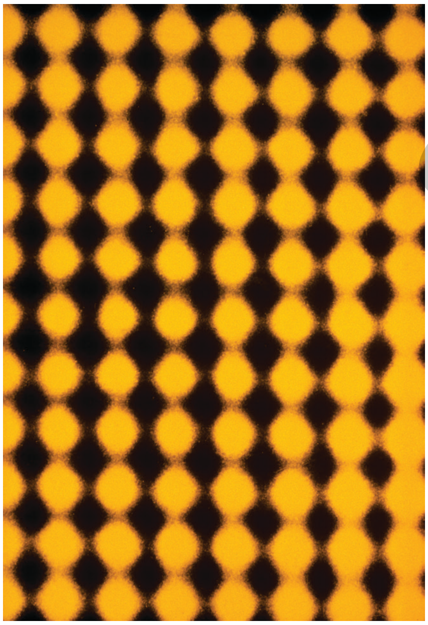


Figure 1.8 Photo of the surface of a gold crystal taken through an electron microscope. Each yellow blob is a separate gold atom – the atoms have been magnified about 35 million times.

1.2 Atomic number and mass number

All the atoms of a particular element have the same number of protons, and atoms of different elements have different numbers of protons.

Hydrogen atoms are the simplest of all atoms – they have just one proton and one electron. The next simplest are atoms of helium with two protons and two electrons, then lithium with three protons, and so on. Large atoms have large numbers of protons and electrons. For example, gold atoms (Figure 1.8) have 79 protons and 79 electrons.

The only atoms with one proton are those of hydrogen; the only atoms with two protons are those of helium; the only atoms with three protons are those of lithium, and so on. This means that the number of protons in an atom decides which element it is. Because of this, scientists have a special name for the number of protons in the nucleus of an atom. They call it the

atomic number and use the symbol *Z* to represent it. So, hydrogen has an atomic number of 1 ($Z = 1$), helium has an atomic number of 2 ($Z = 2$), and so on.

Protons do not account for all the mass of an atom – neutrons in the nucleus also contribute. Therefore, the mass of an atom depends on the number of protons plus neutrons. This number is called the **mass number** of the atom (symbol *A*).

Hydrogen atoms, with one proton and no neutrons, have a mass number of 1. Lithium atoms, with 3 protons and 4 neutrons, have a mass number of 7 and aluminium atoms, with 13 protons and 14 neutrons, have a mass number of 27.

There is an agreed shorthand for showing the mass number and atomic number of an atom. This is shown for a potassium atom, ${}^{39}_{19}\mathrm{K}$, in Figure 1.9. Ions can also be represented using this shorthand. For example, the potassium ion can be written as ${}^{39}_{19}\mathrm{K}^+$.

Key terms

The **atomic number** of an atom is the number of protons in its nucleus. The term 'proton number' is sometimes used for atomic number.

The **mass number** of an atom is the number of protons plus neutrons in its nucleus. Protons and neutrons are sometimes called nucleons, so the term 'nucleon number' is an alternative to mass number.

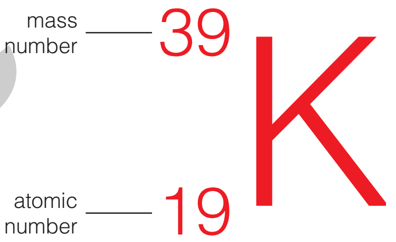


Figure 1.9 The mass number and atomic number can be shown with the symbol of an atom.

Test yourself

8 Use Figure 1.8, and the information in the caption, to estimate the diameter of a gold atom in nanometres.

9 How many protons, neutrons and electrons are there in the following atoms and ions:

- **a)** ${}^{9}_{4}\mathrm{Be}$
- **b)** ${}^{39}_{19}\mathrm{K}$
- **c)** ${}^{235}_{92}\mathrm{U}$
- **d)** ${}^{19}_{9}\mathrm{F}^-$
- **e)** ${}^{40}_{20}\mathrm{Ca}^{2+}$?

10 Write symbols showing the mass number and atomic number for these atoms and ions:

- **a)** an atom of oxygen with 8 protons, 8 neutrons and 8 electrons
- **b)** an atom of argon with 18 protons, 22 neutrons and 18 electrons
- **c)** an ion of sodium with a 1+ charge and a nucleus of 11 protons and 12 neutrons
- **d)** an ion of sulfur with a 2– charge and a nucleus with 16 protons and 16 neutrons.

1.3 Comparing the masses of atoms – mass spectrometry

Individual atoms are far too small to be weighed, but in 1919 F.W. Aston invented the mass spectrometer. This gave scientists an accurate method of comparing the relative masses of atoms and molecules. Since its invention, mass spectrometry has been developed into a sophisticated technique for chemical analysis based on a variety of types of instrumentation.

A mass spectrometer separates atoms and molecules according to their mass, and also shows the relative numbers of the different atoms and molecules present. Figure 1.10 shows a schematic diagram of a mass spectrometer.

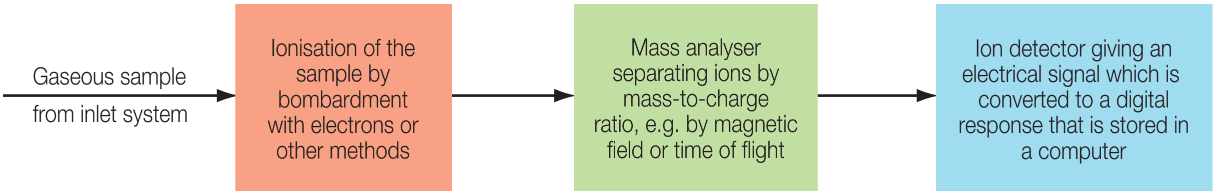


Figure 1.10 A schematic diagram to show the key features of a mass spectrometer.

Before atoms, or molecules, can be separated and detected in a mass spectrometer, they must be converted to positive ions in the gaseous or vapour state. This can be done in various ways. In some mass spectrometers, a beam of high-energy electrons bombards the atoms or molecules of the sample. This turns them into ions by knocking out one or more electrons.

$$\underset{\text{fast-moving electron}}{e^-} + \underset{\text{atom in sample vapour}}{X} \rightarrow \underset{\text{positive ion}}{X^+} + \underset{\text{electron knocked out of X}}{e^-} + \underset{\text{slower-moving electron}}{e^-}$$

Inside a mass spectrometer there is a high vacuum. This allows ionised atoms or molecules from the chemical being tested to be studied without interference from atoms and molecules in the air.

After ionisation, the charged species are separated to produce the mass spectrum, which distinguishes the positive ions on the basis of their **mass-to-charge** ratios.

There are various types of mass spectrometer. They differ in the method used to separate ions with different ratios of mass to charge. One type uses an electric field to accelerate ions into a magnetic field, which then deflects the ions onto the detector. A second type accelerates the ions and then separates them by their flight time through a field-free region. A third type, the so-called transmission quadrupole instrument, is now much the most common because it is very reliable, compact and easy to use. It varies the fields in the instrument in a subtle way to allow ions with a particular mass-to-charge ratio to pass through to the detector at any one time.

The output from the detector of a mass spectrometer is often presented as a 'stick diagram'. This shows the strength of the signal produced by ions of varying mass-to-charge ratio. The scale on the vertical axis shows the relative abundance of the ions. The horizontal axis shows the m/z values.

Each of the four peaks on the mass spectrum of lead in Figure 1.11 represents a lead ion of different mass, and the heights of the peaks give the proportions of the ions present.

Key term

The **mass-to-charge ratio** (m/z) is the ratio of the relative mass, m, of an ion to its charge, z, where z is the number of charges (1, 2 and so on). Spectrometers usually operate so that most ions produced have the value of $z = 1$.

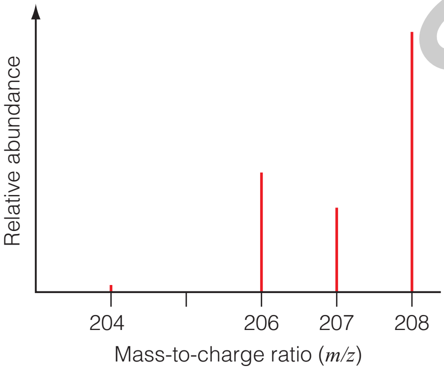


Figure 1.11 A mass spectrum of the element lead. The lead ions that produce the peaks in the mass spectrum are all 1+ ions formed by ionising atoms in a lead vapour at very low pressure. The lead ions that form under these conditions are not the same as the stable lead ions normally found in solid lead compounds or in solutions.

Test yourself

11 Look carefully at Figure 1.11.

a) How many different ions are detected in the mass spectrum of lead?

b) What are the relative masses of these different ions?

c) Make a rough estimate of the relative proportions of these different ions in the sample of lead.

