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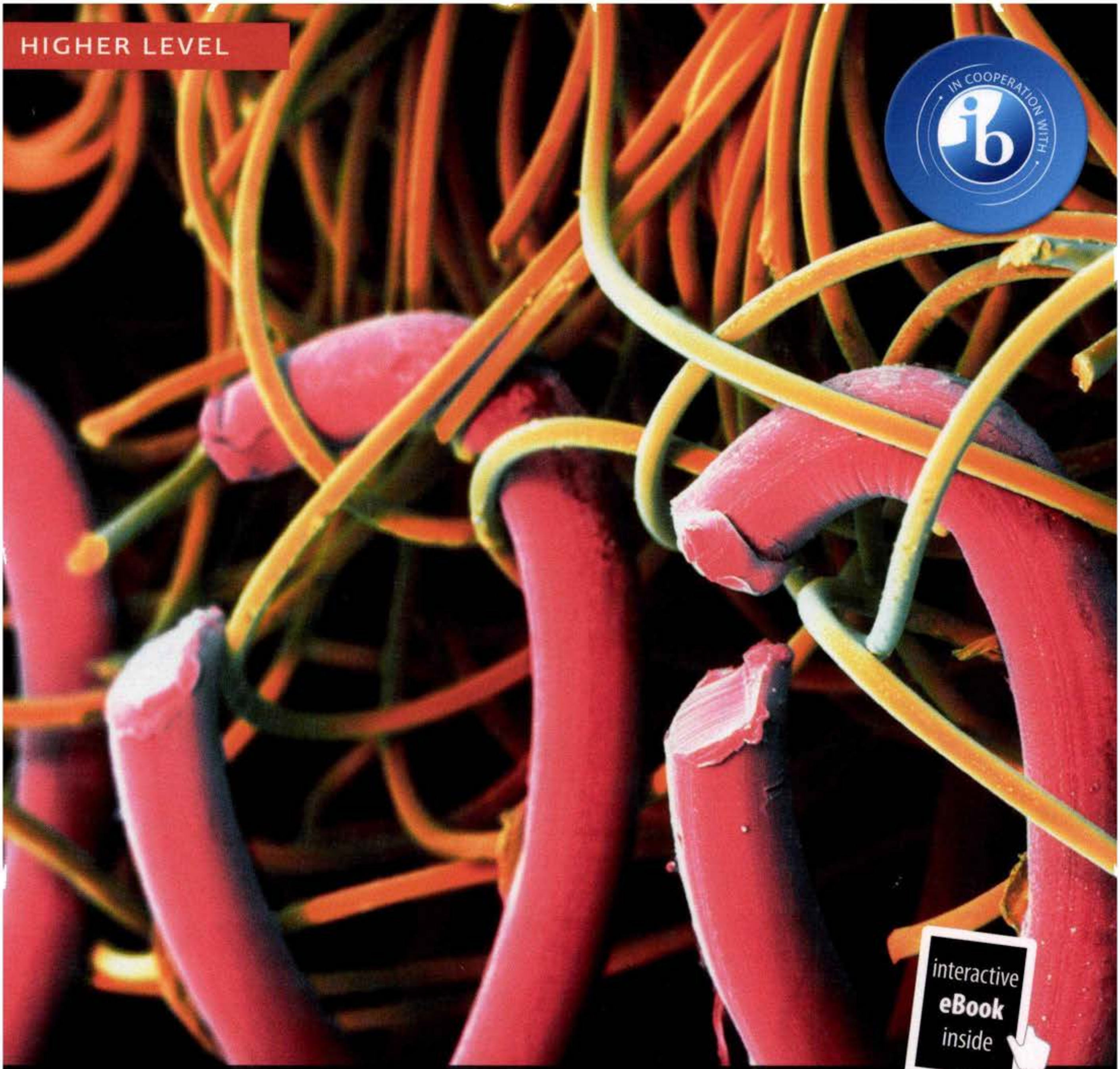

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HIGHER LEVEL

Chemistry

for the IB Diploma Programme

3rd Edition

CATRIN BROWN
MIKE FORD
OLIVER CANNING
ANDREAS ECONOMOU
GARTH IRWIN

Pearson

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 **H** 1.01						Atomic number **Element** Relative atomic mass											2 **He** 4.00
2	3 **Li** 6.94	4 **Be** 9.01											5 **B** 10.81	6 **C** 12.01	7 **N** 14.01	8 **O** 16.00	9 **F** 19.00	10 **Ne** 20.18
3	11 **Na** 22.99	12 **Mg** 24.31											13 **Al** 26.98	14 **Si** 28.09	15 **P** 30.97	16 **S** 32.07	17 **Cl** 35.45	18 **Ar** 39.95
4	19 **K** 39.10	20 **Ca** 40.08	21 **Sc** 44.96	22 **Ti** 47.87	23 **V** 50.94	24 **Cr** 52.00	25 **Mn** 54.94	26 **Fe** 55.85	27 **Co** 58.93	28 **Ni** 58.69	29 **Cu** 63.55	30 **Zn** 65.38	31 **Ga** 69.72	32 **Ge** 72.63	33 **As** 74.92	34 **Se** 78.96	35 **Br** 79.90	36 **Kr** 83.80
5	37 **Rb** 85.47	38 **Sr** 87.62	39 **Y** 88.91	40 **Zr** 91.22	41 **Nb** 92.91	42 **Mo** 95.96	43 **Tc** (98)	44 **Ru** 101.07	45 **Rh** 102.91	46 **Pd** 106.42	47 **Ag** 107.87	48 **Cd** 112.41	49 **In** 114.82	50 **Sn** 118.71	51 **Sb** 121.76	52 **Te** 127.60	53 **I** 126.90	54 **Xe** 131.29
6	55 **Cs** 132.91	56 **Ba** 137.33	57 **La †** 138.91	72 **Hf** 178.49	73 **Ta** 180.95	74 **W** 183.84	75 **Re** 186.21	76 **Os** 190.23	77 **Ir** 192.22	78 **Pt** 195.08	79 **Au** 196.97	80 **Hg** 200.59	81 **Tl** 204.38	82 **Pb** 207.20	83 **Bi** 208.98	84 **Po** (209)	85 **At** (210)	86 **Rn** (222)
7	87 **Fr** (223)	88 **Ra** (226)	89 **Ac ‡** (227)	104 **Rf** (267)	105 **Db** (268)	106 **Sg** (269)	107 **Bh** (270)	108 **Hs** (269)	109 **Mt** (278)	110 **Ds** (281)	111 **Rg** (281)	112 **Cn** (285)	113 **Nh** (286)	114 **Fl** (289)	115 **Mc** (288)	116 **Lv** (293)	117 **Ts** (294)	118 **Og** (294)

†	58 **Ce** 140.12	59 **Pr** 140.91	60 **Nd** 144.24	61 **Pm** (145)	62 **Sm** 150.36	63 **Eu** 151.96	64 **Gd** 157.25	65 **Tb** 158.93	66 **Dy** 162.50	67 **Ho** 164.93	68 **Er** 167.26	69 **Tm** 168.93	70 **Yb** 173.05	71 **Lu** 174.97
‡	90 **Th** 232.04	91 **Pa** 231.04	92 **U** 238.03	93 **Np** (237)	94 **Pu** (244)	95 **Am** (243)	96 **Cm** (247)	97 **Bk** (247)	98 **Cf** (251)	99 **Es** (252)	100 **Fm** (257)	101 **Md** (258)	102 **No** (259)	103 **Lr** (262)

HIGHER LEVEL

Chemistry

for the IB Diploma Programme

Catrin Brown, Mike Ford,
Oliver Canning, Andreas Economou and Garth Irwin

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KEY (t – top, c – center, b – bottom, l – left, r – right)

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Reactivity

Syllabus roadmap

The aim of the syllabus is to integrate concepts, topic content and the Nature of Science through inquiry. Students and teachers are encouraged to personalize their approach to the syllabus according to their circumstances and interests.

Skills in the study of chemistry			
Structure **Structure refers to the nature of matter from simple to more complex forms**		**Reactivity** **Reactivity refers to how and why chemical reactions occur**	
Structure determines reactivity, which in turn transforms structure			
Structure 1 **Models of the particulate nature of matter**	Structure 1.1 – Introduction to the particulate nature of matter	**Reactivity 1** **What drives chemical reactions?**	Reactivity 1.1 – Measuring enthalpy changes
	Structure 1.2 – The nuclear atom		Reactivity 1.2 – Energy cycles in reactions
	Structure 1.3 – Electron configurations		Reactivity 1.3 – Energy from fuels
	Structure 1.4 – Counting particles by mass: The mole		Reactivity 1.4 – Entropy and spontaneity (Additional higher level)
	Structure 1.5 – Ideal gases		
Structure 2 **Models of bonding and structure**	Structure 2.1 – The ionic model	**Reactivity 2** **How much, how fast and how far?**	Reactivity 2.1 – How much? The amount of chemical change
	Structure 2.2 – The covalent model		Reactivity 2.2 – How fast? The rate of chemical change
	Structure 2.3 – The metallic model		Reactivity 2.3 – How far? The extent of chemical change
	Structure 2.4 – From models to materials		
Structure 3 **Classification of matter**	Structure 3.1 – The periodic table: Classification of elements	**Reactivity 3** **What are the mechanisms of chemical change?**	Reactivity 3.1 – Proton transfer reactions
	Structure 3.2 – Functional groups: Classification of organic compounds		Reactivity 3.2 – Electron transfer reactions
			Reactivity 3.3 – Electron sharing reactions
			Reactivity 3.4 – Electron-pair sharing reactions

Authors' introduction to the third edition

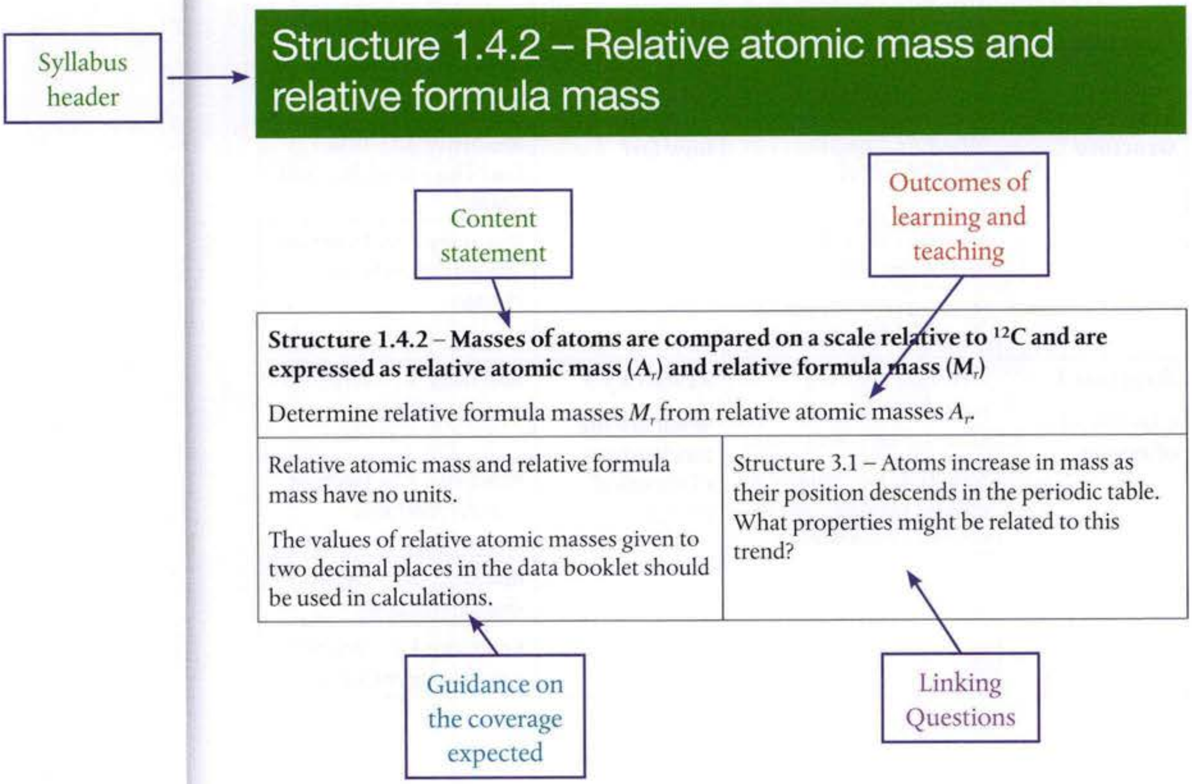
Welcome to your study of IB Diploma Programme chemistry. This is the third edition of Pearson's highly successful Higher Level (HL) chemistry book, first published in 2009. It has been completely rewritten to match the specifications of the new IB chemistry curriculum for first assessments in 2025 and gives thorough coverage of the entire course content. While there is much new and updated material, we have kept and refined the features that made the previous editions so successful. We are delighted to share our enthusiasm for learning chemistry in the IB programme with you!

Content

This book covers the entire HL course. It is divided into the two main themes, **Structure** and **Reactivity**, which in turn are divided into six topics, Structure 1–3 and Reactivity 1–3. Separate chapters cover each sub-topic within each topic. For example, the Structure 1.1 chapter deals with 'Introduction to the particulate nature of matter'.

The syllabus is presented as a sequence of numbered Understandings, which are shown as three-part boxes. We have given the relevant Understanding from the subject guide at the start of each section within a chapter under a brief header. The Table of Contents shows the full list of these Understanding headers, so you can see what is covered in each chapter.

For example:



Structure 1.4.2 – Relative atomic mass and relative formula mass

Structure 1.4.2 – **Masses of atoms are compared on a scale relative to ^{12}C and are expressed as relative atomic mass (A_r) and relative formula mass (M_r)** Determine relative formula masses M_r from relative atomic masses A_r.	
Relative atomic mass and relative formula mass have no units. The values of relative atomic masses given to two decimal places in the data booklet should be used in calculations.	Structure 3.1 – Atoms increase in mass as their position descends in the periodic table. What properties might be related to this trend?

The Understandings are presented in the same sequence as in the subject guide, so that common Standard Level (SL) and HL content is covered first, followed by HL only material. The transition from SL to HL content is shown by icons as follows.

HL

Individual icons to identify HL material such as exercises and practice questions can also be found throughout the book.

The text covers the course content using plain language, with all scientific terms explained and shown in bold as they are first introduced. It follows SI notation, and IUPAC nomenclature and definitions throughout. We have been careful also to apply the same terminology you will see in IB examinations in all worked examples and questions.

Conceptual approach

The syllabus emphasizes a conceptual approach, where the two main themes of chemistry, Structure and Reactivity, are shown to be interdependent. There is no suggested sequence for the coverage of the topics, and many different routes through the syllabus are possible. What is important though, is that the relationships between the different topics are recognized, which leads to an increasing depth of understanding.

There are two features, **Guiding Questions** and **Linking Questions**, which are incorporated into each topic in the syllabus. These are designed to help promote the conceptual approach, and we have emphasized them in the text as follows.

Guiding Question

Guiding Question

How do the nuclei of atoms differ?

Each chapter starts with the Guiding Question for the sub-topic from the IB chemistry subject guide. This is followed by a brief consideration of the question itself, which sets the context for the topic and how it relates to your previous knowledge. It is expected that by the end of the chapter you will be able to answer the Guiding Question more fully.

Guiding Question revisited

Guiding Question revisited

How do we quantify matter on the atomic scale?

At the end of each chapter, the Guiding Question is revisited, and can now be answered with significantly more detail and understanding. It is presented as a bulleted list of the material covered, that may help serve as a checklist of your learning at the end of each chapter. The Guiding Question revisited bulleted lists are available as downloadable PDFs from the eBook to help you with revision.

Reactivity 3.2 – How can oxidation states be used to analyze redox reactions?

Linking Questions

Linking Questions are given in many of the Understandings. Linking Questions have a number which indicates a link from the current chapter to another sub-topic, to Tools or to the Nature of Science (NOS). These questions are designed as prompts to help you build a grasp of unifying concepts and to stimulate further learning. Linking Question boxes can be found in the margin next to the content they link to (see example on the left).

By their very nature, the Linking Questions make reference to different parts of the course, some of which you may not have studied yet. As the questions can be asked in either direction, you may choose to consider them as part of the study of either or both of the linked topics. You will again find that you are able to answer the question more fully as your knowledge and understanding increase.

The Linking Questions are designed to lead to a thoughtful response. For this reason, we have given brief answers alongside the questions in the text, and hope these stimulate further consideration of the question.

The Nature of Science

Throughout the course you are encouraged to think about the nature of scientific knowledge and the scientific process as it applies to chemistry. Examples are given of the evolution of chemical theories as new information is gained, the use of models to conceptualize our understanding, and the ways in which experimental work is enhanced by modern technologies. Ethical considerations, environmental impacts, the importance of objectivity, and the responsibilities regarding scientists' code of conduct are also considered here. The emphasis is not on learning any of these examples, but on appreciating the broader conceptual themes in context. We have included several NOS examples in each chapter, and hope you will come up with your own as you keep these ideas at the forefront of your learning.

Key to feature boxes

You will find different coloured feature boxes interspersed throughout each chapter. These are used to enhance your learning and how it applies to real world examples, as explained below.

Nature of Science

As mentioned this is an overarching theme in the course. Throughout the book you will find NOS themes and questions emerging across different topics. We hope they help you to develop your skills in scientific literacy.

Nature of Science

Magnetism was used in navigation long before it was explained scientifically. Historically, technology emerged before science. Materials were often used practically long before there was an understanding of why they possessed their properties.

In today's world, the reverse is often the case, with scientific understanding leading to technological developments, which in turn drive further developments in scientific ideas.

Global context

The impact of the study of chemistry is global, and includes environmental, political and socio-economic considerations. Examples of this are given to help you to see the importance of chemistry in an international context. These examples also illustrate some of the innovative and cutting-edge aspects of research in chemistry.

A different unit of concentration is known as **ppm**, parts per million. It denotes one part per 10^6 parts of the whole solution, and is useful in describing very low concentrations. This unit is widely used in reporting levels of pollutants in air, water, soil and food. For example, in the USA the FDA has set a maximum permissible level of 1 part of methylmercury in a million parts of seafood (1 ppm).

Skills in the study of chemistry

These boxes indicate links to the Skills section of the course, including ideas for lab work and experiments that will support your learning and help you prepare for the Internal Assessment. These link to further resources in the eBook (look out for the grey icon).

Using spectra to confirm the structure of a compound. Full details of how to carry out this experiment with a worksheet are available in the eBook.

Theory of Knowledge

These questions, which are mostly from the Theory of Knowledge (TOK) guide, stimulate thought and consideration of knowledge issues as they arise in context. The questions are open-ended and will help trigger critical thinking and discussion.

How might developments in scientific knowledge trigger political controversies or controversies in other areas of knowledge?

Key fact

These key facts are drawn out of the main text and highlighted in bold. These boxes will help you to identify the core learning points within each section. They also act as a quick summary for review.

At equilibrium the rate of the forward reaction is equal to the rate of the backward reaction.

Hint for success

These give hints on how to approach questions, and suggest approaches that examiners like to see. They also identify common pitfalls in understanding, and omissions made in answering questions.

Note the definition of bond enthalpy indicates that all the species have to be in the gaseous state.

Challenge yourself

These boxes contain probing questions that encourage you to think about the topic in more depth, and may take you beyond the syllabus content. They are designed to be challenging and to make you think.

Challenge yourself

1. The components of a mixture can usually be separated by physical means. What might be the challenges of trying to separate the metals from an alloy?

Interesting fact

These give background information that will add to your wider knowledge of the topic and make links with other topics and subjects. Aspects such as historic notes on the life of scientists and origins of names are included here.

> Gilbert Lewis (1875–1946), responsible for the electron-pair theory of the covalent bond, was nominated 41 times for the Nobel Prize in Chemistry without winning. In 1946, he was found dead in his laboratory where he had been working with the toxic compound hydrogen cyanide.

Towards the end of the book, there are chapters on Green Chemistry, TOK as it relates to chemistry, the Internal Assessment, the Extended Essay and Strategies for success in IB chemistry.

Questions

There are three types of question in this book.

1. Worked examples with solutions

Worked examples appear at intervals in the text and are used to illustrate the concepts covered.

They are followed by the solution, which shows the thinking and the steps used in solving the problem.

Worked example

Identify the species with 19 protons, 20 neutrons and 18 electrons.

Solution

- the number of protons tells us the atomic number, $Z = 19$, and so the element is potassium, K
- the mass number = p + n = 19 + 20 = 39: ${}^{39}_{19}K$
- the charge = p − e = 19 − 18 = +1 as there is one extra proton: ${}^{39}_{19}K^+$

2. Exercises

These questions are found throughout the text, usually at the end of each Understanding. They allow you to apply your knowledge and test your understanding of what you have just been reading. The answers to these, together with worked solutions, are accessed via icons on the first page of each chapter in the eBook. Exercise answers can also be found at the back of the eBook.

Exercise

Q1. Explain why the relative atomic mass of tellurium is greater than the relative atomic mass of iodine, even though iodine has a greater atomic number.

3. Practice questions

These questions are found at the end of each chapter. They are mostly taken from previous years' IB exam papers. The markschemes used by examiners when marking these questions are accessed via icons in the eBook on the first page of each chapter. Questions which are based on the Understandings for SL are given first, followed by questions which include HL only material. HL questions are clearly marked.

Practice questions

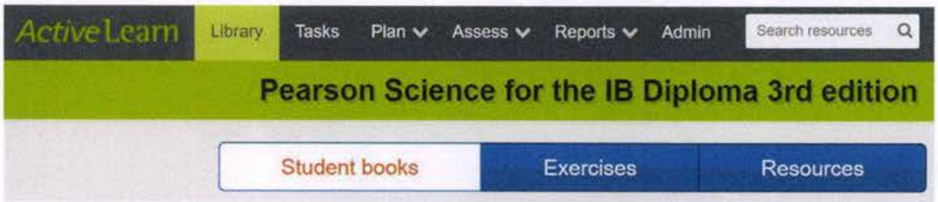
7. **HL** The transition element gold, Au, is used in electrical circuits due to its high electrical conductivity.

   Explain why transition elements are generally better electrical conductors than s and p block metals. (2)

   (Total 2 marks)

eBook

In your eBook you will find more information on the Skills section of the course including detailed suggestions for lab work. You will also find links to videos. In addition, there are auto-marked quizzes in the Exercises tab of your eBook account (see screenshot below).



We hope you enjoy your study of IB chemistry from this textbook.

Catrin Brown, Mike Ford, Oliver Canning, Andreas Economou and Garth Irwin

Introduction to skills in the study of chemistry

"I hear and I forget, I see and I remember, I do and I understand"

Chemistry is an experimental science and its progress continues to be based on the scientific method. The study of chemistry in the IB programme reflects this in the emphasis it places on laboratory work. This approach will help you to understand concepts, learn some practical skills and give you opportunities to explore further through investigations. It is also often the best part about studying chemistry!

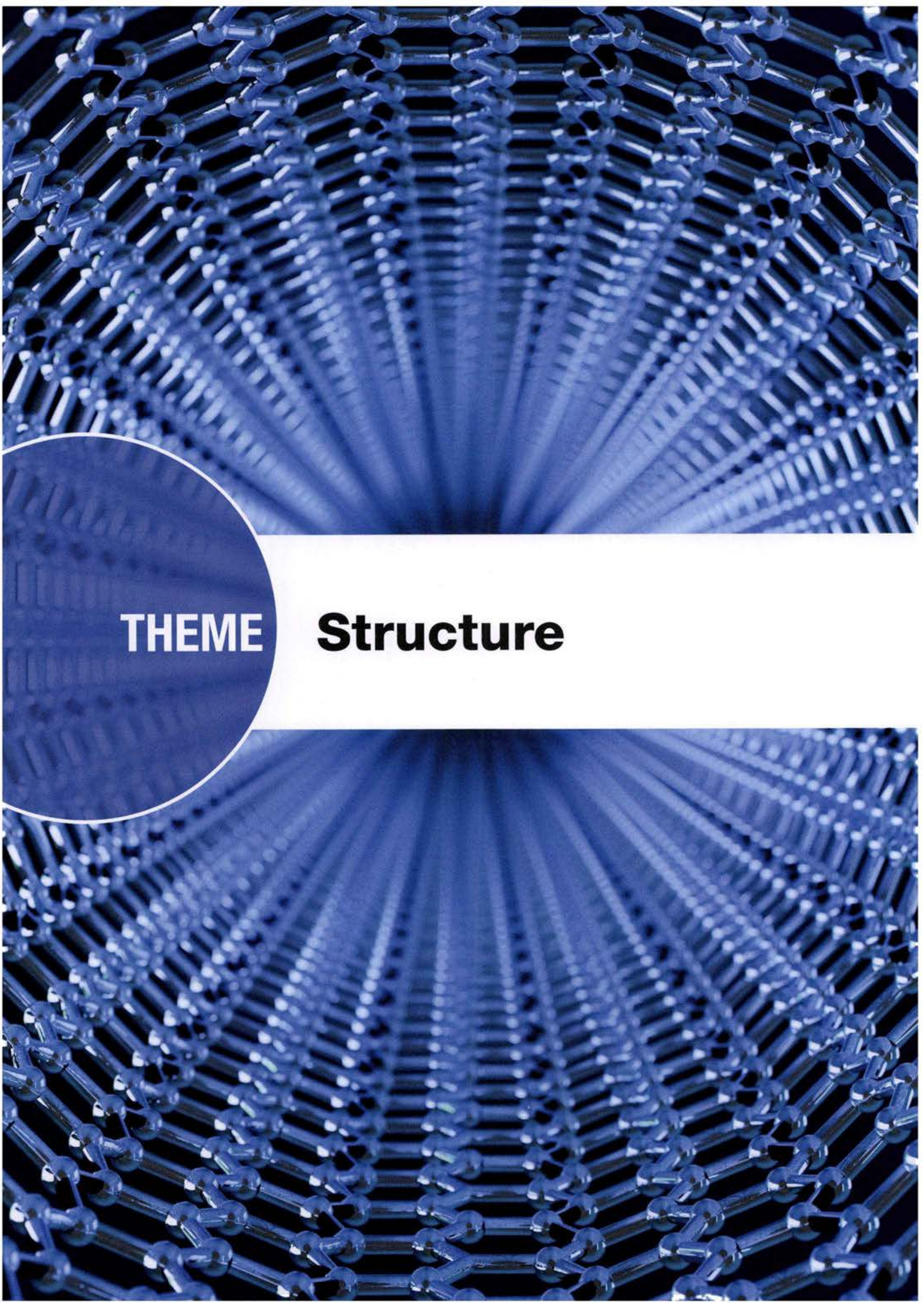
The syllabus roadmap on page vii has 'Skills in the study of chemistry' at the top. This unit is a summary of experimental skills and techniques that should be experienced during the course, including the application of technology and mathematics. It is not intended that these 'Tools' are covered as separate content, but should be integrated into the study of all topics. The 'Skills in the study of chemistry' chapter towards the back of this book includes tables that summarize the details of this unit with references to where in the syllabus content the Tools may be suitably included. There are also many links to experimental work and resources available in the ebook.

Nature of Science

The scientific method consists of systematic observation, the formulation and testing of hypotheses, and the collection of data for analysis and evaluation. Central to this process is a consideration of the limits of the usefulness of the data obtained. The interpretation of results must take into account the precision and accuracy of the measurements, the amount and limitations of data collected and the reproducibility of the results. Effective communication of the results must include this information.

The choice of apparatus for measurement in the laboratory determines the precision of the data collected. Here a pipette is used to deliver a single drop of liquid.

THEME Structure



◀ View of graphene with 3D rendering. Graphene is a relatively modern structure, usually composed of a single layer of carbon atoms. It is considered to be the world's thinnest, strongest and most conductive material, of both electricity and heat. Understanding the structure of graphene has helped develop its applications in many fields such as energy generation, sensors, medical equipment and composite materials.

Structure

Structure refers to the nature of matter. Chemists seek to understand the way in which fundamental particles, the building blocks of all chemical structure, combine to form every chemical structure that exists – from single atoms to the most complex compounds. An understanding of structure leads to the ability to explain and predict chemical properties, as studied in our second theme, *Reactivity*.

A major challenge in the study of structure is that the fundamental particles are too small for us to observe directly. Even the most advanced technology gives us only limited information on the nature and behaviour of these particles. As a result, since the early days of chemical exploration, scientists have used models to help explain and predict the nature of matter. Over time, these models have developed and changed in the light of increasingly detailed observations and new evidence. As we explore the applications of these models, we must also consider their limitations and how they may continue to evolve.

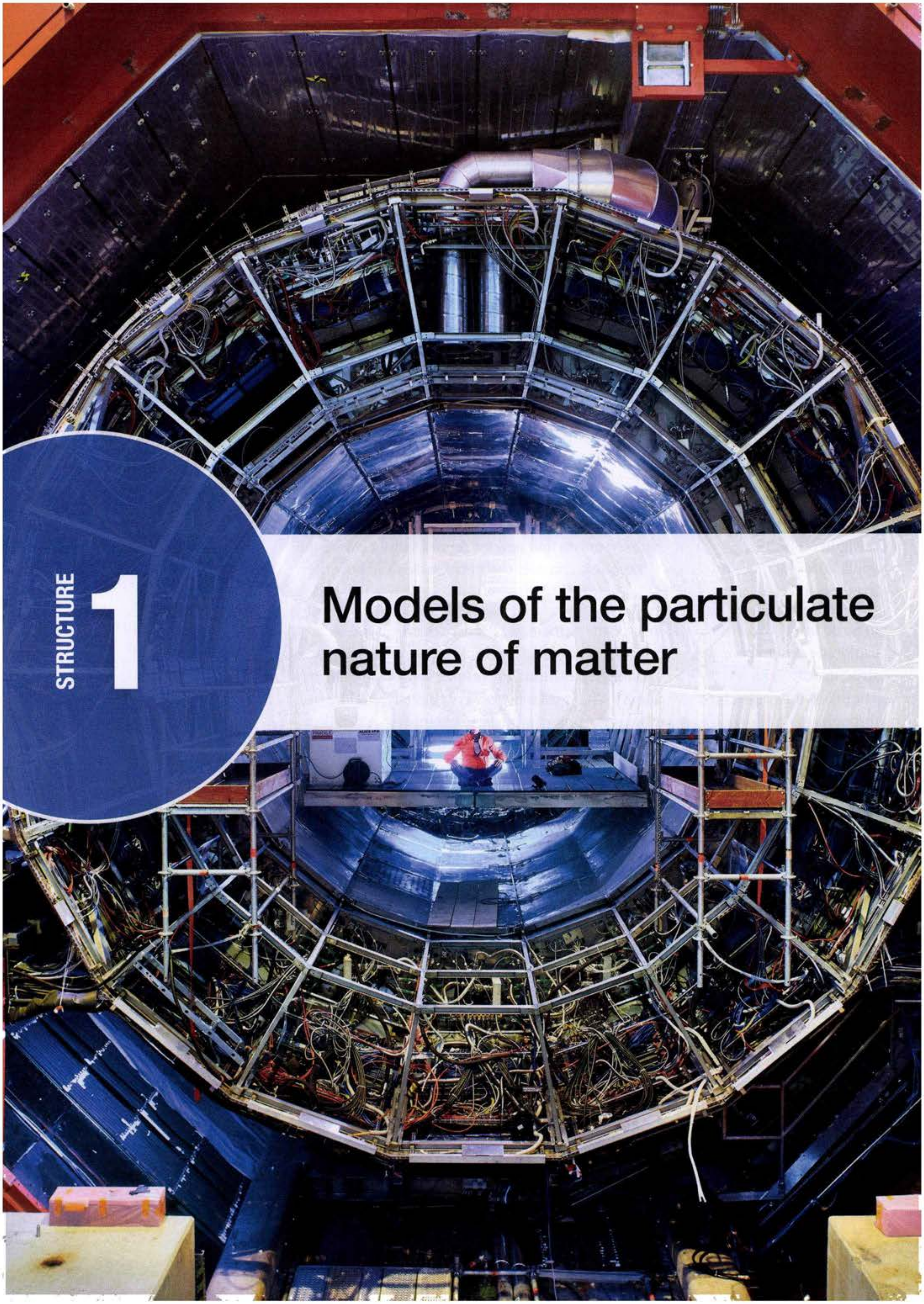
In Structure 1 we consider evidence for the particulate nature of matter. From an exploration of the properties of sub-atomic particles, we build an understanding of the structure of atoms and how they characterize the unique properties of each element. The problem of scale, how we quantify what we cannot observe directly, is addressed through an introduction to the mole as the unit of amount in chemistry. A detailed study of electron configurations helps us to recognize why atoms of different elements differ in their tendency to attract electrons. This leads to descriptions of the models of different chemical bonds – ionic, covalent and metallic – in Structure 2. The organization of elements in the periodic table, as studied in Structure 3, suggests patterns in elements' properties. This gives predictive power to the types of bonds that they will form. As atoms associate through bond formation, the products have different properties, giving rise to an infinite variety of structures. Chemists have developed clear terminology to communicate about chemical structure, and in Structure 3 we are introduced to the IUPAC (International Union of Pure and Applied Chemistry) system of nomenclature, and learn how compounds are given unambiguous and internationally agreed names.

