# 2 Atomic structure

Learning objectives

- Understand that an atom is made up of protons, neutrons and electrons
- Define mass number, atomic number and isotope
- Work out the numbers of protons, neutrons and electrons in atoms and ions
- Discuss the properties of isotopes
- Calculate relative atomic masses and abundances of isotopes
- Understand that a mass spectrometer can be used to determine the isotopic composition of a sample
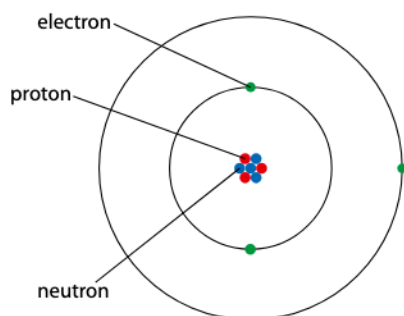
Figure 2.1 A simple representation of a lithium atom (not to scale).

Particle	Relative mass	Relative charge
proton	1	+1
neutron	1	0
electron	5×10^{-4}	−1

Table 2.1 The properties of protons, neutrons and electrons. The mass of an electron is often regarded as negligible.

Protons and neutrons are made up of other particles called quarks.

2.1 The nuclear atom

There are approximately 92 naturally occurring elements, plus several more that have been made artificially in nuclear reactions, and probably a few more that have yet to be discovered. As far as we know, there are no more naturally occurring elements – these are the only elements that make up our universe.

Chemistry is the study of how **atoms** of the various elements are joined together to make everything we see around us. It is amazing when one imagines that the entire Universe can be constructed through combinations of these different elements. With just 92 different building blocks (and in most cases many fewer than this), objects as different as a table, a fish and a piece of rock can be made. It is even more amazing when one realises that these atoms are made up of three subatomic ('smaller than an atom') particles, and so the whole Universe is made up of combinations of just three things – protons, neutrons and electrons.

2.1.1 Atoms

In the simplest picture of the atom the negatively charged electrons orbit around the central, positively charged nucleus (Figure **2.1**). The nucleus is made up of protons and neutrons (except for a hydrogen atom, which has no neutrons).

Protons and neutrons, the particles that make up the nucleus, are sometimes called nucleons.

The actual mass of a proton is 1.67×10^{-27} kg and the charge on a proton is $+1.6 \times 10^{-19}$ C. Relative masses and charges, shown in Table **2.1**, are used to compare the masses of particles more easily. Because the values are relative, there are no units.

From these values it can be seen that virtually all the mass of the atom is concentrated in the nucleus. However, most of the volume of the atom is due to the electrons – the nucleus is very small compared with the total size of the atom.

The diameter of an atom is approximately 1×10^{-10} m and that of a nucleus between about 1×10^{-14} and 1×10^{-15} m, meaning that a nucleus is about 10 000 to 100 000 times smaller than an atom. So, if the nucleus were the size of the full stop at the end of this sentence, the atom would be between 3 and 30 m across.

None of these particles can be observed directly. These particles were originally 'discovered' by the interpretation of experimental data. Do we know or believe in the existence of these particles? If we looked at a science textbook of 200 years ago there would be no mention of protons, electrons and neutrons. If we could look at a chemistry textbook of 200 years in the future will there be any mention of them? Are these particles a true representation of reality, or a device invented by scientists to make sense of experimental data and provide an explanation of the world around them?

Democritus and his teacher Leucippus, fifth-century BC Greek philosophers, are often credited with first suggesting the idea of the atom as the smallest indivisible particle of which all matter is made.

John Dalton (1766–1844) is generally regarded as the founder of modern atomic theory.

The **atomic number (Z)** defines an element – it is unique to that particular element. For example, the element with atomic number 12 is carbon and that with atomic number 79 is gold. This means that we could use the atomic number of an element instead of its name. However, the name is usually simpler and more commonly used in everyday speech.

The overall charge on an atom is zero and therefore:

Atomic number (Z) is the number of protons in the nucleus of an atom.

> **number of protons in an atom = number of electrons**

Atomic number is, however, defined in terms of protons, because electrons are lost or gained when ions are formed in chemical reactions.

> **Mass number (A) is the number of protons plus neutrons in the nucleus of an atom.**

Therefore:

> **number of neutrons in an atom = mass number − atomic number**

The full symbol of an element includes the atomic number and the mass number (see Figure **2.2**). For example, sodium has an atomic number of 11 and a mass number of 23. The nucleus of a sodium atom contains 11 protons and 12 neutrons (23 − 11). Surrounding the nucleus are 11 electrons. The symbol for sodium is $^{23}_{11}$Na.

Ions

> **Ions are charged particles that are formed when an atom loses or gains (an) electron(s).**

A **positive** ion (cation) is formed when an atom **loses** (an) **electron**(s) so that the ion has more protons(+) than electrons(−) (Figure **2.3**). A **negative** ion (anion) is formed when an atom **gains** (an) **electron**(s) so that the ion has more electrons(−) than protons(+).

The electron was discovered in 1897 by J. J. Thompson at the University of Cambridge, UK.
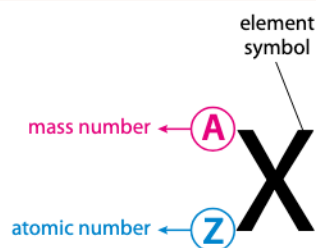
Figure 2.2 Where to place the mass number (A) and atomic number (Z) in the full symbol of an element.
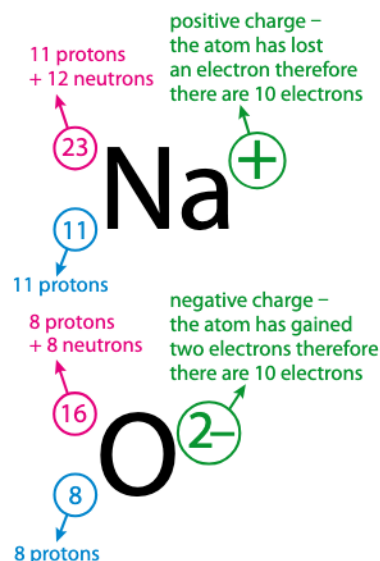
Figure 2.3 The number of subatomic particles in the Na^+ and O^{2-} ions.

2.1.2 Isotopes

The mass number of chlorine is given in many periodic tables as 35.5. It is not possible to have half a neutron – the mass number that is given is an average, taking into account the presence of isotopes.

> **Isotopes** are different atoms of the same element with different mass numbers: i.e. different numbers of neutrons in the nucleus.

The two isotopes of chlorine are ^{35}Cl (chlorine–35) and ^{37}Cl (chlorine–37). Most naturally occurring samples of elements are composed of a mixture of isotopes, but usually one isotope is far more abundant than the others and the mass number of the most common isotope is quoted.

The numbers of protons, neutrons and electrons in some isotopes are shown in Table **2.2**.

> **Isotopes** have the same chemical properties (they react in exactly the same way) but different physical properties (e.g. different melting points and boiling points).

Isotope	Protons	Neutrons	Electrons
$^{1}_{1}$H	1	0	1
$^{2}_{1}$H	1	1	1
$^{3}_{1}$H	1	2	1
$^{12}_{6}$C	6	6	6
$^{13}_{6}$C	6	7	6
$^{14}_{6}$C	6	8	6
$^{35}_{17}$Cl	17	18	17
$^{37}_{17}$Cl	17	20	17

Table 2.2 The numbers of subatomic particles in some common isotopes.

The isotopes of hydrogen are sometimes given different names and symbols: hydrogen–1 is called protium; hydrogen–2 is deuterium (D); and hydrogen–3 is tritium (T).

Isotopes react in the same way because they have the same numbers of electrons, and chemical reactions depend only on the number and arrangement of electrons and not on the composition of the nucleus. For example, both protium and deuterium would react in the same way with nitrogen:

$$N_2 + 3H_2 \rightleftharpoons 2NH_3 \qquad N_2 + 3D_2 \rightleftharpoons 2ND_3$$

Isotopes have different physical properties because, for example, the different masses mean that their atoms move at different speeds. The boiling point of ^{1}H$_2$ is $-253\,°C$, whereas that of ^{2}H$_2$ is $-250\,°C$. Heavy water (D$_2$O) has a melting point of $3.8\,°C$ and a boiling point of $101.4\,°C$.

Nature of science

In science, things change! Science is an ever changing and increasing body of knowledge. This is what Richard Feynman meant when he talked about science as '… *the belief in the ignorance of experts*'.

An important example of how knowledge and understanding have changed is the development of atomic theory. Since the days of John Dalton (1766-1844) our view of the world around us has changed dramatically. These developments have happened through careful observation and experiment and have gone hand–in–hand with improvements in equipment and the development of new technology.

Radioactivity was discovered towards the end of the 19th century and this gave scientists a new tool to probe the atom. In a famous experiment Geiger and Marsden subjected a thin film of metal foil to a beam of alpha particles (helium nuclei, ^{4}He^{2+}) and found that some of the particles were reflected back at large angles. Their experimental data allowed Rutherford to develop the theory of the nuclear atom.

The discovery of subatomic particles (protons, neutrons and electrons) in the late nineteenth and early twentieth centuries necessitated a paradigm shift in science and the development of much more sophisticated theories of the structure of matter.

? Test yourself

1 Give the number of protons, neutrons and electrons in the following atoms:

$^{238}_{92}$U $^{75}_{33}$As $^{81}_{35}$Br

2 Give the number of protons, neutrons and electrons in the following ions:

$^{40}_{20}$Ca^{2+} $^{127}_{53}$I$^-$ $^{140}_{58}$Ce^{3+}

3 If you consider the most common isotopes of elements as given in a basic periodic table, how many elements have more protons than neutrons in an atom?

4 The following table shows the number of protons, electrons and neutrons in a series of atoms and ions.

Symbol	Protons	Neutrons	Electrons
D	27	30	25
X	43	54	42
Q	35	44	35
L	27	32	26
M	35	46	36
Z	54	78	54

a Which symbols represent isotopes?
b Which symbols represent positive ions?

Relative atomic masses

Because of the different isotopes present, it is most convenient to quote an average mass for an atom – this is the **relative atomic mass (A_r)**.

> The relative atomic mass (A_r) of an element is the average of the masses of the isotopes in a naturally occurring sample of the element relative to the mass of $\frac{1}{12}$ of an atom of carbon–12.