1.4 Isotopes and relative isotopic masses

Mass spectrometer traces, like that in Figure 1.11, show that lead and most other elements contain atoms that are not exactly alike. When atoms of these elements are ionised in a mass spectrometer, the ions separate and are detected as two or more peaks with different values of m/z. This shows that the atoms from which the ions formed must have different relative masses. These atoms of the same element with different masses are called **isotopes**.

Look closely at Figure 1.12. It shows a mass spectrometer print out (mass spectrum) for magnesium. The three peaks show that magnesium consists of three isotopes with relative masses of 24, 25 and 26. These relative masses are best described as **relative isotopic masses** because they give the relative mass of particular isotopes.

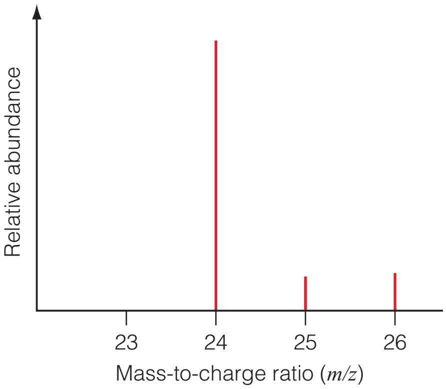


Figure 1.12 A mass spectrum for magnesium.

Chemists originally measured the relative masses of atoms relative to hydrogen. Then, because of the existence of isotopes, it became necessary to choose one particular isotope as the standard. Today, the isotope carbon-12 ($^{12}_{6}C$) is chosen as the standard and given a relative mass of exactly 12.

The heights of the peaks in Figure 1.12 show the relative proportions of the three isotopes. The isotope magnesium-24 has a mass number of 24 with 12 protons and 12 neutrons, whereas magnesium-25 has a mass number of 25 with 12 protons and 13 neutrons. Table 1.2 summarises the important similarities and differences in isotopes.

Table 1.2 Similarities and differences in isotopes.

Isotopes have the same	Isotopes have different
• number of protons • number of electrons • atomic number • chemical properties	• numbers of neutrons • mass numbers • physical properties

Key terms

Isotopes are atoms of the same element which have the same number of protons in the nucleus but a different number of neutrons. So isotopes have the same atomic number but different mass numbers.

Relative isotopic mass is the mass of one atom of an isotope relative to $\frac{1}{12}$th of the mass of an atom of the isotope carbon-12. The values are relative so they do not have units.

Relative atomic mass, A_r, is the average mass of an atom of an element relative to $\frac{1}{12}$th of the mass of an atom of the isotope carbon-12. The values are relative so they do not have units.

Relative atomic masses

The relative atomic mass of an element is the average mass of an atom of the element relative to one twelfth the mass of an atom of the isotope carbon-12. The symbol for **relative atomic mass** is A_r, where 'r' stands for relative.

$$\text{relative atomic mass} = \frac{\text{average mass of an atom of the element}}{\frac{1}{12} \times \text{the mass of one atom of carbon-12}}$$

Using this scale, the relative atomic mass of hydrogen is 1.0, that of helium is 4.0, and that of oxygen is 16.0. This can be written as: $A_r(H) = 1.0$, $A_r(He) = 4.0$ and $A_r(O) = 16.0$, or simply H = 1.0, He = 4.0 and Cl = 35.5 for short (Figure 1.13).

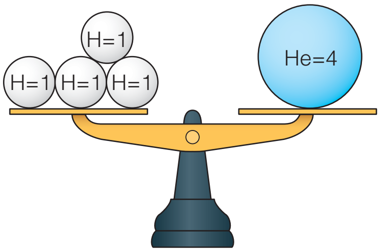


Figure 1.13 If atoms could be weighed, the scales would show that helium atoms are four times as heavy as hydrogen atoms.

The values of relative atomic masses have no units because they are relative. The relative atomic masses of all elements are shown in the Periodic Table on page 652.

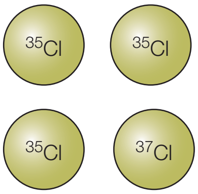


Figure 1.14 On average, for every four chlorine atoms, three are chlorine-35 and one is chlorine-37.

The accurate relative atomic masses of most elements in tables of data are not whole numbers. This is because these elements contain a mixture of isotopes. For example, chlorine contains two isotopes, chlorine-35 and chlorine-37, in the relative proportions of 3 : 1 (Figure 1.14). This is $\frac{3}{4}$, or 75%, chlorine-35 and $\frac{1}{4}$, or 25%, chlorine-37.

So, the average mass of a chlorine atom on the ^{12}C scale is given by:

$$\frac{(3 \times 35) + (1 \times 37)}{4} = 35.5$$

This is the relative atomic mass of chlorine.

Tip

The relative masses of individual isotopes are called **relative isotopic masses**, whereas the relative masses of the atoms in an element (often containing a mixture of isotopes) are called **relative atomic masses**.

Example

The mass spectrum of magnesium (Figure 1.12) shows that it consists of three isotopes with these percentage abundances:

magnesium-24: 78.6%

magnesium-25: 10.1%

magnesium-26: 11.3%

Calculate the relative atomic mass of magnesium.

Notes on the method

The relative atomic mass of magnesium is an average value that takes into account the relative masses of its isotopes and their relative abundance. It is a 'weighted' average (Section A1.4).

The percentages show you how many atoms of each isotope are present in a sample of 100 atoms.

Answer

The total relative mass of 100 atoms of magnesium

$$= (78.6 \times 24) + (10.1 \times 25) + (11.3 \times 26) = 2432.7$$

The average relative mass of a magnesium atom = 2432.7 ÷ 100 = 24.3 (to three significant figures)

Tip

The values for A_r are average values for the mixture of isotopes found naturally. This means that the values of relative atomic masses are often not whole numbers. In calculations you should use A_r values to one decimal place, as in the Periodic Table on page 652.

Test yourself

12 Look up the values of relative atomic masses in the Periodic Table on page 652. How many times heavier (to the nearest whole number) are:

- **a)** C atoms than H atoms
- **b)** Mg atoms than C atoms
- **c)** S atoms than He atoms
- **d)** C atoms than He atoms
- **e)** Fe atoms than N atoms?

13 Silicon consists of three naturally occurring isotopes, ${}^{28}_{14}\mathrm{Si}$ (93.0%), ${}^{29}_{14}\mathrm{Si}$ (5.0%) and ${}^{30}_{14}\mathrm{Si}$ (2.0%).

- **a)** How many protons and neutrons are present in the nuclei of each of these isotopes?
- **b)** What is the relative atomic mass of silicon?

14 Neon has two isotopes with mass numbers of 20 and 22.

- **a)** How do you think the boiling temperature of neon-20 compares with that of neon-22? Explain your answer.
- **b)** Neon in the air contains 90% neon-20 and 10% neon-22. What is the relative atomic mass of neon in the air?

15 Why do isotopes have the same chemical properties, but different physical properties?

Relative molecular and formula masses

Relative atomic masses can also be used to compare the masses of different molecules. The relative masses of molecules are called relative molecular masses (symbol M_r).

The **relative molecular mass** of an element or compound is the sum of the relative atomic masses of all the atoms in its molecular formula.

For oxygen, O_2, $M_r(O_2) = 2 \times A_r(O) = 2 \times 16.0 = 32.0$

and for sulfuric acid, $M_r(H_2SO_4) = 2 \times A_r(H) + A_r(S) + 4 \times A_r(O)$

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

Metal compounds consist of giant structures of ions and not molecules. To avoid the suggestion that their formulae represent molecules, chemists use the term **relative formula mass** (symbol M_r), not relative molecular mass, for ionic compounds and for other compounds with giant structures such as silicon dioxide, SiO_2.

For magnesium nitrate,

$$M_r(Mg(NO_3)_2) = A_r(Mg) + 2 \times [A_r(N) + 3 \times A_r(O)]$$
$$= 24.3 + 2 \times (14.0 + 48.0) = 148.3$$

Key terms

The **relative molecular mass** of an element or compound is the sum of the relative atomic masses of all the atoms in its molecular formula.

The **relative formula mass** of a compound is the sum of the relative atomic masses of all the atoms in its formula.

Tip

Section A1.1 of Appendix A1 on page 626 gives advice on how to work out the value of maths equations with brackets and combinations of multiplication and addition.

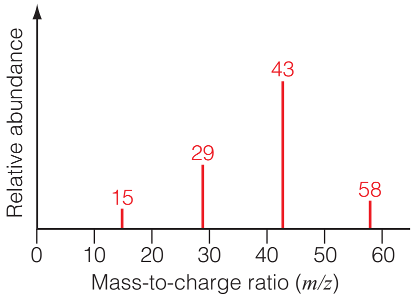


Figure 1.15 The mass spectrum of a hydrocarbon and its fragments.