Our understanding of structure has developed alongside advances in technology and has led to many innovations in materials science. Many modern materials, such as breathable fabrics and biodegradable plastics, and compounds such as therapeutic drugs, are designed for specific functions. You need look no further than your smart phone or clothing to realize how much our lives are influenced by these products. And yet, despite their extraordinary variety and complexity, every chemical structure is based on associations between a relatively small number of different atoms.

Structure determines reactivity, which in turn transforms structure.

STRUCTURE 1

Models of the particulate nature of matter

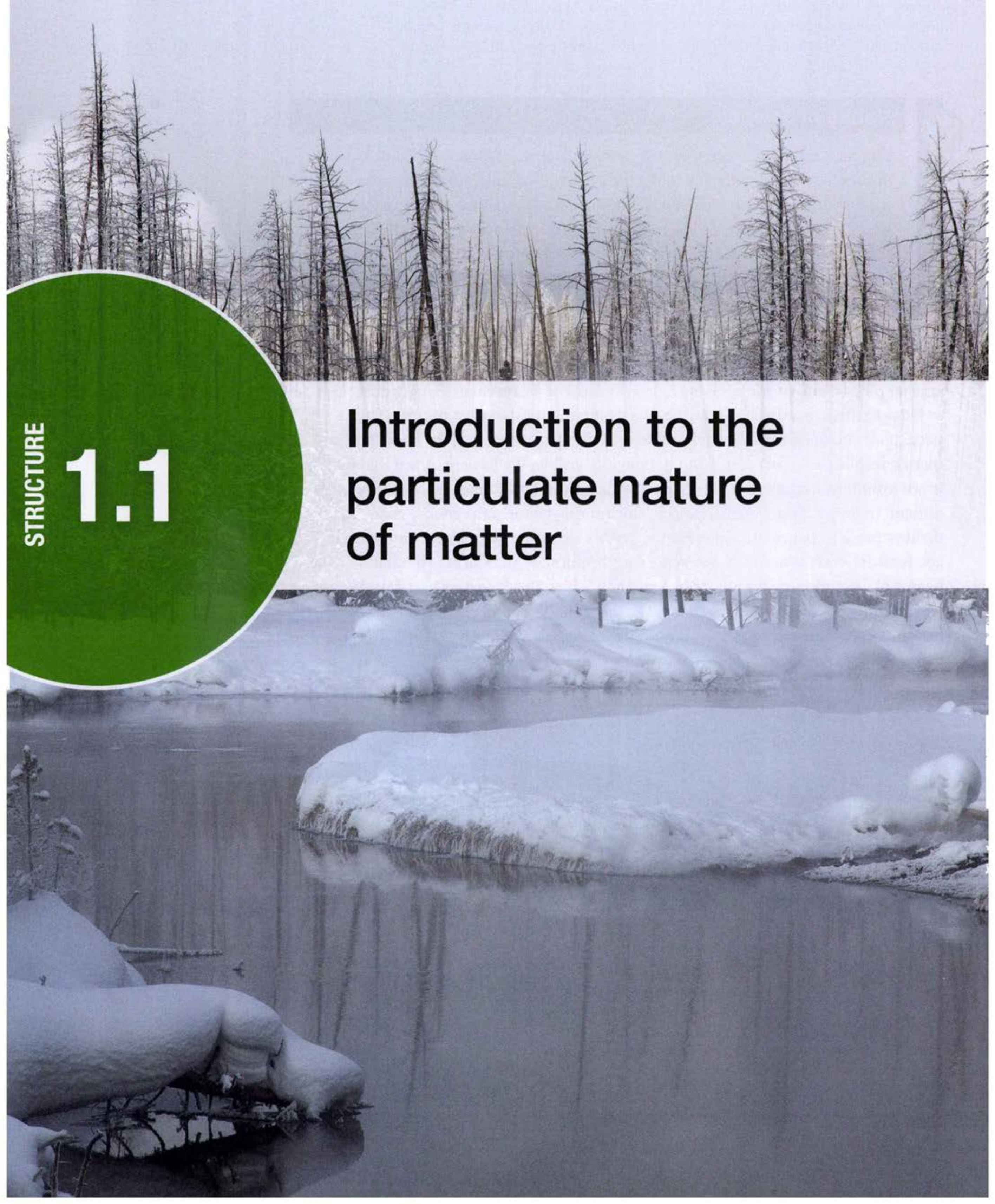


◀ Inside the empty skeleton of the ALICE detector at CERN (the European particle physics laboratory) near Geneva, Switzerland. ALICE (A Large Ion Collider Experiment) is a detector built around the Large Hadron Collider (LHC). The LHC is the world's largest and most powerful particle collider. Beams of ions are accelerated to collide head-on. The collision energy creates new particles that decay into other particles. The LHC energies have allowed the study of exotic materials like quark-gluon plasma, a form of quark matter. CERN announced the Higgs boson discovery on 4 July 2012.

Nature of Science

Progress in science often follows technological developments. The discovery of the Higgs boson was due to the use of particle accelerators, detectors and sophisticated computers. Such technological advances are only possible with international collaboration between scientists. Scientists communicate and collaborate throughout the world. CERN is run by over 20 member states, and many non-European countries are involved in different ways.

One of the earliest questions philosophers asked concerned the divisibility of matter. Could a piece of material be divided again and again continually into smaller and smaller pieces as Aristotle proposed, or would a limit be reached, a single particle, as Democritus argued? The latter idea has generally stood the test of time. This particulate model of matter enables us to explain many aspects of the behaviour of matter despite these particles being not directly visible. We have no proof that matter is not infinitely divisible, but we do have evidence that it becomes increasingly more difficult to divide it into smaller pieces. The limiting factor is the energy required to divide a particle. Experimental evidence for this has come from work with particle accelerators, such as at CERN, referenced in the photo at the start of the chapter, where beams of ions undergo high-energy collisions, which produce new particles. We are still learning about how the world is made up of fundamental particles. The Higgs boson, a key elementary particle, was only discovered as recently as 2012 although its existence had been predicted by scientific models in 1964.



STRUCTURE

1.1 Introduction to the particulate nature of matter

◀ Yellowstone National Park, Wyoming, USA, with mist rising on a cold winter morning from waters warmed by thermal springs. Matter can exist in the solid, liquid and gaseous states. The difference in physical properties of the three states is explained by kinetic molecular theory.

Guiding Question

How can we model the particulate nature of matter?

All things are made from atoms. This is one of the most important ideas that the human race has learned about the universe. Atoms are everywhere and they make up everything. You are surrounded by atoms – they make up the foods you eat, the liquids you drink and the fragrances you smell. Atoms make up you! To understand the world and how it changes, you need to understand atoms.

Atoms are the smallest particle of an element and so are fundamental to chemistry. As they are too small ever to be seen directly by a human eye, scientists have developed a series of models to explain the physical and chemical properties of materials. We can understand many aspects of the world simply by considering how these particles move and interact with each other. This particulate model of matter, which includes atoms, molecules and ions, provides a very strong foundation for our chemical understanding and is a good place to start our explorations.

Nature of Science

Scientists construct models as artificial representations of natural phenomena. All models have limitations that need to be considered in their application.

Structure 1.1.1 – Elements, compounds and mixtures

Structure 1.1.1 – Elements are the primary constituents of matter, which cannot be chemically broken down into simpler substances.

Compounds consist of atoms of different elements chemically bonded together in a fixed ratio.

Mixtures contain more than one element or compound in no fixed ratio, which are not chemically bonded and so can be separated by physical methods.

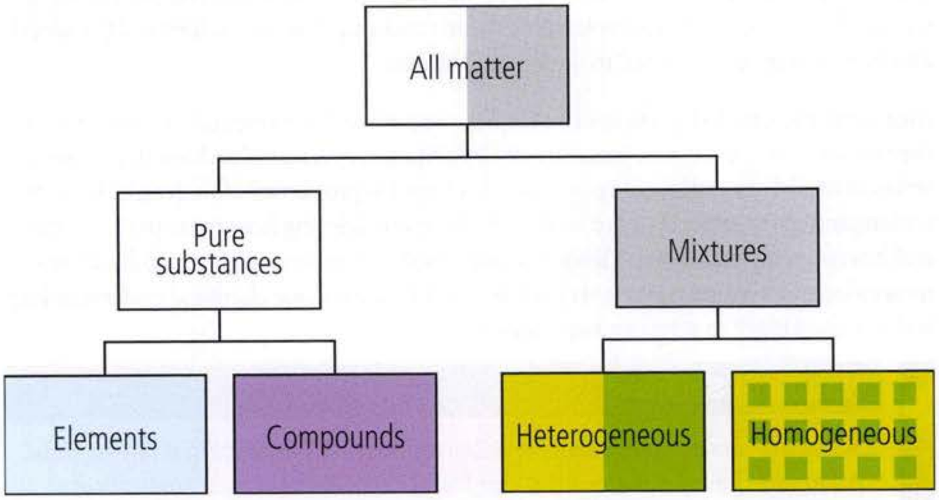
Distinguish between the properties of elements, compounds and mixtures.

Solvation, filtration, recrystallization, evaporation, distillation and paper chromatography should be covered. The differences between homogeneous and heterogeneous mixtures should be understood.	Tool 1 – What factors are considered in choosing a method to separate the components of a mixture? Tool 1 – How can the products of a reaction be purified? Structure 2.2 – How do intermolecular forces influence the type of mixture that forms between two substances? Structure 2.3 – Why are alloys generally considered to be mixtures, even though they often contain metallic bonding?

Matter can be classified into elements, compounds and mixtures

Classifying matter

Matter is present in an infinite number of different forms. The first step to understanding the chemistry of all these substances is an effective classification system. We start with a basic chemical distinction: some matter is made of pure substances, and some is made from mixtures. The chapter will follow the classification outlined in Figure 1.



S1.1 Figure 1 Matter can be classified into pure substances and mixtures. Pure substances can be elements or compounds. Mixtures can be homogeneous or heterogeneous.

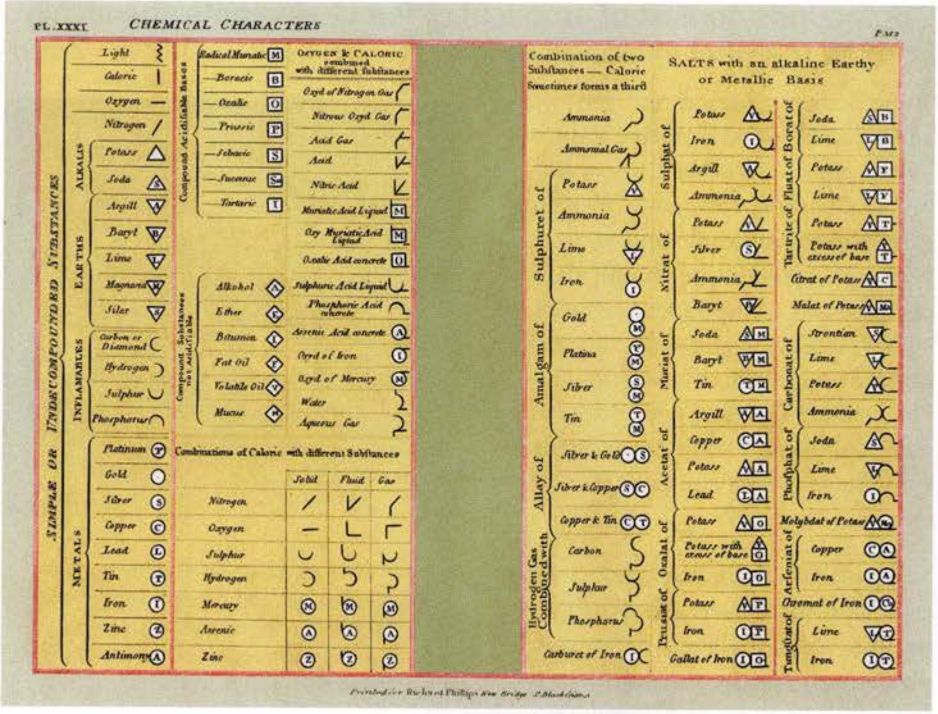
Elements are the primary constituents of matter, which cannot be chemically broken down into simpler substances

An element is a pure chemical substance composed of atoms with the same number of protons in the atomic nucleus.

All languages are based on an alphabet of a limited number of characters. The 26 letters of the English alphabet, for example, can be combined in different ways to form the estimated 600 000 words in the language. In a similar way, the substances known as chemical elements can combine to form the material of our universe. Elements are the primary constituents of matter. They cannot be chemically broken down into simpler substances. The near infinite number of different chemical substances in our world are made from only about 100 known elements.

An atom is the smallest particle of an element to show the characteristic properties of that element.

In Structure 2.1 we will learn about atomic structure, and how each element is made up of a particular type of atom. Atoms of the same element all have the same number of protons in the atomic nucleus and the same number of electrons. The distinct make-up of an element's atoms gives each element its individual properties. An atom is the smallest particle of an element to show the characteristic properties of that element.



Pictographic symbols used at the beginning of the 18th century to represent chemical elements and compounds. They are similar to those of the ancient alchemists. As more elements were discovered during the 18th century, attempts to devise a chemical nomenclature led to the modern alphabetic notational system. This system was devised by the Swedish chemist Berzelius and introduced in 1814.

The number of elements is open to change as new ones can be invented or discovered. It takes time for an element's existence to be confirmed by IUPAC so in the interim, a provisional systematic three-letter symbol is used. Latin abbreviations represent the atomic number. The letters u (un) = 1, b (bi) = 2, t (tri) = 3 and so on are used. The element of atomic number 118 now known as oganesson (Og) was previously known as ununoctium or uuo.

Each element is denoted by a **chemical symbol** and some examples are given below.

Name of element	Symbol
carbon	C
fluorine	F
potassium	K
calcium	Ca
mercury	Hg
tungsten	W

You will notice that often the letter or letters used to represent the elements are derived from its English name, but in some cases, they derive from other languages. For example, Hg for mercury comes from Latin, whereas W for tungsten has its origin in European dialects. These symbols are all accepted and used internationally, which allows for effective global communication between chemists. A complete list of the names of the elements and their symbols is given in Section 6 of the data booklet.

Chemistry is a very exact subject, and it is important to be careful in distinguishing between upper and lower case letters. Cobalt (Co) is a metallic element whereas carbon monoxide (CO) is a poisonous gas.

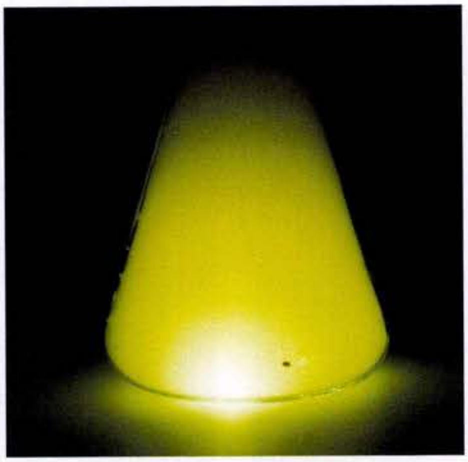
Compounds consist of atoms of different elements chemically bonded together in a fixed ratio

Some elements, such as nitrogen and gold, are found in **native** form, uncombined with other elements in nature. But more commonly, elements exist in chemical combinations with other elements, as **chemical compounds**. Compounds consist of atoms of different elements chemically bonded together in a fixed ratio. The physical and chemical properties of compounds are completely different from those of their component elements.

Sodium chloride, for example, is a white crystalline solid that is added to improve the taste of food, whereas sodium is a dangerously reactive metal that reacts violently with water, and chlorine is a toxic gas.

The **chemical formula** of a compound uses a combination of chemical symbols of its constituent elements. A subscript is used to show the number of atoms of each element in a unit of the compound. Some examples are given below. (The reasons for the different ratios of elements in compounds will become clearer after we have studied atomic structure and bonding in Structure 2.)

▲ Assorted minerals, including elements such as sulfur and silver, and compounds such as Al_2O_3 (sapphire) and CaF_2 (fluorite). Most minerals are impure and exist as mixtures of different elements and compounds.



▲ Sodium, Na, reacts violently with chlorine, Cl_2, to produce white crystals of the compound sodium chloride, NaCl.

$2Na(s) + Cl_2(g) \rightarrow 2NaCl(s)$

The properties of the compound are completely different from those of its component elements.

A compound is a substance made by chemically combining two or more elements in a fixed ratio of atoms. The physical and chemical properties of a compound are different from those of its constituent elements.

Name of compound	Chemical formula	Name of compound	Chemical formula
sodium chloride	NaCl	methane	CH_4
magnesium hydroxide	$Mg(OH)_2$	ammonia	NH_3
copper sulfate	$CuSO_4$	glucose	$C_6H_{12}O_6$
water	H_2O	sulfuric acid	H_2SO_4

Mixtures contain more than one element or compound in no fixed ratio

Chemistry is primarily concerned with understanding the structure and reactivities of pure substances but dealing with mixtures is a practical reality. Although there are a countable number of pure substances, the elements and compounds, which all have distinctive names, there is an infinite number of mixtures. The composition of any one mixture can vary continuously – the relative amounts of ice cream, milk and flavourings in a milkshake can vary depending on the taste of the person preparing the drink. Names for all the mixtures we could make do not exist.

Air is described as a **mixture** of gases because the separate components – different elements and compounds – are interspersed with each other, but not chemically combined. The gases nitrogen and oxygen when mixed in air, for example, have the same properties as they do when they are in pure samples. Substances burn in air because they react with the oxygen in the same way that they react with pure oxygen. As substances can be mixed in any proportion, mixtures, in contrast to compounds, do not have a fixed composition and cannot be represented by a chemical formula. The composition of air for example varies widely around the world due to the presence of different pollutants.

TOK

Our classification systems are embedded in the language we use. To what extent do the classification systems we use affect the knowledge we obtain? To what extent do the names and labels that we use help or hinder the acquisition of knowledge?

Air is an example of a **homogeneous mixture**, as it has uniform composition and properties throughout. A solution of salt in water and a metal alloy such as bronze, which is a mixture of copper and tin, are also homogeneous. To form a homogeneous mixture, the inter-particle attraction within the different components must be similar in nature to those between the components in the mixture. Explanations of the different particle interactions are given in Structure 2.2.

A mixture contains more than one element or compound in no fixed ratio, which are not chemically bonded. The components of a mixture can be separated by physical methods.

Mixture	Component 1	Particle interaction 1	Component 2	Particle interaction 2	Interaction in mixture
air	N_2	dispersion forces	O_2	dispersion forces	dispersion forces
bronze	Cu	metallic bonding	Sn	metallic bonding	metallic bonding
salt water	NaCl	ionic	H_2O	hydrogen bonding	ion-dipole

Making alloys at a steel mill. Alloys are formed by mixing two molten metals that can then form a mixture of uniform composition. There is no chemical reaction between the metallic elements as the metallic bonding present in the individual metals and the alloys is non-directional and not significantly disrupted by the mixing process. Metallic bonding is explored more fully in Structure 2.3.

Structure 2.3 - Why are alloys generally considered to be mixtures, even though they often contain metallic bonding?

Challenge yourself

1. If you add 10 cm^3 of water to 10 cm^3 of water, you get 20 cm^3 of water. Similarly, if you add 10 cm^3 of ethanol to 10 cm^3 of ethanol you get 20 cm^3 of ethanol. Explain why the volume of the solution formed between 10 cm^3 of water and 10 cm^3 ethanol is less than 20 cm^3.

Structure 2.2 - How do intermolecular forces influence the type of mixture that forms between two substances?

A **heterogeneous mixture**, by contrast, such as water and oil, has a non-uniform composition, and its properties are not the same throughout. The interactions between the components of a heterogeneous mixture are different in nature. The water molecules interact by hydrogen bonding and the oil molecules by dispersion forces, as discussed in Structure 2.2.

It is usually possible to see the separate components in a heterogeneous mixture but not in a homogeneous mixture.

Ocean oil spills can occur when oil is extracted or transported. They cause widespread damage to the environment and can have a major impact on local industries such as fishing and tourism. Efforts to reduce the impact of the spill include the use of dispersants, which break up the oil into smaller droplets, allowing it to mix better with water.

Smoke from a controlled burn of the oil spill caused by the explosion of the Deepwater Horizon oil rig, 20th April 2010. Five thousand barrels of oil a day leaked into the Gulf of Mexico, harming local wildlife and fishing industries.

Challenge yourself

2. Does a mixture have the same classification at all scales?

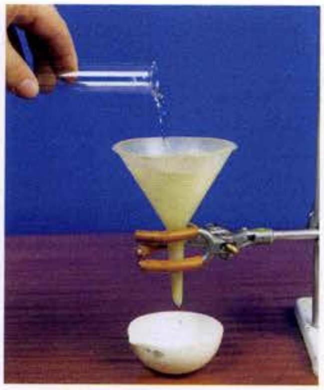
The components in a mixture can be relatively easy to separate if they have a distinct physical property. The technique chosen will depend on this distinct property.

Mixture	Difference in property of components	Technique used
sand and salt	solubility in water	solution and filtration
salt and water	boiling point	distillation
iron and sulfur	magnetism	response to a magnet
pigments in food colouring	adsorption to solid phase	paper chromatography

SKILLS

The required product of a chemical reaction similarly needs to be separated from the reaction mixture, which also contains unreacted reactants and other unwanted products. It is a practical challenge to both maximize the yield and the purity, as some product can be removed with the impurities during the purification process.

Filtration is the process where a solid is separated from a liquid or gas using a membrane. The solid is collected on the membrane as the residue, and the filtrate containing the solute passes through. Sand and salt have different solubilities in water so can be separated by adding water which dissolves the salt – an example of **solvation**. The resulting mixture can be filtered with the insoluble sand removed as the **residue** leaving the salt water solution as the **filtrate**. The water can be separated from the salt by evaporation, which allows the salt crystals to form (**crystallization**).



Filtration apparatus

Tool 1 - What factors are considered in choosing a method to separate the components of a mixture?

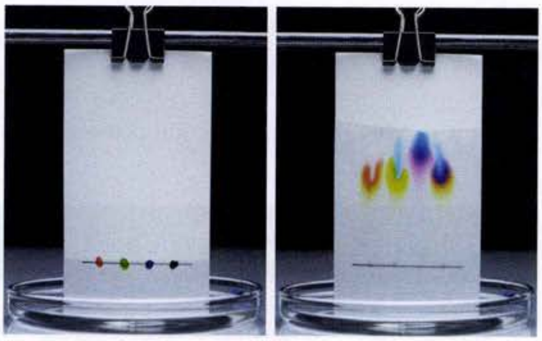
Tool 1 - How can the products of a reaction be purified?

SKILLS Preparation of AgI precipitate from aqueous solutions. Full details of how to carry out this experiment with a worksheet are available in the eBook.

Distillation is used to separate a solvent from a solute. The solvent has a lower boiling point than the solute and so is collected as a gas and passes into the condensing tube, which is surrounded by cold flowing water. The gas is condensed into the pure solvent collected in the beaker at the bottom. This method can be used to separate water from seawater, for example.

Distillation apparatus

In **paper chromatography**, small spots of solutions containing the samples being tested are placed on the baseline. The paper is suspended to ensure that it is saturated **(a)**. The different components have different affinities for the water in the paper (the solvent) and so separate as the solvent moves up the paper **(b)**. This method can be used to investigate the different pigments in food colouring.



(a) **(b)**

Paper chromatography apparatus

Exercise

Q1. Identify the homogeneous mixture.

A water and oil

B sand and water

C salt and water

D sand and salt

Q2. Identify the correct descriptions about mixtures.

I. The components can be elements or compounds.

II. All components must be in the same state.

III. The components retain their individual properties.

A I and II only

B I and III only

C II and III only

D I, II and III

Q3. Identify the homogeneous mixtures.

I. gold
II. bronze
III. steel

A I and II only **B** I and III only
C II and III only **D** I, II and III

Q4. **(a)** River water needs to be purified to make it safe to drink. The water passes through a grid and is then left in a tank where other impurities are removed as they fall to the bottom in a process known as sedimentation. Suggest why pollutants such as fertilizers are not removed in this process.

(b) Drinking water can be obtained from seawater by distillation.

Explain the disadvantages of using distillation to obtain large amounts of drinking water.

Q5. A layer of oil paint is left to dry in the air and it hardens. Suggest what causes the oil to harden.

Q6. Metal coins are made from different metals. The composition of a 20-cent and a 50-cent euro coin is given below.

	Mass/g			
Coin	**Copper**	**Aluminium**	**Zinc**	**Tin**
20 cent	5.11	0.287	0.287	0.057
50 cent	6.94	0.39	0.39	0.080

Compare the chemical compositions of the two coins.

Structure 1.1.2 – The kinetic molecular theory

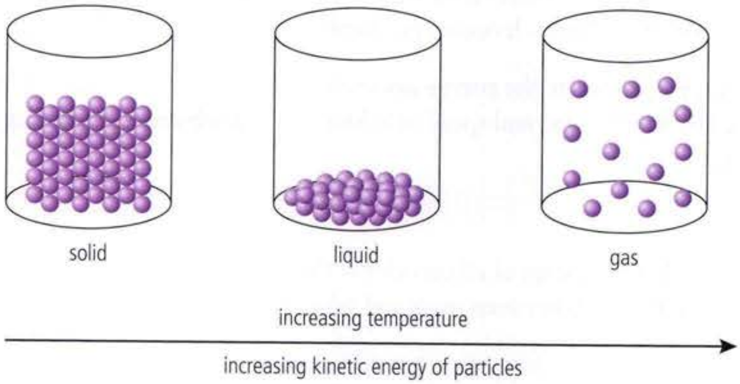
Structure 1.1.2 – The kinetic molecular theory is a model to explain physical properties of matter (solids, liquids and gases) and changes of state. Distinguish the different states of matter. Use state symbols (s, l, g and aq) in chemical equations.	
Names of the changes of state should be covered: melting, freezing, vaporization (evaporation and boiling), condensation, sublimation and deposition.	Structure 2.4 – Why are some substances solid while others are fluid under standard conditions? Structure 2 (all), Reactivity 1.2 – Why are some changes of state endothermic and some exothermic?

The kinetic molecular theory explains physical properties

If you were hit with a bucket of solid water (ice), you could be seriously injured, but the same mass of liquid water would only be annoying. Gaseous water (steam) could also be harmful but for different reasons. These three samples are all made from the same particles: water molecules, H_2O. The difference in physical properties of the three states is explained by **kinetic molecular theory**.

Matter exists in different states as determined by the temperature and the pressure

From our common experience, we know that all matter (elements, compounds, and mixtures) can exist in different forms depending on the temperature and pressure. Liquid water changes into a solid form, such as ice, hail, or snow, as the temperature drops, and it becomes a gas, steam, at higher temperatures. These different forms are known as the **states of matter** and are characterized by the different energies of the particles.



S1.1 Figure 2 Representation of the arrangement of the particles of the same substance in the solid, liquid, and gas states.

A fourth state of matter, plasma, exists only at conditions of very high temperatures and pressures, such as those commonly found in stars such as our Sun.

Solid	Liquid	Gas
• particles closely packed	• particles more spaced	• particles fully spread out
• inter-particle forces strong, particles vibrate in position	• inter-particle forces weaker, particles can slide over each other	• inter-particle forces negligible, particles move freely
• fixed shape	• no fixed shape	• no fixed shape
• fixed volume	• fixed volume	• no fixed volume

This is known as the kinetic molecular theory of matter as the three states are distinguished by the way the particles move. The temperature of the system is directly related to the average kinetic energy of the particles and the state of matter at a given temperature and pressure is determined by the strength of **inter-particle forces** that exist between the particles relative to this average kinetic energy. If the inter-particle forces are sufficiently strong to keep the particles in position at a given temperature and pressure, the substance will be a solid. If not, it will be a liquid or a gas. The different inter-particle forces are explored more fully in Structure 2.

Depending on the chemical nature of the substance, matter may exist as atoms such as Ar(g), as molecules such as $H_2O(l)$, or as ions such as Na^+ and Cl^- in aqueous solution NaCl(aq). The term **particle** is therefore used as an inclusive term that is applied in this text to any or all of these entities of matter.

Challenge yourself

3. What evidence based on simple observations can you think of that supports the idea that water is made from discrete particles?

Temperature is a measure of the average kinetic energy of the particles of a substance.

Structure 2.4 – Why are some substances solid while others are fluid under standard conditions?

Worked example

Which of the following has the highest average kinetic energy?

A He at 100 °C **B** H_2 at 200 °C **C** O_2 at 300 °C **D** H_2O at 400 °C

Solution

D The substance at the highest temperature has the highest average kinetic energy.

Liquids and gases are both referred to as **fluids**, as they have the ability to flow. In the case of liquids, it means that they take the shape of their container. **Diffusion**, the process by which the particles of a substance spread out more evenly, occurs as a result of their random movements. It occurs predominantly in these two fluid states.

▲ Bromine liquid, $Br_2(l)$, has been placed in the lower gas jar only, and its vapour has diffused to fill both jars. Bromine vaporizes readily at room temperature and its distinctive colour allows the diffusion to be observed.

Kinetic energy (E_k) refers to the energy associated with movement or motion. It is determined by the mass (m) and speed or velocity (v) of a substance, according to the relationship:

$$E_k = \frac{1}{2}mv^2$$

As the average kinetic energy of all particles at the same temperature is the same, there is an inverse relationship between mass and velocity:

$$E_k = \frac{1}{2}m_1{v_1}^2 = \frac{1}{2}m_2{v_2}^2$$

$$\frac{m_1}{m_2} = \frac{{v_2}^2}{{v_1}^2}$$

Particles with smaller mass therefore diffuse more quickly than those with greater mass, at the same temperature.

State symbols are used to show the states of the reactants and products taking part in a reaction. These are abbreviations, which are given in parenthesis after each term in an equation, as shown below.

State	Symbol	Example
solid	(s)	$Fe(s)$
liquid	(l)	$Br_2(l)$
gas	(g)	$O_2(g)$
aqueous	(aq)	$H_2SO_4(aq)$

For example:

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

It is good practice to show state symbols in all equations, even when they are not specifically requested.

Sodium hydroxide, NaOH, is produced during this reaction in **aqueous solution.**

Solutions more generally are mixtures of two components. The less abundant component is the **solute** and the more abundant is the **solvent**. The solute can be solid, liquid or gas but the solvent is generally a liquid. Solutions in water are particularly important and are given the state symbol (aq).

Matter changes state reversibly

As the movement or kinetic energy of the particles increases with temperature, they will overcome the inter-particle forces and change state. This occurs at a fixed temperature and pressure for each substance. A solid ($X(s)$) changes to a liquid at a defined **melting point** and a liquid ($Y(l)$) changes to a gas at its **boiling point**.

These changes can be reversed when the substance is cooled: a liquid freezes and becomes solid at the same temperature as the solid melts.

A gas or vapour condenses at the same temperature as the liquid boils.

The reversibility of these changes can be represented by reversible arrows as shown in the table.

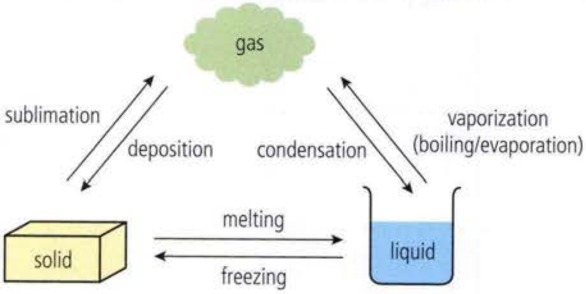
Change of state		Change of state		Reversible equation
melting	$X(s) \rightarrow X(l)$	freezing	$X(l) \rightarrow X(s)$	$X(s) \rightleftharpoons X(l)$
boiling	$Y(l) \rightarrow Y(g)$	condensing	$Y(g) \rightarrow Y(l)$	$Y(l) \rightleftharpoons Y(g)$

The temperature of a state change can be presented from both perspectives:

melting point = freezing point;

boiling point = condensation point.