How to calculate relative atomic mass

Worked examples

2.1 Lithium has two naturally occurring isotopes:

^{6}Li: natural abundance 7% ^{7}Li: natural abundance 93%

Calculate the relative atomic mass of lithium.

Imagine we have 100 Li atoms: 7 will have mass 6 and 93 will have mass 7.

The average mass of these atoms is:

$$\frac{(7 \times 6) + (93 \times 7)}{100} = 6.93$$

Therefore the A_r of Li is 6.93.

2.2 Iridium has a relative atomic mass of 192.22 and consists of Ir–191 and Ir–193 isotopes. Calculate the percentage composition of a naturally occurring sample of iridium.

We will assume that we have 100 atoms and that x of these will have a mass of 191. This means that there will be $(100 - x)$ atoms that have a mass of 193.

The total mass of these 100 atoms will be: $191x + 193(100 - x)$

The average mass of the 100 atoms will be: $\dfrac{191x + 193(100 - x)}{100}$

Therefore we can write the equation: $\dfrac{191x + 193(100 - x)}{100} = 192.22$

$$191x + 193(100 - x) = 19\,222$$

$$191x + 19\,300 - 193x = 19\,222$$

$$-2x = 19\,222 - 19\,300$$

$$-2x = -78$$

Therefore $x = 39$.

This means that the naturally occurring sample of iridium contains 39% Ir–191 and 61% Ir–193.

Alternatively:

$$\frac{A_r - \text{mass number of lighter isotope}}{\text{difference in mass number of two isotopes}} \times 100 = \% \text{ of heavier isotope}$$

In the example here: $\dfrac{(192.22 - 191)}{(193 - 191)} \times 100 = 61\%$
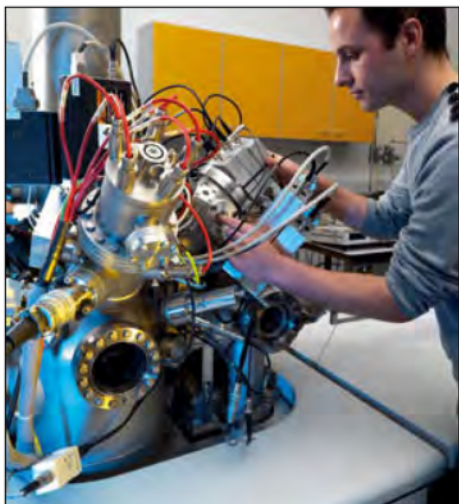

Figure 2.4 Setting up a mass spectrometer.

The mass spectrum of an element and relative atomic mass

The proportion of each isotope present in a sample of an element can be measured using an instrument called a **mass spectrometer** (Figure **2.4**).

The readout from a mass spectrometer is called a mass spectrum. In a mass spectrum of an element, we get one peak for each individual isotope. The height of each peak (more properly, the area under each peak) is proportional to the number of atoms of this isotope in the sample tested. The mass spectrum of magnesium is shown in Figure **2.5**.

78.6 —— area under peak

Mg

10.1   11.3

24   25   26

Mass:charge ratio (m/z)

Abundance/%
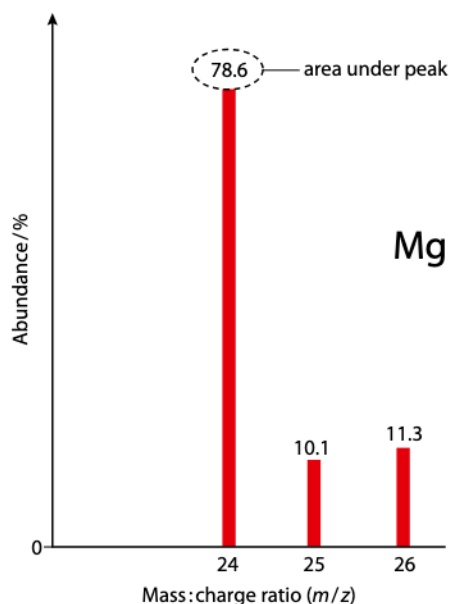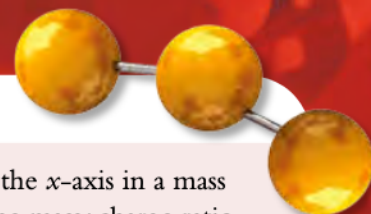
Figure 2.5 The mass spectrum of magnesium showing the amounts of the different isotopes present.

The scale on the x-axis in a mass spectrum is the mass:charge ratio (m/z or m/e). In order to pass through a mass spectrometer, atoms are bombarded with high-energy electrons to produce positive ions. Sometimes more than one electron is knocked out of the atom, which means that the ions behave differently, as if they have smaller masses – hence the use of mass:charge ratio. We can generally ignore this and assume that the horizontal scale refers to the mass of the isotope (the mass of the electron removed is negligible).

The relative atomic mass can be calculated using:

$$A_r = \frac{(78.6 \times 24) + (10.1 \times 25) + (11.3 \times 26)}{100} = 24.3$$

❓ Test yourself

5 Chromium has four naturally occurring isotopes, and their masses and natural abundances are shown in the table below.

Isotope	Natural abundance (%)
^{50}Cr	4.35
^{52}Cr	83.79
^{53}Cr	9.50
^{54}Cr	2.36

Calculate the relative atomic mass of chromium to two decimal places.

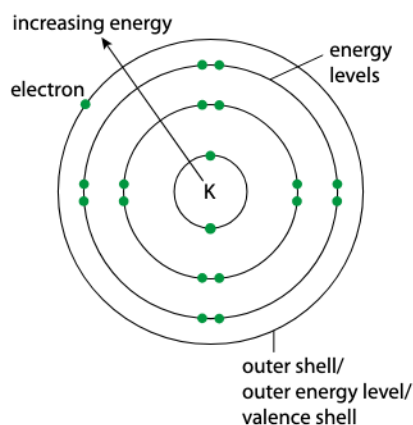6 Silicon has three naturally occurring isotopes and their details are given in the table below.

Isotope	Natural abundance (%)
^{28}Si	92.2
^{29}Si	4.7
^{30}Si	3.1

Calculate the relative atomic mass of silicon to two decimal places.

7 a Indium has two naturally occurring isotopes: indium–113 and indium–115. The relative atomic mass of indium is 114.82. Calculate the natural abundance of each isotope.

  b Gallium has two naturally occurring isotopes: gallium–69 and gallium–71. The relative atomic mass of gallium is 69.723. Calculate the natural abundance of each isotope.

2.2 Electron configuration

2.2.1 The arrangement of electrons in atoms

At the simplest level of explanation, the electrons in an atom are arranged in **energy levels** (**shells**) around the nucleus. For example, the electron arrangement of potassium can be represented as shown in Figure **2.6** and is written as 2,8,8,1 (or 2.8.8.1).

The lowest energy level, called the first energy level or first shell (sometimes also called the K shell), is the one closest to the nucleus. The shells increase in energy as they get further from the nucleus. The maximum number of electrons in each main energy level is shown in Table **2.3**.

The main energy level number is sometimes called the **principal quantum number** and is given the symbol n. The maximum number of electrons in each shell is given by $2n^2$.

Figure 2.6 The electron arrangement of potassium.

main energy level number	1	2	3	4	5
maximum number of electrons	2	8	18	32	50

Table 2.3 Distribution of electrons in energy levels.

The general rule for filling these energy levels is that the electrons fill them from the lowest energy to the highest (from the nucleus out). The first two energy levels must be completely filled before an electron goes into the next energy level. The third main energy level is, however, only filled to 8 before electrons are put into the fourth main energy level. This scheme works for elements with atomic number up to 20.

$$\text{frequency} \propto \frac{1}{\text{wavelength}}$$

$$\text{frequency} \propto \text{energy}$$

The electromagnetic spectrum

Light is a form of energy. Visible light is just one part of the electromagnetic spectrum (Figure **2.7**).
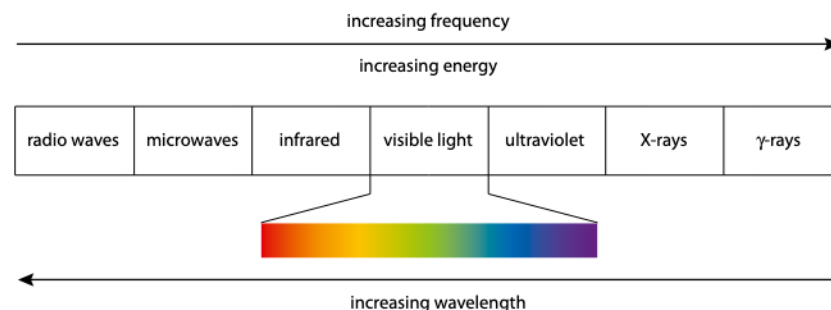
Figure 2.7 The electromagnetic spectrum.

The various forms of electromagnetic radiation are usually regarded as waves that travel at the speed of light in a vacuum $(3.0 \times 10^8 \text{ m s}^{-1})$ but vary in their frequency/energy/wavelength.

Although electromagnetic radiation is usually described as a wave, it can also display the properties of a particle, and we sometimes talk about particles of electromagnetic radiation called **photons**.
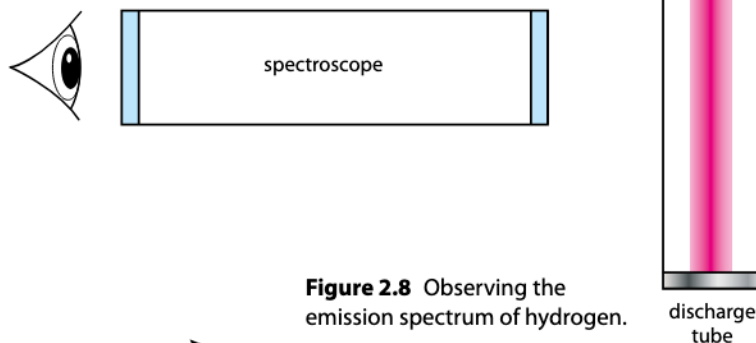
White light is visible light made up of all the colours of the spectrum. In order of increasing energy, the colours of the spectrum are: red < orange < yellow < green < blue < indigo < violet.