Mass spectrometers can also be used to study molecules (Chapter 7). After injecting a sample into the instrument and vaporising it, bombarding electrons not only ionise the molecules but also break them into fragments. Because of the high vacuum inside the mass spectrometer, it is possible to study these molecular fragments and ions which do not normally exist. As a result the mass spectrum consists of a 'fragmentation pattern' (Figure 1.15). When analysing molecular compounds, the peak of the ion with the highest mass is usually the whole molecule ionised. So the mass of this 'parent ion' or 'molecular ion', M^+, is the relative molecular mass of the compound.

$$\underset{\text{high-energy electron}}{e^-} + \underset{\text{molecule in sample}}{M(g)} \longrightarrow \underset{\text{molecular ion}}{M^+} + \underbrace{e^- + e^-}_{\text{electrons}}$$

Test yourself

16 What is the relative molecular mass of:

- **a)** chlorine, Cl_2
- **b)** sulfur, S_8
- **c)** ethanol, C_2H_5OH
- **d)** tetrachloromethane, CCl_4?

17 What is the relative formula mass of:

- **a)** magnesium chloride, $MgCl_2$
- **b)** iron(III) oxide, Fe_2O_3
- **c)** hydrated copper(II) sulfate, $CuSO_4.5H_2O$?

18 Look carefully at Figure 1.15.

- **a)** What is the relative molecular mass of the hydrocarbon?
- **b)** The fragment of the hydrocarbon with relative mass 15 is a CH_3 group. What do you think the fragments are with relative masses of 29 and 43?
- **c)** Draw a possible structure for the hydrocarbon.

Notice that, by carefully interpreting the data from mass spectrometers, chemists can deduce:

- the isotopic composition of elements
- the relative atomic masses of elements
- the relative molecular masses of compounds.

Chemists who separate and synthesise new compounds can also identify the fragments in the mass spectra of these compounds. Then, by piecing the fragments together, they can identify possible structures for the new compounds.

The combination of gas chromatography and mass spectrometry is particularly important in modern chemical analysis. Chromatography is first used to separate the chemicals in an unknown mixture, such as polluted water or similar compounds synthesised for possible use as drugs. Then mass spectrometry is used to detect and identify the separated components.

Activity

Mass spectrometry in sport

Mass spectrometry provides an incredibly sensitive method of analysis in areas such as space research, medical research, monitoring pollutants in the environment and the detection of illegal drugs in sport.

Detecting the use of anabolic steroids in sport

Since the 1980s, unscrupulous sportsmen and sportswomen have tried to improve their performance by using anabolic steroids. These drugs increase muscle size and strength, which increases the chance of winning (Figure 1.16). But anabolic steroids also have serious harmful effects on the body. Women develop masculine features and anyone using them may suffer heart disease, liver cancer and depression leading to suicide.

Figure 1.16 Ben Johnson won the men's 100 m race at the Olympic Games in 1992. Unfortunately, urine tests showed that he had used anabolic steroids – Johnson was stripped of his title and the gold medal.

Sporting bodies, such as the International Olympic Committee, have banned the use of anabolic steroids in all sports and have introduced a rigorous testing regime. The testing procedures involve analysis of urine samples using mass spectrometry. Great care is taken during sampling, transport, storage and analysis to ensure that the results of analysis will stand up in court.

Figure 1.17 shows the molecular ion and the largest fragments in the mass spectrum of a banned chemical that is thought to be dihydrocodeine ($C_{18}H_{23}O_3N$).

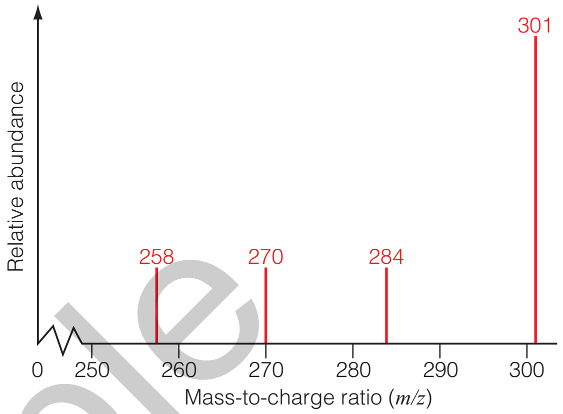


Figure 1.17 The molecular ion and the largest fragments in the mass spectrum of a banned chemical.

1 What is the probable relative molecular mass of the banned chemical on the mass spectrum?

2 Is the probable relative molecular mass consistent with that of dihydrocodeine, ($C_{18}H_{23}O_3N$)? Explain your answer.

3 What is the relative mass of the fragment *lost* from one molecule of the banned substance, leaving the fragment of relative mass 284?

4 Dihydrocodeine contains a CH_3O– group and an –OH group. What evidence does the mass spectrum provide for these two groups?

1.5 Evidence for the electronic structure of atoms

In a mass spectrometer, a beam of electrons can be used to bombard the sample, turning atoms (or molecules) into positive ions. The electrons in the beam must have enough energy to knock electrons off atoms in the sample. By varying the intensity of the beam, it is possible to measure the minimum amount of energy needed to remove electrons from the atoms of an element. From these measurements, scientists can predict the electron structures of atoms.

Key terms

An **ionisation energy** is the energy needed to remove one mole of electrons from one mole of gaseous atoms, or ions, of an element.

Atomic **energy levels** are the energies of electrons in atoms. According to quantum theory, each electron in an atom has a definite energy. When atoms gain or lose energy, the electrons jump from one energy level to another.

Tip

The shells of electrons at fixed or specific levels are sometimes called **quantum shells**. The word 'quantum' is used to describe something related to a fixed amount or a fixed level.

The energy needed to remove one electron from each atom in one mole of gaseous atoms is known as the first **ionisation energy**. The product is one mole of gaseous ions with one positive charge.

So, the first ionisation energy of sodium is the energy required for the process

$\mathrm{Na(g)} \rightarrow \mathrm{Na^{+}(g)} + \mathrm{e^{-}}$ first ionisation energy $= +496\,\mathrm{kJ\,mol^{-1}}$

Ionisation energies like this are always endothermic. Energy is taken in by the reaction so the energy change is given a positive sign.

Scientists can also determine ionisation energies by using a spectroscope to study the light given out by atoms when heated in a flame (as in a flame test). The spectroscope shows up a series of bright lines (Figure 1.18). Heating the atoms gives them energy which makes some of the electrons jump to higher **energy levels**. Each line in the spectrum arises from the energy given out as the electrons drop back from a higher energy level to a lower level.

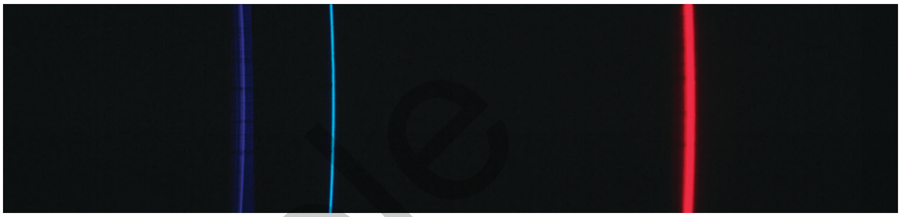


Figure 1.18 The line spectrum of hydrogen in the visible region of the electromagnetic spectrum.

Using data from spectra, it is possible to measure the energy required to remove electrons from ions with increasing charges. A succession of ionisation energies is obtained. For example:

$\mathrm{Na(g)} \rightarrow \mathrm{Na^{+}(g)} + \mathrm{e^{-}}$ first ionisation energy $= +496\,\mathrm{kJ\,mol^{-1}}$

$\mathrm{Na^{+}(g)} \rightarrow \mathrm{Na^{2+}(g)} + \mathrm{e^{-}}$ second ionisation energy $= +4563\,\mathrm{kJ\,mol^{-1}}$

$\mathrm{Na^{2+}(g)} \rightarrow \mathrm{Na^{3+}(g)} + \mathrm{e^{-}}$ third ionisation energy $= +\,6913\,\mathrm{kJ\,mol^{-1}}$

There are 11 electrons in a sodium atom so there are 11 successive ionisation energies for this element.

The successive ionisation energies for an element get bigger and bigger. This is not surprising because, having removed one electron, it is more difficult to remove a second electron from the positive ion formed.

The graph in Figure 1.19 provides evidence to support the theory that the electrons in an atom are arranged in a series of levels or shells around the nucleus.

Tip

Logarithms reduce the range of numbers that vary over several orders of magnitude. Figure 1.19 uses logarithms which work like this: log 10 = 1, log 100 = 2, log 1000 = 3 and so on. A calculator can be used to find the values of the logarithms (log) of other numbers.

