Ensure students understand the bigger picture with a focus on real-world application that builds a foundation for later university study.

Ted Lister and Janet Renshaw

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Figure 1

Define the expression $K_{eqm}$ in Topic 2.5, Balanced equations. There is more about titrations and reversible reactions.

Synoptic link:

Many reactions are reversible and will reach equilibrium with time. The reaction between ethanol, $\text{C}_2\text{H}_5\text{OH}$, and ethanoic acid, $\text{CH}_3\text{CO}_2\text{H}$, is a typical example of a reversible reaction.
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Answers to the Practice Questions and Section Questions are available at
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Section 1
AS Physical chemistry 1

It was only about a century ago that scientists began to discover the nature of atoms, for example, that they were built up from smaller particles. This led to an understanding of how atoms are held together, why the arrangement of the Periodic Table makes sense, and how the properties of elements and compounds can be explained. This unit uses the understanding of how atoms behave to explain some of the most important ideas in chemistry.

**Atomic structure** revises the idea of the atom, looking at some of the evidence for sub-atomic particles. It introduces the mass spectrometer, which is used to measure the masses of atoms. The evidence for the arrangement of electrons is studied and you will see how a more sophisticated model using atomic orbitals rather than circular orbits was developed.

**Amount of substance** is about quantitative chemistry, that is, how much product you get from a given amount of reactants. The idea of the mole is used as the unit of quantity to compare equal numbers of atoms and molecules of different substances, including gases and solutions. Balanced equations are used to describe and measure the efficiency of chemical processes.

**Bonding** revisits the three types of strong bonds that hold atoms together – ionic, covalent, and metallic. It introduces three weaker types of forces that act between molecules, the most significant of these being hydrogen bonding. It examines how the various types of forces are responsible for the solid, liquid, and gaseous states, and explores how the electrons contribute to the shapes of molecules and ions.

**Energetics** revisits exothermic and endothermic reactions and introduces the concept of enthalpy – heat energy measured under specific conditions. It looks at different ways of measuring enthalpy changes and then uses Hess’s law to predict the energy changes of reactions. The idea of bond energies is explored to work out theoretical enthalpy changes by measuring the energy needed to make and break bonds.

**Kinetics** deals with the rate at which reactions take place, reinforcing the idea that reactions only happen when molecules of the reactants collide with enough energy to break bonds. The Maxwell–Boltzmann distribution shows us mathematically what fraction of the reactant molecules have enough collision energy at a given temperature. The role of catalysts is then explored.

**Equilibria** is about reactions that do not go to completion so that the end result is a mixture of reactants and products. It examines how to get the greatest proportion of desired products in the mixture by changing the conditions, and how to calculate the equilibrium composition. Some industrially important reversible reactions are then discussed.
**Oxidation, reduction, and redox reactions** expands the definition of oxidation as addition of oxygen to include reactions that involve electron transfers. It explains the idea of an oxidation state for elements and ions, and uses this to help balance complex redox (reduction–oxidation) equations.

The applications of science are found throughout the chapters, where they will provide you with an opportunity to apply your knowledge in a fresh context.

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**What you already know**

The material in this section builds upon knowledge and understanding that you will have developed at GCSE, in particular the following:

- There are just over 100 elements, all made up of atoms.
- The atoms of any element are essentially the same as each other but they are different from the atoms of any other element.
- Atoms are tiny and cannot be weighed individually.
- Atoms are made of protons, neutrons, and electrons.
- Atoms bond together to obtain full outer shells of electrons.
- Atoms may lose or gain electrons to form ions with full outer electron shells.
- Chemical reactions may give out (exothermic) or take in (endothermic) heat.
- The rates of chemical reactions are affected by temperature, concentration of reactants, surface area of solids, and catalysts.
- Some chemical reactions are reversible – they do not go to completion.
- Reactions can be classified as oxidation (addition of oxygen) or reduction (removal of oxygen).
Developing ideas of the atom

The Greek philosophers had a model in which matter was made up of a single continuous substance that produced the four elements – earth, fire, water, and air. The idea that matter was made of individual atoms was not taken seriously for another 2000 years. During this time alchemists built up a lot of evidence about how substances behave and combine. Their aim was to change other metals into gold. Here are a few of the steps that led to our present model.

1661 Robert Boyle proposed that there were some substances that could not be made simpler. These were the chemical elements, as we now know them.

1803 John Dalton suggested that elements were composed of indivisible atoms. All the atoms of a particular element had the same mass and atoms of different elements had different masses. Atoms could not be broken down.

1896 Henri Becquerel discovered radioactivity. This showed that particles could come from inside the atom. Therefore the atom was not indivisible. The following year, J J Thomson discovered the electron. This was the first sub-atomic particle to be discovered. He showed that electrons were negatively charged and electrons from all elements were the same.

As electrons had a negative charge, there had to be some source of positive charge inside the atom too. Also, as electrons were much lighter than whole atoms, there had to be something to account for the rest of the mass of the atom. Thompson suggested that the electrons were located within the atom in circular arrays, like plums in a pudding of positive charge, see Figure 1.

1911 Ernest Rutherford and his team found that most of the mass and all the positive charge of the atom was in a tiny central nucleus.

So, for many years, it has been known that atoms themselves are made up of smaller particles, called sub-atomic particles. The complete picture is still being built up in ‘atom smashers’ such as the one at CERN, near Geneva.