Some substances can also change directly between the solid and gaseous states.



S1.1 Figure 3 The different state changes between the solid, liquid and gaseous states.

Sublimation is the direct inter-conversion of a solid to a gas without going through the liquid state. It is characteristic of some substances such as iodine, carbon dioxide and ammonium chloride.

Deposition is the reverse of sublimation and occurs when a gas changes directly to a solid. It occurs when snow and frost are formed.

SKILLS

Sublimation of iron and iodine. Full details of how to carry out this experiment with a worksheet are available in the eBook.

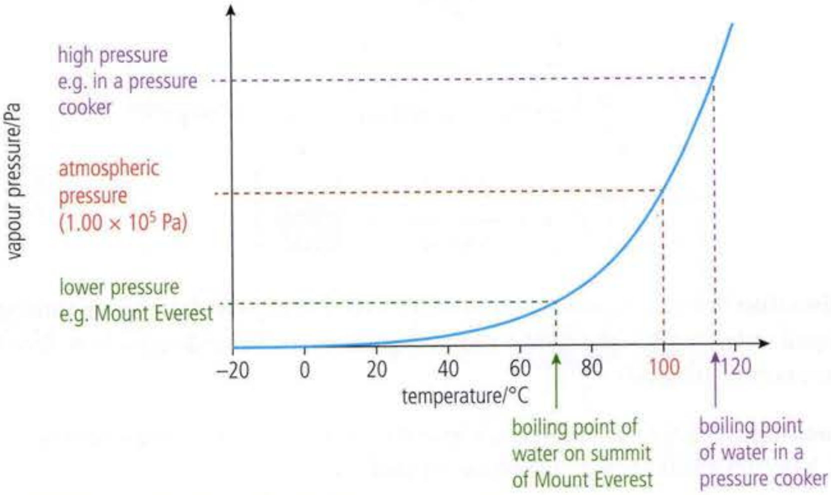
Ice crystals, known as hair ice, formed by deposition on dead wood in a forest on Vancouver Island, Canada.

A liquid can change to gas by two processes: **evaporation** and **boiling**. Boiling occurs at a fixed temperature for a given pressure, when bubbles of gas form throughout the liquid. Evaporation, by contrast, occurs only at the surface and takes place over a range of temperatures below the boiling point.

▲ The heat of the Sun enables all the water to evaporate from the clothes.

More precisely, the boiling point is the temperature at which the vapour pressure is equal to the external pressure. As a liquid is heated, more particles enter the vapour state and the vapour pressure increases. When the vapour pressure reaches the external atmospheric pressure the liquid boils. When the external pressure is lower, the vapour pressure needed to boil is reduced and so boiling occurs at a lower temperature.
The relationship between temperature and vapour pressure and the influence of external pressure on the boiling point is demonstrated in Figure 4.

S1.1 Figure 4 Graph showing the boiling point of water at three different pressures.



A pressure cooker is a sealed container in which a high pressure can be generated. This raises the boiling point of water, allowing cooking time to decrease. Conversely, at altitude, where the atmospheric pressure is lower, the boiling point of water is reduced so it takes much longer to cook food.

◀ A butane gas camping stove. Butane, C_4H_{10}, is stored as a liquid because the high pressure in the canister raises its boiling point. When the valve is opened the release of pressure causes the butane to boil, releasing a gas that can be burned.

Challenge yourself

4. Propane (C_3H_8) and butane (C_4H_{10}) are both commonly used in portable heating devices. Their boiling points are butane −1 °C and propane −42 °C. Suggest why butane is less suitable for use in very cold climates.

Macrophotograph of freeze-dried instant coffee granules.

Freeze-drying is used to preserve food and some pharmaceuticals. It differs from standard methods of dehydration as the energy needed to evaporate water is produced by the sublimation of ice. The substance to be preserved is first frozen, and then warmed gently at very low pressure which causes the ice to change directly to water vapour. The process is slow but has the significant advantage that the composition of the material, and so also its flavour, are largely conserved. The freeze-dried product is stored in a moisture-free package that excludes oxygen, and can be reconstituted by the addition of water.

At night, as the temperature is lowered, the rate of condensation increases. As the air temperature drops below its saturation point, known as the **dew point**, condensed water called **dew** forms. The temperature of the dew point depends on the atmospheric pressure and the water content of the air – that is, the relative humidity.

Exercise

Q7. A mixture of two gases, X and Y, which both have strong but distinct smells, is released. From across the room the smell of X is detected more quickly than the smell of Y. What can you deduce about X and Y?

Q8. Use the kinetic theory to explain whether you would expect the rate of diffusion in a liquid to increase or decrease as the temperature is increased.

Q9. Which is the correct descriptor for the movement of particles in the solid, liquid and gaseous states?

	Solid	Liquid	Gas
A	vibrational movement in one dimension	vibrational movement in two dimensions	vibrational movement in three dimensions
B	no movement, fixed in position	only vibrational movement	free movement in all dimensions
C	free movement in all dimensions	free movement in all dimensions	free movement in all dimensions
D	vibrational movement	limited movement in all dimensions	free movement in all dimensions

Q10. A closed flask contains a pure substance, a brown liquid that is at its boiling point.

(a) Explain what you are likely to observe in the flask.

(b) Distinguish between the inter-particle distances and the average speeds of the particles in the two states present.

Q11. A beaker containing solid carbon dioxide is placed in a fume cupboard at room temperature. The carbon dioxide becomes gaseous. Which process describes this change of state?

A boiling **B** condensation **C** evaporation **D** sublimation

Q12. Water exists in three states: ice, liquid water or steam. Which transition can occur over a range of temperatures at constant pressure?

A freezing **B** melting **C** evaporation **D** boiling

Q13. A liquid is placed in an open dish. Which change increases the rate of evaporation?

I. increased temperature of the liquid

II. increased depth of the liquid

III. increased surface area of the liquid

A I and II **B** I and III **C** II and III **D** I, II and III

Q14. During very cold weather, snow often gradually disappears without melting. Explain how this is possible.

Structure 1.1.3 – Kinetic energy and temperature

Structure 1.1.3 – Temperature (T) in kelvin (K) is a measure of average kinetic energy (E_k) of particles.

Interpret observable changes in physical properties and temperature during changes of state.

Convert between values in the Celsius and Kelvin scales.

The kelvin (K) is the SI unit of temperature and has the same incremental value as the Celsius degree (°C).	Reactivity 2.2 – What is the graphical distribution of kinetic energy values of particles in a sample at a fixed temperature? Reactivity 2.2 – What must happen to particles for a chemical reaction to occur?

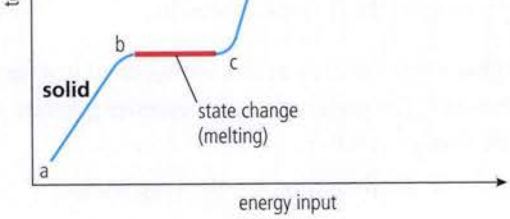
SKILLS

The heat curve of water. Full details of how to carry out this experiment with a worksheet are available in the eBook.

Temperature is constant during changes of state

Matter changes state when it is heated

Simple experiments can be done to monitor the temperature change while a substance is heated and changes state. Figure 5 shows a typical result.



S1.1 Figure 5 Temperature change versus energy input at fixed pressure as a solid substance is heated. The flat regions shown in red are where a change of state is occurring. Heat energy is used to overcome the inter-particle forces.

Ice cubes melting in a beaker of water. Heat from the surroundings breaks some inter-particle forces between the water molecules in the ice. In Structure 2.2.8, we will see that the inter-particle forces in ice are hydrogen bonds.

The graph can be interpreted as follows:

a–b As the solid is heated, the vibrational energy of its particles increases and so the temperature increases.

b–c This is the melting point. The vibrations are sufficiently energetic for the particles to move away from their fixed positions and form a liquid. Energy added during this stage is used to break the inter-particle forces, not to raise the kinetic energy, so the temperature remains constant.

c–d As the liquid is heated, the particles gain kinetic energy and so the temperature increases.

d–e This is the boiling point. There is now sufficient energy to break all of the inter-particle forces and form a gas. Note that this state change needs more energy than melting, as all the inter-particle forces must be broken. The temperature remains constant as the kinetic energy does not increase during this stage. Bubbles of gas are visible through the volume of the liquid.

e–f As the gas is heated under pressure, the kinetic energy of its particles continues to rise, as does the temperature.

▲ Geothermal hot spring, Hveragerdi, Iceland. The geothermal spring provides sufficient energy to separate the water molecules and turn water into steam.

Melting (b to c) and boiling (d to e) are endothermic processes as energy is needed to separate the particles. The reverse processes, freezing (c to b) and condensation (e to d), are exothermic. Energy is given out as the inter-particle forces bring the particles closer together. Energy changes are explored in Reactivity 1.2.

Structure 2 (all), Reactivity 1.2 - Why are some changes of state endothermic and some exothermic?

Challenge yourself

5. Which physical properties determine the gradient of the lines for the different states in Figure 5?

Nature of Science

Scientists analyse their observations looking for patterns, trends or discrepancies. You may have noticed that the volume decreases as ice melts and its density increases. This is unusual as density generally decreases as a solid melts. This discrepancy is explained in Structure 2.2.8.

Temperature in kelvin is known as the absolute temperature

The movement or kinetic energy of the particles of a substance depends on the temperature. If the temperature of a substance is decreased, the average kinetic energy of the particles also decreases. Absolute zero (−273 °C) is the lowest possible temperature attainable as this is the temperature at which all movement stops.

The kelvin is the SI unit of temperature. The absolute temperature is directly proportional to the average kinetic energy of its particles. A temperature increase of 1 °C is also an increase of 1 K. This facilitates conversions between the two scales.

The Celsius scale of temperature is defined relative to the boiling and freezing points of water. The original scale, developed by the Swedish astronomer Anders Celsius, made the boiling point of water zero and the freezing point 100. The modern scale reverses this with the boiling point of water 100 °C and the melting point of ice as 0 °C. The original scale may now seem absurd, but the modern scale is just as arbitrary.

An increase of temperature $\Delta T = 1\ \text{K} = 1\ ^\circ\text{C}$.

More generally $T(\text{K}) = T(^\circ\text{C}) + 273.15$

The kelvin is the SI unit of temperature.

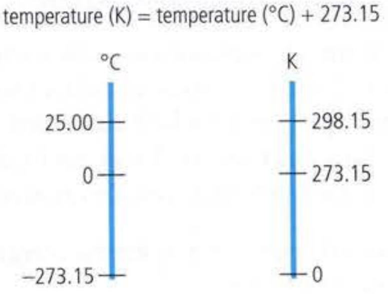
William Thomson (1824–1907), who became known as Lord Kelvin later in life, completed most of his work at the University of Glasgow, Scotland. His concept of the absolute temperature scale followed from his recognition of the relationship between heat energy and the ability to do work. The existence of a minimum possible temperature at which no heat can be extracted from the system and so no work done, led him to the definition of absolute zero in 1848. This in turn led to the formulation of the laws of thermodynamics. Kelvin is considered one of the great scientists of the 19th century, and is buried next to Isaac Newton in London.

Reactivity 2.2 – What is the graphical distribution of kinetic energy values of particles in a sample at a fixed temperature?

Reactivity 2.2 – What must happen to particles for a chemical reaction to occur?

Temperature can be converted from Celsius to the Kelvin scale by the relation:

$$T(\text{K}) = T(^\circ\text{C}) + 273.15 \text{ therefore } T(^\circ\text{C}) = T(\text{K}) - 273.15$$

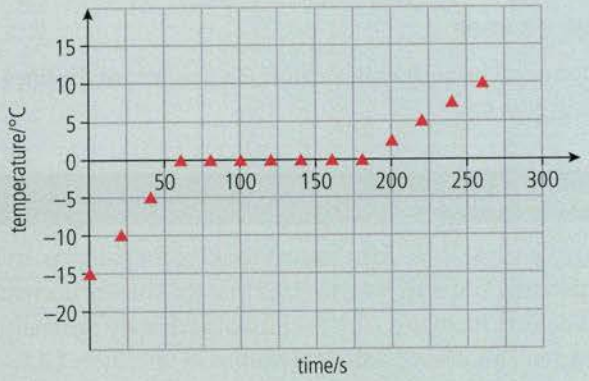


S1.1 Figure 6 The Celsius and Kelvin scales of temperature.

Although we can only relate the average kinetic energy to the temperature, there are many particles in a sample each with a different kinetic energy. The total kinetic energy is conserved in particle collisions, but the kinetic energy of individual particles changes upon each collision. We can however predict the statistical distribution of energies in a sample at a particular temperature, known as the Maxwell–Boltzmann distribution. This distribution will also help us understand the effect of temperature on rates of reaction. To react, particles must collide with sufficient kinetic energy known as the activation energy. Both these points are explored in Reactivity 2.2.

Exercise

Q15. A solid is heated and the temperature is measured every 20 seconds.



(a) Identify the solid.

(b) Describe how the particles in the solid are moving in the interval 0–60 s.

(c) Describe how the particles are moving in the interval after 180 s.

(d) Explain why the temperature does not change in the interval 60–180 s.

(e) Use the graph to predict the temperature after the material has been heated for 600 s.

(f) Use the graph to predict the temperature after 1200 s. Comment on the validity of your prediction.

Q16. Which of the following shows the correct Celsius temperature for the given kelvin temperature?

	Kelvin scale	Celsius scale
A	0	273
B	50	323
C	283	110
D	323	50

Q17. Which of the following occurs at the freezing point when a liquid is converted to a solid?

I. kinetic energy of the particles decreases

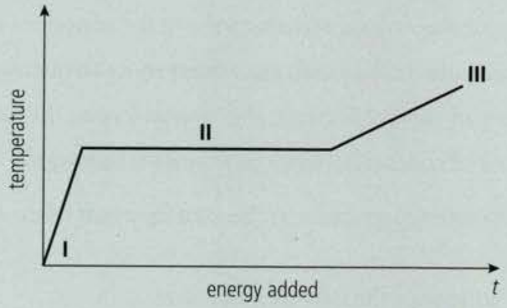
II. separation between the particles decreases

A I only **B** II only **C** I and II **D** neither I nor II

Q18. Two objects made from different masses of iron have the same temperature. Which of the following is the correct comparison of the average kinetic energy and the total energy of the atoms in the objects?

	Average kinetic energy of the atoms	Total energy of the atoms
A	greater in an object of larger mass	same
B	less in an object of larger mass	same
C	same	greater in an object of larger mass
D	same	less in an object of larger mass

Q19. A substance is heated. The graph shows how the temperature changes with the heat energy added.



In which region of the graph must the solid state be present?

A I **B** II **C** III **D** None

Q20. Explain why a burn to the skin caused by boiling water is less harmful than a burn caused by the same amount of steam produced as the water boils.

Guiding Question revisited

How can we model the particulate nature of matter?

In this chapter we have used a particulate model to show:

- All matter is made up from small particles.
- An element is a pure chemical substance composed of the same type of atoms.
- Compounds consist of atoms of different elements chemically bonded together in a fixed ratio.
- Mixtures are made from particles of one substance interspersed between particles of at least one other substance. If this mixing is uniform, it is a homogeneous mixture. If it is not uniform, it is heterogeneous.
- The different states of matter are characterized by the movement and arrangement of the particles.
- Changes of state require energy changes as energy is needed to separate particles and is given out when particles come together.

Practice questions

1. Which statements are correct?

I. Solids have a fixed shape because the particles can only vibrate about a fixed point.

II. Liquids can flow because the particles can move freely.

III. Gases are less dense because the interactions between the particles are very weak.

A I and II **B** I and III **C** II and III **D** I, II and III

2. The temperature of a gas is reduced. Which of the following statements is true?

A The molecules collide with the walls of the container less frequently.

B The molecules collide with each other more frequently.

C The time of contact between the molecules and the wall is reduced.

D The time of contact between molecules is increased.

3. Which of the following occurs at the melting point when a solid is converted to a liquid?

I. kinetic energy of the particles increases

II. separation between the particles increases

A I only **B** II only **C** I and II **D** neither I nor II

4. Identify the change(s) that occur at the boiling point when a liquid is converted to a gas.

I. kinetic energy of the particles increases

II. separation between the particles increases

A I only **B** II only **C** I and II **D** neither I nor II

5. A substance is heated at a constant rate.

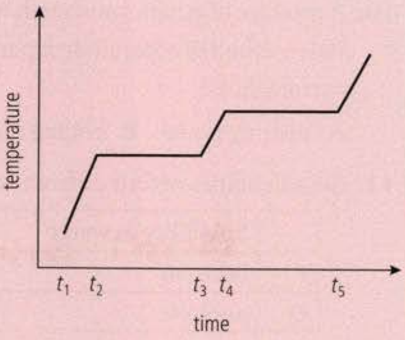
During which interval does the energy of the substance increase the most?

A t_1 to t_2

B t_2 to t_3

C t_3 to t_4

D t_4 to t_5



6. An ice cube of mass 10.0 g with a temperature of 0 °C is placed into a glass containing 90 cm^3 of water at 10 °C.

After 5 minutes some of the ice has melted. What is the temperature of the ice remaining?

A 0 °C **B** 0.5 °C **C** 2.0 °C **D** 5 °C

7. Identify the pair of substances that can form a homogeneous mixture.

A olive oil and vinegar **B** sand and water

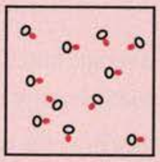
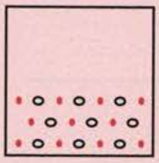
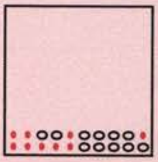
C carbon dioxide and water **D** salt and pepper

8. Identify the equation that represents sublimation.

A $I_2(g) \rightarrow 2I(g)$ **B** $I_2(s) \rightarrow I_2(g)$

C $I_2(s) + I^-(aq) \rightarrow I_3^-(aq)$ **D** $2Al(s) + 3I_2(s) \rightarrow 2AlI_3(s)$

9. Which descriptions are consistent with the diagram?

	Diagram	**Description**
I.		A compound in the gaseous state.
II.		A compound in the liquid state.
III.		A heterogeneous mixture in the solid state.

A I and II only **B** I and III only **C** II and III only **D** I, II and III

10. A mixture of ethanol and methanol can be separated by fractional distillation. This method of separation depends on the difference of which property of the two alcohols?

A melting point **B** boiling point **C** solubility **D** density

11. The solubilities of four different substances in water and ethanol are given.

	Solubility in water	Solubility in ethanol
P	insoluble	insoluble
Q	insoluble	soluble
R	soluble	insoluble
S	soluble	soluble

Some mixtures can be separated by solvation and filtration using water or ethanol as solvents.

Method I uses water as the solvent.

Method II uses ethanol as the solvent.

Which substances can be separated from each other using both methods?

A P and S **B** Q and S **C** R and S **D** Q and P

12. Classify the following mixtures as homogeneous or heterogeneous:

(a) smoke **(b)** sugar and water **(c)** steel (3)

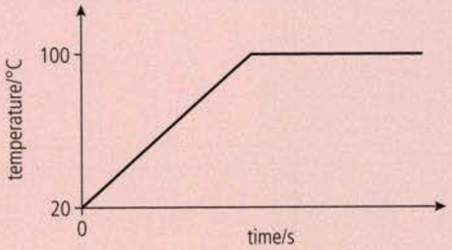
(Total 3 marks)

13. During very cold weather, snow often gradually disappears without melting. Explain how this is possible.

14. **(a)** Describe **two** differences, in terms of particle structure, between a gas and a liquid. (2)

(b) The temperature of a gas is a measure of the average kinetic energy of the gas particles. Suggest why the **average** kinetic energy is specified. (2)

(c) A sample of water was heated. The graph shows how the temperature of the water varied with time.



(i) State why the temperature initially increases. (1)

(ii) State why the temperature remains constant at 100 °C. (2)

(Total 7 marks)

15. **(a)** The physical properties of some halogens are shown in the table.

Element	**Molecular formula**	**Melting point / °C**	**Boiling point / °C**
fluorine	F_2	−220	−188
chlorine	Cl_2	−101	−35
bromine	Br_2		58.8
iodine	I_2	114	184

Predict the melting point of bromine. (1)

(b) Describe the trend in the boiling points of the halogens down the group. (1)

(c) Predict the physical state of iodine at 200 °C. (1)

(d) A simplified diagram of the structure for bromine is shown.

(i) Suggest the state of bromine with this structure and justify your answer. (2)

(ii) Describe the changes that occur to this arrangement when bromine is heated. (2)

(iii) Describe the changes that occur when bromine reacts. (1)

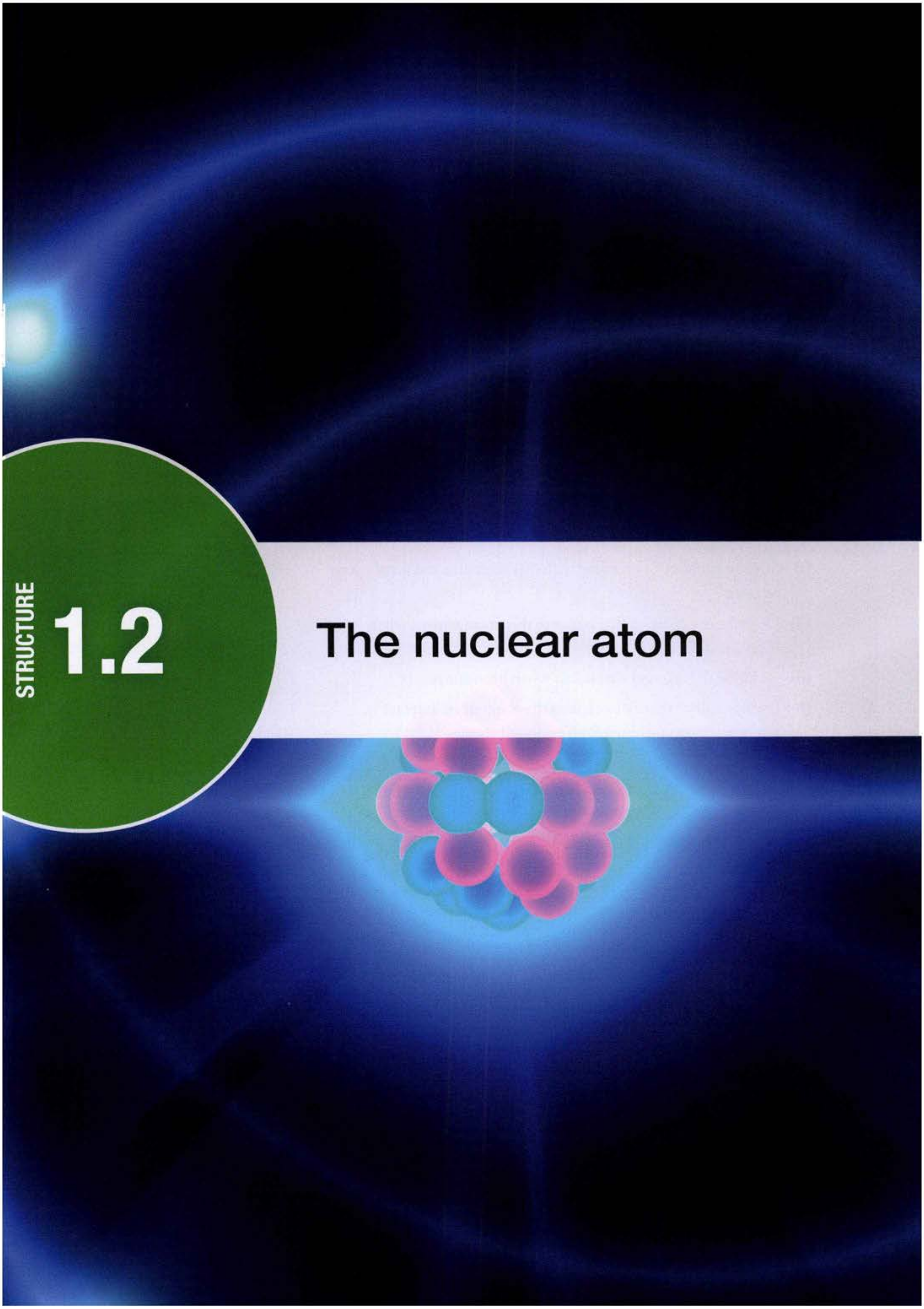
(iv) Use the kinetic theory to explain the effect of an increase in temperature on the rate of diffusion of bromine. (1)

(Total 9 marks)

STRUCTURE

1.2

The nuclear atom



The atomic nucleus is at the centre of the atom. The number of protons in the nucleus gives the atom its identity.

Guiding Question

How do the nuclei of atoms differ?

We saw in Structure 1.1 that all matter is built from no more than about 100 elements. The smallest amount of an element that can exist is an atom, which is the smallest particle of an element to show the element's characteristic properties. It is amazing that particles as small as the atom can have such a huge impact on the universe. Almost all explanations in chemistry refer to the atom, either individually or in the groups we call molecules.

In this chapter we will explore the structure of atoms in more detail. Although the word 'atom' means uncuttable, the atom *can* be split into smaller subatomic particles. All atoms are made from the same basic ingredients: protons, neutrons and electrons, but differ in their composition. If you look at the periodic table, you will see that each element has an atomic number. This was originally used to give the relative position of the element in the table. For example, the first element, hydrogen, has an atomic number of 1. We now know that this number is more fundamental than just a ranking. The atomic number is the defining property of an element as it is the number of protons in the nucleus of the atom.

Although the nucleus is only a small part of the atom, you can think of it as the atom's control centre. As an atom has a neutral charge, the number of protons also determines the number of electrons. The number of protons gives an atom its identity and the number of electrons determines its chemical properties. The mass of an element's atoms can vary due to a difference in the number of neutrons in the nucleus, but this has little impact on the chemistry of the atom. The number of neutrons does, however, affect some physical properties, including the nuclear stability.

TOK Richard Feynman: '... if all of scientific knowledge were to be destroyed, and only one sentence passed on to the next generation of creatures, what statement would contain the most information in the fewest words? I believe it is the atomic hypothesis... that *all things are made of atoms.*'
Are the models and theories that scientists create accurate descriptions of the natural world, or are they primarily useful interpretations for prediction, explanation, and control of the natural world?

Structure 1.2.1 – The atomic model

Structure 1.2.1 – Atoms contain a positively charged, dense nucleus composed of protons and neutrons (nucleons). Negatively charged electrons occupy the space outside the nucleus.

Use the nuclear symbol $({}^{A}_{Z}X)$ to deduce the number of protons, neutrons and electrons in atoms and ions.

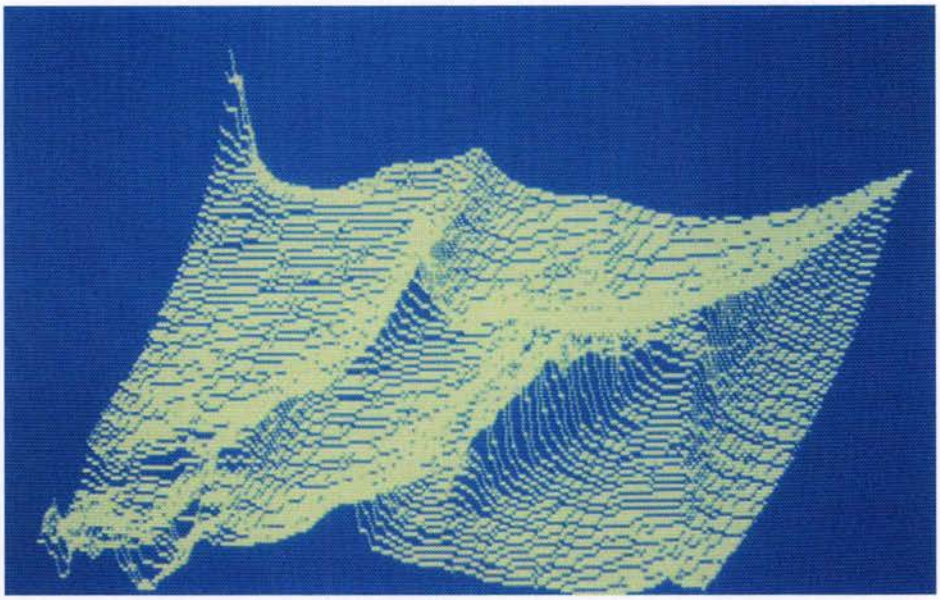
Relative masses and charges of the subatomic particles should be known; actual values are given in the data booklet. The mass of the electron can be considered negligible.	Structure 1.3 – What determines the different chemical properties of atoms? Structure 3.1 – How does the atomic number relate to the position of an element in the periodic table?

Atoms contain a positively charged, dense nucleus

Dalton's model of the atom

One of the first great achievements of chemistry was to show that all matter is built from about 100 **elements.** As mentioned in Structure 1.1, the elements are substances which cannot be broken down into simpler components by chemical reactions. Different elements have different chemical properties but gold foil, for example, reacts in essentially the same way as a single piece of gold dust. Indeed, if the gold dust is cut into smaller and smaller pieces, the chemical properties would remain the same until we reached an **atom**. The atom is the smallest unit of an element. There are only 92 elements which occur naturally on Earth, and they are made up of only 92 different types of atom. (This statement will be qualified when isotopes are discussed later in the chapter.)

The word 'atom' comes from the Greek words for 'not able to be cut'.



Scanning tunnelling microscope (STM) image of the surface of pure gold. STM imaging records the surface structure at the level of the individual atoms. Gold exists in many forms, but all the forms contain the same type of atoms. The 'rolling hills' structure seen here is the result of changes in the surface energy as the gold cooled from its molten state.

Nature of Science

The idea that matter is made up of elements and atoms dates back to the 4th century BCE. This was speculative as there was little evidence to support the idea. Scientists adopt a sceptical attitude to claims and evaluate them using evidence. A significant development for chemistry came with the publication of Robert Boyle's *Sceptical Chymist* in 1661 which emphasized the need for scientific knowledge to be justified by evidence from practical investigations. Boyle was the first person to propose the modern concept of an element as a substance which cannot be changed into anything simpler.

The modern idea of the atom dates from the beginning of the 19th century. John Dalton noticed that the elements hydrogen and oxygen always combined in fixed proportions. To explain this observation, he proposed that:

- all matter is composed of tiny indivisible particles called atoms
- atoms cannot be created or destroyed
- atoms of the same element are alike in every way
- atoms of different elements are different
- atoms can combine together in small numbers to form **molecules**.

Using this model, we can understand how elements react together to make **compounds**. The compound water, for example, is formed when two hydrogen atoms combine with one oxygen atom to produce one water molecule. If we repeat the reaction on a larger scale with $2 \times 6.02 \times 10^{23}$ atoms of hydrogen and 6.02×10^{23} atoms of oxygen, then 6.02×10^{23} molecules of water will be formed. This leads to the conclusion (see Structure 1.4) that 2.02 g of hydrogen will react with 16.00 g of oxygen to form 18.02 g of water. This is one of the observations Dalton was trying to explain.

Nature of Science

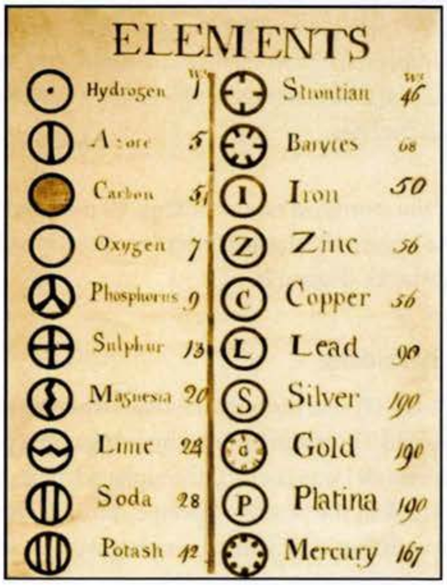
Dalton was a man of regular habits. 'For fifty-seven years… he measured the rainfall, the temperature… Of all that mass of data, nothing whatever came. But of the one searching, almost childlike, question about the weights that enter the construction of simple molecules – out of that came modern atomic theory. That is the essence of science: ask an impertinent question: and you are on the way to the pertinent answer.' (J. Bronowski).