Notice the big jumps in value between the first and second ionisation energies, and between the ninth and tenth ionisation energies in Figure 1.19. This suggests that sodium atoms have one electron in an outer shell or energy level furthest from the nucleus. This outer electron is relatively easily removed because it is **shielded** from the full attraction of the positive nucleus by 10 inner electrons.

Below this outer single electron, sodium atoms appear to have eight electrons in a second shell, all at roughly the same energy level. These eight electrons are closer to the nucleus than the single outer electron.

Finally, sodium atoms have two inner electrons in a shell closest to the nucleus. These two electrons feel the full attraction of the positive nucleus and are hardest to remove with the most endothermic ionisation energies.

This electronic structure for a sodium atom can be represented in an energy level diagram as in Figure 1.20. The electron arrangement in sodium can sometimes be written simply as 2, 8, 1 (but see Section 1.6).

In energy level diagrams such as that in Figure 1.20, the electrons are represented by arrows. When an energy level is filled, the electrons are paired up and in each of these pairs the electrons are spinning in opposite directions. Chemists have found that paired electrons can only be stable when they spin in opposite directions so that the magnetic attraction resulting from their opposite spins can counteract the electrical repulsion from their negative charges.

In energy level diagrams such as Figure 1.20, the opposite spins of the paired electrons are shown by drawing the arrows in opposite directions.

The quantum shells of electrons correspond to the periods of elements in the Periodic Table. By noting where the first big jump comes in the successive ionisation energies of an element, it is possible to predict the group to which the element belongs. For example, the first big jump in the successive ionisation energies for sodium comes after the first electron is removed. This suggests that sodium has just one electron in its outermost shell and, therefore, it must be in Group 1.

Test yourself

19 Write equations to represent:

- **a)** the second ionisation energy of calcium
- **b)** the third ionisation energy of aluminium.

20 The successive ionisation energies of beryllium are 900, 1757, 14 849 and 21 007 kJ mol^{-1}.

- **a)** What is the atomic number of beryllium?
- **b)** Why do successive ionisation energies always get more endothermic?
- **c)** Draw an energy level diagram for the electrons in beryllium, and predict its electron structure.
- **d)** To which group in the Periodic Table does beryllium belong?

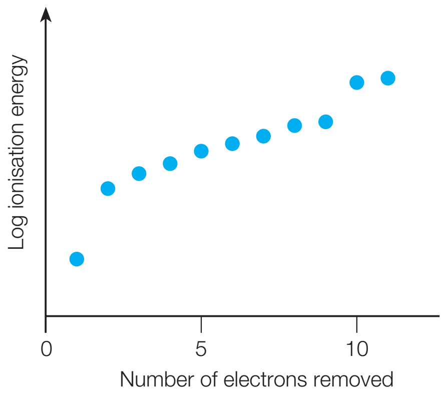


Figure 1.19 Log ionisation energy against the number of electrons removed for sodium. The values for the ionisation energies range from 496 kJ mol^{-1} to 159 079 kJ mol^{-1}. Plotting the logarithms of these values makes it possible to fit them on to the vertical axis, while still showing where there are big jumps in the values.

Key term

Shielding is an effect of inner electrons which reduces the pull of the nucleus on the electrons in the outer shell of an atom. Thanks to shielding, the electrons in the outer shell are attracted by an 'effective nuclear charge' which is less than the full charge on the nucleus.

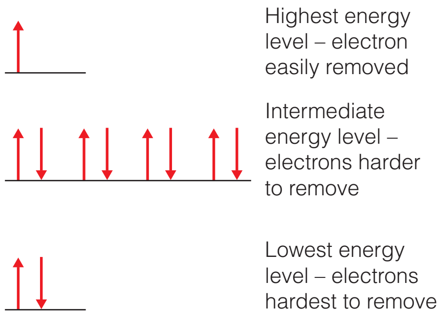


Figure 1.20 The energy levels of electrons in a sodium atom.

Activity

Evidence for sub-shells of electrons

By studying the first ionisation energies of successive elements in the Periodic Table, it is possible to compare how easy it is to remove an electron from the highest energy level in the atoms of these elements. This provides us with evidence for the arrangement of electrons in sub-shells.

1. Refer to the data sheet for Chapter 1, ‘The first ionisation energies of successive elements in the Periodic Table’, which you can access online at www.hoddereducation.co.uk/EdexcelChemistry. Using this data, plot a graph of the first ionisation energy for the first 20 elements in the Periodic Table. Put first ionisation energy on the vertical axis and atomic number on the horizontal axis.
2. When you have plotted the points, draw lines from one point to the next to show a pattern of peaks and troughs. Label each point with the symbol of its corresponding element.
3. **a)** Where do the alkali metals in Group 1 appear in the pattern?
   b) Where do the noble gases in Group 0 appear in the pattern?
4. What similarities do you notice in the pattern for elements in Period 2 (lithium to neon) with that for elements in Period 3 (sodium to argon)?
5. Identify three sub-groups of points in both Period 2 and Period 3. How many elements are there in each sub-group?

1.6 Electrons in energy levels

From the study of ionisation energies and spectra, scientists have found that the electrons in atoms are grouped together in energy levels or quantum shells. The numbers 1, 2, 3, etc. are used to label these main shells, starting nearest to the nucleus.

Each quantum shell can hold only a limited number of electrons:

- the $n = 1$ shell can hold 2 electrons
- the $n = 2$ shell can hold 8 electrons
- the $n = 3$ shell can hold 18 electrons
- the $n = 4$ shell can hold 32 electrons.

These main shells divide into sub-shells labelled s, p, d and f. The labels s, p, d and f are left over from the early studies of the spectra of different elements. These studies used the words ‘sharp’, ‘principal’, ‘diffuse’ and ‘fundamental’ to describe different lines in the spectra. The terms have no special significance now.

Key term

Atomic orbitals are the sub-divisions of the electron shells in atoms. The main shells divide into sub-shells labelled s, p, d and f. The sub-shells are further divided into atomic orbitals. An orbital is a region in space around the nucleus of an atom in which there is a 95% chance of finding an electron, or a pair of electrons with opposite spins.

The sub-shells are further divided into **atomic orbitals** (Figure 1.21). Each orbital is defined by its:

- energy level
- shape
- direction in space.

The shapes and directions in space of the atomic orbitals are found by calculating the *probability* of finding an electron at any point in an atom. These calculations are based on a theoretical model described by the Schrödinger wave equation. The one orbital in the first shell is spherical. It is an example of an s orbital (1s). The four orbitals in the second shell are made up of one s orbital (2s) and three dumbbell-shaped p orbitals. The three p orbitals ($2p_x$, $2p_y$, $2p_z$) are arranged at right angles to each other along the x-, y- and z-axes (Figure 1.22).

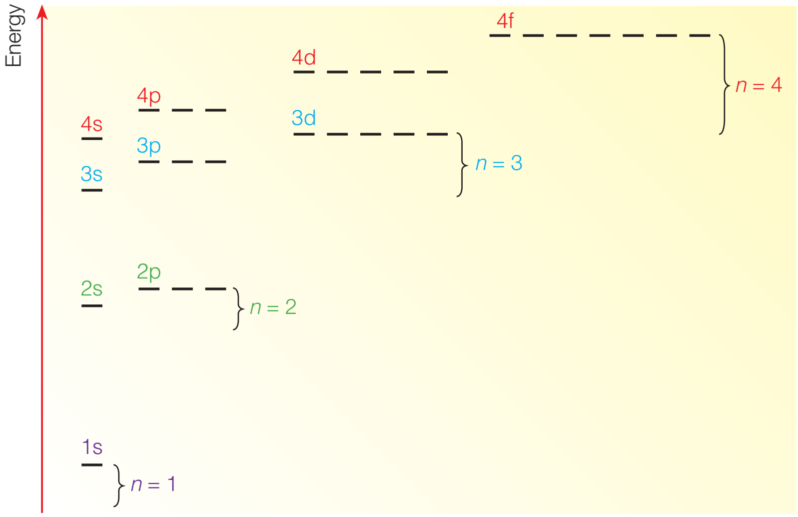


Figure 1.21 The energies of atomic orbitals in atoms. The terms 'energy level' and 'orbital' are often used interchangeably. In a free atom the orbitals in a sub-shell have the same energy.

