PRACTICAL WORK IN CHEMISTRY

While they may not all wear white coats or work in a laboratory, chemists and others who use chemistry in their work carry out experiments and investigations to gather evidence. They may be challenging established chemical ideas and models or using their skills, knowledge and understanding to tackle important problems.

Chemistry is a practical subject. Whether in the laboratory or in the field, chemists use their practical skills to find solutions to problems, challenges and questions. Throughout this course you will learn, develop and use these skills.

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WRITTEN EXAMINATIONS

Your practical skills will be assessed in the written examinations at the end of the course. Questions on practical skills will account for about 15% of your marks at AS and 18% at A-level. The practical skills assessed in the written examinations are:

Independent thinking

- solve problems set in practical contexts
- apply scientific knowledge to practical contexts

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Figure 1 *Most chemists and others who use chemistry in their work spend time in laboratories. Many also use their practical skills outside of a laboratory.*

Use and application of scientific methods and practices

- comment on experimental design and evaluate scientific methods
- present data in appropriate ways
- evaluate results and draw conclusions with reference to measurement uncertainties and errors
- identify variables including those that must be controlled

Numeracy and the application of mathematical concepts in a practical context

- plot and interpret graphs
- process and analyse data using appropriate mathematical skills
- consider margins of error, accuracy and precision of data

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Figure 2 *Chemists record experimental data in laboratory notebooks. They also record, process and present data using computers and tablets.*

Instruments and equipment

- know and understand how to use a wide range of experimental and practical instruments, equipment and techniques appropriate to the knowledge and understanding included in the specification

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Figure 3 *You will need to use a variety of equipment correctly and safely.*

Throughout this book there are questions and longer assignments that will give you the opportunity to develop and practise these skills. The contexts of some of the exam questions will be based on the 'required practical activities'.

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ASSESSMENT OF PRACTICAL SKILLS

Some practical skills, such as handling materials and equipment and making measurements, can only be practised when you are doing experiments. For A-level, these **practical competencies** will be assessed by your teacher when you carry out practical activities:

- follow written procedures
- apply investigative approaches and methods when using instruments and equipment
- safely use a range of practical equipment and materials
- make and record observations and measurements
- research, reference and report findings

You must show your teacher that you consistently and routinely demonstrate the competencies listed above during your course. The assessment will not contribute to your A-level grade, but will appear as a 'pass' alongside your grade on the A-level certificate.

These practical competencies must be demonstrated by using a specific range of **apparatus and techniques**. These are:

- use appropriate apparatus to record a range of measurements (to include mass, time, volume of liquids and gases, temperature)
- use a water bath or electric heater or sand bath for heating
- measure pH using pH charts, or pH meter, or pH probe on a data logger
- use laboratory apparatus for a variety of experimental techniques including:
  - titration, using burette and pipette
  - distillation and heating under reflux, including setting up glassware using retort stand and clamps
  - qualitative tests for ions and organic functional groups
  - filtration, including use of fluted filter paper, or filtration under reduced pressure
- use a volumetric flask, including accurate technique for making up a standard solution
- Use acid–base indicators in titrations of weak/strong acids with weak/strong alkalis
- Purify:
  - a solid product by recrystallization
  - a liquid product, including use of separating funnel
- Use melting point apparatus
- Use thin-layer or paper chromatography
- Set up electrochemical cells and measuring voltages
- Safely and carefully handle solids and liquids, including corrosive, irritant, flammable and toxic substances
- Measure rates of reaction by at least two different methods, for example:
  - an initial rate method such as a clock reaction
  - a continuous monitoring method

Figure 4 *Many chemists analyse material. They are called analytical chemists. Titration is a commonly used technique.*

Figure 5 *pH probe*

For AS, the above will not be assessed but you will be expected to use these skills and these types of

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apparatus to develop your manipulative skills and your understanding of the processes of scientific investigation.

REQUIRED PRACTICAL ACTIVITIES

During the A-level course you will need to carry out twelve **required practical** activities. These are the main sources of evidence that your teacher will use to award you a pass for your competency skills. If you are doing the AS, you will need to carry out the first six in this list.