Evidence for energy levels in atoms

The hydrogen atom spectrum

When hydrogen gas at low pressure is subjected to a very high voltage, the gas glows pink (Figure **2.8**). The glowing gas can be looked at through a **spectroscope**, which contains a diffraction grating and separates the various wavelengths of light emitted from the gas. Because light is emitted by the gas, this is called an **emission spectrum**.

In the visible region, the spectrum consists of a series of sharp, bright lines on a dark background (Figure **2.9**). This is a **line spectrum**, as opposed to a **continuous spectrum**, which consists of all the colours merging into each other (Figure **2.10**).

Would our interpretation of the world around us be different if our eyes could detect light in other regions of the electromagnetic spectrum?

Are there really seven colours in the visible spectrum?

Figure 2.8 Observing the emission spectrum of hydrogen.

hydrogen at low pressure

discharge tube

spectroscope

increasing energy/frequency
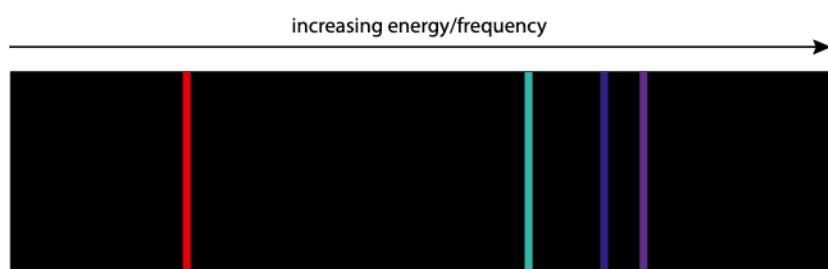
Figure 2.9 A representation of the atomic emission spectrum of hydrogen.

increasing energy/frequency
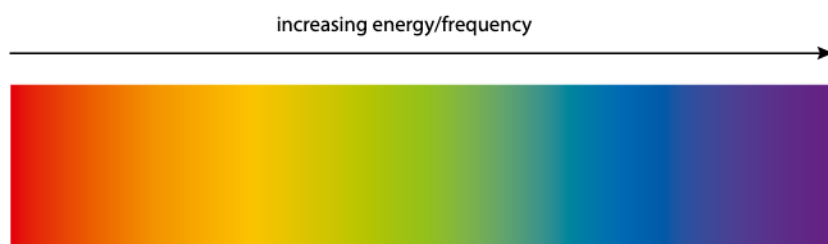
Figure 2.10 A continuous spectrum.
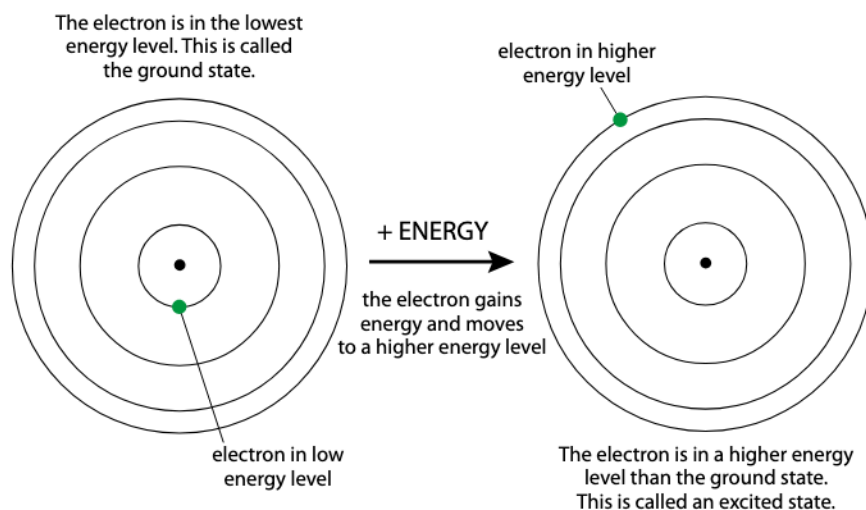
The lines get closer together at higher frequency/energy.

Each element has its own unique emission spectrum, and this can be used to identify the element.

Line spectrum – only certain frequencies/wavelengths of light present.
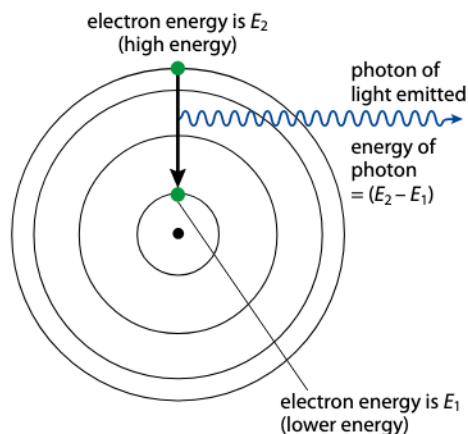Continuous spectrum – **all** frequencies/wavelengths of light present.

How an emission spectrum is formed

Passing an electric discharge through a gas causes an electron to be **promoted to a higher energy level** (shell) (Figure **2.11**).

The electron is in the lowest energy level. This is called the ground state.

electron in higher energy level

+ ENERGY

the electron gains energy and moves to a higher energy level

electron in low energy level

The electron is in a higher energy level than the ground state. This is called an excited state.

Figure 2.11 An electron can be promoted to a higher energy level in a discharge tube.

electron energy is E_2 (high energy)

photon of light emitted

energy of photon = $(E_2 - E_1)$

electron energy is E_1 (lower energy)

Figure 2.12 When an electron falls from a higher to a lower energy level in an atom, a photon of light is emitted.

Because light is given out, this type of spectrum is an emission spectrum.

Each line in the spectrum comes from the transition of an electron **from a high energy level to a lower one**.

The electron is unstable in this higher level and will **fall to a lower energy level** (Figure **2.12**). As it returns from a level at energy E_2 to E_1, the extra energy $(E_2 - E_1)$ is given out in the form of a photon of light. This contributes to a line in the spectrum.

The energy levels can also be shown as in Figure **2.13**.

Increasing energy

6
5
4
3
2
1
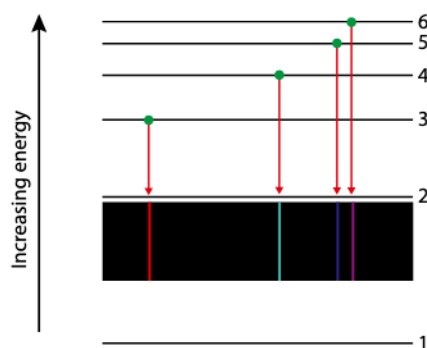
Figure 2.13 How the lines arise in the emission spectrum of hydrogen.

The fact that a line spectrum is produced provides evidence for electrons being in energy levels (shells): i.e. electrons in an atom are allowed to have only certain amounts of energy (Figure **2.14**).
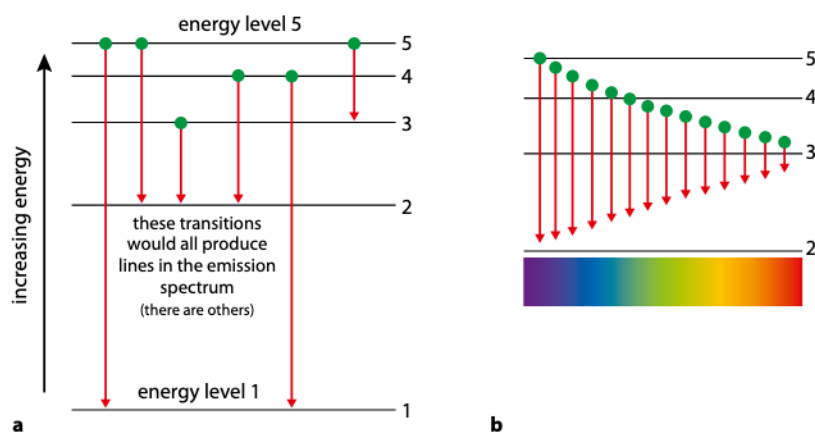
Figure 2.14 a Electrons in energy levels: only transitions between two discrete energy levels are possible, and a line spectrum is produced. **b** If the electrons in an atom could have any energy, all transitions would be possible. This would result in a continuous spectrum.

Different series of lines

Figure **2.15** shows a representation of the emission spectrum of hydrogen across the infrared, visible and ultraviolet regions. The series in each region consists of a set of lines that get closer together at higher frequency. Each series is named after its discoverer.

> The different series of lines occur when electrons fall back down to different energy levels.
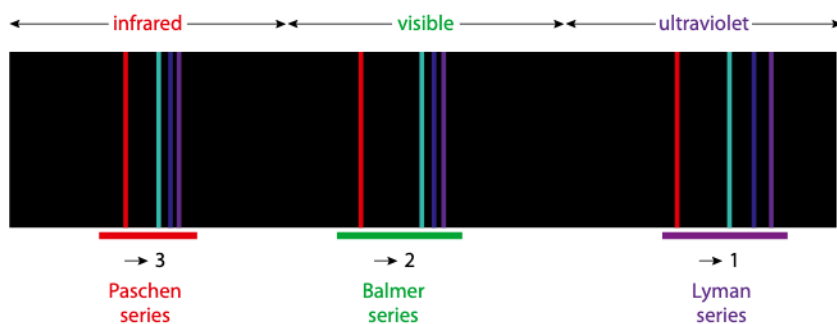
Figure 2.15 A representation of the emission spectrum of hydrogen. The colours and lines in the spectrum in the infrared and ultraviolet regions are just for illustrative purposes.

All the transitions that occur in the visible region of the spectrum (those we can see) involve electrons falling down to level 2 (creating the Balmer series). All transitions down to level 1 occur in the ultraviolet region. Therefore we can deduce that the energy difference between level 1 and any other level is bigger than that between level 2 and any other higher level.

The atomic emission spectrum of hydrogen is relatively simple because hydrogen atoms contain only one electron. Ions such as He^+ and Li^{2+}, which also contain one electron, would have spectra similar to hydrogen – but not exactly the same because the number of protons in the nucleus also influences the electron energy levels.
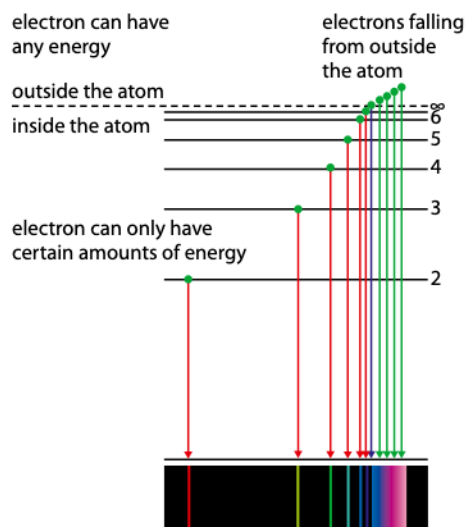
Infrared and ultraviolet radiation can be detected only with the aid of technology – we cannot interact with them directly. Does this have implications as to how we view the knowledge gained from atomic spectra in these regions?