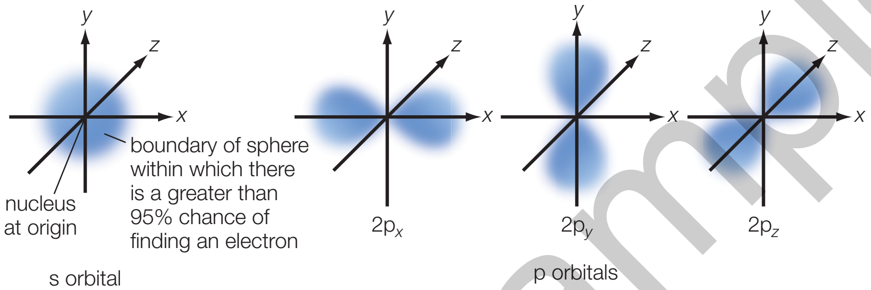


Figure 1.22 The shapes of s and p atomic orbitals. The density of shading indicates the probability of finding an electron at any point.

The electrons in an atom fill the energy levels according to a set of rules which determine electron arrangements in atoms.

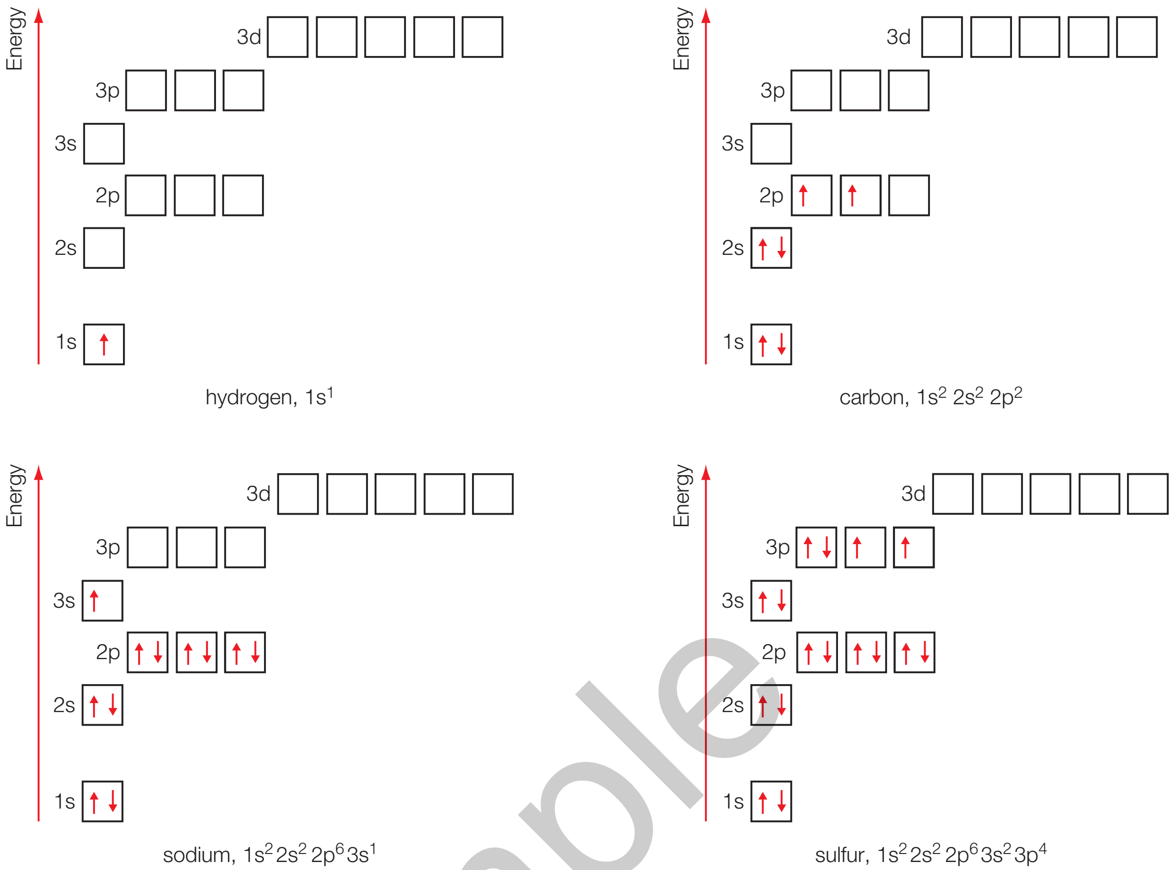
The three rules are:

- electrons go into the orbital with the lowest available energy level first
- each orbital can only contain at most two electrons (with opposite spins)
- where there are two or more orbitals at the same energy, they fill singly before the electrons pair up.

The application of these rules is illustrated for the atoms of four elements in Figure 1.23. These descriptions of the arrangement of electrons in the atoms of elements are called **electronic configurations**. Chemists sometimes use the term 'aufbau principle' for these rules from the German word meaning 'build up'. This is a reminder that electron configurations build up from the bottom. There are several common conventions for representing electron configurations in a shorthand way. Figure 1.24, for example, shows the electrons-in-boxes representations and the s, p, d, f notations for the electronic structures of beryllium, nitrogen and sodium.

Key term

The **electronic configuration** of an element describes the number and arrangement of electrons in an atom of the element. A shortened form of electronic configuration uses the symbol of the previous noble gas, in square brackets, to stand for the inner shells. So, using this convention, the electronic configuration of sodium is $[Ne]3s^1$.



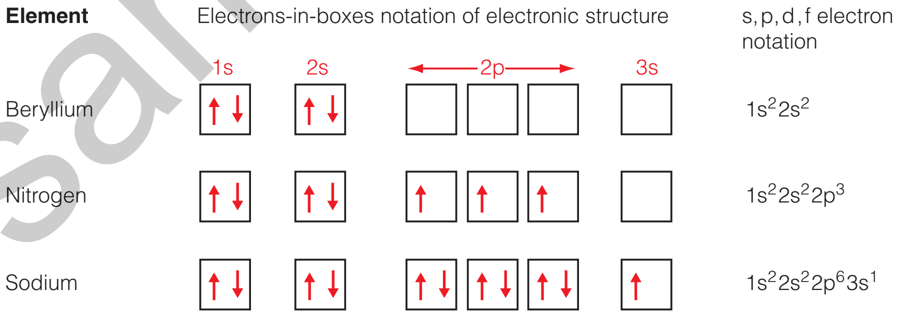
hydrogen, $1s^1$

carbon, $1s^2\ 2s^2\ 2p^2$

sodium, $1s^2 2s^2 2p^6 3s^1$

sulfur, $1s^2 2s^2 2p^6 3s^2 3p^4$

Figure 1.23 Electrons in energy levels for four atoms to show the application of the building-up principle.



Element	Electrons-in-boxes notation of electronic structure						s, p, d, f electron notation
	1s	2s	2p			3s	
Beryllium	↑↓	↑↓					$1s^2 2s^2$
Nitrogen	↑↓	↑↓	↑	↑	↑		$1s^2 2s^2 2p^3$
Sodium	↑↓	↑↓	↑↓	↑↓	↑↓	↑	$1s^2 2s^2 2p^6 3s^1$

Figure 1.24 Electrons-in-boxes representations and s, p, d, f notations for the electronic structure of beryllium, nitrogen and sodium.

Test yourself

21 Sketch a graph of log ionisation energy against number of electrons removed when all the electrons are successively removed from a phosphorus atom. (Sketch the graph in the style of Figure 1.19. There is no need to look up logarithms.)

22 Write out the electron structure in terms of shells (for sodium this would be 2, 8, 1) for the atoms of following elements:

a) lithium	**b)** oxygen
c) neon	**d)** silicon.

23 Write the electronic sub-shell structure for the elements in Question 22 – for sodium this would be $1s^2 2s^2 2p^6 3s^1$.

24 Draw the electrons-in-boxes representations for the following elements:

a) boron **b)** fluorine

c) phosphorus **d)** potassium.

25 Identify the elements with the following electron structures in their outermost shells:

a) $1s^2$ **b)** $2s^2 2p^2$

c) $3s^2$ **d)** $3s^2 3p^4$.

The development of knowledge and understanding about electronic structures illustrates how chemists use the results of their experiments, such as the measurements of ionisation energies, to devise atomic models that they can use to explain the properties of elements. It also illustrates the important distinction between evidence and experimental data on the one hand, and ideas, theories and explanations on the other.

In particular, ionisation energies and spectra have provided chemists with evidence and information that has caused them to develop and modify their models and theories about electron structure. Early ideas about electrons arranged in shells have been developed to take in the evidence for sub-shells, and then modified to include ideas about orbitals.

1.7 Electron structures and the Periodic Table

The Periodic Table helps chemists to bring order and patterns to the vast amount of information they have discovered about all the elements and their compounds.

In the modern Periodic Table, elements are arranged in order of atomic number. The horizontal rows in the table are called **periods** – each period ends with a noble gas. The vertical columns in the table are called **groups** which can be divided into four blocks – the s block, p block, d block and f block – based on the electron structures of the elements (Figure 1.25).