1. Make up a volumetric solution and carry out a simple acid–base titration
2. Measurement of an enthalpy change
3. Investigation of how the rate of a reaction changes with temperature
4. Carry out simple test-tube reactions to identify:
   - cations – Group 2, NH4 +
   - anions – Group 7 (halide ions), OH^-, CO_3^{2-}, SO_4^{2-}
5. Distillation of a product from a reaction
6. Tests for alcohol, aldehyde, alkene and carboxylic acid
7. Measuring the rate of reaction:
   - by an initial rate method
   - by a continuous monitoring method
8. Measuring the EMF of an electrochemical cell
9. Investigate how pH changes when a weak acid reacts with a strong base and when a strong acid reacts with a weak base
10. Preparation of:
    - a pure organic solid and test of its purity
    - a pure organic liquid
11. Carry out simple test-tube reactions to identify transition metal ions in aqueous solution
12. Separation of species by thin-layer chromatography

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Figure 6.

Information about the apparatus, techniques and analysis of required practicals 1 to 6 are found in the relevant chapters of this book, and 7 to 12 in Book 2.

You will be asked some questions in your written examinations (Paper 2 at AS and Paper 3 at A-level) about these required practicals.

Practical skills are really important. Take time and care to learn, practise and use them.

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1 ATOMIC STRUCTURE

PRIOR KNOWLEDGE

You may know that substances are made from atoms and that an element is a substance made from just one sort of atom. You will probably have learnt that an atom consists of a nucleus, made up of protons and neutrons, with electrons moving around it in shells (or energy levels). You may also know about relative electrical charges and masses of protons, neutrons and electrons.

LEARNING OBJECTIVES

In this chapter, you will reinforce and build on these ideas and learn about more sophisticated models of atoms.

(3.1.1.1, 3.1.1.2, 3.1.1.3)

NASA's Curiosity Rover landed in the Gale Crater on Mars in August 2012. Its main mission was to investigate whether Mars has ever possessed the environmental conditions that could support life, as well as finding out about Martian climate and geology. Curiosity Rover contains an on-board science lab, equipped with a sophisticated range of scientific instruments. Many of these instruments have been specially designed for the mission.

The task of the on-board mass spectrometer is to investigate the atoms that are the building blocks of life – carbon, hydrogen, oxygen, phosphorus and sulfur. The spectrometer is making precise measurements of the carbon and oxygen isotopes found in carbon dioxide and methane from the atmosphere and the soil. After one Martian year (687 Earth days) of the mission, scientists have concluded that Mars once had environmental conditions favourable for microbe life.

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1.1 EARLY IDEAS ABOUT THE COMPOSITION OF MATTER

The nature of matter has interested people since the time of the early Greeks. The ideas you have learnt about atomic structure resulted from the work of many people over many centuries. Here are some of the major events since 460BCE that led to our understanding of the atom.

Evidence for atomic structure

460–370BCE, Democritus

The Greek Philosopher Democritus proposed that matter was made up of particles that cannot be divided further. They became known as atoms from the Greek word *atomos*, meaning 'cannot be divided'.

His ideas were based on reasoning – you cannot keep dividing a lump of matter for ever.

384–322BCE, Aristotle

Aristotle was another ancient Greek philosopher, who proposed that all earthly matter was made from four elements: earth, air, fire and water. These elements have their natural place on Earth and when they are out of place, they move. So, rain falls and bubbles of air rise from water.

A tree grows in the earth, and it needs water and air. So, a tree is made from earth, water and air. He could analyse most matter in this way.

1627–1691, Robert Boyle

Robert Boyle was a Fellow of the Royal Society of London. His scientific ideas included the notion that matter is made up of tiny identical particles that cannot be subdivided. These tiny particles made up 'mixt bodies' (we now call them compounds). Putting the particles together in different ways made different compounds. Particles were in fixed positions in solids, but free to move in liquids and gases. Forces between particles made solids solid.

Boyle studied the nature and behaviour of gases, especially the relationship between volume and pressure. His theory of matter supported his experimental observations. He was the first scientist to keep accurate records.

1766–1844, John Dalton

John Dalton was an English chemist and physicist, who named the tiny particles **atoms**. His scientific idea was that atoms are indivisible and indestructible. All atoms of an element are identical and have the same mass and chemical properties. Atoms of different elements have different masses (he called them atomic weights) and different chemical properties. Atoms react together to form 'compound atoms'. These later became known as molecules.