TOK

'What we observe is not nature itself but nature exposed to our mode of questioning.' (Werner Heisenberg).

How does the knowledge we gain about the natural world depend on the questions we ask and the experiments we perform?

Dalton was the first person to assign chemical symbols to the different elements.



ELEMENTS

	Wt		Wt
Hydrogen	1	Strontian	46
Azote	5	Barytes	68
Carbon	5	Iron	50
Oxygen	7	Zinc	56
Phosphorus	9	Copper	56
Sulphur	13	Lead	90
Magnesia	20	Silver	190
Lime	24	Gold	190
Soda	28	Platina	190
Potash	42	Mercury	167

John Dalton's symbols for the elements.

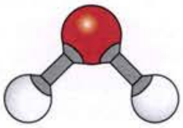
Challenge yourself

1. It is now known that some of these substances are not elements but compounds. Lime, for example, is a compound of calcium and oxygen. Find any other examples of compounds in this list, and explain why the component elements had not been extracted at this time.

Following Dalton's example, you can write the formation of water using modern notation:

$$2H + O \rightarrow H_2O$$

But what are atoms really like? It can be useful to think of them as hard spheres (Figure 1), but this tells us little about how the atoms of different elements differ. To understand this, it is necessary to probe deeper.



S1.2 Figure 1 A model of a water molecule made from two hydrogen atoms and one oxygen atom. Dalton's picture of the atom as a hard ball is the basis behind the molecular models we use today.

Nature of Science

Dalton's atomic theory was not accepted when it was first proposed. Many scientists considered it as nothing more than a useful fiction which should not be taken too seriously. Over time, as the supporting evidence grew, this changed to its widespread acceptance. These revolutions in understanding, or '**paradigm shifts**', are characteristic of the evolution of scientific thinking.

TOK

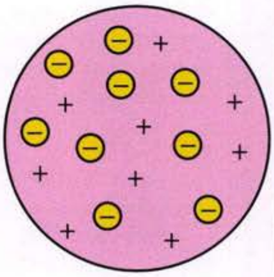
One of the barriers to the acceptance of Dalton's model of the atom was opposition from leading scientists such as Kelvin. In what ways can influential individuals help or hinder the development of scientific knowledge?

Atoms contain electrons

The first indication that atoms were destructible came at the end of the 19th century when the British scientist J. J. Thomson discovered that different metals produce a stream of negatively charged particles when a high voltage is applied across two electrodes. As these particles, which we now know as **electrons**, were the same regardless of the metal, he suggested that they are part of the make-up of all atoms.

Nature of Science

The properties of electrons, or cathode rays as they were first called, could only be investigated once powerful vacuum pumps had been invented – and once advances had been made in the use and understanding of electricity and magnetism. Improved instrumentation and new technology are often the drivers for new discoveries.



▲ **S1.2 Figure 2** Thomson's 'plum pudding' model of the atom. The negatively charged electrons (yellow) are positioned in a positively charged sponge-like substance (pink).

As Thomson knew that the atom had no net charge, he pictured the atom as a 'plum pudding', with the negatively charged electrons positioned in a positively charged sponge-like substance (Figure 2).

Atoms contain a nucleus

Ernest Rutherford (1871–1937) and his research team working at Manchester University in England, tested Thomson's model by firing alpha particles at a piece of gold foil. If Thomson's model was correct, the alpha particles should either pass straight through or get stuck in the positive 'sponge'. Most of the alpha particles did indeed pass straight through, but a very small number were repelled.

TOK

When Rutherford's team reported that they had seen a small number of alpha particles deflected by small angles, he asked them to see if any of the alpha particles had bounced back. This was a very unusual suggestion to make at the time, with little logical justification. What is the role of intuition in the pursuit of scientific knowledge?

The large number of undeflected particles led Rutherford to the conclusion that the atom is mainly empty space. Large deflections occur when the positively charged alpha particles collide with, and are repelled by, a positively charged nucleus. The fact that only a small number of alpha particles bounce back suggests that the nucleus is very small.

Nature of Science

Our knowledge of the nuclear atom came from Rutherford's experiments with the relatively newly discovered alpha particles. Progress in science often follows technological developments that allow new experimental techniques.

Nature of Science

Rutherford used his model of a positively charged nucleus to derive an equation for the scattering pattern of the alpha particles. His derivation assumed that only electrostatic repulsive forces acted between the positive gold nucleus and the positive alpha particles. All models have limitations which need to be considered in their application.

Challenge yourself

2. The derivation of the Rutherford formula is based on the assumption that only electrostatic forces need to be considered during the scattering process. Suggest why the experimental results deviate from this model for high-energy alpha particles.

Subatomic particles

A hundred years or so after Dalton first proposed his model, further experiments showed that the nucleus of an atom is made up of **protons** and **neutrons,** collectively called **nucleons.** Protons and neutrons have almost the same mass and together account for most of the mass of the atom. Electrons, which have a charge equal and opposite to that of the proton, have generally negligible mass and occupy the space in the atom outside of the nucleus.

The absolute masses and charges of these fundamental particles are given in Section 2 of the data booklet and this table gives their relative masses and charges. Note that relative quantities are ratios and so have no units.

Subatomic particle	Relative mass	Relative charge
proton	1	+1
electron	0.0005	−1
neutron	1	0

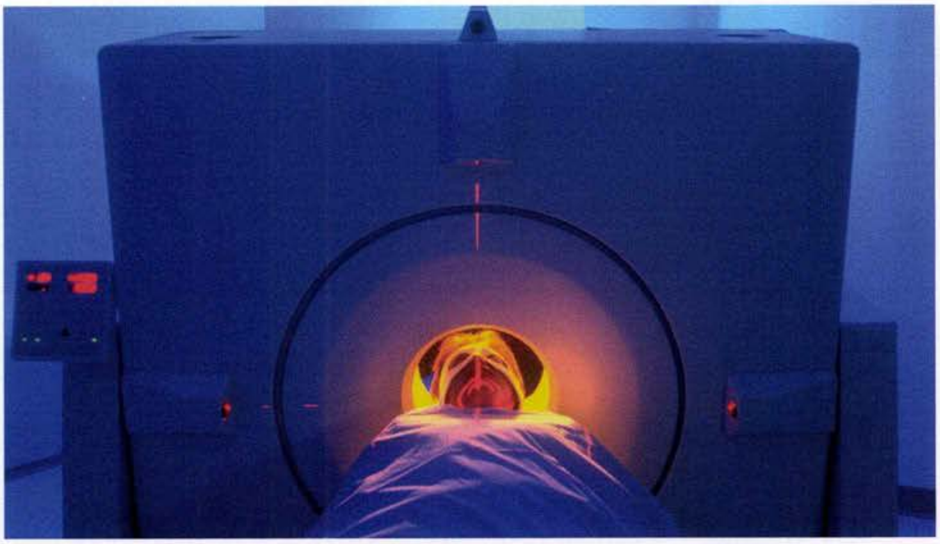
You should know the relative masses and charges of the subatomic particles. Actual values are given in the data booklet. The mass of the electron can generally be considered to be negligible.

Nature of Science

The description of subatomic particles given here is sufficient to understand chemistry but it is incomplete. Although the electron is indeed a fundamental particle, we now know that protons and neutrons are both themselves made up of more fundamental particles called quarks. We also know that all particles have anti-particles. The positron is the anti-particle of an electron; it has the same mass but has an equal and opposite positive charge. When particles and anti-particles collide, they destroy each other and release energy in the form of high-energy **photons** called gamma rays. Our treatment of subatomic particles is in line with the principle of Occam's razor, which states that theories should be as simple as possible while maximizing explanatory power.

PET (positron-emission tomography) scanners give three-dimensional images of tracer concentration in the body, and can be used to detect cancers. The patient is injected with a tracer compound labelled with a positron-emitting isotope. The positrons collide with electrons after travelling a short distance (≈1 mm) within the body. Both particles are destroyed, and two photons are produced. The protons can be collected by the detectors surrounding the patient, and used to generate an image.

As you are made from atoms, you are also mainly empty space. The particles which make up your mass would occupy the same volume as a flea if they were all squashed together, but a flea with your mass. This gives you an idea of the density of the nucleus.



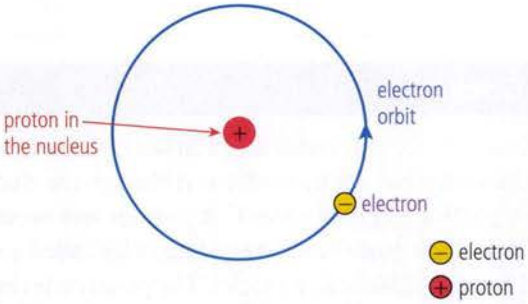
▲ A patient undergoing a positron-emission tomography (PET) brain scan. A radioactive tracer is injected into the patient's bloodstream, which is then absorbed by active tissues of the brain. The PET scanner detects photons emitted by the tracer and produces 'slice' images.

Challenge yourself

3. Construct an equation for the collision of an electron and a positron to give two photons and explain why it is balanced.

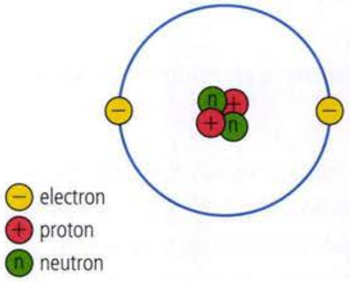
Bohr model of the hydrogen atom

The Danish physicist Niels Bohr pictured the hydrogen atom as a small 'solar system', with an electron moving in an orbit (energy level) around the positively charged nucleus of one proton (Figure 3). The electrostatic force of attraction between the oppositely charged subatomic particles prevents the electron from leaving the atom. The nuclear radius is 10^{-15} m and the atomic radius 10^{-10} m, so most of the volume of the atom is empty space.



▲ **S1.2 Figure 3** The Bohr model of the simplest atom. Only one proton and one electron make up the hydrogen atom. Most of the volume of the atom is empty – the only occupant is the single negatively charged electron. It is useful to think of the electron orbiting the nucleus in a similar way to the planets orbiting the Sun. The absence of a neutron is significant – it would be essentially redundant as there is only one proton.

The existence of neutrally charged neutrons is crucial for the stability of nuclei of elements that have more than one proton (Figure 4). Without the neutrons, the positively charged protons would mutually repel each other and the nucleus would fall apart.



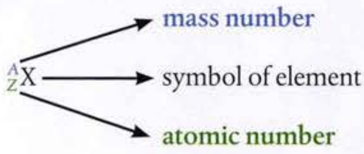
S1.2 Figure 4 The Bohr model of a helium atom. The two neutrons allow the two protons, which repel each other, to stay in the nucleus. A strong nuclear force acts between all the nucleons which is larger than the repulsive electrostatic forces that act between the protons.

Atomic number and mass number

We are now in a position to understand how the atoms of different elements differ. They are all made from the same basic ingredients, the subatomic particles. The only difference is the recipe – how many of each of these subatomic particles are present in the atoms of different elements. If you look at the periodic table, you will see that the elements are each given a number which describes their relative position in the table. This is their **atomic number**. We now know that the atomic number, represented by **Z**, is the defining property of an element as it tells us something about the structure of the atoms of the element. The atomic number is defined as the number of protons in the atom.

As an atom has no overall charge, the positive charge of the protons must be balanced by the negative charge of the electrons. Therefore the atomic number is also equal to the number of electrons in an atom.

The electron has such a very small mass that it is essentially ignored in mass calculations. The mass of an atom depends on the number of protons and neutrons only. The **mass number**, given the symbol **A**, is defined as the number of protons plus the number of neutrons in an atom. An atom is identified in the following way:

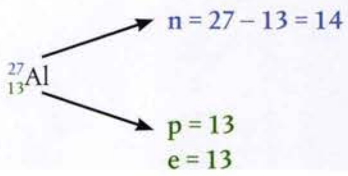


We can use these numbers to find the composition of any atom.

$$\text{number of protons (p)} = \text{number of electrons} = Z$$

$$\text{number of neutrons (n)} = \text{mass number} - \text{number of protons} = A - Z$$

Consider an atom of aluminium:



An aluminium atom has 13 protons and 13 electrons. An atom of gold on the other hand has 79 protons and 79 electrons. Can you find gold in the periodic table? The periodic table arranges the elements in order of their atomic number as discussed in Structure 3.1.

TOK

None of these subatomic particles can be (or ever will be) directly observed.

What assumptions are made when we interpret indirect evidence gained through the use of technology?

The atomic number is defined as the number of protons in the nucleus.

Make sure you have a precise understanding of the terms. The atomic number, for example, is defined in terms of the number of protons, not electrons.

The mass number (*A*) is the number of protons plus the number of neutrons in an atom. It is sometimes called the nucleon number.

SKILLS

Build an atom PhET activity. Full details on how to carry out this activity with a worksheet are available in the eBook.

Structure 3.1 - How does the atomic number relate to the position of an element in the periodic table?

Challenge yourself

4. Explain why the 13 protons in aluminium stay in the nucleus despite their mutual repulsion.

5. Experiments show the nuclear radius R depends on the mass number A according to the expression: $R = 1.2 \times 10^{-15} A^{\frac{1}{3}}$. Deduce an expression for the density of a nucleus and comment on your result.

Worked example

Identify the subatomic particles present in an atom of ^{226}Ra.

Solution

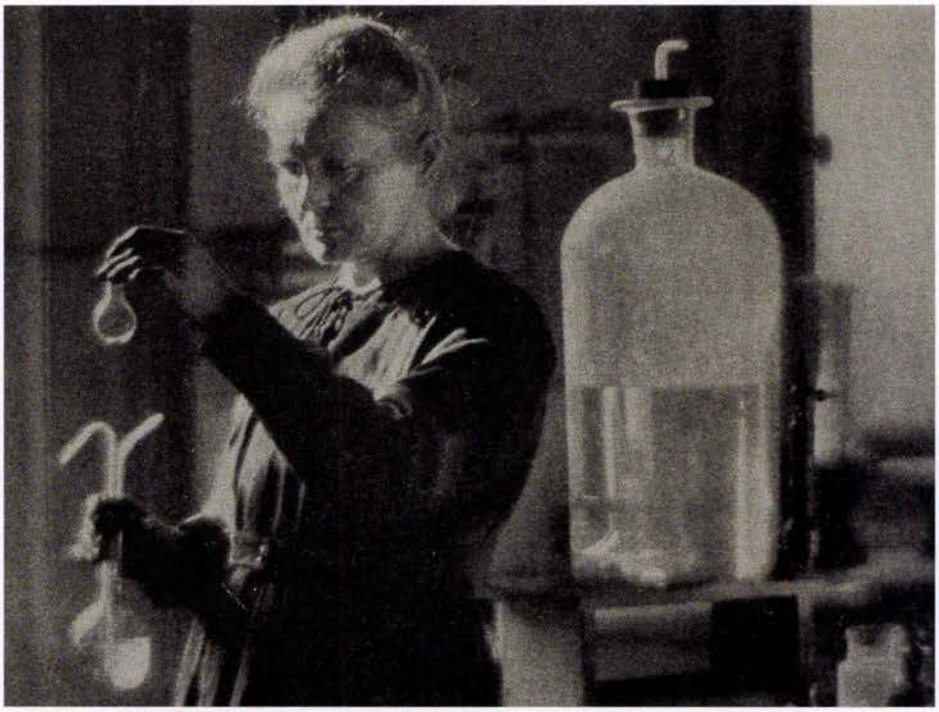
The number identifying the atom is the atomic number. We can find the atomic number from the data booklet (Section 6).

We have $Z = 88$ and $A = 226$

number of protons (p) = 88

number of electrons (e) = 88

number of neutrons (n) = 226 − 88 = 138



The element radium was first discovered by the Polish-French scientist Marie Curie. She is the only person to win Nobel Prizes in both Physics and Chemistry. The Curies were a remarkable family for scientific honours – Marie shared her first prize with her husband Pierre, and her daughter Irène shared hers with her husband Frédéric. All the Curies' prizes were for work on radioactivity.

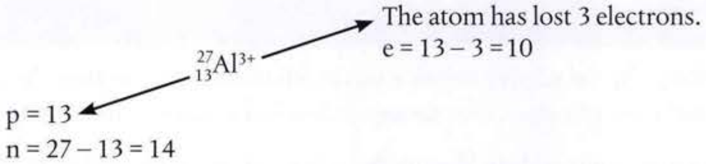
Ions

The atomic number is defined in terms of the number of protons because it is a fixed characteristic of the element. The number of protons identifies the element in the same way your fingerprints identify you. The number of protons and neutrons never changes during a chemical reaction. It is the electrons which are responsible for chemical change. Structure 2.1 examines how atoms can lose or gain electrons to form **ions**. When the number of protons in a particle is no longer balanced by the number of electrons, the particle has a non-zero charge. When an atom loses electrons, it forms a positive ion or **cation**, as the number of protons is now greater than the number of electrons. Negative ions or **anions** are formed when atoms gain electrons. The magnitude of the charge depends on the number of electrons lost or gained. The loss or gain of electrons makes a very big difference to the chemical properties. You swallow sodium ions, Na^+, every time you eat table salt, whereas (as covered in Structure 3.1) sodium atoms, Na, are dangerously reactive.

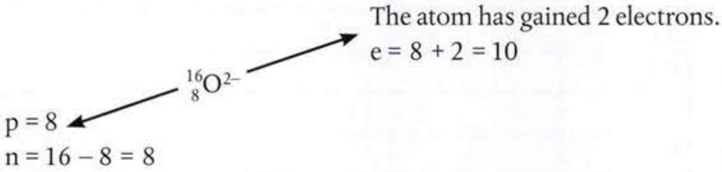
When an atom loses electrons, a positive ion is formed and when an atom gains electrons, a negative ion is formed. Positive ions are called cations and negative ions are called anions.

Structure 1.3 – What determines the different chemical properties of atoms?

An aluminium ion is formed when the atom loses three electrons. There is no change in the atomic or mass numbers of an ion because the number of protons and neutrons remains the same.



Oxygen forms the oxide ion when its atoms gain two electrons.



Worked example

Most nutrient elements in food are present in the form of ions. The calcium ion $^{40}Ca^{2+}$, for example, is essential for healthy teeth and bones. Identify the subatomic particles present in the ion.

Solution

We can find the atomic number from the data booklet (Section 6).
We have Z = 20 and A = 40:

- number of protons (p) = 20
- number of neutrons (n) = 40 – 20 = 20

As the ion has a positive charge of 2+ there are two more protons than electrons:

- number of electrons = 20 – 2 = 18

Worked example

Identify the species with 19 protons, 20 neutrons and 18 electrons.

Solution

- the number of protons tells us the atomic number, $Z = 19$, and so the element is potassium, K
- the mass number = p + n = 19 + 20 = 39: ${}^{39}_{19}\text{K}$
- the charge = p – e = 19 – 18 = +1 as there is one extra proton: ${}^{39}_{19}\text{K}^+$

Challenge yourself

6. We generally make the approximation that the mass of an ion is the same as that of the corresponding atom. To how many significant figures is this approximation valid for the H^+ ion?

Exercise

Q1. Explain why the relative atomic mass of tellurium is greater than the relative atomic mass of iodine, even though iodine has a greater atomic number.

Q2. Use the periodic table to identify the subatomic particles present in the following species.

	Species	No. of protons	No. of neutrons	No. of electrons
(a)	${}^{7}\text{Li}$			
(b)	${}^{1}\text{H}$			
(c)	${}^{14}\text{C}$			
(d)	${}^{19}\text{F}^-$			
(e)	${}^{56}\text{Fe}^{3+}$			

Q3. Isoelectronic species have the same number of electrons. Identify the following isoelectronic species by giving the correct symbol and charge. You will need a periodic table.

The first one has been done as an example.

	Species	No. of protons	No. of neutrons	No. of electrons
	${}^{40}\text{Ca}^{2+}$	20	20	18
(a)		18	22	18
(b)		19	20	18
(c)		17	18	18

Q4. What is the difference between two neutral atoms represented by the symbols ${}^{14}_{6}\text{C}$ and ${}^{14}_{7}\text{N}$?

I. the number of neutrons II. the number of protons
III. the number of electrons

A I and II only **B** I and III only **C** II and III only **D** I, II and III

Structure 1.2.2 – Isotopes

Structure 1.2.2 – Isotopes are atoms of the same element with different numbers of neutrons.

Perform calculations involving non-integer relative atomic masses and abundance of isotopes from given data.

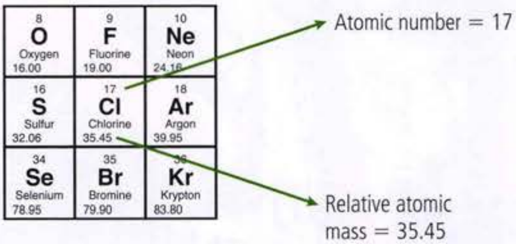
Differences in the physical properties of isotopes should be understood. Specific examples of isotopes need not be learned.	Nature of Science, Reactivity 3.4 – How can isotope tracers provide evidence for a reaction mechanism?

Isotopes are atoms of the same element with different numbers of neutrons

SKILLS

Modelling isotopic abundance. Full details on how to carry out this experiment with a worksheet are available in the eBook.

Find chlorine in the periodic table. There are two numbers associated with the element, as shown below.



How can an element have a fractional relative atomic mass if protons and neutrons each have a relative mass of 1? One reason is that atoms of the same element with different mass numbers exist, and the relative atomic mass given in the periodic table is an average value.

To have different mass numbers, the atoms must have different numbers of neutrons – all the atoms have the same number of protons as they are all chlorine atoms. Atoms of the same element with different numbers of neutrons are called **isotopes**.

Isotopes are atoms of the same element with different mass numbers.

The isotopes show the same chemical properties, as a difference in the number of neutrons makes no difference to how atoms react and so they occupy the same place in the periodic table.

The word 'isotope' derives from the Greek for 'same place'. As isotopes are atoms of the same element, they occupy the same place in the periodic table.

Chlorine exists as two isotopes, $\boxed{^{35}_{17}\text{Cl}}$ and $\boxed{^{37}_{17}\text{Cl}}$. The average relative mass of the isotopes is, however, not 36, but 35.45. This value is closer to 35 as there are more $^{35}_{17}\text{Cl}$ atoms in nature – it is the more *abundant* isotope. In a sample of 1000 chlorine atoms, there are 775 atoms of $^{35}_{17}\text{Cl}$ and 225 atoms of the heavier isotope, $^{37}_{17}\text{Cl}$.

To work out the average mass of one atom, we first have to calculate the total mass of the thousand atoms:

$$\text{total mass} = (775 \times 35) + (225 \times 37) = 35450$$

$$\text{relative average mass} = \frac{\text{(total mass)}}{\text{(number of atoms)}} = \frac{35450}{1000} = 35.45$$

A common error is to misunderstand the meaning of 'physical property'. A difference in the number of neutrons is not a different physical property. A physical property of a substance can be measured without changing the chemical composition of the substance. Density and boiling point are examples of physical properties.

Uranium consists of two natural isotopes: mostly U-238 and less than 1% U-235. The fuel used in nuclear power stations is U-235; its content needs to be increased to around 3-5% of the overall mixture to make a controlled nuclear fission reaction feasible. The enrichment can be carried out by gas diffusion, by heating solid uranium hexafluoride (UF_6). The UF_6 molecules containing U-235 are lighter and diffuse faster through the pipelines and filters, producing a UF_6 gas that is enriched with U-235.

Nature of Science, Reactivity 3.4 - How can isotope tracers provide evidence for a reaction mechanism?

The two isotopes are both atoms of chlorine with 17 protons and 17 electrons.

- $\boxed{^{35}_{17}\text{Cl}}$ number of neutrons = 35 – 17 = 18
- $\boxed{^{37}_{17}\text{Cl}}$ number of neutrons = 37 – 17 = 20

Although both isotopes essentially have the same chemical properties, the difference in mass does lead to different physical properties such as boiling and melting points. As explained in Structure 1.1, heavier particles move more slowly at a given temperature and these differences can be used to separate isotopes.

▲ Gas diffusion machinery in southern France used to enrich uranium for use in nuclear reactors.

Challenge yourself

7. Suggest why isotope nuclear enrichment plants based on gaseous diffusion are so large.

The stability of a nucleus depends on the balance between the number of protons and neutrons. A nucleus which contains either too many or too few neutrons to be stable is radioactive and changes to a more stable nucleus by giving out radiation. As these **radioisotopes** behave chemically in the same way as nonradioactive isotopes, they can be used as tracers to follow the movement of elements or compounds in complex processes such as living systems. The radioisotopes can be located because the radioactivity they emit can be detected. Radioactive isotopes can also provide evidence for the reaction mechanisms explored in Reactivity 3.4.

Human activities have caused increased atmospheric nitrogen pollution, mainly nitrogen oxides and ammonia. This nitrogen is eventually taken up by plants, increasing plant growth. Evidence for this comes from experiments using tracer isotopes of nitrogen ($^{15}_{7}N$) to follow the nitrogen through the air and plants.

▲
Evidence for increased nitrogen pollution comes from experiments using tracer isotopes of nitrogen ($^{15}_{7}N$) in plants.

Challenge yourself

8. Use the periodic table in the data booklet to identify an element with an atomic number of less than 80 which has no stable isotopes.

Exercise

Q5. State two physical properties other than boiling point and melting point that would differ for the two isotopes of chlorine.

Q6. Identify the particles which account for the existence of isotopes.

A electrons **B** nucleons **C** neutrons **D** protons

Q7. Which of the following species contains more electrons than neutrons?

A $^{2}_{1}H$ **B** $^{11}_{5}B$ **C** $^{16}_{8}O^{2-}$ **D** $^{19}_{9}F^{-}$

Q8. Which of the following gives the correct composition of the $^{71}Ga^{+}$ ion?

	Protons	**Neutrons**	**Electrons**
A	31	71	30
B	31	40	30
C	31	40	32
D	32	40	31

Q9. Chromium has an atomic number of 24. The mass numbers of its four stable isotopes are 50, 52, 53 and 54.

Identify the correct statements about the isotopes.

I. All the isotopes have the same chemical properties.
II. All the isotopes have nuclei containing 24 protons.
III. One of the isotopes has 54 neutrons.

A I and II only **B** I and III only **C** II and III only **D** I, II and III

Q10. Identify the atoms which are isotopes.

	Mass number	Atomic number
W	52	24
X	53	25
Y	53	24
Z	52	25

A W and Z **B** X and Y **C** W and Y **D** Y and Z

Q11. The relative atomic mass of silicon is 28.09. Comment on the claim that no atom of silicon exists with this relative mass.

Q12. Deduce the composition of a nucleus of boron-11, $^{11}_{5}B$.

	Protons	Neutrons
A	5	11
B	11	5
C	6	5
D	5	6

Q13. What is the same for an atom of phosphorus-26 and an atom of phosphorus-27?

A atomic number and mass number
B number of protons and electrons
C number of neutrons and electrons
D number of protons and neutrons

HL

Structure 1.2.3 – Mass spectra

Structure 1.2.3 – Mass spectra are used to determine the relative atomic masses of elements from their isotopic composition.

Interpret mass spectra in terms of identity and relative abundance of isotopes.

The operational details of the mass spectrometer will not be assessed.	Structure 3.2 – How does the fragmentation pattern of a compound in the mass spectrometer help in the determination of its structure?

Mass spectra are used to determine the relative atomic masses of elements from their isotopic composition

The mass spectrometer can measure the mass and abundance of isotopes

The masses of the different isotopes and their relative abundance can be measured using a mass spectrometer.

The element to be tested is first vaporized so that individual atoms can be analysed. The atoms are then ionized by high-energy electrons which knock out an electron to produce a positively charged ion:

$$X(g) + e^- \rightarrow X^+(g) + 2e^-$$

The positively charged ions are attracted to a negatively charged plate and deflected by a magnetic field placed at right angles to their path. The amount of deflection is inversely proportional to their **mass/charge** (m/z) ratio. This is equivalent to the mass when the ions have a single positive charge. Single-charge ions with smaller mass are deflected more than heavier ions with the same charge.

If a compound is analysed in a mass spectrometer, the electron collisions during the ionization step are so energetic that they can cause the molecule to break up into different fragments. The resulting **fragmentation pattern** provides useful evidence about the structure of the compound. A chemist pieces together the fragments to form a picture of the complete molecule, in the same way that archaeologists find clues about the past from the pieces of artefacts discovered in the ground. Fragmentation patterns are explored more fully in Structure 3.2.

Structure 3.2 - How does the fragmentation pattern of a compound in the mass spectrometer help in the determination of its structure?

You will not be assessed on the operational details of the mass spectrometer but you should include the positive charge when identifying the ions in a mass spectrum.

The relative atomic mass of an element

The mass of a hydrogen atom is 1.67×10^{-24} g and that of a carbon atom is 1.99×10^{-23} g. As the masses of all elements are in the range 10^{-24} to 10^{-22} g, and as these numbers are beyond our direct experience, it makes more sense to use relative values. The mass needs to be recorded relative to some agreed standard. As carbon is a very common element which is easy to transport and store because it is a solid, its isotope, ^{12}C, was chosen as the standard in 1961. This is discussed in Structure 1.4 and ^{12}C is given a relative mass of exactly 12, as shown below.

Element	**Symbol**	**Relative atomic mass**
carbon	C	12.011
chlorine	Cl	35.453
hydrogen	H	1.008
iron	Fe	55.845
Standard isotope	**Symbol**	**Relative atomic mass**
carbon-12	^{12}C	12.000

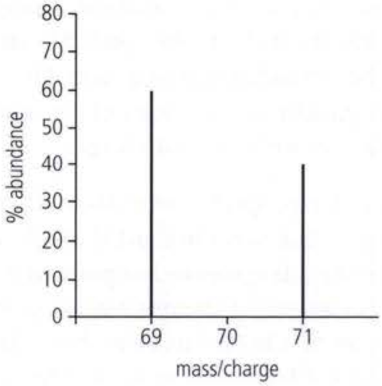
The relative atomic mass of an element (A_r) is the average mass of an atom of the element, taking into account all its isotopes and their relative abundance, compared to one atom of carbon-12.

Carbon-12 is the most abundant isotope of carbon but carbon-13 and carbon-14 also exist. This explains why the average value for the element is greater than 12.

Mass spectra

The results of the analysis by a mass spectrometer are presented in the form of a **mass spectrum**. As discussed earlier, the mass spectrometer measures the mass/charge ratio of the deflected particles and this is displayed on the horizontal axis using the carbon-12 scale. In most cases the charge of the ion is +1 so the horizontal axis generally also gives the mass. The relative abundance of the ions corresponding to different isotopes is shown on the vertical axis.

The mass spectrum of gallium in Figure 5 shows that in a sample of 100 atoms, 60 have a mass of 69 and 40 have a mass of 71. We can use this information to calculate the relative atomic mass of the element.



▲

S1.2 Figure 5 Mass spectrum for gallium. The number of lines indicates the number of isotopes (two in this case), the value on the *x*-axis indicates their mass numbers (69 and 71) and the *y*-axis shows the percentage abundance.

$$\text{total mass of 100 atoms} = (60 \times 69) + (40 \times 71) = 6980$$

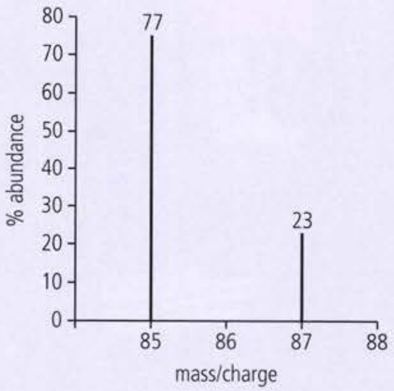
$$\text{relative average mass} = \frac{\text{total mass}}{\text{number of atoms}} = \frac{6980}{100} = 69.80$$

Challenge yourself

9. Suggest how the mass spectrum of gallium changes if the kinetic energy of the electrons used in ionizing the sample in a mass spectrometer is significantly increased.

Worked example

Deduce the relative atomic mass of the element rubidium from the data given in the graph.



Solution

Consider a sample of 100 atoms.

$$\text{total mass of 100 atoms} = (85 \times 77) + (87 \times 23) = 8546$$

$$\text{relative atomic mass} = \text{average mass of atom} = \frac{\text{total mass}}{\text{number of atoms}} = \frac{8546}{100} = 85.46$$

Worked example

Boron exists as two isotopes, ^{10}B and ^{11}B. ^{10}B is used as a control for nuclear reactors. Use your periodic table to find the abundances of the two isotopes.