The sub-atomic particles

Atoms are made of three fundamental particles – protons, neutrons, and electrons.

The protons and neutrons form the nucleus, in the centre of the atom.

- Protons and neutrons are sometimes called nucleons because they are found in the nucleus.
- The electrons surround the nucleus.

The properties of the sub-atomic particles are shown in Table 1.
### Table 1 The properties of the sub-atomic particles

<table>
<thead>
<tr>
<th>Property</th>
<th>Proton p</th>
<th>Neutron n</th>
<th>Electron e</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass / kg</td>
<td>$1.673 \times 10^{-27}$</td>
<td>$1.675 \times 10^{-27}$</td>
<td>$0.911 \times 10^{-30}$ (very nearly 0)</td>
</tr>
<tr>
<td>Charge / C</td>
<td>$+1.602 \times 10^{-19}$</td>
<td>0</td>
<td>$-1.602 \times 10^{-19}$</td>
</tr>
<tr>
<td>Position</td>
<td>in the nucleus</td>
<td>in the nucleus</td>
<td>around the nucleus</td>
</tr>
</tbody>
</table>

These numbers are extremely small. In practice, relative values for mass and charge are used. The relative charge on a proton is taken to be +1, so the charge on an electron is −1. Neutrons have no charge, see Table 2.

### Table 2 The relative masses and charges of the sub-atomic particles

<table>
<thead>
<tr>
<th></th>
<th>Proton p</th>
<th>Neutron n</th>
<th>Electron e</th>
</tr>
</thead>
<tbody>
<tr>
<td>Relative mass</td>
<td>1</td>
<td>1</td>
<td>$\frac{1}{1840}$</td>
</tr>
<tr>
<td>Relative charge</td>
<td>+1</td>
<td>0</td>
<td>−1</td>
</tr>
</tbody>
</table>

In a neutral atom, the number of electrons must be the same as the number of protons because their charge is equal in size and opposite in sign.

### The arrangement of the sub-atomic particles

The sub-atomic particles (protons, neutrons, and electrons) are arranged in the atom as shown in Figure 3.

The protons and neutrons are in the centre of the atom, held together by a force called the strong nuclear force. This is much stronger than the electrostatic forces of attraction that hold electrons and protons together in the atom, so it overcomes the repulsion between the protons in the nucleus. It acts only over very short distances, that is, within the nucleus.

The nucleus is surrounded by electrons. Electrons are found in a series of shells, sometimes referred to as orbits or levels, which get further and further away from the nucleus. This is a simplified picture that will develop in Topic 1.5.

### Summary questions

1. **a** Identify which of the following – protons, neutrons, or electrons:
   - i are nucleons
   - ii have the same relative mass
   - iii have opposite charges
   - iv have no charge
   - v are found outside the nucleus

   **b** Explain why we assume that there are the same number of protons and electrons in an atom.
Mass number and atomic number

**Atomic number Z**

As you have seen in Topic 1.1, atoms consist of a tiny nucleus made up of protons and neutrons that is surrounded by electrons. The number of protons in the nucleus is called the atomic number or the proton number Z.

The number of electrons in the atom is equal to the proton number, so atoms are electrically neutral. The number of electrons in the outer shell of an atom determines the chemical properties of an element (how it reacts) and what sort of element it is. The atomic number defines the chemical identity of an element.

\[
\text{atomic number (proton number) } Z = \text{number of protons}
\]

All atoms of the same element have the same atomic number. Atoms of different elements have different atomic numbers.

**Mass number A**

The total number of protons plus neutrons in the nucleus (the total number of nucleons) is called the mass number A. It is the nucleons that are responsible for almost all of the mass of an atom because electrons weigh virtually nothing.

\[
\text{mass number } A = \text{number of protons} + \text{number of neutrons}
\]

**Isotopes**

Every single atom of any particular element has the same number of protons in its nucleus and therefore the same number of electrons. But the number of neutrons may vary.

- Atoms with the same number of protons but different numbers of neutrons are called isotopes.
- Different isotopes of the same element react chemically in exactly the same way as they have the same electron configuration.
- Atoms of different isotopes of the same element vary in mass number because of the different number of neutrons in their nuclei.

All atoms of the element carbon, for example, have atomic number 6. That is what makes them carbon rather than any other element. However, carbon has three isotopes with mass numbers 12, 13, and 14 respectively (Table 1). All three isotopes will react in the same way, for example, burning in oxygen to form carbon dioxide.

Isotopes are often written like this: $^{13}\text{C}$. The superscript 13 is the mass number of the isotope, and the subscript 6 the atomic number.

Study tip

The mass number of an isotope must always be bigger than the atomic number (except in $^1\text{H}$). Typically it is around twice as big.
Carbon dating

Isotopes of an element have different numbers of neutrons in their nuclei and most elements have some isotopes. Sometimes these isotopes are unstable and the nucleus of the atom itself breaks down giving off bits of the nucleus or energetic rays. This is the cause of radioactivity. Radioactive isotopes have many uses. Each radioactive isotope decays at a rate measured by its half life. This is the time taken for half of its radioactivity to decay.

One well-known radioactive isotope is carbon-14. It has a half life of 5730 years and is produced by cosmic-ray activity in the atmosphere. It is used to date organic matter. Radiocarbon dating can find the age of carbon-based material up to 60 000 years old, though it is most accurate for materials up to 2000 years old.