Exam tip
The names of the series do not have to be learnt for the examination.

electron can have any energy

electrons falling from outside the atom

outside the atom

inside the atom

electron can only have certain amounts of energy
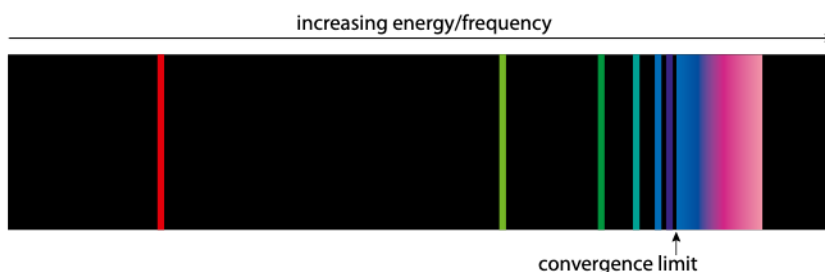
∞
6
5
4
3
2

Figure 2.17 The purple arrow represents the transition giving rise to the convergence limit in the Lyman series for hydrogen.

Convergence

The lines in the emission spectrum get closer together at higher frequency/energy (Figure **2.16**).

increasing energy/frequency

convergence limit

Figure 2.16 A representation of the Lyman series of hydrogen in the ultraviolet region of the electromagnetic spectrum.

Eventually, at the **convergence limit**, the lines merge to form a **continuum**. Beyond this point the electron can have any energy and so must be free from the influence of the nucleus, i.e. the electron is no longer in the atom (Figure **2.17**).

Extension

The convergence limit is not usually observed, but the frequency can be worked out by plotting a graph of the difference in frequency of successive lines against their frequency and extrapolating the graph to give the frequency when the difference in frequency between successive lines is zero.

Nature of science

Advances in technology are often accompanied by advances in science – Bunsen's development of his burner with a high-temperature flame in the 1850s enabled spectroscopic analysis of substances.

Scientific theories often develop from a need to explain natural phenomena. For instance, Niels Bohr, building on the work of Rutherford, proposed a model for the atom in which electrons orbit the nucleus and only exist in certain allowed energy levels. He then used this model to explain the line spectra of hydrogen and other elements.

? Test yourself

8 Arrange the following in order of:
  a increasing energy
  b decreasing wavelength
  ultraviolet radiation   **infrared radiation**
  microwaves   **orange light**   **green light**
9 Describe how a line in the Lyman series of the hydrogen atom spectrum arises.

10 Draw an energy level diagram showing the first four energy levels in a hydrogen atom and mark with an arrow on this diagram one electron transition that would give rise to:
  a a line in the ultraviolet region of the spectrum
  b a line in the visible region of the spectrum
  c a line in the infrared region of the spectrum.

2.2.2 Full electron configurations

The emission spectra of atoms with more than one electron, along with other evidence such as ionisation energy data (see later), suggest that the simple treatment of considering that electrons in atoms occupy only main energy levels is a useful first approximation but it can be expanded.

Sub-energy levels and orbitals

Each main energy level in an atom is made up of **sub–energy levels** (subshells). The first main energy level consists solely of the 1s sub–level, the second main energy level is split into the 2s sub–level and the 2p sub–level. The sub–levels in each main energy level up to 4 are shown in Table **2.4**.

Main energy level	Sub-levels				Number of electrons in each sub-level			
					s	p	d	f
1	1s				2			
2	2s	2p			2	6		
3	3s	3p	3d		2	6	10	
4	4s	4p	4d	4f	2	6	10	14

Table 2.4 The sub-levels in each main energy level up to level 4.

Within any main energy level (shell) the ordering of the sub–levels (subshells) is always s < p < d < f, but there are sometimes reversals of orders between sub–levels in different energy levels. The relative energies of the subshells are shown in Figure **2.18**.

The Aufbau (building-up) principle (part 1)

The **Aufbau principle** is simply the name given to the process of working out the electron configuration of an atom.

> Electrons fill sub–levels from the lowest energy level upwards – this gives the lowest possible (potential) energy.

So the full electron configuration of sodium (11 electrons) can be built up as follows:
- The first two electrons go into the 1s sub–level → $1s^2$: this sub–level is now full.
- The next two electrons go into the 2s sub–level → $2s^2$: this sub–level is now full.
- The next six electrons go into the 2p sub–level → $2p^6$: this sub–level is now full.
- The last electron goes into the 3s sub level → $3s^1$.

The full electron configuration of sodium is therefore $1s^2 2s^2 2p^6 3s^1$ (Figure **2.19**). This can also be abbreviated to $[Ne]3s^1$, where the electron configuration of the previous noble gas is assumed and everything after that is given in full.

Learning objectives

- Determine the full electron configuration of atoms with up to 36 electrons
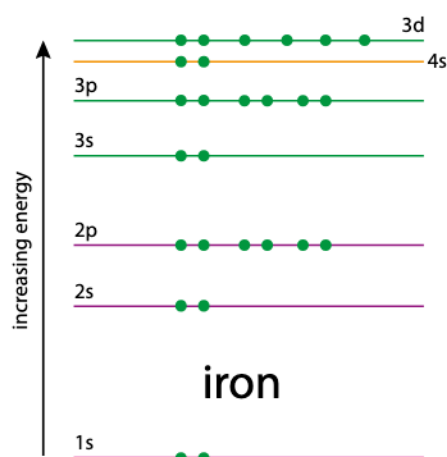- Understand what is meant by an orbital and a subshell (sub–energy level)
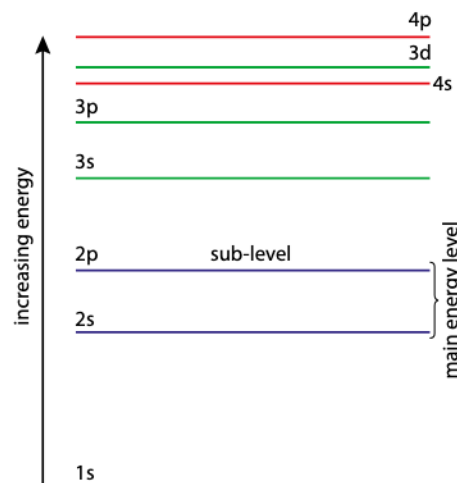
Figure 2.18 The ordering of the energy levels and sub-levels within an atom. The sub-levels within a main energy level are shown in the same colour.
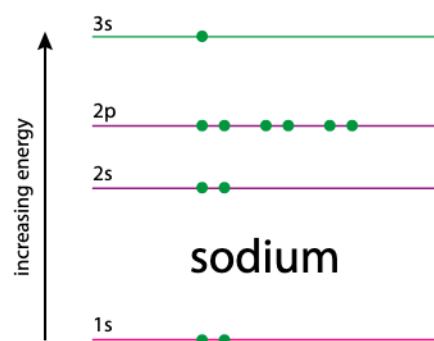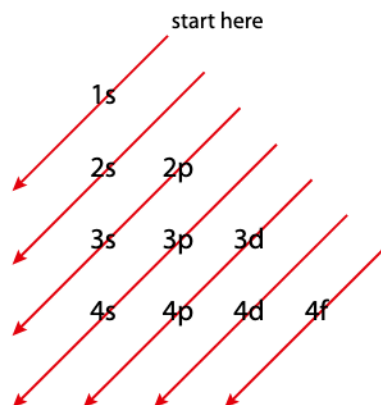

Figure 2.19 The arrangement of electrons in energy levels for a sodium atom.

$[1s^2\ 2s^2\ 2p^6]\ 3s^1$

from neon

Figure 2.20 The arrangements of electrons in energy levels for an iron atom.

iron

start here

Figure 2.22 Draw out the sub-levels in each main energy level. Starting at 1s, follow the arrows to give the ordering of the sub-levels.

The full electron configuration of iron (26 electrons) is: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$ (Figure **2.20**). Note that because the 4s sub–level is lower in energy than the 3d sub–level, it is filled first. In other words, two electrons go into the fourth main energy level before the third main energy level is filled. This can be written as $[Ar]4s^2 3d^6$.

> This is sometimes written as $[Ar]3d^6 4s^2$ to keep the sub–levels in order of the main energy levels.

The full electronic configuration of germanium (32 electrons) is: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^2$. Or, in abbreviated form: $[Ar]4s^2 3d^{10} 4p^2$.

The order in which the sub–levels are filled can be remembered most easily from the periodic table. For example, Selenium (Se) is in period 4 and 4 along in the p block – therefore the last part of the electron configuration is $4p^4$. The full electron configuration can be worked out by following the arrows in Figure **2.21**:

H→He $\quad 1s^2$
Li→Be $\quad 2s^2$ $\qquad\qquad\qquad\qquad$ B→Ne $\quad 2p^6$
Na→Mg $\quad 3s^2$ $\qquad\qquad\qquad\qquad$ Al→Ar $\quad 3p^6$
K→Ca $\quad 4s^2$ $\quad$ Sc→Zn $\quad 3d^{10}$ $\quad$ Ga→Se $\quad 4p^4$
(remember to go down 1 in the d block)

Therefore the electron configuration of selenium is: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^4$.

Figure **2.22** shows an alternative way of remembering the order in which sub–levels are filled.

> Note: all the atoms in the same group (vertical column) of the periodic table have the same outer shell electron configuration. For example, all the elements in group 16 (like Se) have the outer shell electron configuration $ns^2 np^4$, where n is the period number.

Figure 2.21 Electron configurations can be worked out from the periodic table. The 'p block' is so named because the highest occupied sub-level is a p sub-level. The period number indicates the highest occupied main energy level. Some exceptions to the general rules for filling sub-levels are highlighted in pink. Helium has the configuration $1s^2$ and has no p electrons, despite the fact that it is usually put in the p block.

11 Give the full electron configurations of the following atoms:
   a N   **c** Ar   **e** V
   b Si   **d** As

Orbitals

Electrons occupy atomic orbitals in atoms.