So, the modern arrangement of elements in the Periodic Table reflects the underlying electronic structures of the atoms, while the more sophisticated model of electron structure in terms of orbitals allows chemists to explain the properties of elements more effectively. The four blocks in the Periodic Table are shown in different colours in Figure 1.25.

- The *s block* comprises the reactive metals in Group 1 and Group 2 – such as potassium, sodium, calcium and magnesium. In these metals, the outermost electron is in an s orbital in the outer shell.
- The *p block* comprises the elements in Groups 3, 4, 5, 6, 7 and 0 on the right of the Periodic Table. These elements include relatively unreactive metals such as tin and lead, plus all the non-metals. In these elements, the last electron added goes into a p orbital in the outer shell.

Key terms

A **period** is a horizontal row of elements in the Periodic Table.

A **group** is a vertical column of elements in the Periodic Table. Elements in the same group have similar properties because they have the same outer electronic configuration.

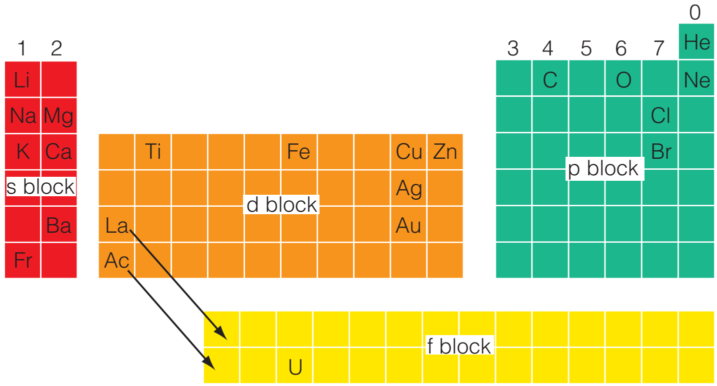


Figure 1.25 The s, p, d and f blocks in the Periodic Table.

Tip

The International Union of Pure and Applied Chemistry (IUPAC) now recommends that the groups in the Periodic Table should be numbered from 1 to 18. Groups 1 and 2 are the same as before. Groups 3 to 12 are the vertical families of d-block elements. The groups traditionally numbered 3 to 7 and 0 then become Groups 13 to 18.

- The *d-block* elements occupy a rectangle across Periods 4, 5, 6 and 7 between Group 2 and Group 3. The d-block elements are all metals – including titanium, iron, copper and silver – in which the last electron added goes into a d orbital. These metals are much less reactive than the s-block metals in Groups 1 and 2. Within the d block there are marked similarities across the periods, as well as the usual vertical similarities. The d-block elements are sometimes loosely called 'transition metals'.
- The *f-block* elements occupy a low rectangle across Periods 6 and 7 within the d block, but they are usually placed below the main table to prevent it becoming too wide to fit the page. Like the d-block elements, those in the f block are all metals. Here, the last added electron is in an f orbital. The f-block elements are often called the lanthanoids and actinoids, or lanthanides and actinides, because they are the 14 elements immediately following lanthanum, La, and actinium, Ac, in the Periodic Table. Another name used for the f-block elements is the 'inner transition elements'.

As the shells of electrons around the nuclei of atoms get further from the nucleus, they become closer in energy (see Figure 1.21). Therefore, the difference in energy between the second and third shells is less than that between the first and second. When the fourth shell is reached there is, in fact, an overlap between the orbitals of highest energy in the third shell (the 3d orbital) and that of lowest energy in the fourth shell (the 4s orbital) (Figure 1.26). As a result the orbitals that fill in the fourth period are the 4s, 3d and 4p orbitals in that order. This accounts for the position of the d-block elements in the Periodic Table.

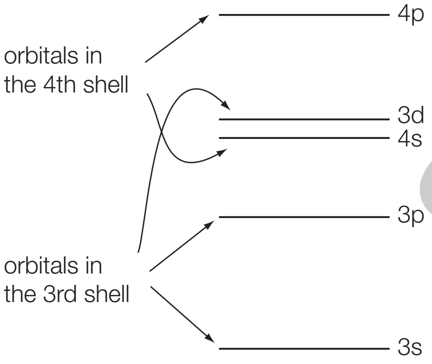


Figure 1.26 The relative energy levels of orbitals in the third and fourth shells.

Tip

The 4s orbital fills before the 3d orbital because it has a lower energy. However, the 4s orbital is the outer orbital and it is the electrons in the 4s orbital that are lost first when a d-block element ionises. Chromium and copper each only have one 4s electron in their atoms. The explanation for the irregularities lies in the stability of half-filled and filled sub-shells. So the electronic structure of chromium is $[Ar]3d^5 4s^1$ and that of copper is $[Ar]3d^{10} 4s^1$.

Table 1.3 shows the electron configurations of four elements in the fourth period. The rules for the order in which electrons fill orbitals still apply.

Element and symbol	**Electronic structure**										
	spdf notation	**Electrons-in-boxes notation**									
			3d					4s	4p		
Potassium K	[Ar]$4s^1$	[Ar]						↑			
Vanadium V	[Ar]$3d^3 4s^2$	[Ar]	↑	↑	↑			↑↓			
Iron Fe	[Ar]$3d^6 4s^2$	[Ar]	↑↓	↑	↑	↑	↑	↑↓			
Bromine Br	[Ar]$3d^{10} 4s^2 4p^5$	[Ar]	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑

Table 1.3 Electron configurations of four elements in the fourth period. [Ar] represents the electronic configuration of argon: $1s^2 2s^2 2p^6 3s^2 3p^6$.

Test yourself

26 Write the electronic sub-shell structure for the atoms of these elements using spdf notation:

a) scandium **b)** manganese

c) zinc **d)** germanium.

27 Identify the elements with the following electron structures:

a) $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$

b) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^8 4s^2$

c) $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$

28 Write the electronic sub-shell structure for these ions using spdf notation:

a) Al^{3+} **b)** S^{2-}

c) Zn^{2+} **d)** Br^-

Groups

The elements in each group have similar properties because they have similar electron structures. This important point is well illustrated by the alkali metals in Group 1. Look at Figure 1.27 – notice that each alkali metal has one s electron in its outer shell. This similarity in their electron structures explains why they have similar properties.

Alkali metals:

- are very reactive because they lose their single outer electron so easily
- form ions with a charge of 1+ (Li^+, Na^+, K^+, etc.) so the formulae of their compounds are similar
- form very stable ions with an electron structure like that of a noble gas.

The chemical properties of all other elements are also determined by their electronic structures. Chemistry is largely about the electrons in the outer shells of atoms. The reactivity of an element depends on the number of electrons in the outer shell and how strongly they are held by the nuclear charge. This is a fundamental feature of chemistry and an essential principle which governs the way in which chemists think and work.

Group 1
The alkali metals
Lithium Li 2, 1 ($1s^2 2s^1$)
Sodium Na 2, 8, 1 ($1s^2 2s^2 2p^6 3s^1$)
Potassium K 2, 8, 8, 1 ($1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$)

Figure 1.27 Electron structures of the first three alkali metals.

Test yourself

29 Why are sodium and potassium so alike?

30 Why are the noble gases so unreactive?

31 **a)** Write down the electron shell structures and sub-shell structures of fluorine and chlorine in Group 7.

b) Why do you think fluorine and chlorine are so reactive with metals?

c) Why do the compounds of fluorine and chlorine with metals have similar formulae?

1.8 Periodic properties

Modern versions of the Periodic Table are all based on the one suggested by the Russian chemist Dmitri Mendeléev in 1869. When Mendeléev arranged the elements in order of atomic mass, he saw repeating patterns in their properties. A repeating pattern is a periodic pattern – hence the terms 'periodic properties' and 'periodicity'.

Perhaps the most obvious repeating pattern in the Periodic Table is from metals on the left, through elements with intermediate properties (called metalloids), to non-metals on the right. Graphs of the physical properties of the elements – such as melting temperatures, electrical conductivities and first ionisation energies – against atomic number, also show repeating patterns. Using the models of bonding between atoms and molecules, chemists can explain the properties of elements and the repeating patterns in the Periodic Table.

Melting temperatures of the elements

Figure 1.28 shows the periodic pattern revealed by plotting the melting temperatures of elements against atomic number.