There is always a tiny fixed proportion of carbon-14 in all living matter. All living matter takes in and gives out carbon in the form of food and carbon dioxide, respectively. As a result, the level of carbon-14 stays the same. Once the living matter dies, this stops happening. The radioactive carbon breaks down and the level of radioactivity slowly falls. So, knowing the half life of carbon-14, scientists work backwards. They work out how long it has taken for the level of radioactivity to fall from what it is in a living organism to what it is in the sample. So, a sample with half the level of radioactivity expected in a living organism would have been dead for 5730 years, while one with a quarter of the expected level would have been dead for twice as long.

The radioactivity in a wooden bowl was found to be \( \frac{1}{8} \) of that found in a sample of living wood.

1. How old is the wood from the bowl?
2. Does this tell us the age of the bowl? Explain your answer.

Carbon-14

Radiocarbon dating was introduced in 1949 by the American Willard Libby who won the Nobel Prize for the technique. Carbon-14 is produced in the atmosphere by a nuclear reaction in which a neutron (from a cosmic ray) hits a nitrogen atom and ejects a proton:

\[ ^{14}_{7}N + _{0}^{1}n \rightarrow ^{14}_{6}C + _{1}^{1}P \]

If the half life of \(^{14}\text{C}\) is taken to be 6000 years, 24 000 years is four half lives so the remaining radioactivity will be

\[ \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} \times \frac{1}{2} = \frac{1}{16} \]

of the original activity.

Suggest why 60 000 years is the practical limit for \(^{14}\text{C}\) dating.
Learning objectives:

➔ Explain how a mass spectrometer works and what it measures.

Specification reference: 3.1.1

The mass spectrometer

The mass spectrometer is the most useful instrument for the accurate determination of relative atomic masses $A_r$. Relative atomic masses are measured on a scale on which the mass of an atom of $^{12}\text{C}$ is defined as exactly 12. No other isotope has a relative atomic mass that is exactly a whole number. This is because neither the proton nor the neutron has a mass of exactly 1.

relative atomic mass $A_r = \frac{\text{average mass of 1 atom of an element}}{\frac{1}{12} \text{ mass of 1 atom of } ^{12}\text{C}}$

relative molecular mass $M_r = \frac{\text{average mass of a molecule}}{\frac{1}{12} \text{ mass of 1 atom of } ^{12}\text{C}}$

The mass spectrometer determines the mass of separate atoms (or molecules). Mass spectrometers are an essential part of a chemist’s toolkit of equipment. For example, they are used by forensic scientists to help identify substances such as illegal drugs.

There are several types of mass spectrometer, but all work on the principle of forming ions from the sample and then separating the ions according to the ratio of their charge to their mass. The type described here is called an electro spray ionisation time of flight (TOF) instrument. The layout of this type of mass spectrometer is shown in Figure 2.

What happens in a time of flight mass spectrometer?

In outline, the substance(s) in the sample are converted to positive ions, accelerated to high speeds (which depend on their mass to charge ratio), and arrive at a detector. The steps are described in more detail below.

- **Vacuum** The whole apparatus is kept under a high vacuum to prevent the ions that are produced colliding with molecules from the air.
- **Ionisation** The sample to be investigated is dissolved in a volatile solvent and forced through a fine hollow needle that is connected

Synoptic link

Mass spectrometry can also be used to measure relative molecular masses and much more, as you will see in Topic 16.2, Mass spectrometry.

Synoptic link

You will find out more about relative atomic mass in Topic 2.1, Relative atomic and molecular masses, the Avogadro constant, and the mole.
to the positive terminal of a high voltage supply. This produces tiny positively charged droplets which have lost electrons to the positive charge of the supply. The solvent evaporates from the droplets into the vacuum and the droplets get smaller and smaller until they may contain no more than a single positively charged ion of mass $m$.

- **Acceleration** The positive ions are attracted towards a negatively charged plate and accelerate towards it. Lighter ions and more highly charged ions achieve a higher speed.

- **Ion drift** The ions, all of which have the same kinetic energy, KE, pass through a hole in the negatively charged plate, forming a beam and travel along a tube, called the flight tube, to a detector with velocity, $v$.

- **Detection** When ions with the same charge arrive at the detector, the lighter ones are first as they have higher velocities. The flight times are recorded. The positive ions pick up an electron from the detector, which causes a current to flow.

- **Data analysis** The signal from the detector is passed to a computer which generates a mass spectrum like those in Figures 3 and 4.

### Mass spectrometers

The mass spectrometer can be used to identify the different isotopes that make up an element. It detects individual ions, so different isotopes are detected separately because they have different masses. This is how the data for the neon, germanium, and chlorine isotopes in Figures 3, 4, and 5 were obtained. The peak height gives the relative abundance of each isotope and the horizontal scale gives the mass to charge ratio, $m/z$, which, for a singly charged ion is numerically the same as the mass number $A$.

Mass spectrometers can measure relative atomic masses to five decimal places of an atomic mass unit – this is called high resolution mass spectrometry. However, most work is done to one decimal point – this is called low resolution mass spectrometry.