> An **orbital** is a region of space in which there is a high probability of finding an electron. It represents a discrete energy level.

There are four different types of atomic orbital: **s**   **p**   **d**   **f**

The first shell (maximum number of electrons 2) consists of a 1s orbital and this makes up the entire 1s sub-level. This is spherical in shape (Figure 2.23a).

The 1s orbital is centred on the nucleus (Figure 2.23b). The electron is moving all the time and the intensity of the colour here represents the probability of finding the electron at a certain distance from the nucleus. The darker the colour the greater the probability of the electron being at that point. This represents the electron density.

The electron can be found anywhere in this region of space (except the nucleus – at the centre of the orbital) but it is most likely to be found at a certain distance from the nucleus.

The second main energy level (maximum number of electrons 8) is made up of the 2s sub-level and the 2p sub-level. The 2s sub-level just consists of a 2s orbital, whereas the 2p sub-level is made up of three 2p orbitals. The 2s orbital (like all other s orbitals) is spherical in shape and bigger than the 1s orbital (Figure 2.24).

p orbitals have a 'dumb-bell' shape (Figure 2.25). Three p orbitals make up the 2p sub-level. These lie at 90° to each other and are named appropriately as p_x, p_y, p_z (Figure 2.26). The p_x orbital points along the x-axis. The three 2p orbitals all have the same energy – they are described as **degenerate**.
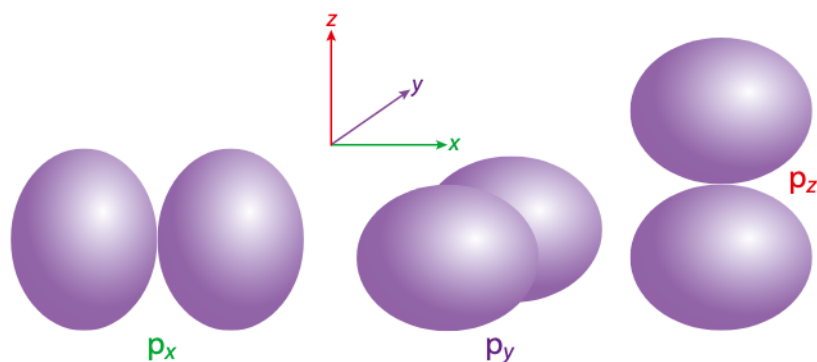
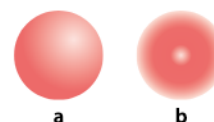> An orbital can contain a maximum of two electrons.

Figure 2.23 a The shape of a 1s orbital; **b** the electron density in a 1s orbital.
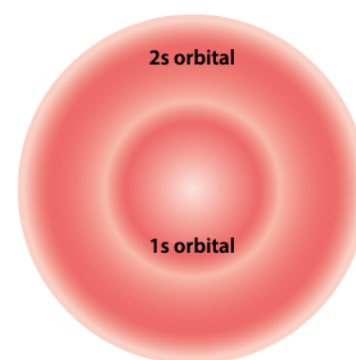

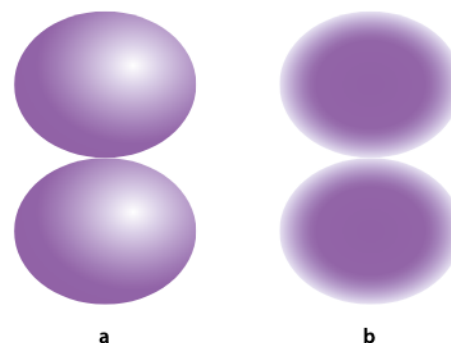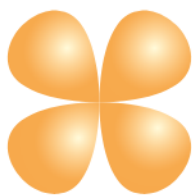**Figure 2.24** A cross section of the electron density of the 1s and 2s orbitals together.

Figure 2.25 a The shape of a 2p orbital; **b** the electron density in a 2p orbital.

Figure 2.26 The three p orbitals that make up a p sub-level point at 90° to each other.

Figure 2.28 One of the five d orbitals in the 3d sub-level.

Figure 2.29 One of the f orbitals in the 4f sub-level.

Main energy level (shell)	s	p	d	f
1	1			
2	1	3		
3	1	3	5	
4	1	3	5	7

Table 2.5 The number of orbitals in each energy level.

Figure 2.27 The 2s and 2p sub-levels in the second main energy level.

Figure **2.27** shows the orbitals that make up the 2s and 2p sub-levels in the second main energy level.

The third shell (maximum 18 electrons) consists of the 3s, 3p and 3d sub-levels. The 3s sub-level is just the 3s orbital; the 3p sub-level consists of three 3p orbitals; and the 3d sub-level is made up of five 3d orbitals. One of the five 3d orbitals is shown in Figure **2.28**.

The fourth shell (maximum 32 electrons) consists of one 4s, three 4p, five 4d and seven 4f orbitals. The seven 4f orbitals make up the 4f sub-level. One of the f orbitals is shown in Figure **2.29**.

> Within any subshell, all the orbitals have the same energy (they are **degenerate**) – e.g. the three 2p orbitals are degenerate and the five 3d orbitals are degenerate.

The number of orbitals in each energy level is shown in Table **2.5**.

The diagrams of atomic orbitals that we have seen here are derived from mathematical functions that are solutions to the Schrödinger equation. Exact solutions of the Schrödinger equation are only possible for a system involving one electron, i.e. the hydrogen atom. It is not possible to derive exact mathematical solutions for more complex atoms. What implications does this have for the limit of scientific knowledge? When we describe more complex atoms in terms of orbitals, we are actually just extending the results from the hydrogen atom and gaining an approximate view of the properties of electrons in atoms.

Electrons can be regarded as either spinning in one direction (clockwise);

or in the opposite direction (anticlockwise).

Putting electrons into orbitals – the Aufbau principle (part 2)

As well as moving around in space within an orbital, electrons also have another property called **spin**.

There are two rules that must be considered before electrons are put into orbitals.

1 **The Pauli exclusion principle**: the maximum number of electrons in an orbital is two. If there are two electrons in an orbital, they must have opposite spin.
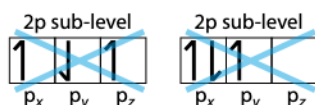
2 Hund's rule: electrons fill orbitals of the same energy (degenerate orbitals) so as to give the maximum number of electrons with the same spin.

Here we can see how three electrons occupy the orbitals of the 2p sub-level:

2p sub-level

p_x p_y p_z
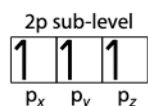
By contrast, these higher energy situations do not occur:

Figures **2.30a** and **b** show the full electron configuration of oxygen and silicon atoms, respectively.

There are a small number of exceptions to the rules for filling sub-levels – i.e. electron configurations that are not quite as expected. Two of these exceptions are **chromium** and **copper**, which, instead of having electron configurations of the form $[Ar]3d^n4s^2$ have only one electron in the 4s sub-level:

$_{24}Cr: [Ar]3d^54s^1$ $_{29}Cu: [Ar]3d^{10}4s^1$

The reasons for this are complex and beyond the level of the syllabus – but in general, having the maximum number of electron spins the same within a set of degenerate orbitals gives a lower energy (more stable) situation.

Figure 2.30 Electron configuration: **a** oxygen; **b** silicon.

Nature of science

Scientific theories are constantly being modified, improved or replaced as more data become available and the understanding of natural phenomena improves. The most up-to-date theory of the structure of the atom involves quantum mechanics and this has replaced previous theories.

Developments in apparatus and techniques have been essential in the advancement of science. For instance, J.J. Thomson used electric and magnetic fields to investigate the properties of cathode rays, which led to the discovery of the electron.
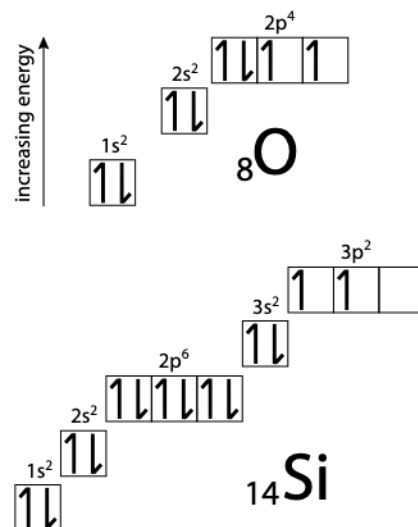
? Test yourself

12 Draw out the full electron configurations of the following atoms, showing electrons in boxes:
  a C   **b** P   **c** Cr

- Solve problems using $E = h\nu$
- Explain successive ionisation data for elements
- Explain the variation in first ionisation energy across a period and down a group
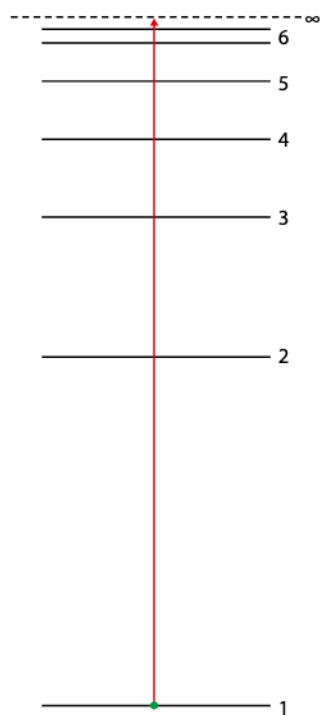
Figure 2.31 The ionisation process in a hydrogen atom.

2.3 Electrons in atoms (HL)

2.3.1 Ionisation energy and the convergence limit

As discussed on page **66**, the lines in the emission spectrum of an atom get closer together at higher frequency/energy.

Eventually, at the convergence limit, the lines merge to form a continuum. Beyond this point the electron can have any energy and so must be free from the influence of the nucleus, i.e. the electron is no longer in the atom (Figure **2.17** on page **66**). Knowing the frequency of the light emitted at the convergence limit enables us us to work out the **ionisation energy** of an atom – the energy for the process:

$$M(g) \rightarrow M^+(g) + e^-$$

> The ionisation energy is the minimum amount of energy required to remove an electron from a gaseous atom.

The ionisation energy for hydrogen represents the minimum energy for the removal of an electron (from level 1 to ∞) (Figure **2.31**), and the frequency of the convergence limit in the Lyman series represents the amount of energy given out when an electron falls from outside the atom to level 1 (∞ to 1). These are therefore the same amount of energy.