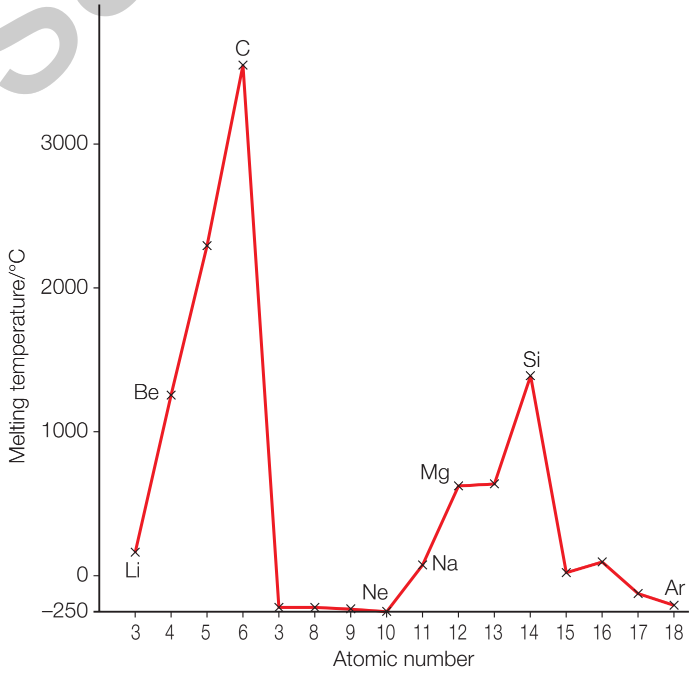


Figure 1.28 Periodicity in the melting temperatures of the elements.

The melting temperature of an element depends on both its structure and the type of bonding between its atoms. In metals, the bonding between atoms is strong (Section 2.9), so their melting temperatures are usually high. The more electrons each atom contributes from its outermost shell to the shared delocalised electrons, the stronger the bonding and the higher the melting temperature.

Therefore, melting temperatures rise from Group 1 to Group 2 to Group 3. In Group 4, the elements carbon and silicon have giant covalent structures. The bonds in these structures are strong and highly directional, so most of the bonds must break before the solid melts. This means that the melting temperatures of Group 4 elements are very high and at the peaks of the graph in Figure 1.28.

The non-metal elements in Groups 5, 6, 7 and 0 form simple molecules. The intermolecular forces between these simple molecules are weak, so these elements have low melting temperatures (Section 2.3).

First ionisation energies of the elements

Figure 1.29 shows the clear periodic trend in the first ionisation energies of the elements. The general trend is that first ionisation energies increase from left to right across a period.

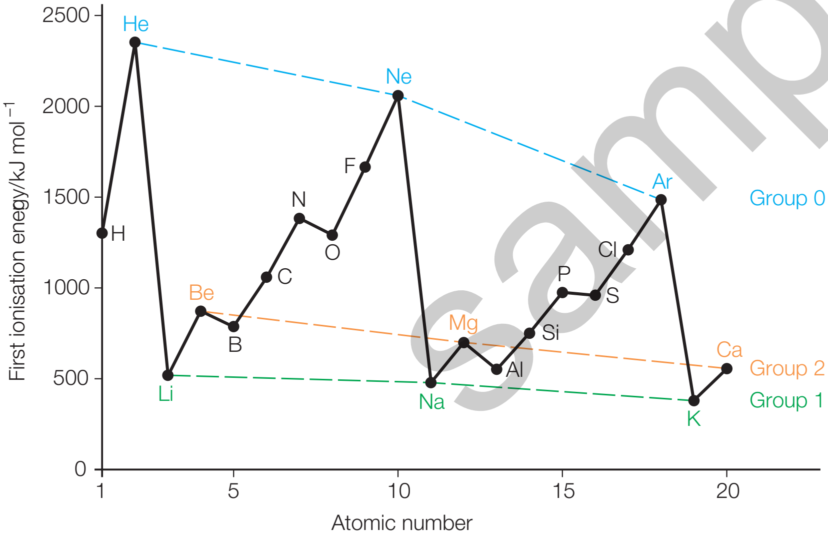


Figure 1.29 Periodicity in the first ionisation energies of the elements.

The ionisation energy of an atom is determined by three atomic properties.

- *The size of the positive nuclear charge*. As the positive nuclear charge increases, its attraction for outermost electrons increases and this tends to increase the ionisation energy.
- *The distance of the outermost electron from the nucleus*. As this distance increases, the attraction of the positive nucleus for the negative electron decreases and this tends to reduce the ionisation energy.

- *The shielding effect of electrons.* Electrons in inner shells exert a repelling effect on electrons in the outer shells of an atom. This reduces the pull of the nucleus on the electrons in the outer shell. Thanks to shielding, the 'effective nuclear charge' attracting electrons in the outer shell is much less than the full positive charge of the nucleus. As expected, the shielding effect increases as the number of inner shells increases.

Moving from left to right across any period, the nuclear charge increases as electrons are added to the same outer shell. The increasing nuclear charge tends to pull the outer electrons closer to the nucleus. The shielding effect of full inner shells is constant, the extra electrons in the same outer shell do not shield each other well so shielding hardly changes across the period. The increased nuclear charge and the reduced distance of the outer electrons from the nucleus makes the outer electrons more difficult to remove and, in general, the first ionisation energy increases.

But notice in Figure 1.29 that the rising trend in ionisation energies across a period is not smooth. There is a 2–3–3 pattern, which reflects the way in which electrons feed into s and p orbitals. The first ionisation energy decreases from beryllium to boron and again from nitrogen to oxygen.

A beryllium atom loses one of the $2s^2$ electrons from its outer shell when it ionises. The electronic configuration of boron is $2s^22p^1$, so the electron lost when a boron atom ionises is a 2p electron. The 2p electron is in a higher energy sub-shell than a 2s electron, so it takes less energy to remove the boron 2p electron, despite the increase in nuclear charge.

The electronic configuration of oxygen is $1s^22s^22p^4$. This means that one of the paired 2p electrons is removed on ionisation. In a nitrogen atom the electronic configuration is $1s^22s^22p^3$ and all three p electrons are unpaired. Ionisation of nitrogen involves losing an unpaired electron. The repulsion between the negative electrons is greater for the paired electrons in the same sub-shell of an oxygen atom than between the unpaired electrons in a nitrogen atom. As a result it is easier to ionise an oxygen atom despite the increase in nuclear charge.

Test yourself

32 Why do the first ionisation energies of elements decrease with increasing atomic number in every group of the Periodic Table?

Chapter summary

Chapter 1 Atomic structure and the Periodic Table

- The nucleus of an atom consists of protons (charge +1, relative mass 1) and neutrons (charge 0, relative mass 1).
- The atomic (proton) number gives the number of protons in the nucleus. The mass number is the number of protons plus the number of neutrons.
- The isotopes of an element have the same atomic number but different mass numbers.
- Relative isotopic mass is the mass of one atom of an isotope relative to 1/12th of the mass of an atom of carbon-12.
- Mass spectrometry measures the relative mass and relative abundance of the isotopes of an element. The output is often presented as a 'stick diagram' showing the relative abundance of the ions of differing mass-to-charge ratios.
- Data from a mass spectrum can be used to calculate the relative atomic mass of the element, which is the average mass of the atoms of the element relative to 1/12th of the mass of an atom of carbon-12.
- The relative molecular mass of an element or compound is the sum of the relative atomic masses of all the atoms in its molecular formula.
- The mass spectrum of a molecular substance consists of a fragmentation pattern in which the peak of the highest m/z value is that of the 'molecular ion', M^+. The relative mass of this ion is the relative molecular mass of the compound.
- An ionisation energy measures the energy needed to remove one mole of electrons from one mole of gaseous atoms or ions.
- The study of successive ionisation energies and spectra shows that electrons are grouped in energy levels, or quantum shells. These shells are divided into sub-shells labelled s, p, d and f.
- Each s sub-shell has one spherical s-orbital; each p sub-shell has three dumbbell-shaped p-orbitals.
- Electrons in an atom fill energy levels according to rules: electrons go into the orbital with the lowest available energy; each orbital can only contain at most two electrons; where there are two or more orbitals with the same energy, they fill singly before they pair up; electrons in the same orbital have opposite spins.
- In the Periodic Table, the elements are arranged in order of atomic number: the horizontal rows are periods and the vertical columns are groups.
- Electronic configuration determines the chemical properties of the elements, and the division of the Periodic Table into s, p and d blocks reflects the underlying electron configurations of the atoms.
- There are properties of elements that show repeating (periodic) patterns in the Periodic Table: these include atomic radii, melting and boiling temperatures and first ionisation energies.
- The melting temperature of an element depends on both its structure and the type of bonding between its atoms.
- The sizes of ionisation energies are related to the number of protons in the nucleus, shielding and the electron sub-shell (orbital) from which the electron is removed. These factors can account for the general rise of first ionisation energies across a period and the fall in first ionisation energies down a group.