### Low resolution mass spectrometry

The low resolution mass spectrum of neon is shown in Figure 3. This shows that neon has two isotopes, with mass numbers 20 and 22, and abundances to the nearest whole number of 90% and 10%, respectively. From this we can say that neon has an average relative atomic mass of:

$$\frac{(90 \times 20) + (10 \times 22)}{100} = 20.2$$

When calculating the relative atomic mass of an element, you must take account of the relative abundances of the isotopes. The relative atomic mass of neon is not 21 because there are far more atoms of the lighter isotope.

Another example is the mass spectrum of the element germanium, which is shown in Figure 4.

### Isotopes of chlorine

Chlorine has two isotopes. They are $^{35}\text{Cl}$, with a mass number of 35, and $^{37}\text{Cl}$, with a mass number of 37. They occur in the ratio of almost exactly 3 : 1.

$$^{35}\text{Cl} \quad ^{35}\text{Cl} \quad ^{35}\text{Cl} \quad ^{37}\text{Cl}$$

three of these to every one of this
So there are 75% $^{35}$Cl and 25% $^{37}$Cl atoms in naturally occurring chlorine gas (see Figure 5).

The average mass of these is 35.5, as shown below.

Mass of 100 atoms = $(35 \times 75) + (37 \times 25) = 3550$

Average mass = $\frac{3550}{100} = 35.5$

This explains why the relative atomic mass of chlorine is approximately 35.5.

### Identifying elements

All elements have a characteristic pattern that shows the relative abundances of their isotopes. This can be used to help identify any particular element. Chlorine, for example, shows two peaks at mass 35 and mass 37. The peak of mass 35 is three times the height of the peak of mass 37 because there are three times as many $^{35}$Cl atoms in chlorine.

The spectrum will also show peaks caused by ionised Cl$_2$ molecules. These are called molecular ions. There will be three of these:

- at $m/z$ 70, due to $^{35}$Cl$^{35}$Cl
- at $m/z$ 72, due to $^{35}$Cl$^{37}$Cl
- at $m/z$ 74, due to $^{37}$Cl$^{37}$Cl

High resolution mass spectrometers can measure the masses of atoms to several decimal places. This allows us to identify elements by the exact masses of their atoms that (apart from carbon-12 whose relative atomic mass is exactly 12) are not exactly whole numbers.

What will be the relative abundances of the three Cl$_2^+$ ions of $m/z$ 70, 72, and 74 respectively? The relative abundances of the atoms are $^{35}$Cl : $^{37}$Cl = 3 : 1. i.e., $\frac{3}{4} : \frac{1}{4}$

### Mass spectrometers in space

Space probes such as the Mars Rover Curiosity carry mass spectrometers. They are used to identify the elements in rock samples. The Huygens spacecraft that landed on Titan, one of the moons of Saturn, in January 2005 carried a mass spectrometer used to identify and measure the amounts of the gases in Titan’s atmosphere. After landing, it also analysed vaporised samples of the surface.

Relative atomic masses are weighted averages of the mass numbers of the isotopes of the element, taking account of both the masses and their abundances, relative to the $^{12}$C isotope, which is exactly 12. Chlorine has isotopes of mass number 35 and 37 but the relative atomic mass of chlorine is not 36, it is 35.5.
Summary questions

1. Explain why the ions formed in a mass spectrometer have a positive charge.
2. Explain what causes the ions to accelerate through the mass spectrometer.
3. Describe what forms the ions into a beam.
4. State which ions will arrive at the detector first.
5. Use the information about germanium in Figure 4 to calculate its relative atomic mass.
6. Figure 8 shows the mass spectrum of copper. Calculate the relative atomic mass of copper.

Mini-mass spectrometer

The latest development in mass spectrometry is a unit small enough to carry as a back pack. The unit, including rechargeable batteries, weighs 10 kg, light enough to be carried by scene of crime officers looking for drugs, explosives, or chemical weapons. Other uses include investigating chemical spills.

Figure 7  The mini-mass spectrometer

The mass spectrometer includes software to match spectra of samples investigated with a library of spectra and so identify them. The instrument can be used by operators with little or no chemical knowledge.

Figure 8  The mass spectrum of copper
The atom and electrons

During the early years of the twentieth century, physicists made great strides in understanding the structure of the atom. These are some of the landmarks.

1913 Niels Bohr put forward the idea that the atom consisted of a tiny positive nucleus orbited by negatively-charged electrons to form an atom like a tiny solar system. The electrons orbited in shells of fixed size and the movement of electrons from one shell to the next explained how atoms absorbed and gave out light. This was the beginning of what is called quantum theory.

1926 Erwin Schrödinger, a mathematical physicist, worked out an equation that used the idea that electrons had some of the properties of waves as well as those of particles. This led to a theory called quantum mechanics, which can be used to predict the behaviour of sub-atomic particles.

1932 James Chadwick discovered the neutron.

At the same time, chemists were developing their ideas about how electrons allowed atoms to bond together. One important contributor was the American, Gilbert Lewis. He put forward the ideas that:

- the inertness of the noble gases was related to their having full outer shells of electrons
- ions were formed by atoms losing or gaining electrons to attain full outer shells
- atoms could also bond by sharing electrons to form full outer shells.

Lewis' theories are the basis of modern ideas of chemical bonding, and explain the formulae of many simple compounds using the idea that atoms tend to gain the stable electronic structure of the nearest noble gas.