The relationship between the energy of a photon and the frequency of electromagnetic radiation

Light, and other forms of electromagnetic radiation, exhibit the properties of both waves and particles – this is known as wave–particle duality.

The energy (E) of a photon is related to the frequency of the electromagnetic radiation:

$$E = h\nu$$

where

ν is the frequency of the light (Hz or s^{-1})

h is Planck's constant (6.63×10^{-34} J s)

This equation can be used to work out the differences in energy between various levels in the hydrogen atom.

Worked example

2.3 The frequency of a line in the visible emission spectrum of hydrogen is 4.57×10^{14} Hz. Calculate the energy of the photon emitted.

$E = h\nu$

Therefore $E = 6.63 \times 10^{-34} \times 4.57 \times 10^{14}$

$\qquad\qquad = 3.03 \times 10^{-19}$ J

This line in the spectrum represents an electron falling from level 3 to level 2 and so the energy difference between these two levels is 3.03×10^{-19} J.

The wavelength of the light can be worked out from the frequency using the equation:

$$c = \nu\lambda$$

where
    λ is the wavelength of the light (m)
    c is the speed of light ($3.0 \times 10^8\,ms^{-1}$)

    The two equations $E = h\nu$ and $c = \nu\lambda$ can be combined:

$$E = \frac{hc}{\lambda}$$

This relates the energy of a photon to its wavelength.

Worked example

2.4 If the frequency of the convergence limit in the Lyman series for hydrogen is 3.28×10^{15} Hz, calculate the ionisation energy of hydrogen in $kJ\,mol^{-1}$.

$E = h\nu$

Therefore $E = 6.63 \times 10^{-34} \times 3.28 \times 10^{15}$

            $= 2.17 \times 10^{-18}\,J$

This represents the minimum amount of energy required to remove an electron from just one atom of hydrogen, but we are required to calculate the total energy required to remove one electron from each atom in 1 mole of hydrogen atoms – therefore we must multiply by Avogadro's constant.

The energy required is $2.17 \times 10^{-18} \times 6.02 \times 10^{23}$, or 1.31×10^6 $J\,mol^{-1}$.

Dividing by 1000 gives the answer in $kJ\,mol^{-1}$, so the ionisation energy of hydrogen is $1.31 \times 10^3\,kJ\,mol^{-1}$.

The ionisation energy of hydrogen can be obtained only from a study of the series of lines when the electron falls back to its ground state (normal) energy level – in other words, only the Lyman series, where the electron falls back down to level 1.
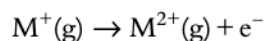
Ionisation energy and evidence for energy levels and sub-levels

The **first** ionisation energy for an element is the energy for the process:
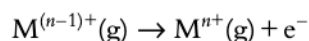
$$M(g) \rightarrow M^+(g) + e^-$$

The full definition is **the energy required to remove one electron from each atom in one mole of gaseous atoms under standard conditions**, but see later.
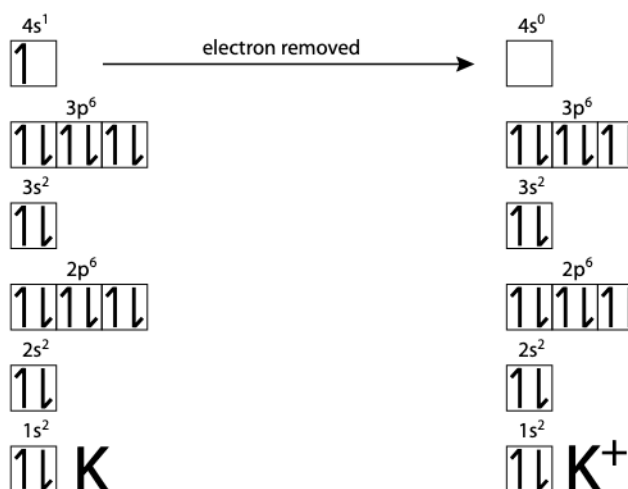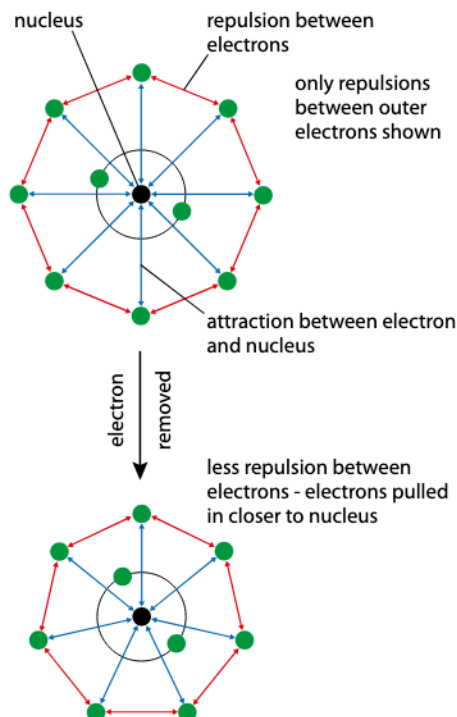
The **second** ionisation energy is:

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

The **nth** ionisation energy is:

$$M^{(n-1)+}(g) \rightarrow M^{n+}(g) + e^-$$

The highest energy electrons are removed first. Figure **2.32** shows this for potassium, in which the highest energy electron is the $4s^1$, and this is the first to be removed:

Figure 2.32 The first ionisation of potassium.

The second ionisation energy is always higher than the first, and this can be explained in two ways:

1. Once an electron has been removed from an atom, a positive ion is created. A positive ion attracts a negatively charged electron more strongly than a neutral atom does. More energy is therefore required to remove the second electron from a positive ion.
2. Once an electron has been removed from an atom, there is less repulsion between the remaining electrons. They are therefore pulled in closer to the nucleus (Figure **2.33**). If they are closer to the nucleus, they are more strongly attracted and more difficult to remove.

Successive ionisation energies of potassium

The graph in Figure **2.34** shows the energy required to remove each electron in turn from a gaseous potassium atom.

The simple electron arrangement of potassium is 2,8,8,1 and this can be deduced directly from Figure **2.34**. The large jumps in the graph occur between the main energy levels (shells).

The outermost electron in potassium is furthest from the nucleus and therefore least strongly attracted by the nucleus – so this electron is easiest to remove. It is also **shielded** (screened) from the full attractive force of the nucleus by the other 18 electrons in the atom (Figure **2.35**).

Figure 2.33 When an electron is removed from an atom, the remaining electrons are drawn closer to the nucleus due to reduced repulsion.
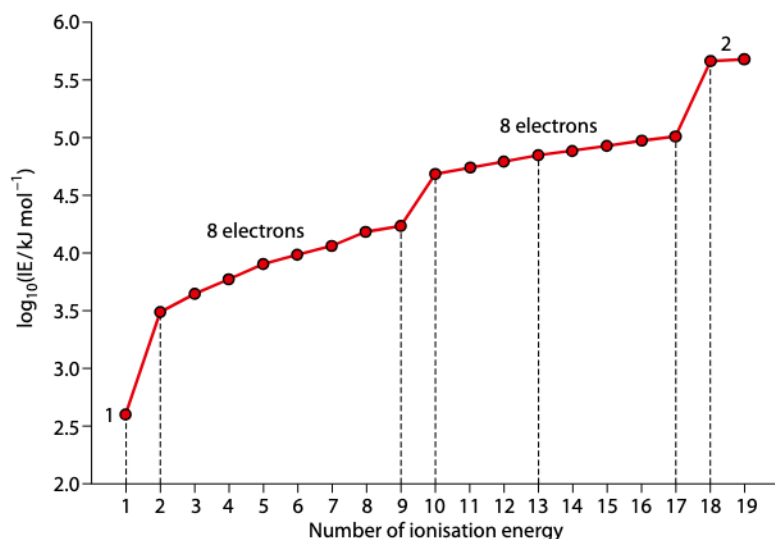
Figure 2.34 Successive ionisation energies (IE) for potassium.

Plotting $\log_{10}$ of these numbers reduces the range. The 1st ionisation energy of potassium is $418\,\mathrm{kJ\,mol^{-1}}$, whereas the 19th is $475\,000\,\mathrm{kJ\,mol^{-1}}$. It would be very difficult to plot these values on a single graph.

A log scale is used here to allow all the data to be plotted on one graph, but although on one level this has made the data easier to interpret and support the explanations that have been given, it has also distorted the data. The difference between the first and second ionisation energies of potassium is about $2600\,\mathrm{kJ\,mol^{-1}}$, but the difference between the 18th and 19th ionisations energies is over $30\,000\,\mathrm{kJ\,mol^{-1}}$! How can the way data are presented be used by scientists to support their theories? Can you find examples where the scale on a graph has been chosen to exaggerate a particular trend – is scientific knowledge objective or is it a matter of interpretation and presentation? The arguments for and against human-made climate change are a classic example of where the interpretation and presentation of data are key in influencing public opinion.

Complete shells of electrons between the nucleus and a particular electron reduce the attractive force of the nucleus for that electron. There are three full shells of electrons between the outermost electron and the nucleus, and if this shielding were perfect the **effective nuclear charge** felt by the outer electron would be 1+ (19+ in nucleus −18 shielding electrons). This shielding is not perfect, however, and the effective nuclear charge felt by the outermost electron is higher than +1.

An alternative view of shielding is that the outer electron is attracted by the nucleus but repelled by the inner electrons.
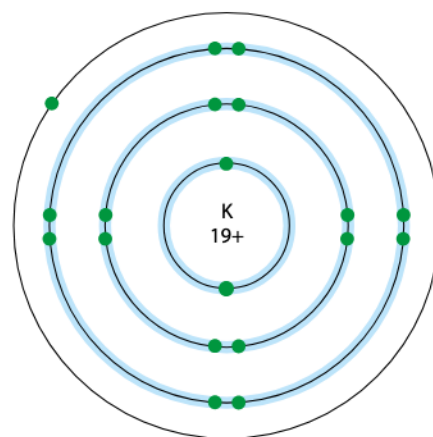

Figure 2.35 The outer electron in a potassium atom is shielded from the full attractive force of the nucleus by the inner shells of electrons (shaded in blue).

In electrostatics, a sphere of charge behaves like a point charge at its centre; therefore relative to the outer electron, spheres of charge inside (the electron shells) behave as if their charge is at the nucleus. The charge felt by the outer electron is $(19+) + (18-) = 1+$ acting at the nucleus.