Solution

Consider a sample of 100 atoms.

Let x atoms be ^{10}B atoms. The remaining atoms are ^{11}B.

number of ^{11}B atoms $= 100 - x$

total mass of 100 atoms $= [x \times 10] + [(100 - x) \times 11] = 10x + 1100 - 11x = 1100 - x$

$$\text{average mass} = \frac{\text{total mass}}{\text{number of atoms}} = \frac{1100 - x}{100}$$

From the periodic table, the relative atomic mass of boron = 10.81.

$$10.81 = \frac{1100 - x}{100}$$

$1081 = 1100 - x$

$x = 1100 - 1081 = 19$

The abundances are $^{10}B = 19\%$ and $^{11}B = (100 - 19) = 81\%$

A mass spectrometer used in radiocarbon dating. The ratio of radioactive ^{14}C to stable ^{12}C is related to the time since the death of the animal or plant being investigated.

Carbon-14 has eight neutrons, which is too many to be stable. It can reduce the neutron-to-proton ratio by radioactive decay. The relative abundance of carbon-14 present in living plants is constant as the carbon atoms are continually replenished from the carbon present in atmospheric carbon dioxide. When organisms die, however, no more carbon-14 is absorbed and the levels of carbon-14 fall as they decay. As this process occurs at a regular rate, it can be used to date carbon-containing materials.

Exercise

Q14. A sample of chromium has the following isotopic composition by mass.

Isotope	^{50}Cr	^{52}Cr	^{53}Cr	^{54}Cr
Relative abundance / %	4.31	83.76	9.55	2.38

Calculate the relative atomic mass of chromium based on these data, giving your answer to two decimal places.

Q15. Use the periodic table to find the percentage abundance of neon-20, if neon has only one other isotope, neon-22.

Q16. Magnesium has three stable isotopes: ^{24}Mg, ^{25}Mg, and ^{26}Mg. The lightest isotope has an abundance of 78.90%. Calculate the percentage abundance of the other isotopes.

Q17. The relative abundances of the two isotopes of chlorine are shown in this table:

Isotope	**Relative abundance**
^{35}Cl	75%
^{37}Cl	25%

Use this information to deduce the mass spectrum of chlorine gas, Cl_2.

In 1911, a 40 kg meteorite fell in Egypt. Isotopic and chemical analyses of oxygen extracted from this meteorite showed a different relative atomic mass to that of oxygen normally found on Earth. The relative atomic mass value did however match measurements made of the Martian atmosphere by the Viking landing in 1976. This provides strong evidence that the meteorite had originated from Mars.

Challenge yourself

10. Oxygen atoms in water molecules from two different samples in an ice core were analysed.

	Sample 1		**Sample 2**	
isotope	^{16}O	^{18}O	^{16}O	^{18}O
relative abundance / %	99.759	0.241	99.757	0.243

Determine the relative mass of oxygen in the two samples and identify which sample originated from higher historic temperatures.

11. Bromine is a mixture of two isotopes with mass numbers 79 and 81. They are naturally present in equal amounts.

The relative abundances of the two isotopes of chlorine are ^{35}Cl (75%) and ^{37}Cl (25%).

Calculate the percentage of naturally occurring CH_2BrCl molecules with a relative molecular mass of 128.

You can assume that the carbon atoms have a mass number of 12 and the hydrogen atoms have a mass number of 1.

HL end

Guiding Question revisited

How do the nuclei of atoms differ?

In this chapter we explored the structure of the atom and how the nuclei of atoms differ.

- All atoms are made up of protons, neutrons and electrons.
- The protons and neutrons, which contribute most of the mass of the atom, are in a small dense nucleus surrounded by electrons which occupy most of the volume of the atom.
- The atomic number gives the atom its identity. This is the number of protons in the nucleus. In a neutral atom this is also the number of electrons.
- The mass number is the number of nucleons: the number of protons and neutrons in the nucleons.
- Evidence shows that most elements have more than one isotope: atoms with the same number of protons but a different number of neutrons.
- The relative atomic mass, which is the average mass of an atom, can be determined from the relative abundance of its isotopes.

HL

- The mass of individual atomic masses can be measured by a mass spectrometer.
- A mass spectrum shows the relative abundance of the different isotopes of an element.

HL end

Practice questions

1. Which statements about the isotopes of chlorine, $^{35}_{17}Cl$ and $^{37}_{17}Cl$, are correct?

   I. They have the same chemical properties.

   II. They have the same atomic number.

   III. They have the same physical properties.

   A I and II only **B** I and III only

   C II and III only **D** I, II and III

2. Which statement about the numbers of protons, electrons and neutrons in an atom is always correct?

   A The number of neutrons minus the number of electrons is zero.

   B The number of protons plus the number of neutrons equals the number of electrons.

   C The number of protons equals the number of electrons.

   D The number of neutrons equals the number of protons.

3. Which quantities are the same for all atoms of chlorine?

   I. number of protons

   II. number of neutrons

   III. number of electrons

   A I and II only **B** I and III only

   C II and III only **D** I, II and III

4. How many electrons does the ion $^{31}_{15}P^{3-}$ contain?

   A 12 **B** 15 **C** 16 **D** 18

4. Deduce the number of elementary particles present in the $^{55}_{25}Mn^{2+}$ ion. (3)

   (Total 3 marks)

6. A sample of iron has the following isotopic composition by mass.

Isotope	^{54}Fe	^{56}Fe	^{57}Fe
Relative abundance / %	5.95	91.88	2.17

   Calculate the relative atomic mass of iron based on these data, giving your answer to two decimal places. (2)

   (Total 2 marks)

7. **(a)** Explain why the relative atomic mass of cobalt is greater than the relative atomic mass of nickel, even though the atomic number of nickel is greater than the atomic number of cobalt. (1)

   (b) Deduce the numbers of protons and electrons in the Co^{2+} ion. (1)

   (Total 2 marks)

8. The table below refers to a sample of silicon.

Mass number of isotope	28	29	30
Relative abundance / %	92.18	4.70	3.12

(a) Explain why atoms of an element can have different mass numbers. (1)

(b) Compare the chemical properties of the four isotopes and justify your answer. (1)

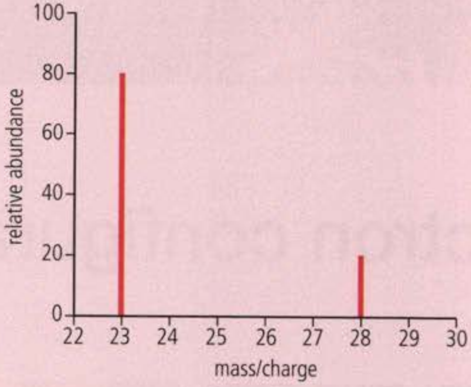
(c) HL Identify the instrument used to collect these data. (1)

(d) Calculate the relative atomic mass of this sample of silicon. (2)

(Total 5 marks)

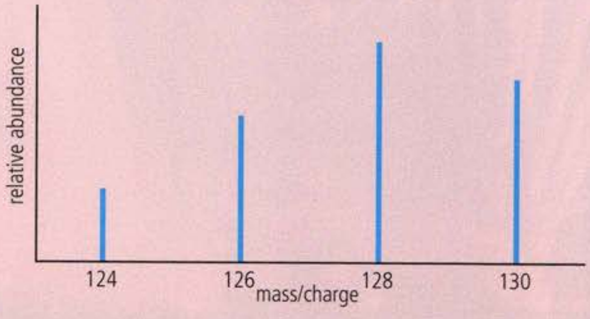
HL

9. What is the relative atomic mass of an element with the following mass spectrum?



A 24 **B** 25 **C** 26 **D** 27

10. The mass spectrum of an element is shown below.



(a) Identify the element and justify your answer. (2)

(b) Estimate the percentage of the total mass of the element due to neutrons. (2)

(Total 4 marks)

HL end

STRUCTURE

1.3

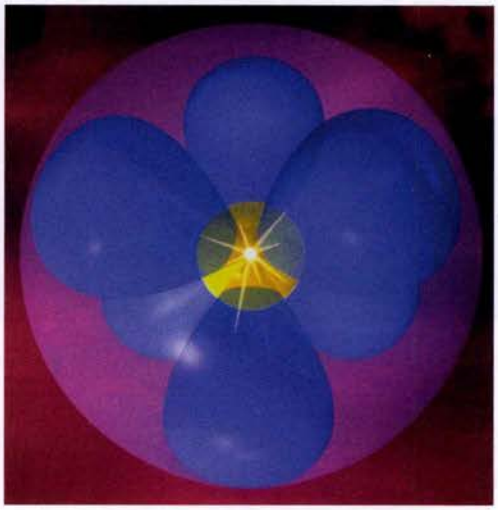
Electron configurations

The dazzling colours observed during a firework display are a result of electrons moving between different energy states.

Guiding Question

How can we model the energy states of electrons in atoms?

The chemical behaviour of an atom is determined by its electron configuration. As we cannot look inside the atom directly, we have to look elsewhere for evidence of how the electrons are arranged. The analysis of light emitted from an atom gives us valuable information about the electron configuration within it. It shows that an electron can exist only in certain discrete energy states. This cannot be understood with reference to our everyday experience and demands a new perspective. The notion of particles following fixed trajectories does not apply to the microscopic world of the atom. We can only give a probability description of electron behaviour and use quantum theory to adopt a wave description of the electron. The possible positions of an electron are spread out in space in the same way as a wave spreads through space. We will see how the energy states of electrons are best explained in terms of atomic orbitals. These are regions in space where an electron is likely to be found. Within one atom, there are an infinite number of orbitals of different shapes, sizes and energies. These ideas are revolutionary. As Niels Bohr, one of the principal scientists involved in the development of quantum theory said, 'Anyone who is not shocked by quantum theory has not understood it'.



Electrons occupy atomic orbitals of different energy states. The atomic orbitals in an atom of neon, Ne, are represented here. The nucleus is shown by a flash of light and the 1s orbital as a yellow sphere. The 2s orbital is shown as a pink sphere, and the 2p orbitals as blue lobes.

Structure 1.3.1 and 1.3.2 – Emission spectra

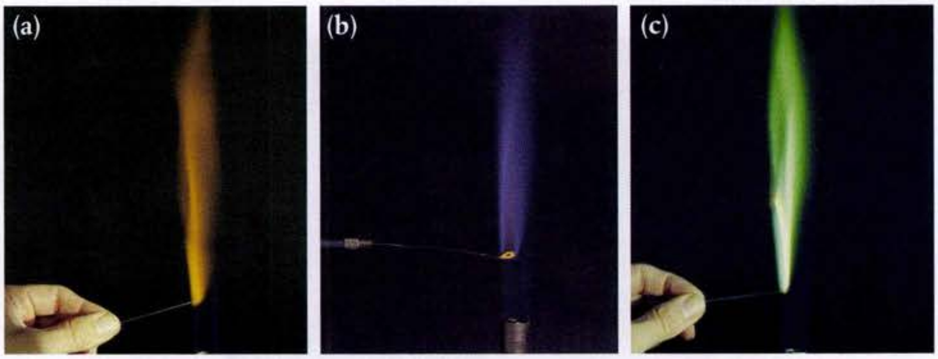
Structure 1.3.1 – Emission spectra are produced by atoms emitting photons when electrons in excited states return to lower energy levels. Qualitatively describe the relationship between colour, wavelength, frequency and energy across the electromagnetic spectrum. Distinguish between a continuous and a line spectrum.	
Details of the electromagnetic spectrum are given in the data booklet.	

Structure 1.3.2 – The line emission spectrum of hydrogen provides evidence for the existence of electrons in discrete energy levels, which converge at higher energies. Describe the emission spectrum of the hydrogen atom, including the relationships between the lines and energy transitions to the first, second and third energy levels.	
The names of the different series in the hydrogen emission spectrum will not be assessed.	Inquiry 2 – In the study of emission spectra from gaseous elements and from light, what qualitative and quantitative data can be collected from instruments such as gas discharge tubes and prisms? Nature of Science, Structure 1.2 – How do emission spectra provide evidence for the existence of different elements?

Atoms of different elements give out light of distinctive colours

Atoms of different elements give out light of a distinctive colour when an electric discharge is passed through a vapour of the element. Similarly, metals can be identified by the colour of the flame produced when their compounds are heated in a Bunsen burner. Analysis of the light emitted by different atoms gives us insights into the electron configurations within the atom.

Flame tests on the compounds of (a) sodium, (b) potassium and (c) copper.



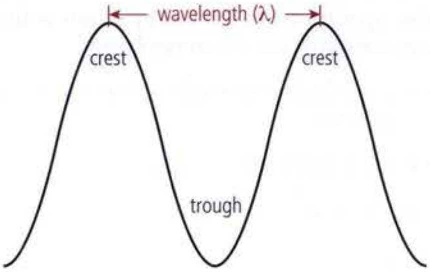
Flame colours can be used to identify unknown compounds. Full details of how to carry out a flame test experiment with a worksheet are available in the eBook.

To interpret these results, we must consider the nature of electromagnetic radiation.

Electromagnetic radiation is emitted in different forms of differing energies

Electromagnetic radiation comes in different forms of differing energy. The visible light we need to see the world is only a small part of the full spectrum, which ranges from low-energy radio waves to high-energy gamma (γ) rays. All electromagnetic waves travel at the same **speed (c)** but can be distinguished by their different **wavelengths (λ)** (Figure 1).

S1.3 Figure 1 Snapshot of a wave at a given instant. The distance between successive crests or peaks is called the wavelength (λ).



Different colours of visible light have different wavelengths; red light, for example, has a longer wavelength than blue light. The full electromagnetic spectrum is given in Section 5 of the data booklet.

The number of waves that pass a particular point in 1 s is called the **frequency (f)**; the shorter the wavelength, the higher the frequency. Blue light has a higher frequency than red light.

The precise relation is:

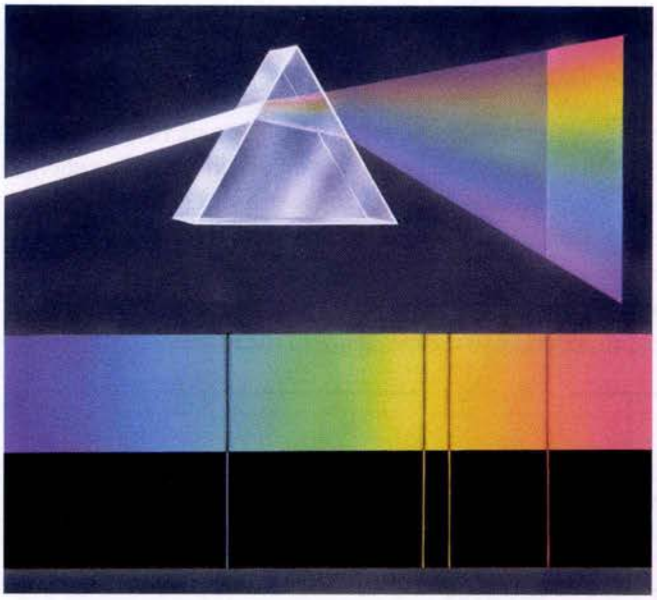
$$c = f\lambda$$

where c is the speed of light.

All electromagnetic waves travel at the same speed, $c = 3.00 \times 10^8\,\mathrm{m\,s^{-1}}$. This is the cosmic speed limit as, according to Einstein's Theory of Relativity, nothing in the universe can travel faster than this in a vacuum.

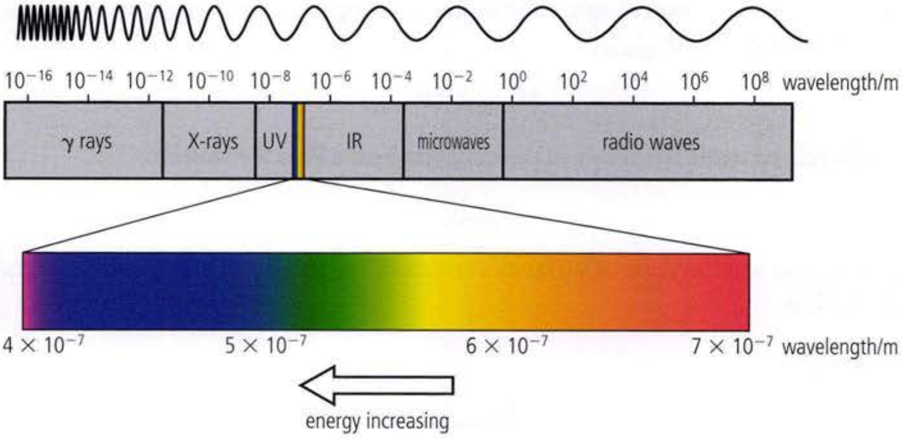
The distance between two successive crests (or troughs) is called the wavelength (λ). The frequency (f) of the wave is the number of waves that pass a point in one second. The wavelength and frequency are related by the equation $c = f\lambda$ where c is the speed of light.

White light is a mixture of light waves of differing wavelengths or colours. We see this when sunlight passes through a prism to produce a **continuous spectrum** or when light is scattered through water droplets in the air.



A continuous spectrum is produced when white light is passed through a prism. The different **colours** merge smoothly into one another. The two spectra below the illustration of the prism show (top) a continuous spectrum with a series of discrete absorption lines, and (bottom) a line emission spectrum. Details of the absorption spectrum will not be assessed.

As well as visible light, atoms emit infrared (IR) radiation, which has a longer wavelength than red light, and ultraviolet radiation, which has a shorter wavelength than violet light. The complete electromagnetic spectrum is shown in Figure 2.



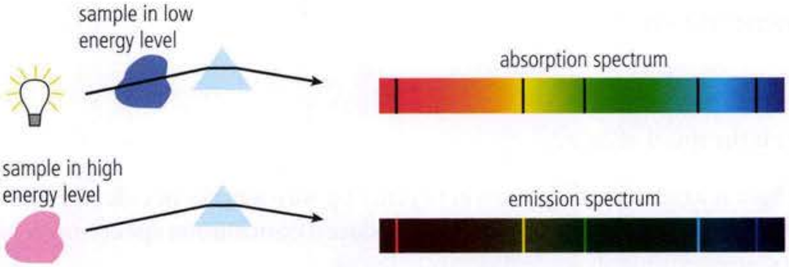
S1.3 Figure 2 The changing wavelength (in m) of electromagnetic radiation through the spectrum is shown by the trace across the top. At the short wavelength end (on the left) of the spectrum are gamma rays, X-rays, and ultraviolet light. In the centre of the spectrum are wavelengths that the human eye can see, known as visible light. Visible light comprises light of different wavelengths, energies, and colours. At the longer wavelength end of the spectrum (on the right) are infrared radiation, microwaves, and radio waves. The visible spectrum gives us only a small window to see the world.

TOK

Electromagnetic waves allow energy to be transferred across the universe. They also carry information. Low-energy radio waves are used in radar and television, for example, and higher energy gamma rays are used as medical tracers. The precision with which we view the world is limited by the wavelengths of the colours we can see. This is why we will never be able to see an atom directly; it is too small to interact with the relatively long waves of visible light. What are the implications of this for human knowledge?

An emission spectrum is produced when an atom moves from a higher to a lower energy level

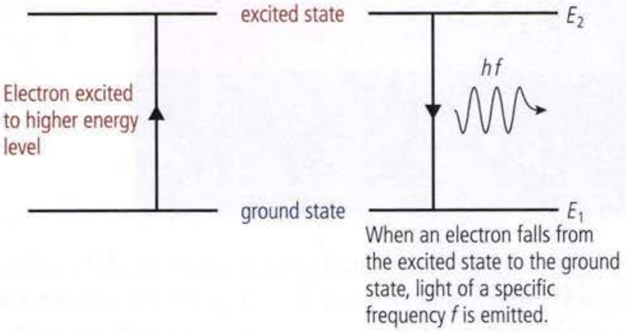
When electromagnetic radiation is passed through a collection of atoms, some of the radiation is absorbed and used to excite the atoms from a lower energy level to a higher energy level. A spectrometer analyses the transmitted radiation relative to the incident radiation and an absorption spectrum is produced (Figure 3).



S1.3 Figure 3 The origin of absorption and emission spectra. An absorption spectrum shows the radiation absorbed as atoms move from a lower to a higher energy level. An emission spectrum is produced when an atom moves from a higher to a lower level.

Gases produce a characteristic **emission line spectrum** when they are heated to a high temperature or if a high voltage is applied. Atoms are excited into a higher energy level, which is unstable, so the electron soon falls back to the **ground state**. The energy the electron gives out when it falls into lower levels is in the form of electromagnetic radiation. One packet of energy, a **photon,** is released for each electron transition (Figure 4). Photons of ultraviolet light have more energy than photons of infrared light. The energy of the photon is proportional to the frequency of the radiation.

S1.3 Figure 4 Emission spectra are the result of electrons falling from an excited state E_2 to a lower energy level E_1.



- **A continuous spectrum shows an unbroken sequence of frequencies, such as the spectrum of visible light.**
- **A line emission spectrum has only certain frequencies of light because it is produced by excited atoms and ions as they fall back to a lower energy level.**

The energy of the photon of light emitted (E_{photon}) is equal to the energy change of the electron in the atom ($\Delta E_{\text{electron}}$):

$$\Delta E_{\text{electron}} = E_{\text{photon}}$$

It is also related to the frequency of the radiation by the Planck equation:

$$E_{\text{photon}} = hf$$

This equation and the value of h (Planck's constant) are given in Sections 1 and 2 of the data booklet.

This leads to:

$$\Delta E_{\text{electron}} = hf$$

This is a very significant equation because it shows that line spectra allow us to glimpse inside the atom. The atoms emit photons of certain energies, which give lines of certain frequencies because the electron can only occupy certain energy levels. You can think of the energy levels as a staircase. The electron cannot change its energy in a continuous way, in the same way that you cannot stand between steps; it can only change its energy by discrete amounts. This energy of the atom is said to be **quantized**. The line spectrum is crucial evidence for quantization: if the energy were not quantized, the emission spectrum would be continuous.

Nature of Science

The idea that you can think of electromagnetic waves as a stream of photons, or quanta, is one aspect of quantum theory. The theory has implications for human knowledge and technology. The key idea is that energy can only be transferred in discrete amounts or quanta. Quantum theory shows us that our everyday experience cannot be transferred to the microscopic world of the atom. It has led to great technological breakthroughs such as the modern computer. It has been estimated that 30% of the gross national product of the USA depends on the application of quantum theory. Our scientific understanding has led to many technological developments. These new technologies in turn drive developments in science. The implications of quantum theory for the electron are discussed in more detail later (page 60). Note that 'discrete' has a different meaning to 'discreet'.

As different elements have different line spectra, they can be used like barcodes to identify unknown elements. They give us valuable information about the electron configurations of different atoms.

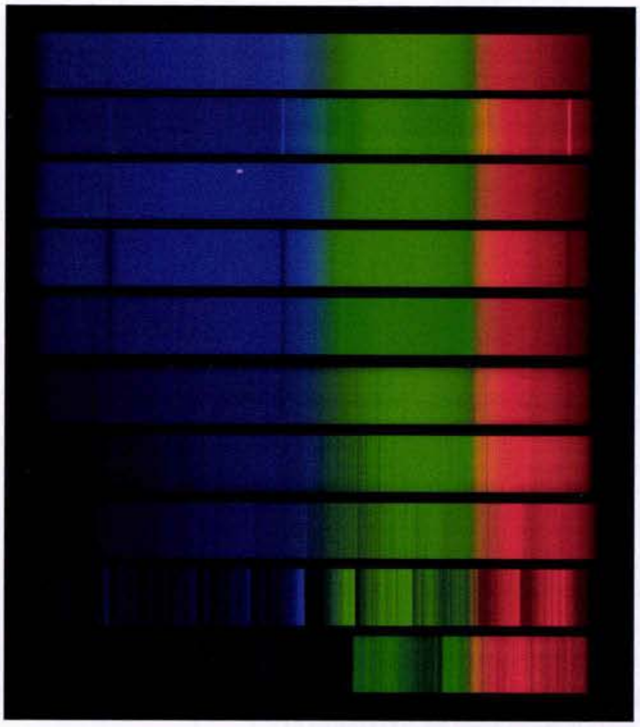


Diagram of the spectra of stars, showing a set of dark absorption lines, which indicate the presence of certain elements, such as hydrogen and helium, in the outer atmosphere of the star.

The words 'discrete' meaning 'separate', and 'discreet' meaning 'unobtrusive' both come from the Latin word 'discretus' for 'to keep separate'.

When asked to distinguish between a line spectrum and a continuous spectrum, references should be made to discrete or continuous energy levels and to specific colours, wavelengths or frequencies.

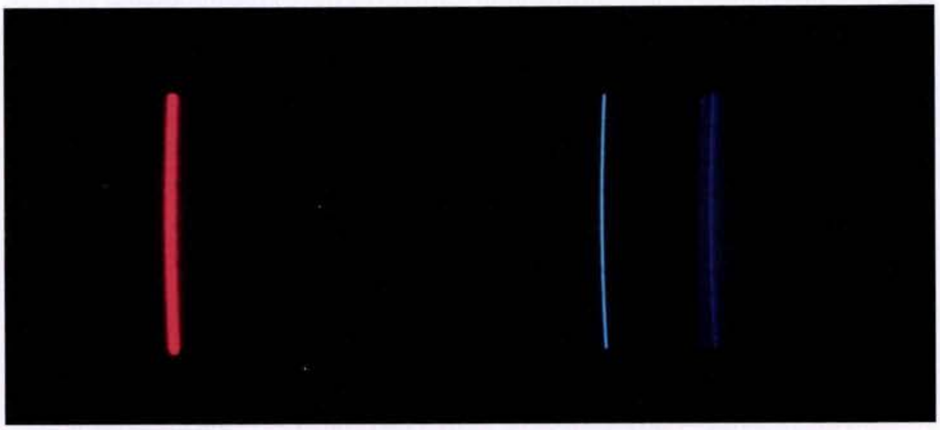
Elements discovered from their line spectra and named from their flame colours include rubidium (red), caesium (sky blue), thallium (green), and indium (indigo). Emission spectroscopy was a key tool in the discovery of new elements.

Nature of Science, Structure 1.2 – How do emission spectra provide evidence for the existence of different elements?

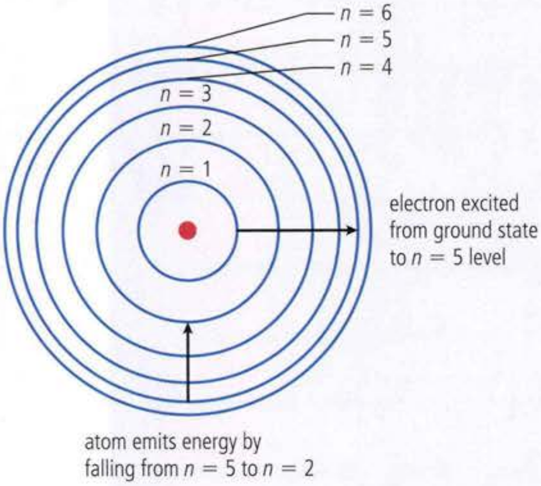
The elemental composition of stars can be determined by analysing their spectra. The gases that surround the center of a star absorb some wavelengths of the star's emitted radiation, producing dark absorption lines in the spectrum. These dark bands can be used to identify the elements present. The Sun's spectrum shows dark lines that represent absorbed radiation due to the presence of hydrogen and helium.

The line emission spectrum of hydrogen provides evidence for discrete energy levels

As discussed earlier, a line emission spectrum provides evidence for the electrons in an atom occupying discrete energy levels. A simple picture of the hydrogen atom was considered in Structure 1.2 with the electron orbiting the nucleus in a circular energy level. Niels Bohr proposed that an electron moves into an orbit further from the nucleus (a higher energy level) when an atom absorbs energy. This energy is given out in the form of electromagnetic radiation when the electron falls back from a higher to a lower energy level. In any sample of hydrogen many transitions can occur with each line corresponding to a particular transition. Visible light is produced when the electron falls to the second energy level ($n = 2$; see Figure 5).

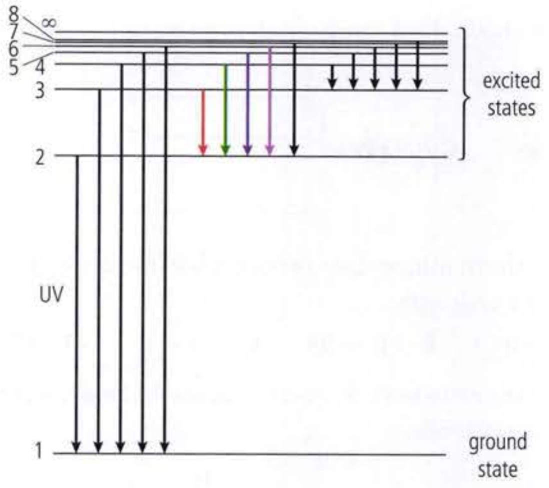


▲ Visible emission spectrum of hydrogen. The energy of lines increases from left to right. They converge at higher energies. Similar series are found in the UV and IR regions.



▲ **S1.3 Figure 5** An electron is excited from the ground state to a higher energy level. If the unstable electron then falls to a lower $n = 2$ energy level, visible light is emitted.

The transitions to the first energy level ($n = 1$) correspond to the highest energy change and are in the ultraviolet region of the spectrum. Infrared radiation is produced when an electron falls to the third or higher energy levels (Figure 6).



▲

S1.3 Figure 6 Energy levels of the hydrogen atom showing the transitions. The transition 1 → ∞ corresponds to ionization:

$$H(g) \rightarrow H^{+}(g) + e^{-}$$

HL This is discussed in more detail later.

The pattern of the lines in Figure 6 gives us a picture of the energy levels in the atom. The lines converge at higher energies because the energy levels inside the atoms are closer together. When an electron is at the highest energy $n = \infty$, it is no longer in the atom and the atom has been ionized. The energy needed to remove an electron from the ground state of one mole of gaseous atoms, ions, or molecules is called the **ionization energy**. Ionization energies can also be used to support this model of the atom (see page 74).

SKILLS

Emission spectra can be observed using discharge tubes of different gases and a spectroscope. The colours and relative intensities of the lines should be observed. The wavelengths can be measured.

Inquiry 2 – In the study of emission spectra from gaseous elements and from light, what qualitative and quantitative data can be collected from instruments such as gas discharge tubes and prisms?

Exercise

Q1. Emission spectra provide evidence for:

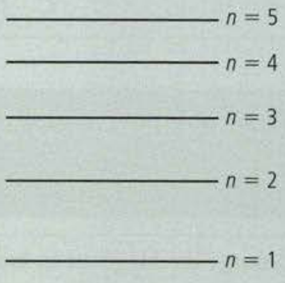
A the existence of neutrons

B the existence of isotopes

C the existence of atomic energy levels

D the nuclear model of the atom

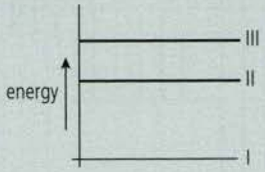
Q2. The diagram shows the lowest five electron energy levels in the hydrogen atom.



Deduce how many different frequencies in the visible emission spectrum of atomic hydrogen would arise as a result of electron transitions between these levels.

A 3 **B** 4 **C** 6 **D** 10

Q3. The diagram shows three energy levels of an atom.

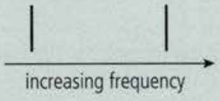


(a) Identify the transition that corresponds to the emission of light with the shortest wavelength.

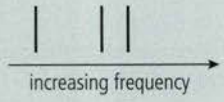
A I → II **B** II → III **C** III → I **D** III → II

(b) Identify the emission line spectra that results from transitions between these energy levels.

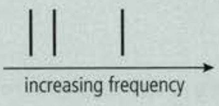
A



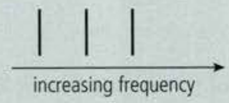
B



C



D

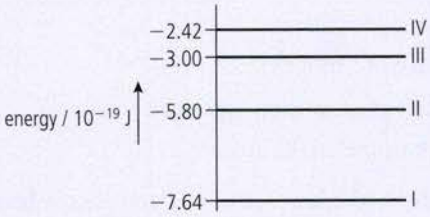


Q4. The visible emission spectrum for hydrogen includes a red line with a wavelength of 657 nm corresponding to the transition 3 → 2. State if the transition from 4 → 2 corresponds to a higher or lower wavelength and justify your answer.

Challenge yourself

1. One of the wavelengths in the emission spectrum of helium occurs at 588 nm.

Some energy levels of the helium atom are shown. The energies of the levels are given in joules. Identify the transition that produces the line at 588 nm.