Evolving ideas

Early theories model the electron as a minute solid particle. Later theories suggest you can also think of electrons as smeared out clouds of charge, so you can never say exactly where an electron is at any moment. You can merely state the probability that it can be found in a particular volume of space that has a particular shape. However, chemists still use different models of the atom for different purposes.

- Dalton’s model can still be used to explain the geometries of crystals.
- Bohr’s model can be used for a simple model of ionic and covalent bonding.
- The charge cloud idea is used for a more sophisticated explanation of bonding and the shapes of molecules.
- The simple model of electrons orbiting in shells is useful for many purposes, particularly for working out bonding between atoms.

You will be familiar with the electron diagrams in this section from GCSE. They lead on to the more sophisticated models of electron structure described in Topic 1.5. However, they can still be useful, for example, in predicting and explaining the formulae of simple compounds and the shapes of molecules.
Electron shells
The first shell, which is closest to the nucleus, fills first, then the second, and so on. The number of electrons in each shell = \(2n^2\), where \(n\) is the number of the shell, so:

- the first shell holds up to two electrons
- the second shell holds up to eight electrons
- the third shell holds up to 18 electrons.

Electron diagrams
If you know the number of protons in an atom, you also know the number of electrons it has. This is because the atom is neutral. You can therefore draw an electron diagram for any element. For example, carbon has six electrons. The four electrons in the outer shell are usually drawn spaced out around the atom (Figure 1).

Sulfur has 16 electrons. It has six electrons in its outer shell. It helps when drawing bonding diagrams to space out the first four (as in carbon), and then add the next two electrons to form pairs (Figure 2).

You can also draw electron diagrams of ions, as long as you know the number of electrons. For example, a sodium atom, Na, has 11 electrons, but its ion has 10, so it has a positive charge, Na\(^+\) (Figure 3).

An oxygen atom has eight electrons, but its ion has 10, so it has a negative charge, O\(^2-\) (Figure 4).

You can write electron diagrams in shorthand:

- write the number of electrons in each shell, starting with the inner shell and working outwards
- separate each number by a comma.

For carbon you write 2,4; for sulfur 2,8,6; for Na\(^+\) 2,8.

Summary questions

1. Draw the electron arrangement diagrams of atoms that have the following numbers of electrons:
   - a 3   b 9   c 14

2. State, in shorthand, the electron arrangements of atoms with:
   - a 4 electrons   b 13 electrons   c 18 electrons

3. Identify which of the following are atoms, positive ions, or negative ions. Give the size of the charge on each ion, including its sign. Use the Periodic Table to identify the elements A–E.

<table>
<thead>
<tr>
<th>Number of protons</th>
<th>Number of electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>12</td>
</tr>
<tr>
<td>B</td>
<td>2</td>
</tr>
<tr>
<td>C</td>
<td>17</td>
</tr>
<tr>
<td>D</td>
<td>10</td>
</tr>
<tr>
<td>E</td>
<td>3</td>
</tr>
</tbody>
</table>
As you have seen in Topic 1.4, in a simple model of the atom the electrons are thought of as being arranged in shells around the nucleus. The shells can hold increasing numbers of electrons as they get further from the nucleus – the pattern is 2, 8, 18, and so on.

**Energy levels**

Electrons in different shells have differing amounts of energy. They can therefore be represented on an energy level diagram. The shells represent energy levels and they are labelled 1, 2, 3, and so on (Figure 1). Each main shell can hold up to a maximum number of electrons given by the formula $2n^2$, where $n$ is the number of the main shell. So, you can have two electrons in the first main shell, eight in the next, 18 in the next, and so on.

Apart from the first shell, these main energy levels are divided into sub-shells, called s, p, d, and f, which have slightly different energies (Figure 2). Shell 2 has an s-sub-shell and a p-sub-shell. Shell 3 an s-sub-shell, a p-sub-shell, and a d-sub-shell.

**Quantum mechanics**

For a more complete description of the electrons in atoms a theory called quantum mechanics is used, which was developed during the 1920s. This describes the atom mathematically with an equation (the Schrödinger equation). The solutions to this equation give the probability of finding an electron in a given volume of space called an atomic orbital.

**Atomic orbitals**

The electron is no longer considered to be a particle but a cloud of negative charge. An electron fills a volume in space called its atomic orbital. The concept of the main shells and the sub-shells is then included in the following way.

- Different atomic orbitals have different energies. Each orbital has a number that tells us the main energy shell that it corresponds to: 1, 2, 3, and so on.
- The atomic orbitals of each main shell have different shapes, which in turn have slightly different energies. These are the sub-shells. They are described by the letters s, p, d, and f.
The shapes of the s-, p-, and d-orbitals are shown in Figure 3. The shapes of f-orbitals are even more complicated.

- These shapes represent a volume of space in which there is a 95% probability of finding an electron and they influence the shapes of molecules.
- The first main shell consists of a single s-orbital. The second main shell has a single s-orbital and three p-orbitals of a slightly higher energy, the third main shell has a single s-orbital, three p-orbitals of slightly higher energy, and five d-orbitals of slightly higher energy still, and so on, see Figure 4.
- Any single atomic orbital can hold a maximum of two electrons.
- s-orbitals can hold up to two electrons.
- p-orbitals can hold up to two electrons each, but always come in groups of three of the same energy, to give a total of up to six electrons in the p-sub-shell.
- d-orbitals can hold up to two electrons each, but come in groups of five of the same energy to give a total of up to 10 electrons in the d-sub-shell.