Exam practice questions

1 Antimony has two main isotopes – antimony-121 and antimony-123. A forensic scientist was asked to help a crime investigation by analysing the antimony in a bullet. This was found to contain 57.3% of ^{121}Sb and 42.7% of ^{123}Sb.

a) State what is meant by the term 'relative atomic mass'. *(3)*

b) Calculate the relative atomic mass of the sample of antimony from the bullet. Write your answer to an appropriate number of significant figures. *(3)*

c) State one similarity and one difference, in terms of sub-atomic particles, between the isotopes. *(2)*

2 This question concerns the following five species:

$^{16}_{8}O^{2-}$ $^{19}_{9}F^{-}$ $^{20}_{10}Ne$ $^{23}_{11}Na$ $^{25}_{12}Mg^{2+}$

a) Identify two species that have the same number of neutrons. *(2)*

b) Identify two species that have the same ratio of neutrons to protons. *(2)*

c) Identify the species that does not have 10 electrons. *(1)*

3 a) Identify the elements with these electron configurations as s-, p- or d-block elements.

i) $1s^22s^22p^63s^2$

ii) $1s^22s^22p^63s^23p^4$

iii) $1s^22s^22p^63s^23p^63d^64s^2$ *(3)*

b) Give the electrons-in-boxes notation for the electron configurations of:

i) a nitrogen atom

ii) a sodium ion

iii) a sulfide ion. *(3)*

4 The isotopes of magnesium, ^{24}Mg, ^{25}Mg and ^{26}Mg, can be separated by mass spectrometry.

a) State what is meant by the term 'isotope'. *(2)*

b) Copy and complete the table below to show the composition of the ^{24}Mg and ^{26}Mg isotopes. *(2)*

	Protons	**Neutrons**	**Electrons**
^{24}Mg			
^{26}Mg			

c) Copy and complete the electronic configuration of an atom of ^{24}Mg.

$1s^2$ __________ *(1)*

5 The table shows the melting temperatures of the elements in Period 3 of the Periodic Table.

Element	**Melting temperature/°C**
Na	98
Mg	649
Al	660
Si	1410
P	44
S	119
Cl	−101
Ar	−189

The trend in the melting temperatures across Period 3 and other periods is described as a periodic property.

a) Give the general pattern in melting temperatures across periods in the Periodic Table. *(2)*

b) Show that this general trend is related to the different types of elements. *(1)*

c) State what is meant by the term 'periodic property'. *(2)*

d) State two other properties which can be described as periodic in relation to the Periodic Table. *(2)*

6 The table shows the first and second ionisation energies of lithium and sodium in Group 1 of the Periodic Table.

Element	**First ionisation energy/kJ mol⁻¹**	**Second ionisation energy/kJ mol⁻¹**
Lithium	520	7298
Sodium	496	4563

a) Write an equation, with state symbols, for the second ionisation energy of sodium. *(2)*

b) Explain why the second ionisation energies of lithium and sodium are larger than their first ionisation energies. *(3)*

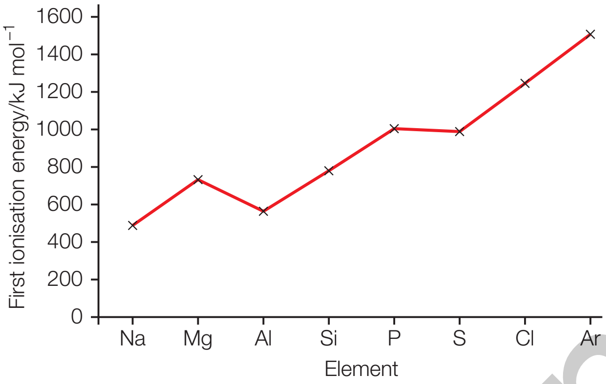
c) Explain why the first and second ionisation energies of sodium are smaller than those of lithium. *(4)*

d) The first five successive ionisation energies, in kJ mol^{-1}, of an element, X, in Period 3 of the Periodic Table are 578, 1817, 2745, 11 578, 14 831.

- **i)** Identify element X. *(1)*
- **ii)** Explain how you obtained your answer. *(2)*

e) Predict which element in the Periodic Table has the highest first ionisation energy and explain your answer. *(3)*

7 The graph shows the first ionisation energies of the elements in Period 2 of the Periodic Table.



a) Describe and explain the *general* trend in first ionisation energies from Na to Ar. *(3)*

b) Explain why aluminium, Al, has a lower first ionisation energy than magnesium, Mg. *(2)*

c) Explain why the ionisation energy decreases from phosphorus, P, to sulfur, S. *(2)*

d) Predict the value for the first ionisation energy of potassium and explain your answer. *(2)*

e) The first five ionisation energies of an element are 738, 1451, 7733, 10 541, 13 629 kJ mol^{-1}. Explain why the element cannot have an atomic number less than 12. *(3)*

8 a) Bromine consists of two isotopes bromine-79 and bromine-81 which are equally abundant. Explain why the mass spectrum of bromine includes:

- **i)** two lines with *m/z* values of 79 and 81 with heights in the ratio 1 : 1 *(3)*
- **ii)** three lines with *m/z* values of 158, 160 and 162 with heights in the ratio 1 : 2 : 1. *(3)*

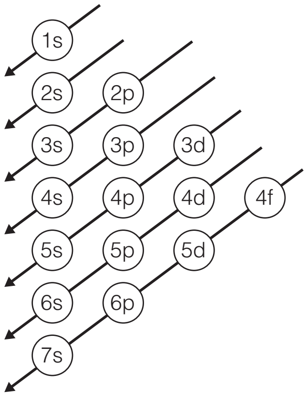
b) Chlorine consists of two isotopes chlorine-35 and chlorine-37. Explain why the mass spectrum of chlorine includes:

- **i)** two lines with *m/z* values of 35 and 37 with heights in the ratio 3 : 1 *(2)*
- **ii)** three lines with *m/z* values of 70, 72 and 74 with heights in the ratio 9 : 6 : 1. *(3)*

c) Explain these features of the mass spectrum of dichloroethene, $C_2H_2Cl_2$ ($M_r = 97$):

- **i)** the absence of a peak at *m/z* = 97 *(2)*
- **ii)** the presence of three peaks at *m/z* values of 96, 98 and 100 with intensities in the ratio 9 : 6 : 1 *(3)*
- **iii)** the presence of two peaks at *m/z* values of 61 and 63 with intensities in the ratio 3 : 1. *(3)*

9 This diagram shows the order in which sub-shells are filled by electrons according to the Aufbau principle which accounts for the arrangement of elements in the modern form of the Periodic Table.



a) Show that this diagram accounts for the position of the d-block elements in the Periodic Table. *(2)*

b) Give the electronic configuration of tin (atomic number 50). *(1)*

c) Explain why this diagram cannot account for elements with atomic numbers greater than 88. *(2)*

d) Predict the number of orbitals in the 4f sub-shell. Show how you decide on your answer. *(2)*

e) Comment on the relative energies of the 4f and 5d orbitals given the electron configurations of the four elements with atomic numbers from 57 to 60.

Lanthanum: $[Xe]4f^0 5d^1 6s^2$
Cerium: $[Xe]4f^2 5d^0 6s^2$
Praseodymium: $[Xe]4f^3 5d^0 6s^2$
Neodymium: $[Xe]4f^4 5d^0 6s^2$

Show that this information, and the diagram above, can account for the position of the elements with atomic numbers 58–71 in the Periodic Table. *(4)*

10 The table below shows the groups, formulae and boiling temperatures of chlorides for the elements in Periods 2 and 3.

a) Explain why are there no entries in the table for Group 0. *(2)*

b) i) Describe the pattern shown by the formulae of the chlorides in Periods 2 and 3. *(2)*

ii) Suggest an explanation for the pattern you describe. *(4)*

c) Explain why formulae OCl_2 and FCl are normally written as Cl_2O and ClF, respectively. *(1)*

d) i) Describe the pattern in the boiling temperatures of the chlorides of the elements in Periods 2 and 3. *(2)*

ii) Explain the pattern you describe. *(4)*

e) Phosphorus forms a second chloride, PCl_5, but nitrogen only forms the one chloride. Explain this difference in terms of the electron configurations of the atoms of phosphorus and nitrogen. *(5)*

11* Discuss the following statements using examples to show the extent to which you think that they are true or false:

a) The atomic number of an element is a better guide to its atomic structure and is more useful in its classification than its relative atomic mass. *(6)*

b) The chemical properties of an element are largely determined by the number of electrons in the outer shell of its atoms. *(6)*

	Group						
	1	**2**	**3**	**4**	**5**	**6**	**7**
Period 2							
Formula of chloride	LiCl	$BeCl_2$	BCl_3	CCl_4	NCl_3	OCl_2	FCl
Boiling temperature of chloride/°C	1340	520	13	77	71	4	−101
Period 3							
Formula of chloride	NaCl	$MgCl_2$	$AlCl_3$	$SiCl_4$	PCl_3	S_2Cl_2	Cl_2
Boiling temperature of chloride/°C	1413	1412	423	58	76	136	−35