A I → III **B** III → I **C** II → IV **D** IV → II

Structure 1.3.3, 1.3.4 and 1.3.5 – Electron configuration

Structure 1.3.3 – The main energy level is given an integer number, *n*, and can hold a maximum of $2n^2$ electrons.

Deduce the maximum number of electrons that can occupy each energy level.

	Structure 3.1 – How does an element's highest main energy level relate to its period number in the periodic table?

Structure 1.3.4 – A more detailed model of the atom describes the division of the main energy level into s, p, d and f sublevels of successively higher energies. Recognize the shape and orientation of an s atomic orbital and the three p atomic orbitals.	
	Structure 3.1 – What is the relationship between energy sublevels and the block nature of the periodic table?

Structure 1.3.5 – Each orbital has a defined energy state for a given electron configuration and chemical environment, and can hold two electrons of opposite spin. **Sublevels contain a fixed number of orbitals, regions of space where there is a high probability of finding an electron.** Apply the Aufbau principle, Hund's rule and the Pauli exclusion principle to deduce electron configurations for atoms and ions up to $Z = 36$.	
Full electron configurations and condensed electron configurations using the noble gas core should be covered. Orbital diagrams, i.e. arrow-in-box diagrams, should be used to represent the filling and relative energy of orbitals. The electron configurations of Cr and Cu as exceptions should be covered.	

A more sophisticated model is needed for atoms with more than one electron

Wave and particle models of light and the electron

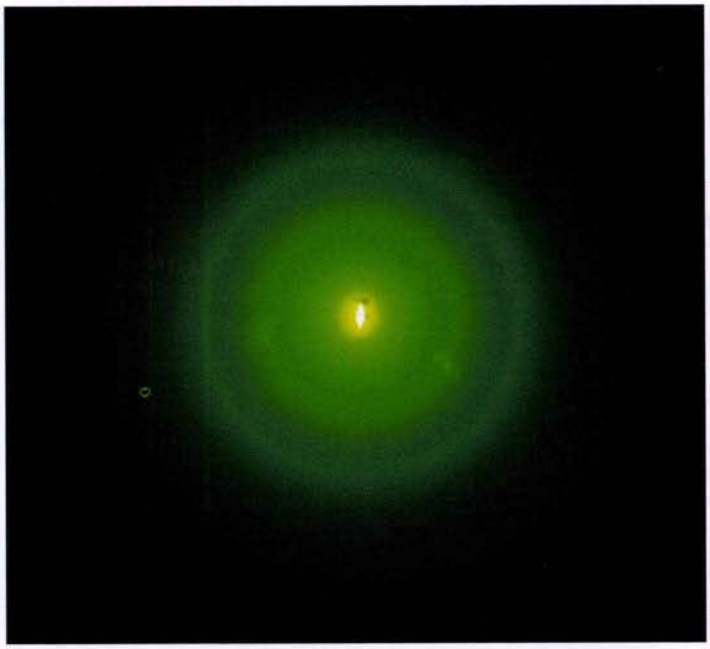
Although the Bohr model of the atom was able to predict the wavelengths of lines in the emission spectrum of hydrogen with great success, it failed to predict the spectral lines of atoms with more than one electron. The model is a simplification. To develop the model of the atom further, we need to reconsider the nature of light and matter.

We saw earlier that light could either be described by its frequency, f, which is a wave property, or by the energy of individual particles, E (called photons, or quanta, of light), which make up a beam of light. The two properties are related by the Planck equation $E = hf$. Both wave and particle models have traditionally been used to explain scientific phenomena and you may be tempted to ask which model gives the 'true' description of light. We now realize that neither model gives a complete explanation of light's properties – both models are needed.

- The diffraction, or spreading out, of light that occurs when light passes through a small slit can only be explained by a wave model.
- The scattering of electrons that occurs when light is incident on a metal surface is best explained using a particle model of light.

TOK We have outlined the plum pudding and Bohr models of the atom even though we now know they are incorrect. How can a model be useful even if it is obviously false?

In a similar way, quantum theory suggests that it is sometimes preferable to think of an electron (or indeed any particle) as having wave properties. The diffraction pattern produced when a beam of electrons is passed through a thin sheet of graphite demonstrates the wave properties of electrons. To understand the electron configurations of atoms, it is useful to consider a wave description of the electron.



Demonstration of wave-particle duality. An electron gun is fired at a thin sheet of graphite. The electrons pass through the graphite and hit a luminescent screen, producing the pattern of rings associated with diffraction. Diffraction occurs when a wave passes through an aperture similar in size to its wavelength. Quantum theory shows that electrons have wavelengths inversely proportional to their momentum (momentum is the product of their mass and velocity).

Nature of Science

Scientists use models to explain processes that may not be observable. The models can be simple or complex in nature but must match the experimental evidence if they are to be accepted. The power of the wave and particle models is that they are based on our everyday experience, but this is also their limitation. We should not be too surprised if this way of looking at the world breaks down when applied to the atomic scale, as this is beyond our experience. The model we use depends on the phenomena we are trying to explain.

When differences occur between the theoretical predictions and experimental data, the models must be modified or replaced. Bohr's model of the hydrogen atom was very successful in explaining the line spectra of the hydrogen atom but could not explain the spectra of more complex atoms, or the relative intensities of the lines in the hydrogen spectra. It also suffered from a fundamental weakness in that it was based on postulates, which combined ideas from classical and quantum physics in an ad hoc manner, with little experimental justification. Ideally, models should be consistent with the assumptions and premises of other theories. A modification of Bohr's model could only be achieved at the expense of changing our model of the electron as a particle. Dalton's atomic model and quantum theory are both examples of such radical changes of understanding, often called **paradigm shifts**.

TOK

What role do paradigm shifts play in the progression of scientific knowledge? Do they play a similar role in other areas of knowledge?

The electron's trajectory cannot be precisely described

Another fundamental problem with the Bohr model is that it assumes the electron's trajectory can be precisely described. This is now known to be impossible, as any attempt to measure an electron's position will disturb its motion. The act of focusing radiation to locate the electron sends it hurtling off in a random direction.

According to Heisenberg's **Uncertainty Principle** we cannot know where an electron is at any given moment in time – the best we can hope for is a probability picture of where the electron is *likely* to be. The possible positions of an electron are spread out in space in the same way as a wave is spread across a water surface.

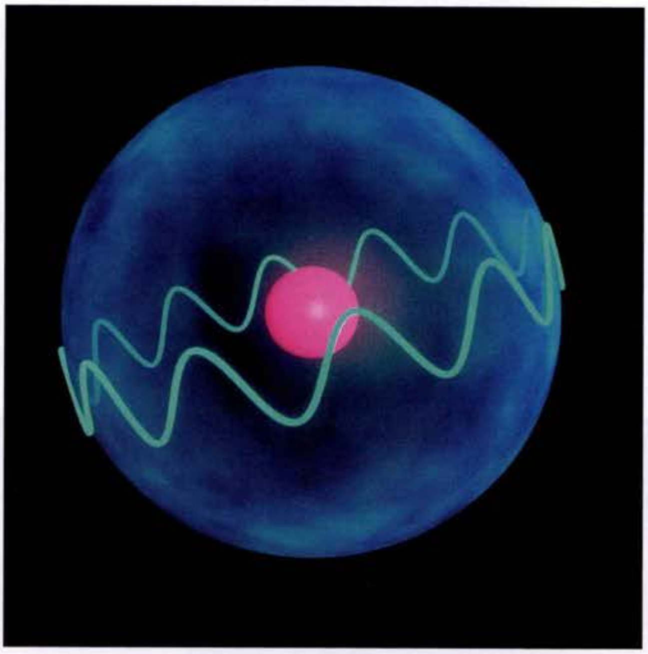
TOK

The Uncertainty Principle states that it is impossible to make an exact and simultaneous measurement of both the position and momentum of any given body. It can be thought of as an extreme example of the observer effect discussed on page 887. The significance of the Uncertainty Principle is that it shows the effect cannot be decreased indefinitely by improving the apparatus. There is an inherent uncertainty in our measurements. What are the implications of this for the limits of human knowledge?

Electrons occupy atomic orbitals

Schrödinger model of the hydrogen atom

We have seen that the electron can be considered to have wave properties and that only a probability description of its location is possible at a given time. Both of these ideas are encapsulated in the Schrödinger model of the hydrogen atom. Erwin Schrödinger (1887–1961) proposed that a wave equation could be used to describe the behaviour of an electron in the same way that a wave equation could be used to describe the behaviour of light. The equation can be applied to multi-electron systems and its solutions are known as **atomic orbitals.** An atomic orbital is a region around an atomic nucleus in which there is a 90% probability of finding the electron. The shape of the orbitals will depend on the energy of the electron. When an electron is in an orbital of higher energy, it will have a higher probability of being found further from the nucleus.



The hydrogen atom shown as a nucleus (a central proton, pink), and an electron orbiting in a wavy path (light blue). It is necessary to consider the wave properties of the electron to understand atomic structure in detail. According to Heisenberg's Uncertainty Principle, the exact position of an electron cannot be defined; atomic orbitals represent regions where there is a high probability of finding an electron.

Challenge yourself

2. State **two** ways in which the Schrödinger model of the hydrogen atom differs from that of the Bohr model.

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The progressive nature of scientific knowledge about the atom is illustrated by the Nobel Prizes awarded between 1922 and 1933 to Bohr, Heisenberg and Schrödinger.

Our model of the atom owes a great deal to the work of Niels Bohr and Werner Heisenberg, who worked together in the early years of quantum theory before World War II. But they found themselves on different sides when war broke out. The award-winning play and film *Copenhagen* is based on their meeting in the city in 1941 and explores their relationship, the uncertainty of the past, and the moral responsibilities of the scientist.

The Pauli exclusion principle states that no more than two electrons can occupy any one orbital, and if two electrons are in the same orbital, they must spin in opposite directions.

An electron is uniquely characterized by its atomic orbital and spin. If two electrons occupied the same orbital spinning in the same direction, they would be the same electron – which is impossible!

An orbital shows the volume of space in which the electron is likely to be found.

An orbital can hold two electrons of opposite spin

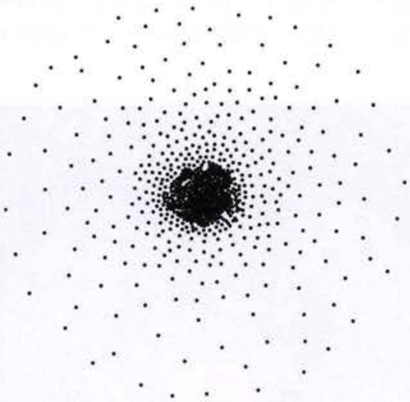
The Schrödinger model of the hydrogen spectrum does not fully explain the fine details of the hydrogen spectrum. The model needs to be further refined: in addition to moving around the nucleus, electrons can also be thought to **spin** on their own axis. They can spin in either a clockwise direction, represented by an upward arrow, or an anti-clockwise direction, represented by a downward arrow. Spin is an important factor in electron–electron interactions. Electrons can occupy the same region of space despite their mutual repulsion if they spin in opposite directions. This leads to the **Pauli exclusion principle**, which states that an orbital can hold only two electrons of opposite spin.

Atomic orbitals have different shapes and sizes

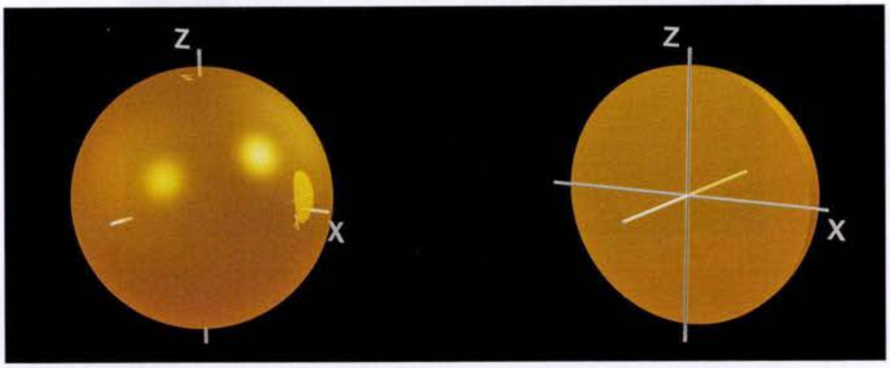
The first energy level has one 1s orbital

We saw that the electron in hydrogen occupies the first energy level in the ground state. This energy level can hold a maximum of two electrons. To highlight the distinction between this wave description of the electron provided by the Schrödinger model and the circular orbits of the Bohr atom, we say the electron occupies a 1s orbital.

The dots in Figure 7 represent locations where the electron is most likely to be found. The denser the arrangement of dots, the higher the probability that the electron occupies this region of space. The electron can be found anywhere within a spherical space surrounding the nucleus.



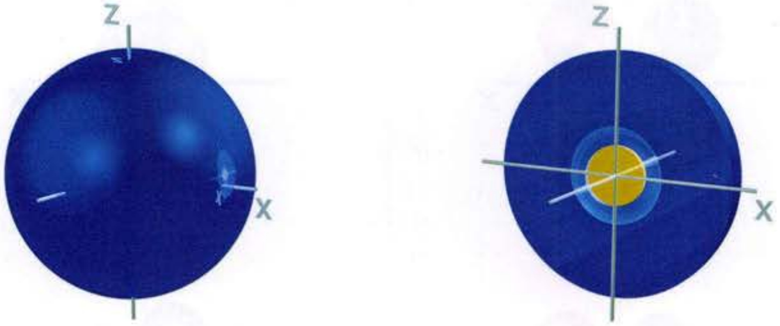
S1.3 Figure 7 An electron in a 1s atomic orbital. The density of the dots gives a measure of the probability of finding the electron in this region.



The first energy level consists of a 1s atomic orbital, which is spherical in shape.

The second energy level has a 2s and 2p sublevel

The second energy level of the Bohr model is split into two **sublevels** in the Schrödinger model. Further evidence of sublevels comes from a consideration of patterns in first ionization energies, which is discussed on page 74. The 2s sublevel is one 2s orbital and can hold a maximum of two electrons, and the 2p sublevel is three 2p orbitals and can hold six electrons. The 2s orbital has the same symmetry as a 1s orbital but extends over a larger volume. An electron in a 2s orbital is, on average, further from the nucleus than an electron in a 1s orbital and has higher energy.

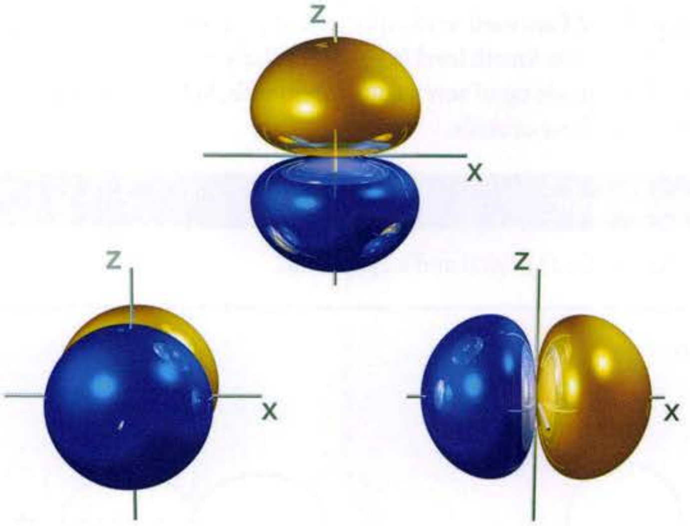


The 2s electron orbital. Just as a water wave can have crests and troughs, an orbital can have positive and negative areas. The blue area shows positive values, and the gold area negative. As it is the magnitude of the wave, not the sign, which determines the probability of finding an electron at particular positions, the sign is often not shown.

The three 2p atomic orbitals in the 2p sublevel have equal energy and are said to be **degenerate**. They all have the same dumbbell shape; the only difference is their orientation in space. They are arranged at right angles to each other with the nucleus at the centre.

SKILLS

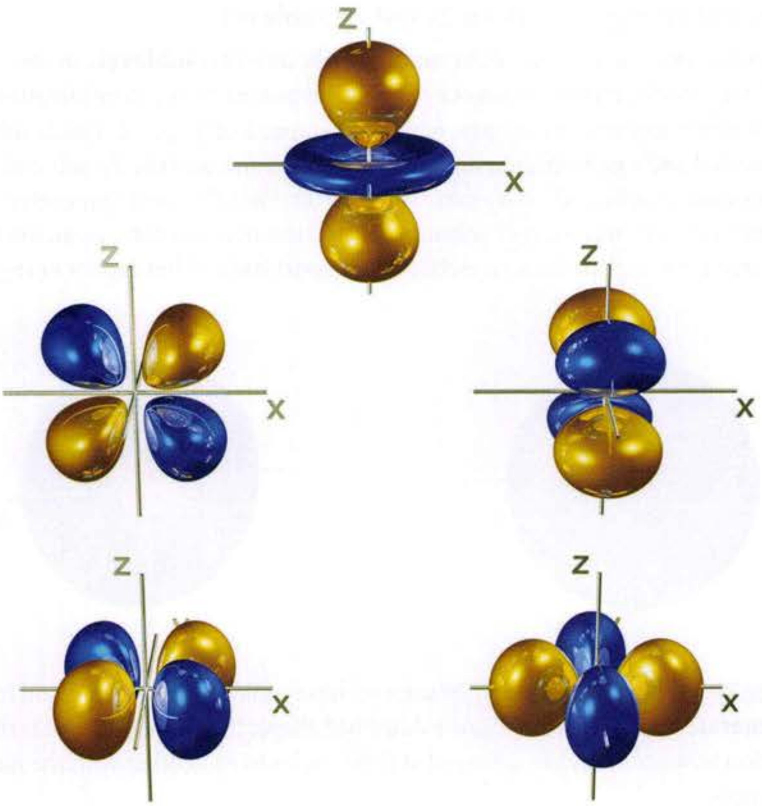
Investigating orbital shapes with modelling clay. Full details of how to carry out this experiment with a worksheet are available in the eBook.



From left to right, the p_y, p_z, and p_x atomic orbitals, localized along the *y*, *z*, and *x*-axes respectively (the *y*-axis comes out of the page). As they have the same energy, they are said to be degenerate. They form the 2p sublevel.

d and f orbitals

We have seen that the first energy level is made up of one sublevel and the second energy level is made up of two sublevels. This pattern can be generalized; the *n*th energy level of the atom is divided into *n* sublevels. The third energy level is made up of three sublevels: the 3s, 3p and 3d. The d sublevel is made up of five d atomic orbitals.



The five electron orbitals found in the 3d sublevel. Four of the orbitals are made up of four lobes, centred on the nucleus.

You are expected to know the shapes and names of the s and p atomic orbitals, but not of the d atomic orbitals.

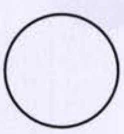
The labels s, p, d and f relate to the nature of the spectral lines the model was attempting to explain. The corresponding spectroscopic terms are *sharp*, *principal*, *diffuse* and *fine*.

The letters **s**, **p**, **d**, and **f** are used to identify different sublevels and the atomic orbitals that comprise them. The fourth level ($n = 4$) is similarly made up from four sublevels. The 4f sublevels are made up of seven f atomic orbitals, but you are not required to know the shapes of these orbitals.

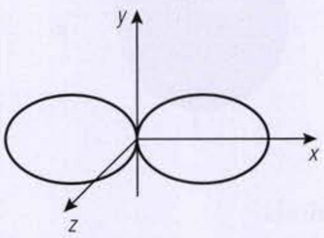
Worked example

Draw the shapes of a 1s orbital and a $2p_x$ orbital.

Solution



1s orbital

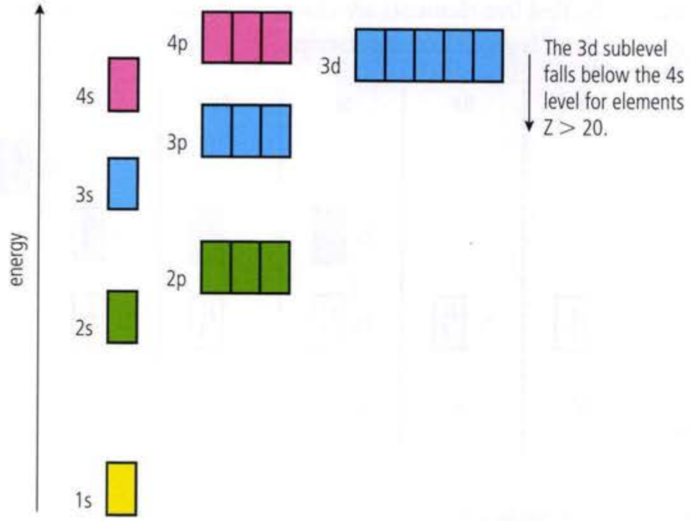


$2p_x$ orbital

The shapes of a 1s orbital and a $2p_x$ orbital. A simple two-dimensional drawing is sufficient.

Each main energy level is divided into sublevels

The atomic orbitals associated with the different energy levels are shown in Figure 8. This diagram is a simplification, as the relative energy of the orbitals depends on the atomic number. The relative energies of the 4s and 3d atomic orbitals are particularly significant and will be discussed in more detail later.



S1.3 Figure 8 The relative energies of the atomic orbitals up to the 4p sublevel. The 3d sublevel falls below the 4s level for elements $Z > 20$.

Degenerate orbitals of the same energy form a sublevel; three p orbitals form a p sublevel, five d orbitals form a d sublevel and seven f orbitals form an f sublevel. A single s orbital makes up an s sublevel.

The number of electrons in the sublevels of the first four energy levels are shown in the table.

Level	Sublevel	Maximum number of electrons in sublevel	Maximum number of electrons in level
$n = 1$	1s	2	2
$n = 2$	2s	2	8
	2p	6	
$n = 3$	3s	2	18
	3p	6	
	3d	10	
$n = 4$	4s	2	32
	4p	6	
	4d	10	
	4f	14	

We can see the following from the table:

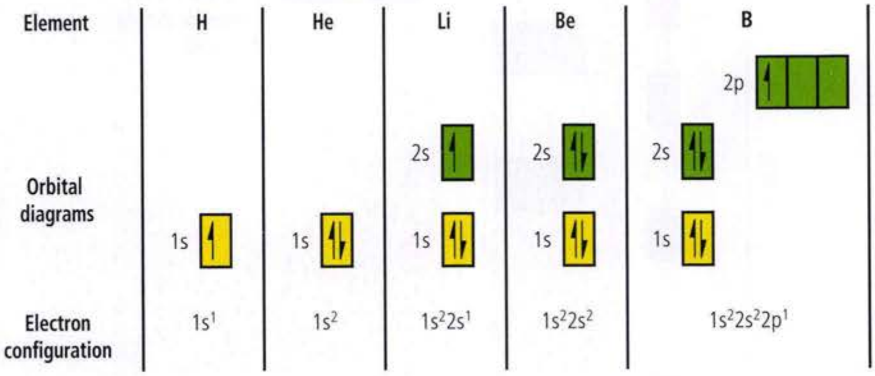
- The nth energy level of the atom is divided into n sublevels. For example, the fourth level ($n = 4$) is made up of four sublevels.
- Each main level can hold a maximum of $2n^2$ electrons. The 3rd energy level, for example, can hold a maximum of 18 electrons ($2 \times 3^2 = 18$).
- s sublevels can hold a maximum of 2 electrons.
- p sublevels can hold a maximum of 6 electrons.
- d sublevels can hold a maximum of 10 electrons.
- f sublevels can hold a maximum of 14 electrons.

Models are simplifications of complex systems. Details of the historic atomic models of Dalton, Bohr, Schrödinger and Heisenberg will not be assessed.

The Aufbau principle: constructing arrow-in-box diagrams

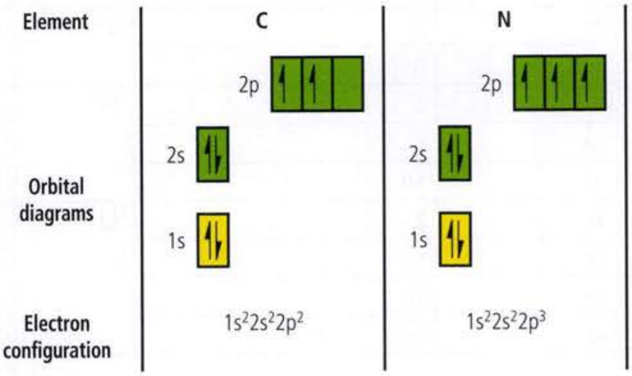
Aufbau means 'building up' in German.

The electron configuration of the ground state of an atom of an element can be determined using the **Aufbau principle**, which states that electrons are placed into orbitals of lowest energy first. Boxes can be used to represent the atomic orbitals, with single-headed arrows to represent the spinning electrons. The **electron configurations** of the first five elements are shown in Figure 9. The number of electrons in each sublevel is given as a superscript.



▲ **S1.3 Figure 9** The electron configuration of the first five elements.

The next element in the periodic table is carbon. It has two electrons in the 2p sublevel. These could either pair up, and occupy the same p orbital, or occupy separate p orbitals. Following **Hund's third rule**, we place the two electrons in separate orbitals because this configuration minimizes the mutual repulsion between them. As the 2p orbitals are perpendicular to each other and do not overlap, the two 2p electrons are unlikely to approach each other too closely. The electrons in the different 2p orbitals have parallel spins, as this leads to lower energy. The electron configurations of carbon and nitrogen are shown in Figure 10.



▲ **S1.3 Figure 10** Electron configurations of carbon and nitrogen.

Hund's rule: If more than one orbital in a sublevel is available, electrons occupy different orbitals with parallel spins.

The 2p electrons begin to pair up for oxygen ($1s^22s^22p_x^{\,2}2p_y^{\,1}2p_z^{\,1}$) and fluorine ($1s^22s^22p_x^{\,2}2p_y^{\,2}2p_z^{\,1}$). The 2p sub-shell is completed for neon ($1s^22s^22p_x^{\,2}2p_y^{\,2}2p_z^{\,2}$).

Worked example

Deduce the electron configuration of sulfur.

Solution

Sulfur has an atomic number of 16. Therefore it has 16 electrons.

Two electrons occupy the 1s: $1s^2$

Two electrons occupy the 2s: $2s^2$

Six electrons occupy the 2p: $2p^6$

Two electrons occupy the 3s: $3s^2$

Four electrons occupy the 3p: $3p^4$

So the electron configuration is $1s^2\,2s^2 2p^6\,3s^2\,3p^4$

Exercise

Q5. List the 4d, 4f, 4p, and 4s atomic orbitals in order of increasing energy.

Q6. State the number of 4d, 4f, 4p, and 4s atomic orbitals.

Q7. Apply the *orbital diagram* method to determine the electron configuration of calcium.

Q8. Deduce the number of unpaired electrons present in a phosphorus atom.

Q9. Deduce the number of orbitals in the $n = 4$ level and explain your answer.

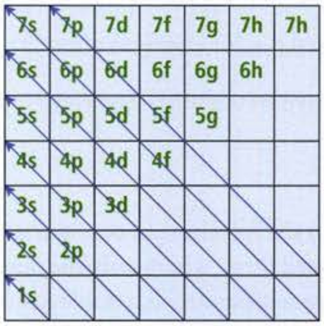
Challenge yourself

3. Which of the following provide evidence to support the Bohr model of the hydrogen atom?

I. The energy of the lines in the emission spectra of atomic hydrogen.

II. The relative intensity of the different spectral lines in the emission spectrum of atomic hydrogen.

A I only **B** II only **C** I and II **D** Neither I nor II



S1.3 Figure 11 Order of filling sublevels: 1s, 2s, 2p, 3s, 3p, 4s, 3d, 4p, 5s, 4d, 5p, 6s, 4f, 5d, 6p, 7s, 5f, 6d, 7p.

Can you think of a mnemonic for the order of filling orbitals? Figure 11 shows orbitals filled to sublevel 7s. Follow the arrows to see the order in which the sublevels are filled.

The mathematical nature of the orbital description is illustrated by some simple relationships:

- number of sublevels at nth main energy level = n
- number of orbitals at nth energy level = n^2
- number of electrons at nth energy level = $2n^2$
- number of orbitals at lth sublevel = $(2l + 1)$ where n and l are sometimes known as quantum numbers.

Sublevel	s	p	d	f
l	0	1	2	3

TOK

The abstract language of mathematics provides a powerful tool for describing the behaviour of electrons in the atom. The shapes and equations it generates have elegance and symmetry. What do such results tell us about the relationship between the natural sciences, mathematics, and the natural world? Why are many of the laws in the natural sciences stated using the language of mathematics?

The relative energy of the orbitals depends on the atomic number

The energy of an orbital depends on the attraction between the electrons and the nucleus and inter-electron repulsions. As these interactions change with the nuclear charge and the number of electrons – that is, the atomic number – so does the relative energy of the orbitals. All the sublevels in the third energy level (3s, 3p, and 3d), for example, have the same energy for the hydrogen atom and only become separated as extra protons and electrons are added. The situation is particularly complicated when we reach the d block elements. The 3d and 4s levels are very close in energy and their relative separation is very sensitive to inter-electron repulsion. For the elements potassium and calcium, the 4s orbitals are filled before the 3d sublevel. Electrons are, however, first lost from the 4s sublevel when transition metals form their ions, as once the 3d sublevel is occupied the 3d electrons push the 4s electrons to higher energy.

When the transition metal atoms form ions they lose electrons from the 4s sublevel before the 3d sublevel.

Worked example

State the full electron configuration of vanadium and deduce the number of unpaired electrons.

Solution

The atomic number of vanadium gives the number of electrons: Z = 23.

So the electron configuration is: $1s^22s^22p^63s^23p^64s^23d^3$. Note: the 3d sublevel is filled *after* the 4s sub level.

It is useful, however, to write the electron configuration with the 3d sub-shell before the 4s: $1s^22s^22p^63s^23p^63d^34s^2$ as the 3d sublevel falls below the 4s orbital once the 4s orbital is occupied (i.e. for elements after Ca).

The three 3d orbitals each have an unpaired electron. Number of unpaired electrons = 3.

The worked example asked for the full electron configuration. Sometimes it is convenient to use an abbreviated form, where only the outer electrons are explicitly shown. The inner electrons are represented as a noble gas core. Using this notation, the electron configuration of vanadium is written [Ar] $3d^34s^2$, where [Ar] represents the electron configuration of Ar, which is $1s^22s^22p^63s^23p^6$.

The electron configurations of the first 30 elements are shown in the table.

Element	Electron configuration	Element	Electron configuration
${}_{1}$H	$1s^1$	${}_{16}$S	$1s^2 2s^2 2p^6 3s^2 3p^4$
${}_{2}$He	$1s^2$	${}_{17}$Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$
${}_{3}$Li	$1s^2 2s^1$	${}_{18}$Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$
${}_{4}$Be	$1s^2 2s^2$	${}_{19}$K	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^1$
${}_{5}$B	$1s^2 2s^2 2p^1$	${}_{20}$Ca	$1s^2 2s^2 2p^6 3s^2 3p^6 4s^2$
${}_{6}$C	$1s^2 2s^2 2p^2$	${}_{21}$Sc	[Ar] $3d^1 4s^2$
${}_{7}$N	$1s^2 2s^2 2p^3$	${}_{22}$Ti	[Ar] $3d^2 4s^2$
${}_{8}$O	$1s^2 2s^2 2p^4$	${}_{23}$V	[Ar] $3d^3 4s^2$
${}_{9}$F	$1s^2 2s^2 2p^5$	${}_{24}$Cr	[Ar] $3d^5 4s^1$
${}_{10}$Ne	$1s^2 2s^2 2p^6$	${}_{25}$Mn	[Ar] $3d^5 4s^2$
${}_{11}$Na	$1s^2 2s^2 2p^6 3s^1$	${}_{26}$Fe	[Ar] $3d^6 4s^2$
${}_{12}$Mg	$1s^2 2s^2 2p^6 3s^2$	${}_{27}$Co	[Ar] $3d^7 4s^2$
${}_{13}$Al	$1s^2 2s^2 2p^6 3s^2 3p^1$	${}_{28}$Ni	[Ar] $3d^8 4s^2$
${}_{14}$Si	$1s^2 2s^2 2p^6 3s^2 3p^2$	${}_{29}$Cu	[Ar] $3d^{10} 4s^1$
${}_{15}$P	$1s^2 2s^2 2p^6 3s^2 3p^3$	${}_{30}$Zn	[Ar] $3d^{10} 4s^2$

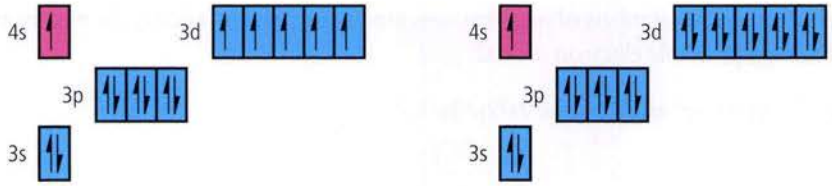
The electrons in the outer energy level are mainly responsible for compound formation and are called **valence electrons**. Lithium has one valence electron in the outer second energy level ($2s^1$), beryllium has two ($2s^2$), boron has three ($2s^2 2p^1$), and so on. The number of valence electrons follows a periodic pattern, which is discussed fully in Structure 3.1. Atoms can have many other electron configurations when in an excited state. Unless otherwise instructed, assume that you are being asked about ground-state configurations.