Table 1 summarises the number of electrons in the different shells and sub-shells.

<table>
<thead>
<tr>
<th>Main energy level (shell)</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
</tr>
</thead>
<tbody>
<tr>
<td>sub-shell(s)</td>
<td>s</td>
<td>s</td>
<td>p</td>
<td>s</td>
</tr>
<tr>
<td>number of orbitals in sub-shell</td>
<td>1 (2 electrons)</td>
<td>1 (2e⁻)</td>
<td>3 (6e⁻)</td>
<td>1 (2e⁻)</td>
</tr>
<tr>
<td>total number of electrons in main shell</td>
<td>2</td>
<td>8</td>
<td>18</td>
<td>32</td>
</tr>
</tbody>
</table>

The energy level diagram in Figure 5 shows the energies of the orbitals for the first few elements of the Periodic Table. Notice that the first main shell has only an s-orbital. The second main shell has an s- and p-sub-shell, and the p-sub-shell is composed of three p-orbitals of equal energy. The third main shell has an s-, p-, and d-sub-shell, and the d-sub-shell is composed of five atomic orbitals of equal energy.

- Each ‘box’ in Figure 5 represents an orbital of the appropriate shape that can hold up to two electrons.
- Notice that 4s is actually of slightly lower energy than 3d for neutral atoms, though this can change when ions are formed.

**Spin**

Electrons also have the property called spin.

- Two electrons in the same orbital must have opposite spins.
- The electrons are usually represented by arrows pointing up or down to show the different directions of spin.

**Putting electrons into atomic orbitals**

Remember that the label of an atomic orbital tells us about the energy (and shape) of an electron cloud. For example, the atomic orbital 3s means the main shell is 3 and the sub-level (and therefore the shape) is spherical.
There are three rules for allocating electrons to atomic orbitals:

1. Atomic orbitals of lower energy are filled first – so the lower main shell is filled first and, within this shell, sub-shells of lower energy are filled first.
2. Atomic orbitals of the same energy fill singly before pairing starts. This is because electrons repel each other.
3. No atomic orbital can hold more than two electrons.

The electron diagrams for the elements hydrogen to sodium are shown in Figure 6.

Study tip
Practise working out the shorthand electronic structure of all the elements at least up to krypton (atomic number 36).

Summary questions
1. a. Give the full electron arrangement for phosphorus.
   b. Give the electron arrangement for phosphorus using an inert gas symbol as a shorthand.
2. a. Give the full electron arrangements of:
   i. Ca²⁺
   ii. F⁻
   b. Give their electron arrangements using an inert gas symbol as a shorthand.

▲ Figure 6 The electron arrangements for the elements hydrogen to sodium – note how they obey the rule above

Writing electronic structures

A shorthand way of writing electronic structures is as follows, for example, for sodium which has 11 electrons:

\[\begin{align*}
1s^2 & \quad 2s^2 \quad 2p^6 \quad 3s^1 \\
2 & \quad 8 & \quad 1
\end{align*}\]

Note how this matches the simpler 2,8,1 you used at GCSE.

Calcium, with 20 electrons would be:

\[\begin{align*}
1s^2 & \quad 2s^2 \quad 2p^6 \quad 3s^2 \quad 3p^6 \quad 4s^2
\end{align*}\]

which matches 2,8,8,2

Notice how the 4s orbital is filled before the 3d orbital because it is of lower energy.

After calcium, electrons begin to fill the 3d orbitals, so vanadium with 23 electrons is: 1s² 2s² 2p⁶ 3s² 3p⁶ 3d³ 4s²

Krypton with 36 electrons is: 1s² 2s² 2p⁶ 3s² 3p⁶ 3d¹⁰ 4s² 4p⁶

Sometimes it simplifies things to use the previous noble gas symbol. So the electron arrangement of calcium, Ca, could be written [Ar] 4s² as a shorthand for [1s² 2s² 2p⁶ 3s² 3p⁶ 3d³ 4s²] 4s² because 1s² 2s² 2p⁶ 3s² 3p⁶ is the electron arrangement of argon.

You can use the same notation for ions. So a sodium ion, Na⁺, would have the electron arrangement 1s² 2s² 2p⁶, one less than a sodium atom, 1s² 2s² 2p⁶ 3s¹.

Synoptic link

You will learn how electron arrangements affect the properties of the transition metals in Topic 23.1, The general properties of transition metals.
The patterns in first ionisation energies across a period provide evidence for electron sub-shells.

**Ionisation energy**

Electrons can be removed from atoms and the energy it takes to remove them can be measured. This is called ionisation energy because as the electrons are removed, the atoms become positive ions.

- Ionisation energy is the energy required to remove a mole of electrons from a mole of atoms in the gaseous state, and is measured in kJ mol$^{-1}$.
- Ionisation energy has the abbreviation IE.

**Removing the electrons one by one**

You can measure the energies required to remove the electrons one by one from an atom, starting from the outer electrons and working inwards.

- The first electron needs the least energy to remove it because it is being removed from a neutral atom. This is the first IE.
- The second electron needs more energy than the first because it is being removed from a +1 ion. This is the second IE.
- The third electron needs even more energy to remove it because it is being removed from a +2 ion. This is the third IE.
- The fourth needs yet more, and so on.