The electrons do not form perfect spheres of charge, and the movement of the outer electron is not simply in an orbit around the nucleus as shown, and this is why the effective nuclear charge felt by the outer electron in potassium is greater than 1. There are various ways of estimating or calculating the effective nuclear charge for a particular electron in an atom (e.g. Slater's rules). Calculations suggest that the effective nuclear charge felt by the outer electron in potassium is about 3.5+.

a

b   9th electron

c   10th electron
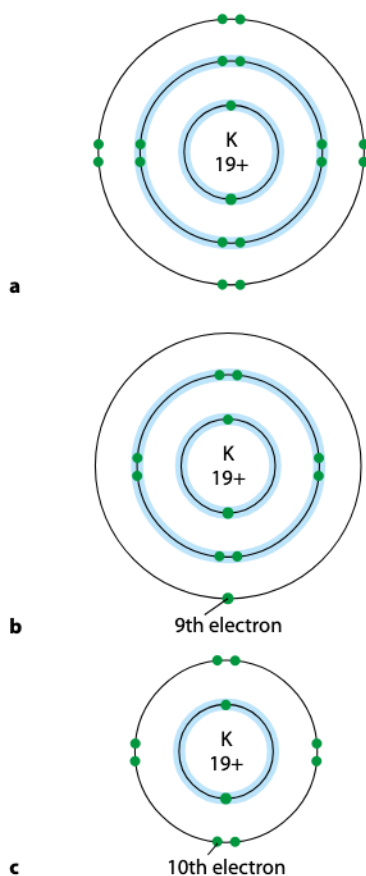
Figure 2.36 The ionisation energy depends on which main energy level the electron is removed from.

Once the first electron has been removed from a potassium atom, the next electron is considerably more difficult to remove (there is a large jump between first and second ionisation energies). This is consistent with the electron being removed from a new main energy level (shell). This electron is closer to the nucleus and therefore more strongly attracted (Figure **2.36a**). It is also shielded by fewer electrons (the ten electrons in the inner main energy levels), because electrons in the same shell do not shield each other very well (they do not get between the electron and the nucleus).

The ionisation energy now rises steadily as the electrons are removed successively from the same main energy level. There is no significant change in shielding, but as the positive charge on the ion increases it becomes more difficult to remove a negatively charged electron (less electron–electron repulsion, so the electrons are pulled in closer to the nucleus).

There is another large jump in ionisation energies between the ninth and the tenth (Figure **2.36b** and **c**) because the ninth electron is the last to be removed from the third main energy level but the tenth is the first to be removed from the second level. The tenth electron is significantly closer to the nucleus and is less shielded than the ninth electron to be removed.

Graphs of successive ionisation energy give us information about how many electrons are in a particular energy level. Consider the graph
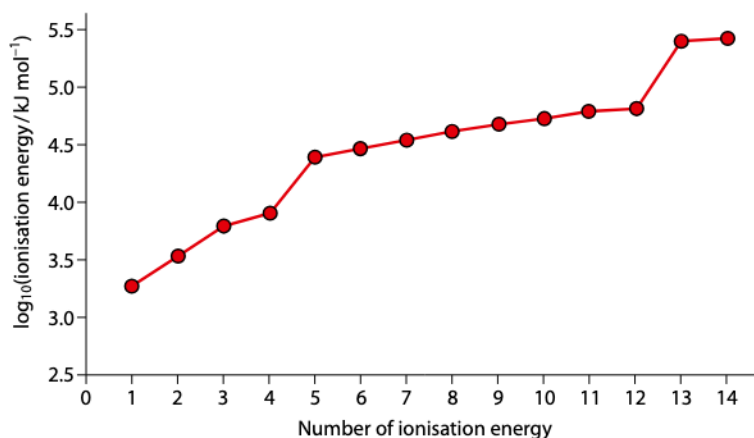
Figure 2.37 The successive ionisation energies of silicon.

for silicon shown in Figure **2.37**. There is a large jump in the ionisation energy between the fourth and the fifth ionisation energies, which suggests that these electrons are removed from different main energy levels. It can therefore be deduced that silicon has four electrons in its outer main energy level (shell) and is in group 14 of the periodic table.

If a graph of ionisation energy (rather than $\log_{10}$ ionisation energy) is plotted for the removal of the first few electrons from a silicon atom, more features can be seen (Figure **2.38**). For example there is a larger jump in the ionisation energy between the second and third ionisation energies.

The full electron configuration of silicon is $1s^2 2s^2 2p^6 3s^2 3p^2$. The first two electrons are removed from the 3p sub–level (subshell), whereas the third electron is removed from the 3s sub–level (Figure **2.39**). The 3p sub–level is higher in energy than the 3s sub–level, and therefore less energy is required to remove the electron. This provides evidence for the existence of sub energy levels (subshells) in an atom.

Figure 2.38 The first four ionisation energies of silicon.

? Test yourself

13 a The frequency of a line in the emission spectrum of hydrogen is 7.31×10^{14} Hz. Calculate the energy of the photon emitted.
 b The energy of a photon is 1.53×10^{-18} J. Calculate the frequency of the electromagnetic radiation.

14 The table shows the successive ionisation of some elements. Deduce which group in the periodic table each element is in.

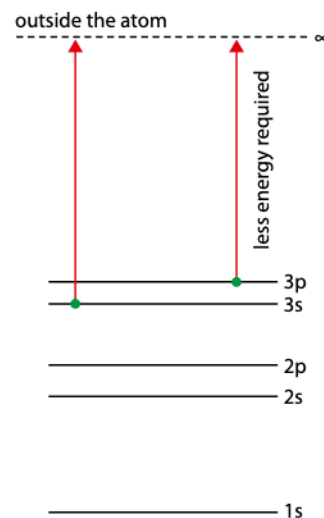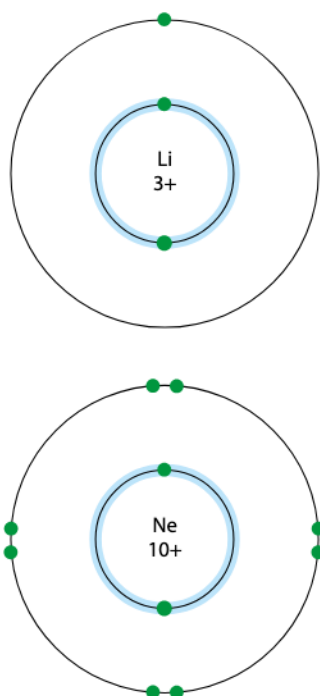| Number of ionisation energy	Ionisation energy / kJ mol⁻¹		
	Element X	**Element Z**	**Element Q**
1	1 085	736	1 400
2	2 349	1 448	2 851
3	4 612	7 719	4 570
4	6 212	10 522	7 462
5	37 765	13 606	9 429
6	47 195	17 964	53 174

Figure 2.39 More energy is required to remove an electron from the 3s sub-level of silicon than from the 3p sub-level.
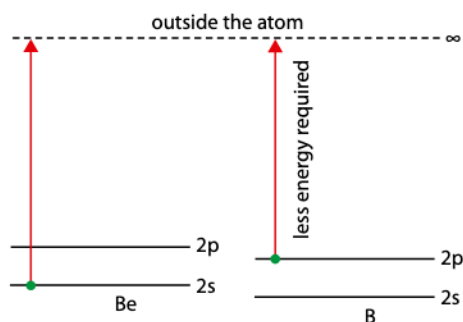
We are using reasoning to deduce the existence of energy levels in an atom. Do we **know** that energy levels exist?

Variation in ionisation energy across a period

The first ionisation energies for the elements in period 2, from lithium to neon, are plotted in Figure **2.40**.

Figure 2.40 The first ionisation energies for the period 2 elements.

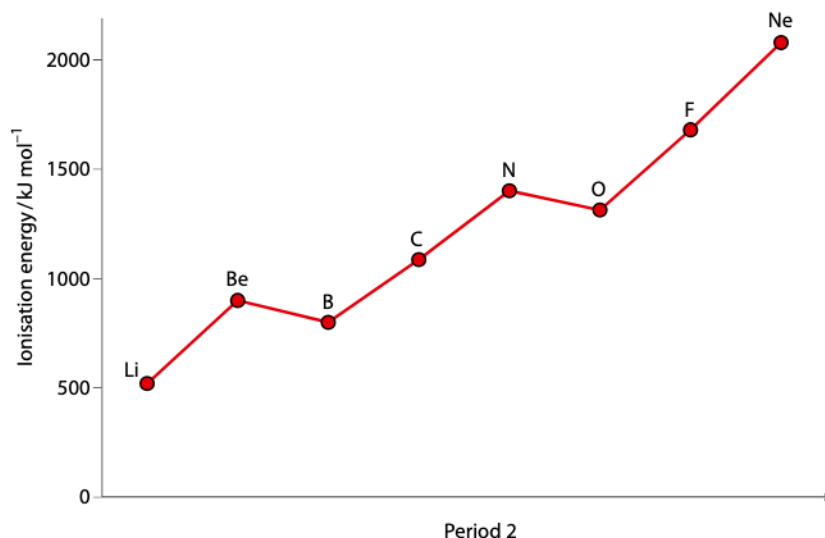**Figure 2.41** Ne has more protons in the nucleus, but the amount of shielding from inner electrons is roughly the same as in lithium.

The nuclear charge increases from lithium (3+) to neon (10+) as protons are added to the nucleus (Figure **2.41**). The electrons are all removed from the same main energy level and, because electrons in the same energy level do not shield each other very well, there is no big change in shielding. Therefore the attractive force on the outer electrons increases from left to right across the period, and the outer electron is more difficult to remove for neon. The neon atom is also smaller than the lithium atom, and so the outer electron is closer to the nucleus and more strongly held.

This can also be explained in terms of the effective nuclear charge felt by the outer electron in neon being higher.

There are two exceptions to the general increase in ionisation energy across a period.

Despite the fact that boron has a higher nuclear charge (more protons in the nucleus) than beryllium the ionisation energy is lower. The electron configurations of beryllium and boron are:

Be $1s^2 2s^2$ B $1s^2 2s^2 2p^1$

The major difference is that the electron to be removed from the boron atom is in a 2p sub-level, whereas it is in a 2s sub-level in beryllium. The 2p sub-level in B is higher in energy than the 2s sub-level in beryllium (Figure **2.42**), and therefore less energy is required to remove an electron from boron.
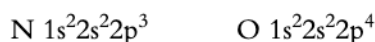

Figure 2.42 The 2p subshell in boron is higher in energy than the 2s subshell in beryllium.