The term 'valence' is derived from the Latin word for 'strength'.

For the d block elements, three points should be noted:

- the 3d sublevel is written with the other $n = 3$ sublevels because it falls below the 4s orbital once the 4s orbital is occupied (i.e. for elements after Ca), as discussed earlier
- chromium has the electron configuration [Ar] $3d^5 4s^1$
- copper has the electron configuration [Ar] $3d^{10} 4s^1$.

To understand the electron configurations of copper and chromium, it is helpful to consider the electrons-in-boxes arrangements in Figure 12. As the 4s and 3d orbitals are close in energy, the electron configuration for chromium, with a half-full d sublevel, is relatively stable as it minimizes electrostatic repulsion, with six singly occupied atomic orbitals. This would be the expected configuration using Hund's rule if the 4s and 3d orbitals had exactly the same energy. Half-filled and filled sublevels seem to be particularly stable: the configuration for copper is similarly due to the stability of the full d sublevel.



chromium: [Ar]$3d^5 4s^1$

copper: [Ar]$3d^{10} 4s^1$

S1.3 Figure 12 The electron configurations of the 3rd and 4th energy levels for chromium and copper.

Exercise

Q10. Identify the sublevel that does not exist.

A 5d **B** 4d **C** 3f **D** 2p

Q11. Which is the correct order of orbital filling according to the Aufbau principle?

A 4s 4p 4d 4f **B** 4p 4d 5s 4f

C 4s 3d 4p 5s **D** 4d 4f 5s 5p

Q12. State the full ground-state electron configuration of the following elements.

(a) V **(b)** K **(c)** Se **(d)** Sr

Q13. Determine the total number of electrons in d orbitals in a single iodine atom.

A 5 **B** 10 **C** 15 **D** 20

Q14. Identify the excited state (i.e. not a ground state) in the following electron configurations.

A [Ne] $3s^2 3p^3$ **B** [Ne] $3s^2 3p^3 4s^1$

C [Ne] $3s^2 3p^6 4s^1$ **D** [Ne] $3s^2 3p^6 3d^1 4s^2$

Q15. Deduce the number of unpaired electrons present in the ground state of a titanium atom.

A 1 **B** 2 **C** 3 **D** 4

Q16. Identify the atom that possesses the most unpaired electrons.

A O **B** Mg **C** Ti **D** Fe

Electron configuration of ions

As discussed earlier, positive ions are formed by the loss of electrons. These electrons are lost from the outer sublevels. For example, the electron configurations of the different aluminium ions formed when electrons are successively removed are as follows:

- Al^+ is $1s^2 2s^2 2p^6 3s^2$
- Al^{2+} is $1s^2 2s^2 2p^6 3s^1$
- Al^{3+} is $1s^2 2s^2 2p^6$, etc.

When positive ions are formed for transition metals, the outer 4s electrons are removed before the 3d electrons, as discussed earlier.

For example, Cr is [Ar] $3d^5 4s^1$ and Cr^{3+} is [Ar] $3d^3$

The electron configurations of negative ions are determined by adding the electrons into the next available electron orbital:

S is $1s^2 2s^2 2p^6 3s^2 3p^4$ and S^{2-} is $1s^2 2s^2 2p^6 3s^2 3p^6$

Worked example

Deduce the ground-state electron configuration of the Fe^{3+} ion.

Solution

First find the electron configuration of the atom. Fe has 26 electrons:
$1s^22s^22p^63s^23p^64s^23d^6$

As the 3d sublevel is below the 4s level for elements after calcium, we write this as
$1s^22s^22p^63s^23p^63d^64s^2$

Now remove the two electrons from the 4s sublevel and one electron from the 3d sublevel.

Electron configuration of Fe^{3+} is $1s^22s^22p^63s^23p^63d^5$

Note the abbreviated electron configuration using the noble gas core is not acceptable when asked for the *full* electron configuration.

Exercise

Q17. State the full ground-state electron configuration of the following ions.

(a) O^{2-} **(b)** Cl^- **(c)** Ti^{3+} **(d)** Cu^{2+}

Q18. State the electron configuration of the following transition metal ions by filling in the boxes below. Use arrows to represent the electron spin.

	Ion	**3d**					**4s**
(a)	Ti^{2+}						
(b)	Fe^{2+}						
(c)	Ni^{2+}						
(d)	Zn^{2+}						

Q19. **(a)** State the full electron configuration for neon.

(b) State the formulas of two oppositely charged ions which have the same electron configuration as neon.

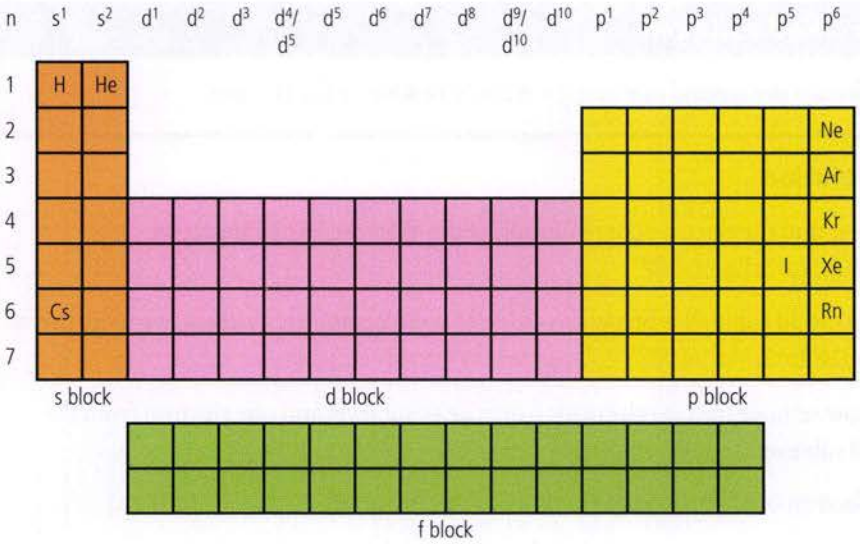
Q20. State the abbreviated electron configuration using the previous noble gas core for:

(a) Ni^{2+} **(b)** Pb^{2+} **(c)** S^{2-} **(d)** Si^{4+}

Electron configuration and the periodic table

We are now in a position to understand the structure of the periodic table (Figure 13):

- elements whose valence electrons occupy an s sublevel make up the s block
- elements with valence electrons in p orbitals make up the p block
- the d block and the f block are similarly made up of elements with outer electrons in d and f orbitals.



S1.3 Figure 13 The block structure of the periodic table is based on the sublevels of the atom. H and He are difficult elements to classify. Although they have electron configurations that place them in the s block, their chemistry is not typical of group 1 or group 2 elements.

Structure 3.1 - What is the relationship between energy sublevels and the block nature of the periodic table?

The *ns* and *np* sublevels are filled for elements in period *n*. However the (*n* - 1)d sublevel is filled for elements in period *n*.

Structure 3.1 - How does an element's highest main energy level relate to its period number in the periodic table?

Some versions of the periodic table use the numbering 3-7 for groups 13-17. In this version, group 3 elements have three valence electrons and group 7 elements have seven valence electrons. Although this is simpler, in some respects it can lead to problems. After extensive discussions, the IUPAC concluded that the 1 to 18 numbering provides the clearest and most unambiguous labelling system.

The position of an element in the periodic table is based on the occupied sublevel of highest energy in the ground-state atom. Conversely, the electron configuration of an element can be deduced directly from its position in the periodic table.

Here are some examples.

- Caesium is in group 1 and period 6 and has the electron configuration: $[Xe]\ 6s^1$.
- Iodine is in group 17 and in period 5 and has the configuration: $[Kr]\ 5s^2 4d^{10} 5p^5$. Placing the 4d sublevel before the 5s gives $[Kr]\ 4d^{10} 5s^2 5p^5$. Iodine has 7 valence electrons, in agreement with the pattern discussed on page 69.

Exercise

Q21. Use the periodic table to find the full ground-state electron configuration of the following elements.

(a) Cl **(b)** Nb **(c)** Ge **(d)** Sb

Q22. Identify the elements that have the following ground-state electron configurations.

(a) $[Ne]\ 3s^2 3p^2$ **(b)** $[Ar]\ 3d^5 4s^2$

(c) $[Kr]\ 5s^2$ **(d)** $1s^2 2s^2 2p^6 3s^2 3p^6 3d^1 4s^2$

Q23. State the total number of p orbitals containing one or more electrons in tin.

Q24. How many electrons are there in all the d orbitals in an atom of barium?

Q25. State the electron configuration of the ion Cd^{2+}.

Q26. State the full electron configuration of U^{2+}.

Challenge yourself

4. State the electron configuration of thorium.

5. Only a few atoms of element 109, meitnerium, have ever been made. Isolation of an observable quantity of the element has never been achieved and may well never be. This is because meitnerium decays very rapidly.

  (a) Suggest the electron configuration of the ground-state atom of the element.

  (b) There is no g block in the periodic table as no elements with outer electrons in g orbitals exist in nature or have been made artificially. Suggest a minimum atomic number for such an element.

6. Consider how the shape of the periodic table is related to the three-dimensional world we live in.

  (a) How many 3p and 3d orbitals would there be if only the x and y dimensions existed?

  (b) How many groups in the p and d block would there be in such a two-dimensional world?

TOK

Do atomic orbitals exist or are they primarily useful inventions to aid our understanding? What consequences might questions about the reality of scientific entities have for the public perception and understanding of the subject? If they are only inventions, how is it that they can yield such accurate predictions?

Nature of Science

We have seen how the model of the atom has changed over time. All these theories are still used today. Dalton's model adequately explains many properties of the states of matter, the Bohr model is used to explain chemical bonding, and the structure of the periodic table is explained by the wave description of the electron. In science, we often follow Occam's razor and use the simplest explanation that can account for the phenomena. As Einstein said 'Explanations should be made as simple as possible, but not simpler'.

HL

Structure 1.3.6 and 1.3.7 – Ionization energies

Structure 1.3.6 – In an emission spectrum, the limit of convergence at higher frequency corresponds to ionization.

Explain the trends and discontinuities in first ionization energy (IE) across a period and down a group.

Calculate the value of the first IE from spectral data that gives the wavelength or frequency of the convergence limit.

The value of the Planck constant h and the equations $E = hf$ and $c = \lambda f$ are given in the data booklet.	Structure 3.1 – How does the trend in IE values across a period and down a group explain the trends in properties of metals and non-metals? Nature of Science, Tool 3, Reactivity 3.1 – Why are log scales useful when discussing $[H^+]$ and ionization energies?

Structure 1.3.7 – Successive ionization energy (IE) data for an element give information about its electron configuration.

Deduce the group of an element from its successive ionization data.

Databases are useful for compiling graphs of trends in IEs.	Structure 3.1 – How do patterns of successive IEs of transition elements help to explain the variable oxidation states of these elements?

In an emission spectrum, the limit of convergence at higher frequency corresponds to ionization

The first ionization energy of an element is the energy needed to remove one mole of electrons from the ground state of one mole of the gaseous atom. For hydrogen it corresponds to the following change, with the electron being removed from the 1s orbital:

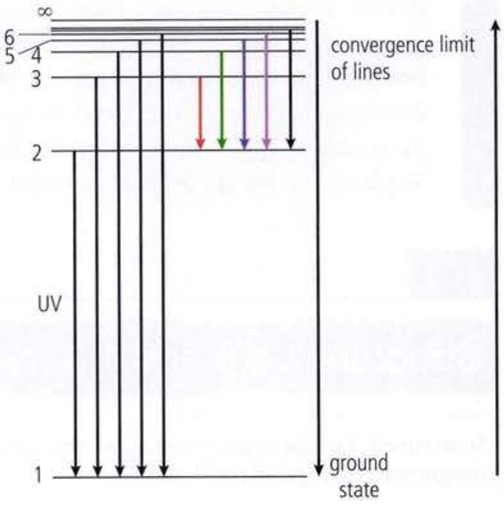
$$H(g) \longrightarrow H^{+}(g) + e^{-}$$

Once removed from the atom, the electron is an infinite distance away from the nucleus and can be considered to be in the $n = \infty$ energy level.

The first ionization energy of an element is the minimum energy needed to remove one mole of electrons from one mole of gaseous atoms in their ground state.

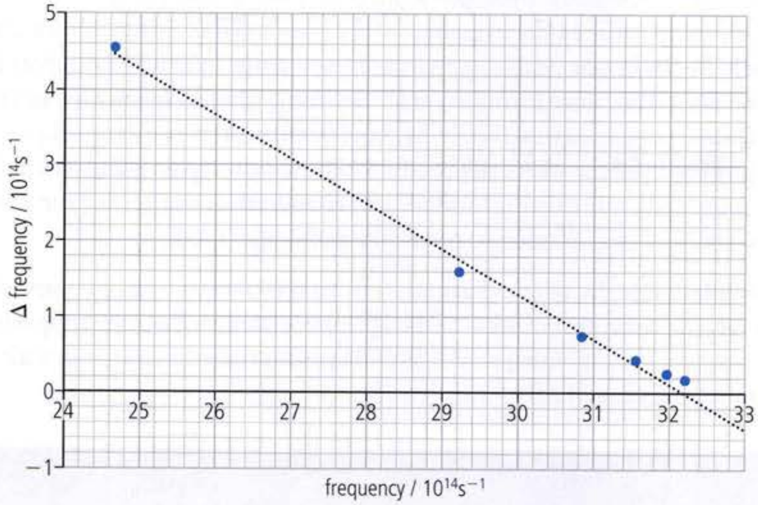
We saw earlier that the energy levels in hydrogen converge at higher energy. This allows us to calculate the ionization energy from the convergence limit at higher frequency.

The frequency at which convergence occurs can be obtained graphically. The frequencies of the lines where the transitions involve the electron falling from the excited levels with $n \geq 1$ to the $n = 1$ energy level are shown below. The difference between the frequencies in successive lines is given in the third column.



Excited energy level (n)	Frequency, f / × 10^{-14} s^{-1}	Δf / × 10^{-14} s^{-1}
2	24.66	4.57
3	29.23	1.60
4	30.83	0.74
5	31.57	0.40
6	31.97	0.24
7	32.21	0.16
8	32.37	

A graph of f against Δf ($f_{n+1} - f_n$) gives an approximate best-fit straight line with the intercept on the x axis giving the frequency at which convergence occurs.



A graph showing the frequency of the line emitted against the difference in frequency between successive lines in the UV region of the hydrogen atom.

From the graph, convergence occurs when $\Delta f = 0$ at $f = 32.3 \times 10^{-14}\,\text{s}^{-1}$

Using the equation $E = hf$ we have the ionization energy for one atom:

$$E = 32.3 \times 10^{-14}\,\text{s}^{-1} \times 6.63 \times 10^{-34}\,\text{J s}$$

So for one mole, the ionization energy is given by:

$$\text{IE} = 32.3 \times 10^{-14}\,\text{s}^{-1} \times 6.63 \times 10^{-34}\,\text{J s} \times 6.02 \times 10^{23}\,\text{mol}^{-1}$$

$$= 1290\,\text{kJ mol}^{-1}$$

This is close to the value of 1312 kJ mol^{-1} given in Section 9 of the data booklet.

Nature of Science

The best data for making accurate and precise descriptions are often quantitative as you can use this for mathematical analysis. The data can often be presented in a variety of formats that can be analysed. Scientists look for patterns in an attempt to discover relationships.

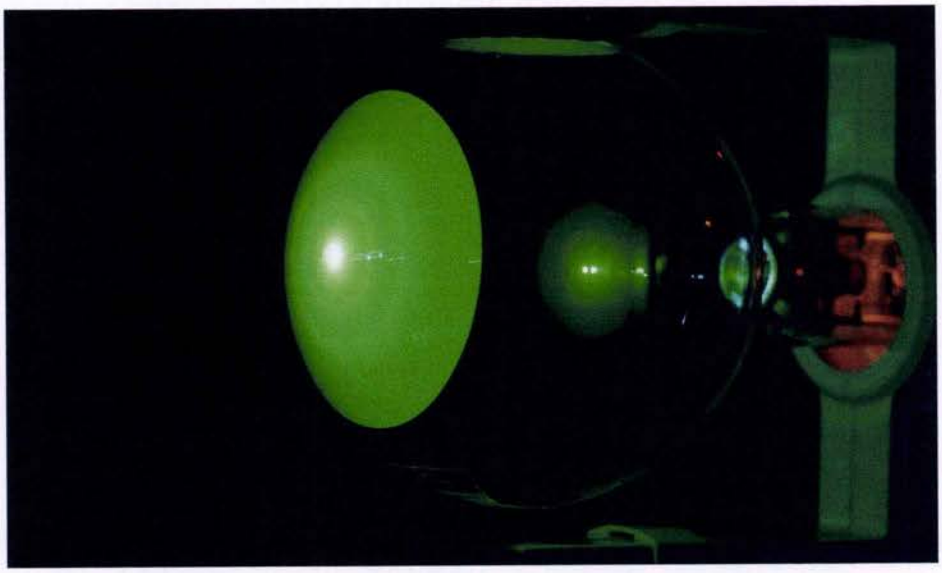
Challenge yourself

7. A more accurate value for the convergence limit can also be found by plotting a graph of the frequencies of the lines against $\frac{1}{n^2}$. Determine the ionization energy of hydrogen using this method and explain why this method is more accurate.

Nature of Science

The Bohr model of the hydrogen atom (1913) was able to explain the relationship between the frequency of the lines and the *n* values for the energy levels, but Bohr was unable to provide experimental evidence to support his postulates. They were inconsistent as they came from an unjustified mixture of classical and quantum theory. In general, scientists strive to develop hypotheses and theories that are compatible with accepted principles and that simplify and unify existing ideas. A deeper understanding needed the wave description of the electron suggested by de Broglie (1926).

Many scientific discoveries have come from speculation or simple curiosity about particular phenomena. De Broglie speculated on the wave properties of particles by combining results from Einstein's theory of relativity with Planck's quantum theory.



An electron diffraction tube. The electrons fired at a thin sheet of graphite produce the patterns of rings associated with diffraction. De Broglie (1892–1987) correctly deduced that the electrons would have wavelengths inversely proportional to their momentum ($\lambda = h/p$).

TOK

The de Broglie equation ($\lambda = h/p$) shows that macroscopic particles have too short a wavelength for their wave properties to be observed. Is it meaningful to talk of properties which can never be observed from sense perception?

Ionization energies can also be used to support this model of the atom.

Exercise

Q27. Sodium lamps used for street lighting emit a distinctive orange light with a wavelength of 590 nm. Calculate the energy produced by one mole of excited sodium atoms when they give out orange light of this wavelength.

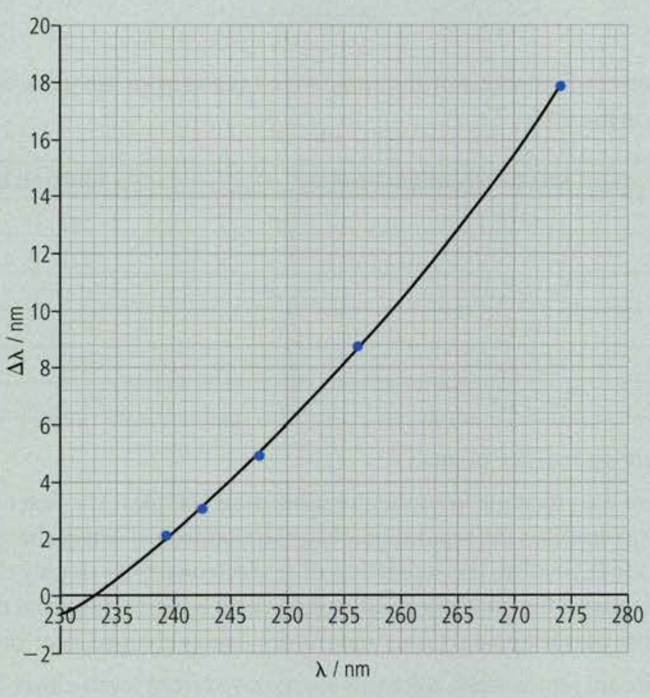
Q28. Some frequencies of the lines in the spectrum of He^+ ion are shown in the table. Determine the convergence limit and ionization energy of the He^+ ion.

Excited energy level (*n*)	Frequency, f / $\times 10^{-15}\ s^{-1}$
2	9.87
3	11.72
4	12.36
5	12.66
6	12.82

Q29. The convergence limits in the spectra of two single electron ions are shown in the table. Use these values to calculate the ionization energy of the ions.

	Frequency of convergence limit/ s^{-1}
Li^{2+}	2.97×10^{16}
Be^{3+}	5.27×10^{16}

Q30. The emission spectrum of lithium includes a number of lines corresponding to the transitions involving the valence electron falling from excited states back to the 2s orbital. The graph shows the wavelength λ_n of a number of these lines in the spectrum, plotted against the difference in wavelength between consecutive lines ($\Delta\lambda = \lambda_n - \lambda_{n+1}$).



Determine the wavelength that corresponds to ionization of lithium and calculate the ionization energy.

Successive ionization energy (IE) data for an element give information about its electron configuration

Additional evidence for the electron configuration of an atom comes from looking at patterns of successive ionization energies. As discussed earlier for aluminium, the first ionization energy corresponds to the following process:

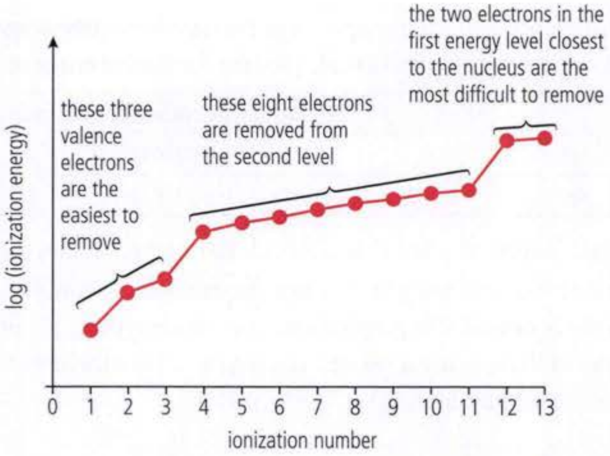
$$Al(g) \rightarrow Al^{+}(g) + e^{-}$$

The second ionization energy corresponds to the change:

$$Al^{+}(g) \rightarrow Al^{2+}(g) + e^{-}$$

and so on.

The ionization energies for aluminium are shown in Figure 14.



S1.3 Figure 14 Successive ionization energies for aluminium. Note the jumps between the 3rd and 4th and between the 11th and 12th ionization energies as electrons are removed from lower energy levels. As there is a wide range of values, they are best presented on a log scale.

The electron configurations of aluminium ions as electrons are successively removed are shown in the table.

	Electron configuration		Electron configuration
Al	$1s^22s^22p^63s^23p^1$	Al^{6+}	$1s^22s^22p^3$
Al^{+}	$1s^22s^22p^63s^2$	Al^{7+}	$1s^22s^22p^2$
Al^{2+}	$1s^22s^22p^63s^1$	Al^{8+}	$1s^22s^22p^1$
Al^{3+}	$1s^22s^22p^6$	Al^{9+}	$1s^22s^2$
Al^{4+}	$1s^22s^22p^5$	Al^{10+}	$1s^22s^1$
Al^{5+}	$1s^22s^22p^4$	Al^{11+}	$1s^2$

TOK

How does the method of data presentation influence how the data are interpreted? The use of scale can clarify important relationships but can also be used to manipulate data. How can you as a knower distinguish between the use and abuse of data presentation?

Nature of Science, Tool 3, Reactivity 3.1 - Why are log scales useful when discussing $[H^+]$ and ionization energies?

Figure 14 shows two key points.

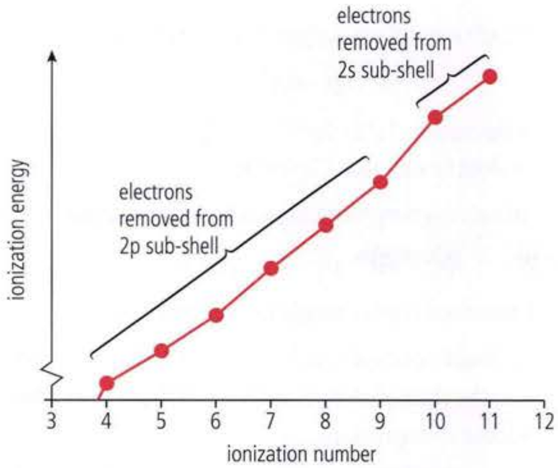
- There is an increase in successive ionization energies. The first ionization energy involves the separation of an electron from a singly charged ion and the second IE involves the separation of an electron from a doubly charged ion. The process becomes more difficult as there is increasing attraction between the higher charged positive ions and the oppositely charged electron.
- There are jumps when electrons are removed from levels closer to the nucleus. The first three ionization energies involve the removal of electrons from the third level. The 3p electron is removed first, followed by the electrons from the 3s orbital. An electron is removed from the second level for the fourth ionization energy. This electron is closer to the nucleus and is more exposed to the positive charge of the nucleus and so needs significantly more energy to be removed. There is similarly a large jump for the 12th ionization energy as it corresponds to an electron being removed from the 1s orbital.

TOK

Which of Dalton's five proposals (page 30) do we now hold to be 'true'? How does scientific knowledge change with time? Are the models and theories of science accurate descriptions of the natural world, or just useful interpretations to help predict and explain the natural world?

A closer look at successive ionization energies gives evidence for sublevels in the atom

A closer look at the successive ionization energies shows evidence of the sublevels present with each level. The log graph of all 13 ionization energies showed a 2, 8, 3 pattern in successive ionization energies, which reflects the electron arrangement of the atom, with two electrons in the first level, eight electrons at the second energy level, and three valence electrons in the outer shell. Now we consider the fourth to eleventh ionization energies in more detail. These correspond to the removal of the eight electrons in the second energy level (Figure 15).



S1.3 Figure 15 Successive ionization energies for aluminium. The jump between the ninth and tenth ionization energies indicates that the second energy level is divided into sublevels. The smaller jump between the sixth and seventh ionization energies should also be noted and is discussed more fully in the text.

The jump between the ninth and tenth ionization energies shows that the eleventh electron is more difficult to remove than we would expect from the pattern of the six previous electrons. This suggests that the second energy level is divided into two sublevels.

This evidence confirms that the **2s sublevel** can hold a maximum of two electrons, and the **2p sublevel** can hold six electrons.

SKILLS

Successive ionization energies database investigation. Full details of how to carry out this activity with a worksheet are available in the eBook.

Worked example

A graph of some successive ionization energies of aluminium is shown in Figure 15.

(a) Explain why there is a large increase between the ninth and tenth ionization energies.

(b) Explain why the increase between the sixth and seventh values is greater than the increase between the fifth and sixth values.

Solution

(a) The ninth ionization energy corresponds to the change:

$$Al^{8+}(g) \rightarrow Al^{9+}(g) + e^-$$

Al^{8+} has the configuration $1s^22s^22p^1$. The electron is removed from a 2p orbital.

The tenth ionization energy corresponds to the change:

$$Al^{9+}(g) \rightarrow Al^{10+}(g) + e^-$$

Al^{9+} has the configuration $1s^22s^2$. The electron is removed from a 2s orbital.

Electrons in a 2s orbital are of lower energy than those is 2p orbitals. They are closer to the nucleus and experience a stronger force of electrostatic attraction and so are more difficult to remove.

(b) The sixth ionization energy corresponds to the change:

$$Al^{5+}(g) \rightarrow Al^{6+}(g) + e^-$$

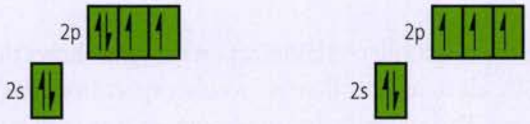
Al^{5+} has the configuration $1s^22s^22p^4$ ($1s^22s^22p_x^{\ 2}2p_y^{\ 1}2p_z^{\ 1}$). The electron is removed from a doubly occupied 2p orbital.

The seventh ionization energy corresponds to the change:

$$Al^{6+}(g) \rightarrow Al^{7+}(g) + e^-$$

The electron is removed from a singly occupied 2p orbital.

An electron in a doubly occupied orbital is repelled by its partner, and so is easier to remove than electrons in half-filled orbitals, which do not experience this force of repulsion.



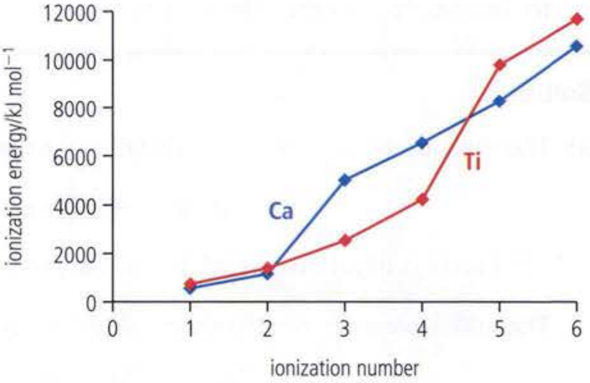
Al^{5+}: $1s^22s^22p_x^{\ 2}2p_y^{\ 1}2p_z^{\ 1}$ **Al^{6+}: $1s^22s^22p_x^{\ 2}2p_y^{\ 1}2p_z^{\ 1}$**

▲ The electron removed from the Al^{5+} ion is from a doubly occupied 2p orbital. This is easier to remove than an electron in a singly occupied orbital because it is repelled by its partner.

Successive ionization energies of transition elements

One of the key features of transition metal chemistry is the wide range of oxidation states that the metals display in their compounds. Calcium, for example, only shows the +2 state whereas titanium shows the +4 , +3, and +2 states. The difference in behaviour can be related to patterns in successive ionization energies (Figure 16).

Element	Electron configuration
Ca	$1s^22s^22p^63s^23p^64s^2$
Ti	$1s^22s^22p^63s^23p^63d^24s^2$



S1.3 Figure 16 Successive ionization energies for Ca and Ti.

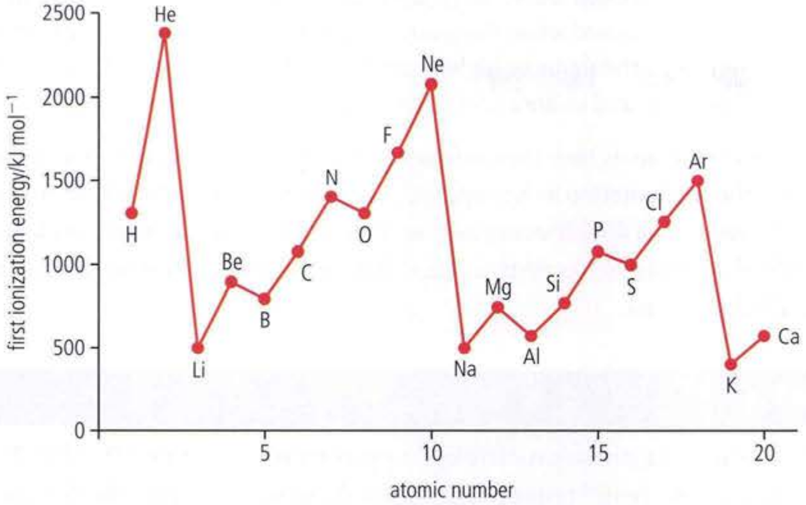
Structure 3.1 – How do patterns of successive IEs of transition elements help to explain the variable oxidation states of these elements?