These are called **successive ionisation energies**.

For example, sodium:

- $\text{Na}(g) \rightarrow \text{Na}^{+}(g) + e^{-}$ first IE $= + 496$ kJ mol$^{-1}$
- $\text{Na}^{+}(g) \rightarrow \text{Na}^{2+}(g) + e^{-}$ second IE $= + 4563$ kJ mol$^{-1}$
- $\text{Na}^{2+}(g) \rightarrow \text{Na}^{3+}(g) + e^{-}$ third IE $= + 6913$ kJ mol$^{-1}$

and so on, see Table 1.

Notice that the second IE is not the energy change for

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

The energy for this process would be (first IE + second IE).

If you plot a graph of the values shown in Table 1 you get Figure 1.

Notice that one electron is relatively easy to remove, then comes a group of eight that are more difficult to remove, and finally two that are very difficult to remove.
This suggests that sodium has:
- **one** electron furthest away from the positive nucleus (easy to remove)
- **eight** electrons nearer in to the nucleus (harder to remove)
- **two** electrons very close to the nucleus (very difficult to remove because they are nearest to the positive charge of the nucleus).

This tells you about the number of electrons in each main shell or orbit: 2, 8, 1. The eight electrons in shell 2 are in fact sub-divided into two further groups that correspond to the $2s^2, 2p^6$ electrons in the second main shell, but this is not visible on the scale of Figure 1.

You can find the number of electrons in each main shell of any element by looking at the jumps in successive ionisation energies.

**Trends in ionisation energies across a period in the Periodic Table**

The trends in first ionisation energies moving across a period in the Periodic Table can also give information about the energies of electrons in main shells and sub-shells. Ionisation energies generally increase across a period because the nuclear charge is increasing and this makes it more difficult to remove an electron.

The data for Period 3 are shown in Table 2.

<table>
<thead>
<tr>
<th></th>
<th>Na</th>
<th>Mg</th>
<th>Al</th>
<th>Si</th>
<th>P</th>
<th>S</th>
<th>Cl</th>
<th>Ar</th>
</tr>
</thead>
<tbody>
<tr>
<td>1st IE</td>
<td>496</td>
<td>738</td>
<td>578</td>
<td>789</td>
<td>1012</td>
<td>1000</td>
<td>1251</td>
<td>1521</td>
</tr>
</tbody>
</table>

Plotting a graph of these values shows that the increase is not regular (Figure 2). In going from magnesium ($1s^2, 2s^2, 2p^6, 3s^2$) to aluminium ($1s^2, 2s^2, 2p^6, 3s^2, 3p^1$), the ionisation energy actually goes down, despite the increase in nuclear charge. This is because the outer electron in aluminium is in a $3p$ orbital which is of a slightly higher energy than the $3s$ orbital. It therefore needs less energy to remove it, see Figure 3.
In Figure 2, notice the small drop between phosphorus (1s², 2s², 2p⁶, 3s², 3p³) and sulfur (1s², 2s², 2p⁶, 3s², 3p⁴). In phosphorus, each of the three 3p orbitals contains just one electron, while in sulfur, one of the 3p orbitals must contain two electrons. The repulsion between these paired electrons makes it easier to remove one of them, despite the increase in nuclear charge, see Figure 4.

Both these cases, which go against the expected trend, are evidence that confirms the existence of s- and p-sub-shells. These were predicted by quantum theory and the Schrödinger equation.

**Trends in ionisation energies down a group in the Periodic Table**

Figure 5 shows that there is a general decrease in first ionisation energy going down Group 2, and the same pattern is seen in other groups. This is because the outer electron is in a main shell that gets further from the nucleus in each case.

**Summary questions**

1. State why the second ionisation energy of any atom is larger than the first ionisation energy.

2. Sketch a graph similar to Figure 1 of the successive ionisation energies of aluminium (electron arrangement 2,8,3).

3. An element X has the following values (in kJ mol⁻¹) for successive ionisation energies: 1093, 2359, 4627, 6229, 37 838, 47 285.
   
   a. Identify which group in the Periodic Table it is in.
   
   b. Explain your answer to a.

Going down a group, the nuclear charge increases. At first sight you might expect that this would make it more difficult to remove an electron. However, the actual positive charge ‘felt’ by an electron in the outer shell is less than the full nuclear charge. This is because of the effect of the inner electrons shielding the nuclear charge.
1. The diagram to the right shows the first ionisation energies of some Period 3 elements.

(a) Draw a cross on the diagram to show the first ionisation energy of aluminium.

(b) Write an equation to show the process that occurs when the first ionisation energy of aluminium is measured.

(c) State which of the first, second, or third ionisations of aluminium would produce an ion with the electron configuration $1s^2\ 2s^2\ 2p^6\ 3s^1$.

(d) Explain why the value of the first ionisation energy of sulfur is less than the value of the first ionisation energy of phosphorus.

(e) Identify the element in Period 2 that has the highest first ionisation energy and give its electron configuration.

(f) State the trend in first ionisation energies in Group 2 from beryllium to barium. Explain your answer in terms of a suitable model of atomic structure.

2. (a) One isotope of sodium has a relative mass of 23.
   (i) Define, in terms of the fundamental particles present, the meaning of the term *isotopes*.
   (ii) Explain why isotopes of the same element have the same chemical properties.