The second exception is that the first ionisation energy of oxygen is lower than that of nitrogen.

The electron configurations for nitrogen and oxygen are:

N $1s^2 2s^2 2p^3$ O $1s^2 2s^2 2p^4$

The major difference is that oxygen has two electrons paired up in the same p orbital, but nitrogen does not (Figure **2.43**). An electron in the same p orbital as another electron is easier to remove than one in an orbital by itself because of the repulsion from the other electron.

When two electrons are in the same p orbital they are closer together than if there is one in each p orbital. If the electrons are closer together, they repel each other more strongly. If there is greater repulsion, an electron is easier to remove.

Down a group in the periodic table the ionisation energy **decreases**.
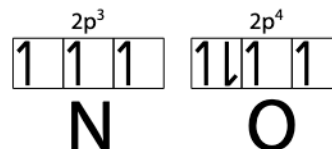
Figure 2.43 Electrons in the 2p sub-level of nitrogen and oxygen.

The variation in first ionisation energy down a group is discussed on page **92**.

The transition metals

The transition metals will be considered in more detail in a later topic, but they are mentioned here for completeness. These elements represent a slight departure from the 'last in, first out' rule for ionisation energy. Although the sub-levels are filled in the order 4s and then 3d, the 4s electrons are always removed before the 3d electrons.

The full electron configuration for an iron atom is $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^6$. The electron configuration for Fe^{2+} is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^6$. The electron configuration for Fe^{3+} is $1s^2 2s^2 2p^6 3s^2 3p^6 3d^5$.

Nature of science

Theories in science must be supported by evidence. Experimental evidence from emission spectra and ionisation energy is used to support theories about the electron arrangements of atoms.

? **Test yourself**

15 Work out the full electron configurations of the following ions:
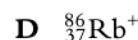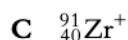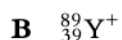   **a** Ca^{2+} **b** Cr^{3+} **c** Co^{2+} **d** Rb^{+}

Exam-style questions

1 Which of the following contains 50 neutrons?

    A $^{50}_{23}V$ **B** $^{89}_{39}Y^+$ **C** $^{91}_{40}Zr^+$ **D** $^{86}_{37}Rb^+$
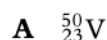
2 Which of the following has more electrons than neutrons?

    A $^{9}_{4}Be^{2+}$ **B** $^{31}_{15}P^{3-}$ **C** $^{79}_{35}Br^-$ **D** $^{40}_{20}Ca^{2+}$
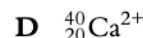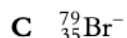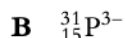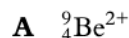
3 Rhenium has two naturally occurring isotopes, ^{185}Re and ^{187}Re. The relative atomic mass of rhenium is 186.2. What are the natural abundances of these isotopes?

    A 40% ^{185}Re and 60% ^{187}Re
    B 60% ^{185}Re and 40% ^{187}Re
    C 12% ^{185}Re and 88% ^{187}Re
    D 88% ^{185}Re and 12% ^{187}Re

4 Which of the following electron transitions in the hydrogen atom will be of highest energy?

    A $n=8 \rightarrow n=4$ **C** $n=9 \rightarrow n=3$
    B $n=7 \rightarrow n=2$ **D** $n=6 \rightarrow n=2$
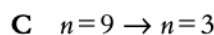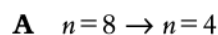
HL 5 Within any main energy level the correct sequence, when the sub-energy levels (subshells) are arranged in order of increasing energy, is:

    A s   p   f   d   **C** s   p   d   f
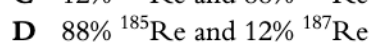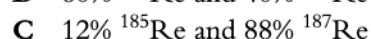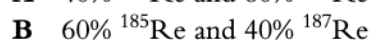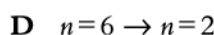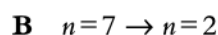   **B** d   s   f   p   **D** s   d   p   f
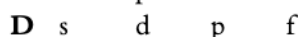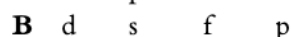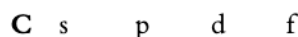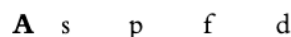
HL 6 Which of the following electron configurations is **not** correct?

    A Mg: $1s^2 2s^2 2p^6 3s^2$ **C** Ge: $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^2$
    B Cu: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^9$ **D** Br: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^5$
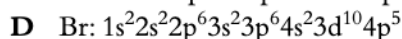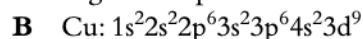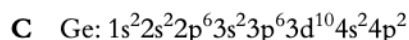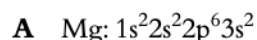
HL 7 Planck's constant is $6.63 \times 10^{-34} J s$. The energy of a photon of light with frequency $5.00 \times 10^{14} Hz$ is:

    A $7.54 \times 10^{47} J$ **C** $3.32 \times 10^{-19} J$
    B $1.33 \times 10^{-48} J$ **D** $1.33 \times 10^{-20} J$
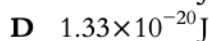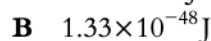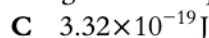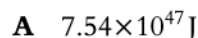
HL 8 Which of the following does **not** have three unpaired electrons?

    A P   **B** V   **C** Mn^{3+} **D** Ni^{3+}

HL 9 In which of the following does the second element have a lower first ionisation energy than the first?

    A Si   C
    B Na   Mg
    C Be   B
    D Ar   Ne

10 The first four ionisation energies of a certain element are shown in the table below.

Number of ionisation energy	Ionisation energy / kJ mol^{-1}
1	418
2	3046
3	4403
4	5866

In which group in the periodic table is this element?

       A group 1   **B** group 2   **C** group 13   **D** group 14

11 a Define the terms **atomic number** and **isotopes**.   **[3]**

  b State the number of protons, neutrons and electrons in an atom of $^{57}_{26}$Fe.   **[2]**

  c A sample of iron from a meteorite is analysed and the following results are obtained.

Isotope	Abundance / %
^{54}Fe	5.80
^{56}Fe	91.16
^{57}Fe	3.04

     i Name an instrument that could be used to obtain this data.   **[1]**
     ii Calculate the relative atomic mass of this sample, giving your answer to two decimal places.   **[2]**

12 a Describe the difference between a **continuous spectrum** and a **line spectrum**.   **[2]**

  b Sketch a diagram of the emission spectrum of hydrogen in the visible region, showing clearly the relative energies of any lines.   **[2]**

  c Explain how a line in the visible emission spectrum of hydrogen arises.   **[3]**

d The frequencies of two lines in the emission spectrum of hydrogen are given in the table.
    Calculate the energy difference between levels 5 and 6 in a hydrogen atom.   **[2]**

Higher level	Lower level	Frequency / Hz
5	3	2.34×10^{14}
6	3	2.74×10^{14}

13 a Write the full electron configuration of an atom of potassium.   **[1]**

b Write an equation showing the second ionisation energy of potassium.   **[2]**

c Explain why the second ionisation energy of potassium is substantially higher than its first ionisation energy.   **[3]**

d State and explain how the first ionisation energy of calcium compares with that of potassium.   **[3]**

14 a Write the full electron configuration of the O^{2-} ion. **[1]**

    b Give the formula of an atom and an ion that have the same number of electrons as an O^{2-} ion. **[2]**

(HL) **c** Explain why the first ionisation energy of oxygen is lower than that of nitrogen. **[2]**

(HL) **d** Sketch a graph showing the variation of the **second** ionisation energy for the elements in period 2 of the periodic table from lithium to neon. **[3]**

Summary

ATOMS —*contain*— nucleus —*contains*— protons — number of protons = atomic number
                          electrons   neutrons — number of neutrons + protons = mass number

filled from lowest to highest energy —— arranged in energy levels (shells) —— **To SUBSHELLS on next page**

Isotopes are atoms of the same element that have different mass numbers.

can be separated by mass spectrometry

Atomic emission spectra are caused by electrons falling from a higher energy level to a lower one.

line spectra – only certain frequencies are present

series of lines

spectrum becomes continuous at the **convergence limit**

HL $E = h\nu$ can be used to work out the ionisation energy of hydrogen from the convergence limit of the Lyman series

HL To IONISATION ENERGY on next page

Lyman series – electron falls to energy level 1

Balmer series – electron falls to energy level 2

Paschen series – electron falls to energy level 3

emitted radiation is ultraviolet

emitted radiation is visible light

emitted radiation is infrared

all part of the electromagnetic spectrum

Summary – continued

SUBSHELLS ——— *contain* ——— orbitals ——— *types* ——— s (spherical)
└— p (dumb-bell shaped)

p_x p_y p_z

s (max 2e⁻)
p (max 6e⁻)   increasing energy
d (max 10e⁻)   in a shell
f (max 14e⁻)   ↓

example ——— The full electron configuration of an atom shows the distribution of its electrons over its subshells.

The **Pauli exclusion principle**:
The maximum number of electrons in an orbital is 2. If there are 2 electrons in an orbital, they must have opposite spins.

Ge: $1s^2 2s^2 2p^6 3s^2 3p^6 4s^2 3d^{10} 4p^2$

remember

Hund's rule:
Electrons fill degenerate orbitals to give the maximum number of electrons with the same spin.

$_{24}$Cr: [Ar]$3d^5 4s^1$ $_{29}$Cu: [Ar]$3d^{10} 4s^1$

HL

IONISATION ENERGY ——— The electron with the highest energy is removed first. ——— The 4s electrons are removed first from transition metals.

first ionisation energy (energy required to remove the first electron)

*n*th ionisation energy (energy required to remove the *n*th electron) ——— *n*th ionisation energy > (*n* – 1)th ionisation energy because the electron is removed from a more positive ion

(in general) increases across a period as the nuclear charge increases

large jump when an electron is removed from a new main energy level (shell) ——— The electron in the new energy level is closer to the nucleus and so more strongly attracted.

BUT!

B has a lower 1st ionisation energy than Be because the electrons are removed from different subshells.

O has a lower 1st ionisation energy than N because O has 2e⁻ paired in the same p orbital.