The Ca^{3+} ion is energetically unstable because there is a large jump in ionization energy as the third electron is removed from the inner 3p orbital. The increase in successive energies for titanium is more gradual as the 3d and 4s orbitals are close in energy. Titanium shows the +2, +3, and +4 oxidation states. A large jump occurs between the fourth and fifth ionization energies, as the inner 3p electron is removed, so titanium does not form the +5 state.

Further evidence of sub-shells comes from a consideration of patterns in first ionization energies.

Trends in first ionization energy across periods account for the existence of main energy levels and sublevels in atoms

The periodic arrangement of the elements in the periodic table is also reflected by patterns in the first ionization energies.



▲ The first ionization energies of the first 20 elements.

- Ionization energies generally increase from left to right across a period, as the nuclear charge increases. The electrons are removed from the same main energy level, but there is an increase in the force of electrostatic attraction between the nucleus and outer electrons.
- Ionization energy decreases down a group as a new energy level, which is further from the nucleus, is occupied. Less energy is required to remove outer electrons that are further from the attractive pull of the nucleus.
- There are regular discontinuities in the trend across a period, which are explored below. These provide further evidence for the existence of sub-shells.

The metals on the left of the periodic table have low ionization energies and generally form stable positive ions. The non-metals on the right of the periodic table have high ionization energies and do not lose electrons readily. They generally form negative ions. This is explored in more detail in Structure 3.1.

Structure 3.1 - How does the trend in IE values across a period and down a group explain the trends in properties of metals and non-metals?

Worked example

Further evidence for the existence of sub-shells comes from a study of first ionization energies.

(a) In period 2, there is a decrease in first ionization energies between Be and B, and in period 3, there is a decrease between Mg and Al. Explain this decrease in ionization energies between group 2 and group 13 elements.

(b) In period 2, there is a decrease in first ionization energies between N and O, and in period 3, there is a decrease between P and S. Explain the decrease in ionization energies between group 15 and group 16 elements.

Solution

(a) The group 2 elements have the electron configuration ns^2. The group 13 elements have the electron configuration ns^2np^1.

The electron removed when the group 13 elements are ionized is a p electron. The electron removed when the group 2 elements are ionized is an s electron. Electrons in p orbitals are of higher energy and further away from the nucleus than s electrons and so are easier to remove.

(b) Group 15 elements have the configuration $ns^2np_x^1np_y^1np_z^1$. Group 16 elements have the configuration $ns^2np_x^2np_y^1np_z^1$. For group 16 elements, the electron is removed from a doubly occupied p orbital. An electron in a doubly occupied orbital is repelled by its partner and so is easier to remove than an electron in a half-filled orbital.

SKILLS

Databases can be used for compiling graphs of trends in ionization energies.

Exercise

Q31. The first four ionization energies for a particular element are 738, 1450, 7730, and 10 550 kJ mol^{-1} respectively. Deduce the group number of the element.

A 1 **B** 2 **C** 3 **D** 4

Q32. Successive ionization energies for an unknown element are given in the table.

First ionization energy / kJ mol^{-1}	Second ionization energy / kJ mol^{-1}	Third ionization energy / kJ mol^{-1}	Fourth ionization energy / kJ mol^{-1}
590	1145	4912	6491

Identify the element.

A K **B** Ca **C** S **D** Cl

Q33. The successive ionization energies (in kJ mol^{-1}) for carbon are shown in the table.

1st	2nd	3rd	4th	5th	6th
1086	2352	4619	6220	37820	47280

(a) Explain why there is a large increase between the fourth and fifth values.

(b) Explain why there is an increase between the second and third values.

Q34. Sketch a graph to show the expected pattern for the first seven ionization energies of fluorine.

Q35. The first ionization energies of the period 3 elements Na to Ar are given in Section 9 of the data booklet.

(a) Explain the general increase in ionization energy across the period.

(b) Explain why the first ionization energy of magnesium is greater than that of aluminium.

(c) Explain why the first ionization energy of sulfur is less than that of phosphorus.

Nature of Science

This chapter has highlighted the need for experimental evidence to support our scientific theories.

Scientific ideas often start as speculations which are only later confirmed experimentally. The existence of the Higgs' boson was, for example, first suggested by the physicist Peter Higgs in 1964. It was, however, only detected in 2012 when two separate international teams working at the Large Hadron Collider at CERN independently announced that they had collected evidence to support its existence.

TOK

The discovery of the Higgs boson was greatly facilitated by growth in computing power and sensor technology. Experiments in CERN's Large Hadron Collider regularly produce 23 petabytes of data per second, equivalent to 13.3 years of high-definition TV content per second. How does computation help people to process data to gain knowledge?

HL end

Guiding Question revisited

How can we model the energy states of electrons in atoms?

In this chapter we have developed models of the energy states of electrons in atoms to explain atomic emission line spectra and patterns in successive ionization energies of an element, and first ionizations.

- Electromagnetic radiation can be described using a wave model or a particle model. The speed of the wave (c) is related to the frequency (f) and wavelength (λ) by the expression: $c = f\lambda$
- The existence of lines in an emission spectrum indicates that the electron can only exist in discrete energy levels. The lines in the spectra converge at high energies because the gaps between energy levels in the atom decrease at higher energies.
- In the Bohr model of the hydrogen atom, the electron travels in orbits of discrete radii around the nucleus. This model correctly predicts the frequencies and wavelengths of the line spectra but does not apply to more complex systems with more than one electron.
- According to the quantum theory, an electron's trajectory can only be described in terms of probabilities and a wave model of the electron is needed.
- Electrons in the atom occupy atomic orbitals, which are regions in which the electron is most likely to be found. Two electrons of opposite spin can occupy one orbital.
- Atomic orbitals have different shapes, sizes and energies. Orbitals of the same energy form sublevels. The first energy level is made up of one sublevel, the second has two sublevels and so on.
- The ground state configuration of an atom is obtained using the Aufbau principle, with electrons occupying the available orbitals of lowest energy.
- The periodic table reflects the periodicity of the electron configuration. Elements with valence electrons in s orbitals are in the s block, elements with valence electrons in p orbitals are in the p block, and so on.
- The energy of a photon (E_{photon}) depends on the frequency (f) according to Planck's equation: $E_{\text{photon}} = hf$.
- When an excited electron in an atom loses energy, the energy is given out as a photon. $\Delta E_{\text{atom}} = E_{\text{photon}}$

Practice questions

1. What is the electron configuration of the Cr^{2+} ion?

A [Ar] $3d^5 4s^1$ **B** [Ar] $3d^3 4s^1$

C [Ar] $3d^6 4s^1$ **D** [Ar] $3d^4 4s^0$

2. Which is correct for the following regions of the electromagnetic spectrum?

	Ultraviolet (UV)		**Infrared (IR)**	
A	high energy	short wavelength	low energy	low frequency
B	high energy	low frequency	low energy	long wavelength
C	high frequency	short wavelength	high energy	long wavelength
D	high frequency	long wavelength	low frequency	low energy

3. An ion has the electron configuration $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$.
Which ion could it be?

A Ni^{2+} **B** Cu^+ **C** Cu^{2+} **D** Co^{3+}

4. In the emission spectrum of hydrogen, which electron transition would produce a line in the visible region of the electromagnetic spectrum?

A $n = 2 \rightarrow n = 1$ **B** $n = 3 \rightarrow n = 2$

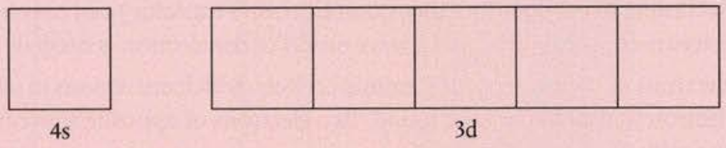
C $n = 2 \rightarrow n = 3$ **D** $n = \infty \rightarrow n = 1$

5. The electron configuration of chromium can be expressed as $[Ar]4s^x 3d^y$.

(a) Explain what the square brackets around argon, [Ar], represent. (1)

(b) State the values of x and y. (1)

(c) Annotate the diagram below to show the 4s and 3d orbitals for a chromium atom. Use an arrow, ↿ and ⇂, to represent a spinning electron.



(1)

(Total 3 marks)

6. **(a)** List the following types of electromagnetic radiation in order of increasing wavelength (shortest first).

I. Yellow light II. Red light

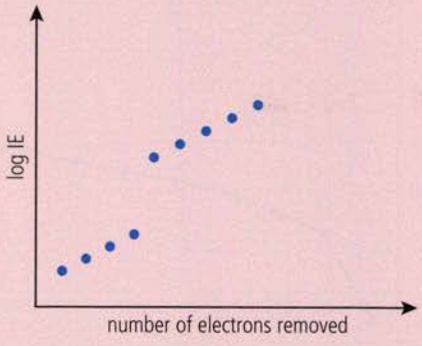
III. Infrared radiation IV. Ultraviolet radiation (1)

(b) Distinguish between a continuous spectrum and a line spectrum. (1)

(Total 2 marks)

HL

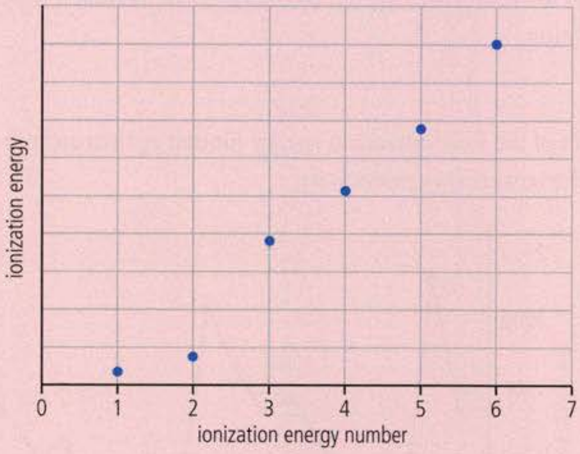
7. The graph represents the energy needed to remove nine electrons, one at a time, from an atom of an element. Not all of the electrons have been removed.



Which element could this be?

A C **B** Si **C** P **D** S

8. The graph gives the successive ionization energies for an element X.



Deduce the charge of the most stable ion formed by X.

A X^+ **B** X^{2+} **C** X^{3+} **D** X^{4+}

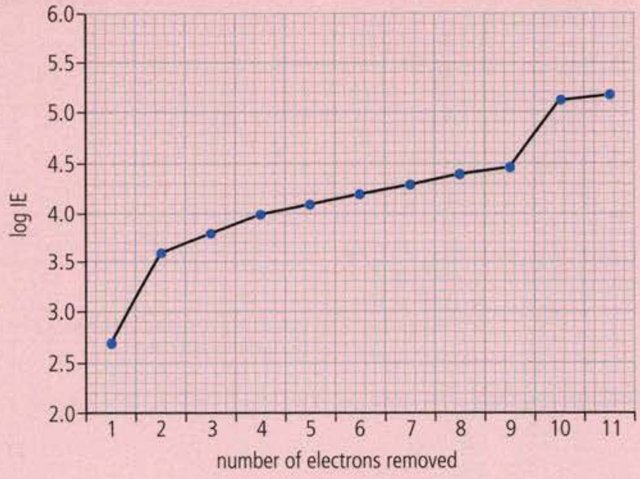
9. The successive ionization energies of an element, Y, are shown in the table.

	1st	2nd	3rd	4th	5th	6th	7th
Ionization energy / kJ mol^{-1}	788	1577	3232	4356	16091	19805	23780

Identify the type of orbital from which the first electron is removed when the first ionization energy is determined.

A s orbital **B** p orbital **C** d orbital **D** f orbital

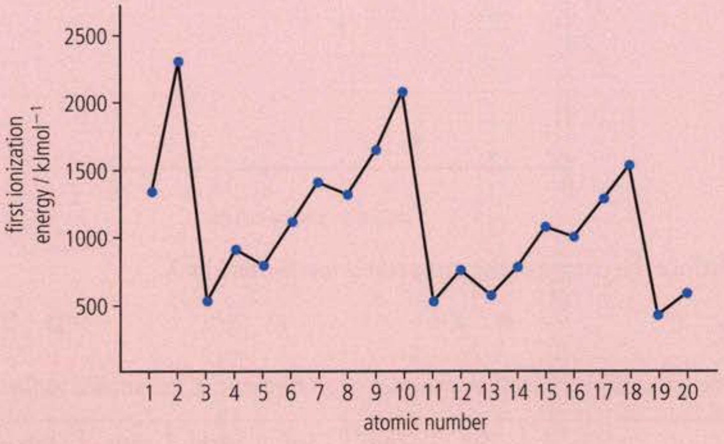
10. The graph represents the successive ionization energies of sodium. The vertical axis plots log(ionization energy) instead of ionization energy to allow the data to be represented without using an unreasonably long vertical axis.



State the full electron configuration of sodium and explain how the successive ionization energy data for sodium are related to its electron configuration. (4)

(Total 4 marks)

11. The graph of the first ionization energy plotted against atomic number for the first 20 elements shows periodicity.

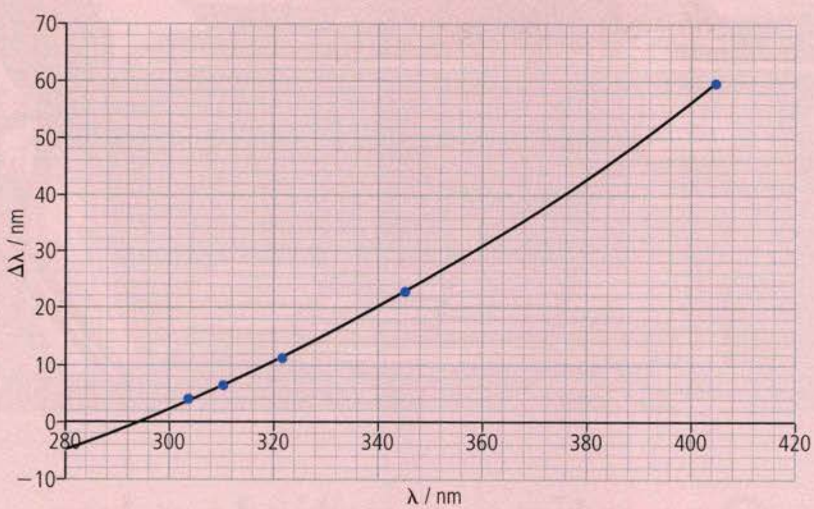


(a) Explain how information from this graph provides evidence for the existence of main energy levels and sublevels within atoms. (4)

(b) State what is meant by the term *second ionization energy*. (1)

(Total 5 marks)

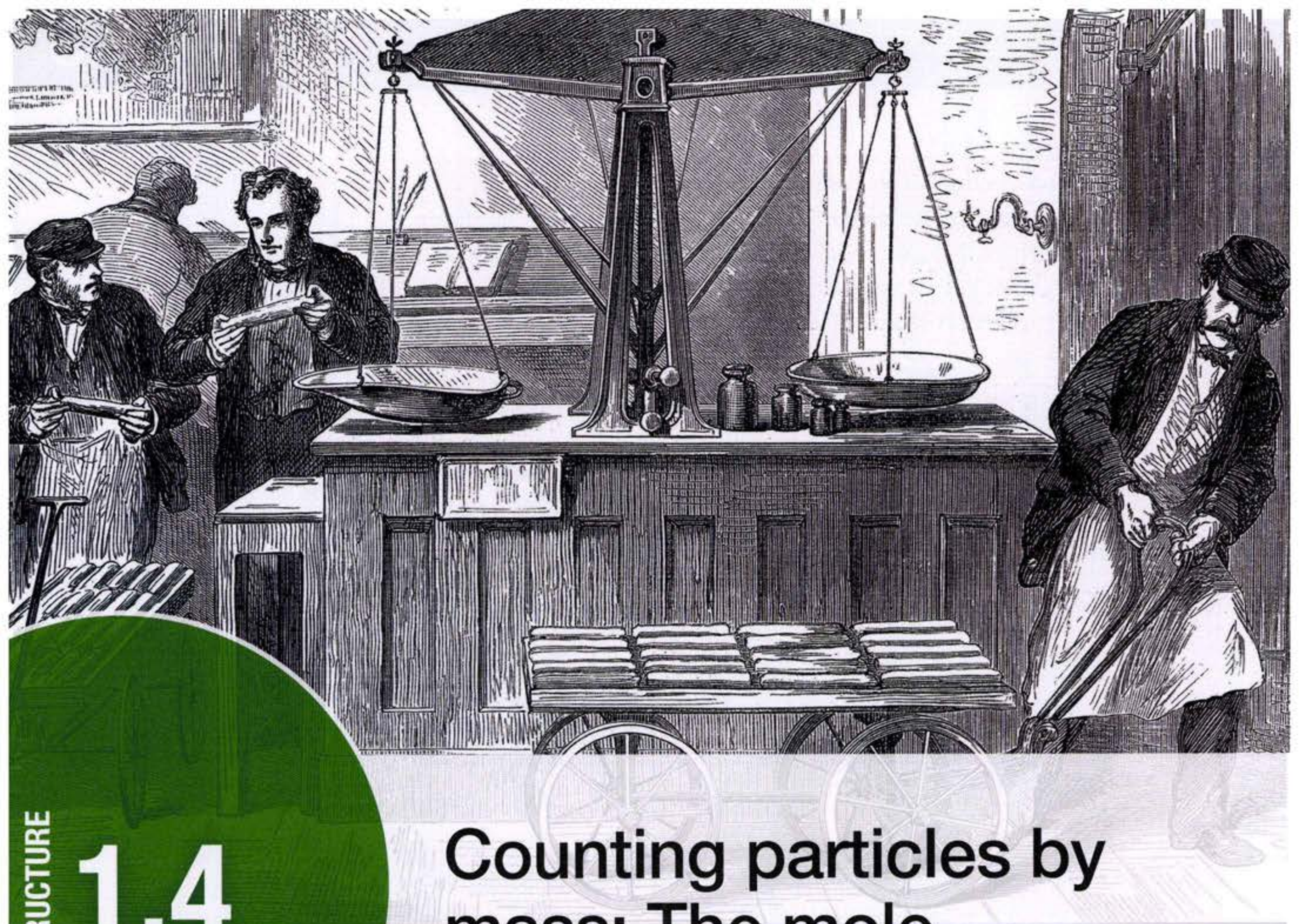
12. The emission spectrum of potassium includes a number of lines corresponding to the transitions involving the valence electron falling from excited states back to the 4s orbital. The graph shows the wavelength λ_n of a number of these lines in the spectrum plotted against the difference in wavelength between consecutive lines ($\Delta\lambda = \lambda_n - \lambda_{n+1}$).



Determine the wavelength that corresponds to ionization of potassium and calculate the ionization energy in kJ mol^{-1}. (2)

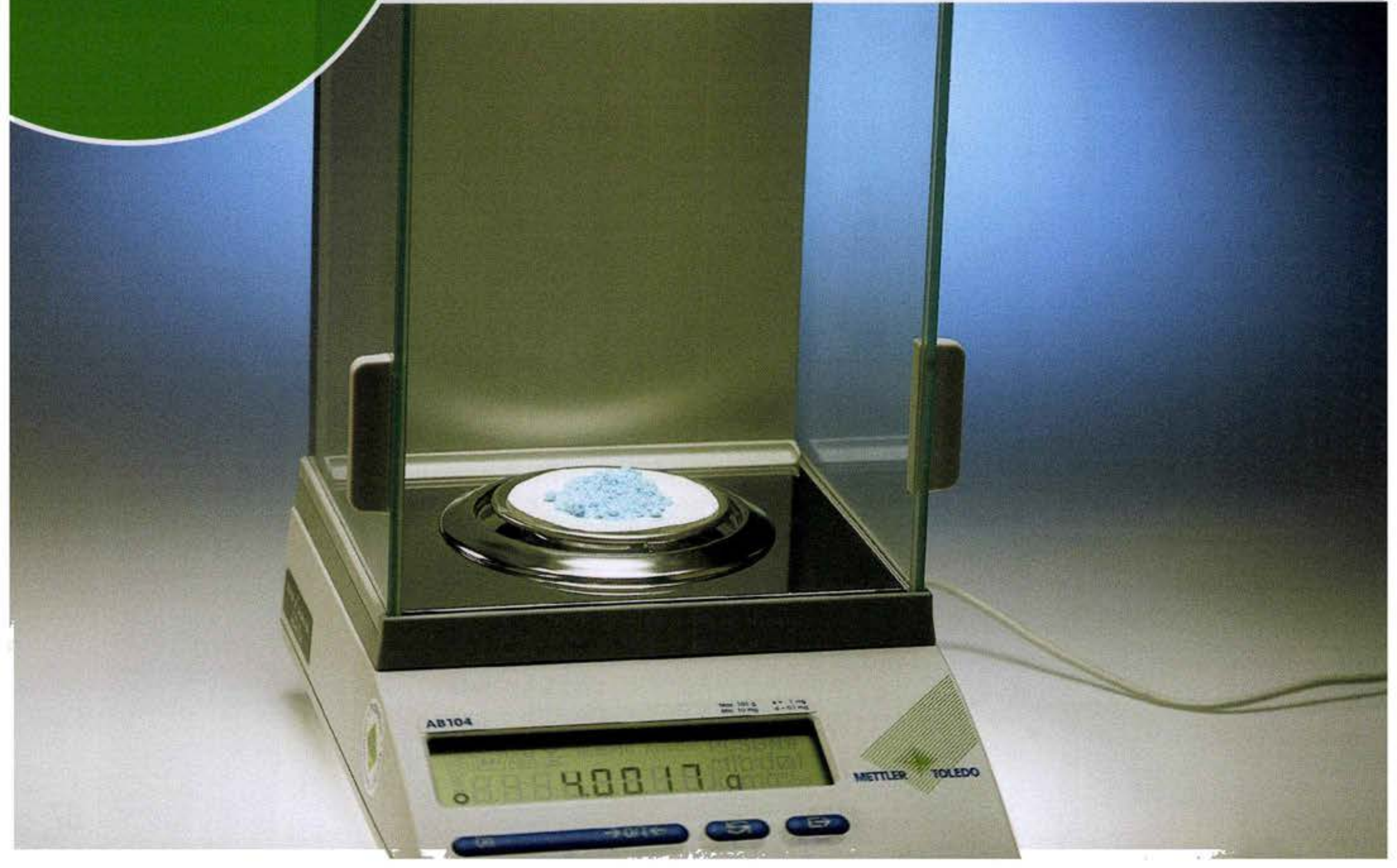
(Total 2 marks)

HL end



STRUCTURE 1.4

Counting particles by mass: The mole



◀ **(Top)** Entrance to the Bank of England, London, 1872. Samples of precious metals such as gold and silver are being checked for mass on the balance in the centre. **(Bottom)** A modern analytical instrument that measures mass to a high degree of precision, accounting for small factors such as dust and airflow.

Nature of Science

Advances in technology have led to increasingly precise ways of measuring mass, as well as units derived from it, such as concentration. This means that values which were previously too low to be detected can now be reported accurately. This makes possible changes in regulations and laws, such as levels of pollutants in fluids and of illegal drugs in the bloodstream. Authorities and governments often depend on measurements such as these in making judgements and enforcing the law. It is therefore essential that the data collected are reliable and include clearly stated uncertainties.

Guiding Question

How do we quantify matter on the atomic scale?

Chemical change involves interactions between atoms that have fixed mass. Yet the mass of an individual atom is so small that it is not practical to measure it directly in a laboratory. The upper limit of precision of very high quality analytical balances is generally about 1×10^{-8} kg, whereas, for example, a single atom of carbon weighs 1.99×10^{-26} kg.

Clearly, we need a way to close the gap between what can be measured and what is happening on the atomic scale. In this chapter we will learn how solving this problem led to the development of the chemical unit of amount, the mole. The mole is a fundamental unit in the SI system and is one of the most widely used tools in chemistry. It allows a form of book-keeping at the atomic level, making that important link between the measurable mass and the number of reacting particles.

Structure 1.4.1 – The mole as the unit of amount

Structure 1.4.1 – The mole (mol) is the SI unit of amount of substance. One mole contains exactly the number of elementary entities given by the Avogadro constant.

Convert the amount of substance, *n*, to the number of specified elementary entities.

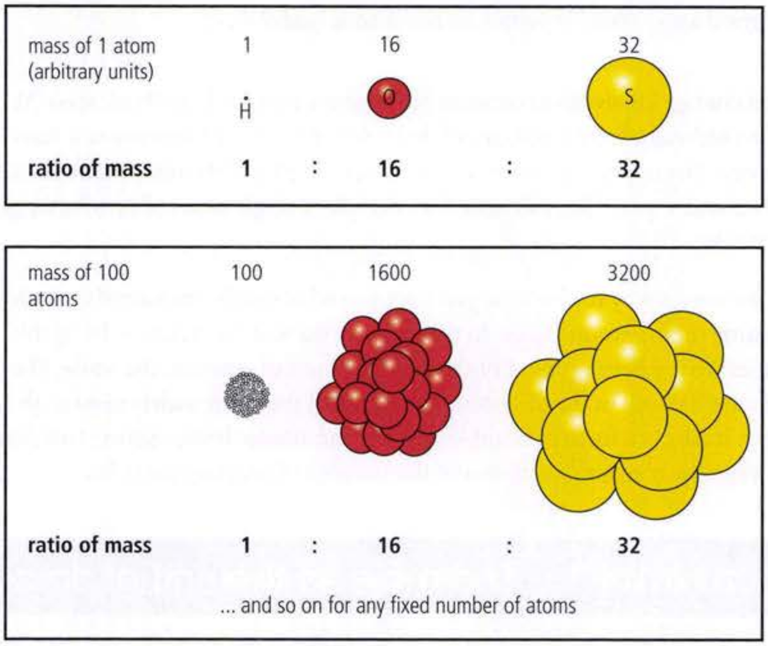
An elementary entity may be an atom, a molecule, an ion, an electron, any other particle or a specified group of particles. Avogadro's constant (N_A) is given in the data booklet. It has the units mol^{-1}.	

The Avogadro constant defines the mole as the unit of amount in chemistry

SKILLS The mole. Full details of how to carry out this activity with a worksheet are available in the eBook.

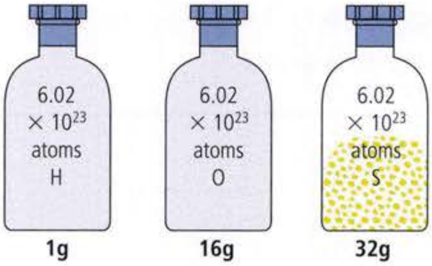
We know that even with the very best experimental apparatus available, we are unable to measure the mass of individual atoms in the laboratory directly. They are simply too small. This is not really a problem because all we need to do is to weigh an appropriately large number of atoms to give a mass that will be a useful quantity in grams. As atoms do not react individually but in very large numbers, this approach makes sense. So how many atoms shall we lump together in our 'appropriately large number'?

Let us first consider that atoms of different elements have different masses because they contain different numbers of particles, mostly **nucleons** in their nucleus, as discussed in Structure 1.2. This means we can compare their masses with each other in relative terms. For example, an atom of oxygen has a mass approximately 16 times greater than an atom of hydrogen, and an atom of sulfur has a mass about twice that of an atom of oxygen. The good news is that these ratios will stay the same when we increase the number of atoms, *so long as we ensure we have the same number of each type of atom.*



100 atoms of H, O and S have the same mass ratio as one atom of each element, 1 : 16 : 32.

If we could take 6×10^{23} atoms of hydrogen, it would have a mass of 1 g. It follows from the ratios above that *the same number of atoms* of oxygen would have a mass of 16 g, while *the same number of atoms* of sulfur would have a mass of 32 g. We now have a quantity of atoms that we can measure in grams (Figure 1).



S1.4 Figure 1 6.02×10^{23} atoms of H, O and S have the same mass ratio as one atom of each element. This number of atoms gives an amount that we can see and measure in grams.

This number, accurately stated as $6.02214129 \times 10^{23}$, is known as the Avogadro number and it is the basis of the unit of **amount** used in chemistry known as the **mole**. In other words, one mole of a substance contains the Avogadro number of particles. Mole, the unit of amount, is one of the base units in the SI system and has the unit symbol **mol.**

The example in Figure 1 is illustrative only, as in reality hydrogen and oxygen do not occur stably as single atoms, but as diatomic molecules, H_2 and O_2, as explained in Structure 2.2. Other substances exist as particles of different types, so the term **elementary entity** is used to cover the broad range of possible particles. An elementary entity may be an atom, a molecule, an ion, an electron, any other particle or a specified group of particles.

In 2019, the International Union of Pure and Applied Chemistry (IUPAC) published a change to the definition of the mole. The new definition emphasizes that the quantity 'amount of substance' is concerned with counting entities, rather than measuring the mass of a sample.

The SI refers to the metric system of measurement based on seven base units. These are metre (m) for length, kilogram (kg) for mass, second (s) for time, ampere (A) for electric current, kelvin (K) for temperature, candela (cd) for luminous intensity and mole (mol) for amount. All other units are derived from these. The SI system is the world's most widely used system of measurement.

The International Bureau of Weights and Measures (BIPM according to its French initials) is an international standards organization, which aims to ensure uniformity in the application of SI units around the world. The BIPM officially introduced updated definitions to these base units, including the mole, in 2019.

So 'mole' is simply a word that represents a number, just as 'couple' is a word for 2 and 'dozen' is a word for 12. A mole is a very large number, bigger than we can easily imagine or ever count, but it is nonetheless a fixed number. So a mole of any substance contains the Avogadro number, 6.02×10^{23}, of entities. It can refer to atoms, molecules, ions, electrons and so on – it can be applied to any entity because it is just a number. And from this, we can easily calculate the number of particles in any fraction or multiple of a mole of a substance.

Amedeo Avogadro (1776–1856) was an Italian scientist who made several experimental discoveries. He clarified the distinction between atoms and molecules, and used this to propose the relationship between gas volume and number of molecules. His ideas were not accepted in his time, largely due to a lack of consistent experimental evidence. After his death, when his theory was confirmed by fellow Italian Cannizzaro, his name was given in tribute to the famous constant that he helped to establish.

The mole is the SI unit of amount of substance. One mole contains exactly 6.022×10^{23} elementary entities. This number is the fixed numerical value of the Avogadro constant, N_A.

Each sample contains one mole, 6.02×10^{23} particles, of a specific element. Each has a characteristic mass, known as its molar mass. Clockwise from upper left the elements are: carbon (C), sulfur (S), iron (Fe), copper (Cu) and magnesium (Mg).

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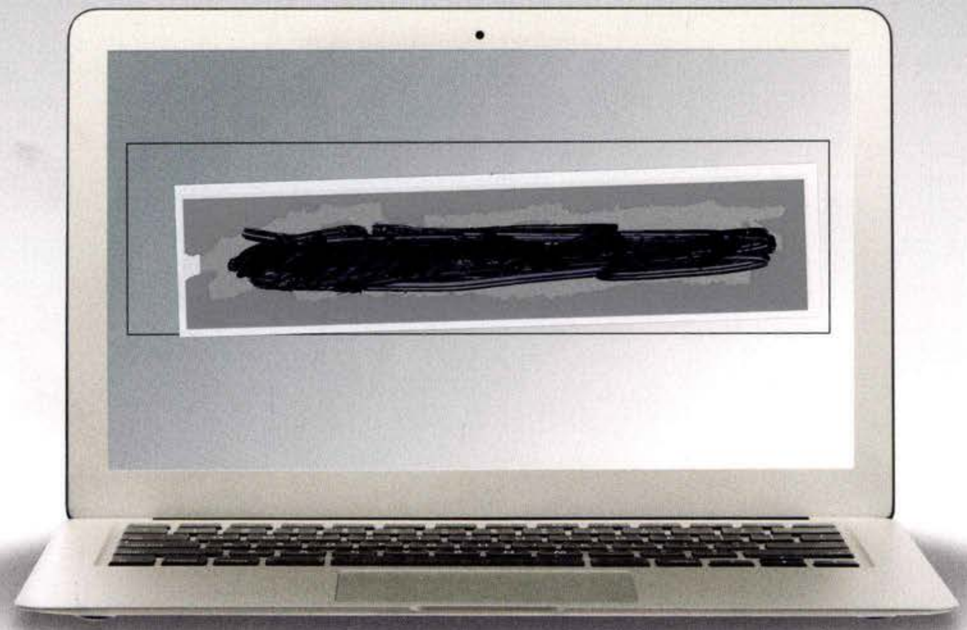

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