(b) Give the electronic configuration, showing all sub-shells, for a sodium atom.

(c) An atom has half as many protons as an atom of $^{28}\text{Si}$ and also has six fewer neutrons than an atom of $^{28}\text{Si}$. Give the symbol, including the mass number and the atomic number, of this atom.

3. The values of the first ionisation energies of neon, sodium, and magnesium are 2080, 494, and 736 kJ mol$^{-1}$, respectively.

(a) Explain the meaning of the term *first ionisation energy* of an atom.

(b) Write an equation using state symbols to illustrate the process occurring when the *second* ionisation energy of magnesium is measured.

(c) Explain why the value of the first ionisation energy of magnesium is higher than that of sodium.

(d) Explain why the value of the first ionisation energy of neon is higher than that of sodium.
4 A sample of iron from a meteorite was found to contain the isotopes $^{54}$Fe, $^{56}$Fe, and $^{57}$Fe.  
(a) The relative abundances of these isotopes can be determined using a mass spectrometer. In the mass spectrometer, the sample is first vaporised and then ionised.  
(i) State what is meant by the term isotopes.  
(ii) Explain how, in a mass spectrometer, ions are detected and how their abundance is measured.  

(b) (i) Define the term relative atomic mass of an element.  
(ii) The relative abundances of the isotopes in this sample of iron were found to be as follows.  

<table>
<thead>
<tr>
<th>m/z</th>
<th>Relative abundance</th>
<th>Relative abundance %</th>
</tr>
</thead>
<tbody>
<tr>
<td>54</td>
<td></td>
<td>5.80</td>
</tr>
<tr>
<td>56</td>
<td></td>
<td>91.60</td>
</tr>
<tr>
<td>57</td>
<td></td>
<td>2.60</td>
</tr>
</tbody>
</table>

Use the data above to calculate the relative atomic mass of iron in this sample. Give your answer to the appropriate number of significant figures.  

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5 The diagram shows the layout of a time of flight mass spectrometer.  

(a) Explain how positive ions are formed from the sample.  

(b) Explain why the instrument is kept under vacuum.  

(c) Explain how the ions are accelerated and separated by mass in the instrument.  

(d) Explain how an electric current is produced when an ion arrives at the detector.  

(e) The low resolution mass spectrum of magnesium shows three peaks.  

<table>
<thead>
<tr>
<th>Mass / charge</th>
<th>Relative abundance / %</th>
</tr>
</thead>
<tbody>
<tr>
<td>24</td>
<td>79.0%</td>
</tr>
<tr>
<td>25</td>
<td>10.0%</td>
</tr>
<tr>
<td>26</td>
<td>11.0%</td>
</tr>
</tbody>
</table>

(i) Give the numbers of protons and neutrons in the nuclei of each isotope.  

(ii) Calculate the relative atomic mass of a sample of magnesium. Give your answer to the appropriate number of significant figures.
6.3 The equilibrium constant $K_e$

Learning objectives:
- Define the term chemical equilibrium.
- Define the expression $K_e = \frac{[C][D]}{[A][B]}$ for a reaction $A + B \rightleftharpoons C + D$.
- Ensure students understand the bigger picture with a focus on real-world application that builds a solid foundation for university study.
- Strengthen mathematical skills, with Maths skills tips, a dedicated Maths chapter, worked examples and practice questions.
- Support those students who don’t speak English as a first language with clear language, an extensive glossary and highlighted key terms.

The equation tells you that when 1 mol of CH$_3$CO$_2$H is used up, 1 mol of C$_2$H$_5$OH and 1 mol of H$_2$O are produced. So, there must be 0.10 mol of C$_2$H$_5$OH and 0.10 mol of H$_2$O. From this you can work out the number of moles of each component present at equilibrium.

To find the value of $K_e$ for the reaction between ethanol and ethanoic acid:

At start:

- CH$_3$CO$_2$H (l) + C$_2$H$_5$OH (l) $\rightleftharpoons$ CH$_3$CO$_2$C$_2$H$_5$ (l) + H$_2$O (l)

To find $K_e$ for this reaction (where $c$ is the equilibrium constant for the reaction):

$K_e = \frac{[C][D]}{[A][B]}$ where $A + B \rightleftharpoons C + D$

As you have seen, many reactions are reversible and do not go to completion in a single step. Instead, they can be used to produce a reaction mixture in which the concentrations of the substances involved do not change. An example of such a reaction is:

$A + B \rightleftharpoons C + D$

At equilibrium, the concentrations of the reactants and products are constant. The rate at which they react is equal to the rate at which they are produced. The equilibrium constant $K_e$ is a measure of the extent to which this reaction has occurred. It is defined as:

$K_e = \frac{[C][D]}{[A][B]}$ where $A + B \rightleftharpoons C + D$

where $A$ and $B$ are the reactants and $C$ and $D$ are the products.

The value of $K_e$ is a measure of the extent to which the reaction has occurred. It is defined as:

$K_e = \frac{[C][D]}{[A][B]}$ where $A + B \rightleftharpoons C + D$

The value of $K_e$ varies with the temperature. The higher the temperature, the greater the value of $K_e$. This is because the reaction is more likely to proceed in the forward direction at higher temperatures. The value of $K_e$ can be used to calculate the equilibrium concentrations of the reactants and products, and to predict whether the reaction will proceed in the forward or reverse direction.