He studied the physical properties of air and gases. This led him to analytical work on ethene (olefiant gas), methane (carburetted hydrogen) and others. His atomic theory explained his chemical analysis. He summed up 150 years of ideas with his atomic theories.

1850–1930, Eugen Goldstein

The German physicist Eugen Goldstein's scientific idea was that cathode rays contained negatively charged particles with mass. He assumed these particles were produced when the gas particles in the cathose ray tube were split. Cathode rays could be deflected by a magnetic field. Goldstein also detected heavier positive particles.

He experimented with electrical discharge tubes – he passed an electric current between a cathode and an anode in a sealed tube containing gas at a very low pressure. He adapted his experiment, inserting a perforated cathode, as in Figure 1.

1856–1937, Joseph John Thomson

Thomson's idea was that atoms contained **electrons**. He proposed that atoms could be divided into smaller particles. Electrons have very small mass, about one two-thousandths of the mass of a hydrogen atom.

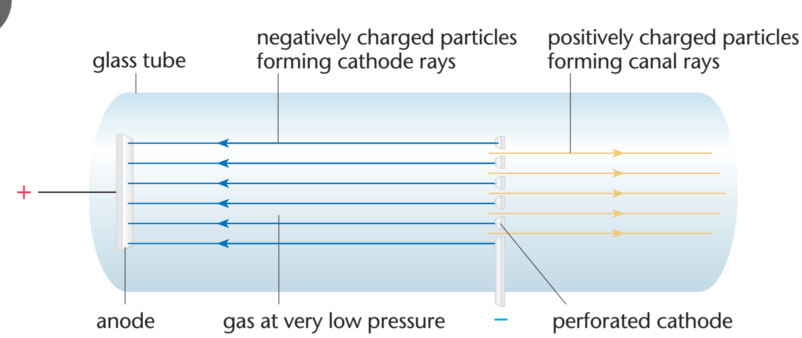

Figure 1 *An electrical discharge tube with a perforated cathode as used by Goldstein*

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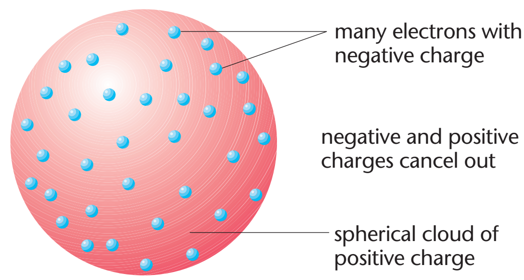

Figure 2 *Thomson's plum pudding model of the atom*

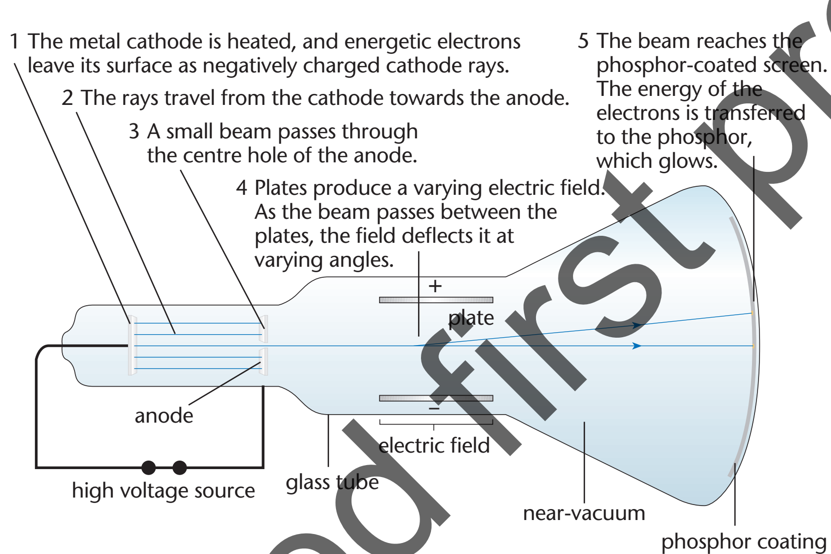

Figure 3 *Cathode ray tubes used to be used in televisions and computers before flat screens.*

They are negatively charged. The negative charge is cancelled out by a sphere of positively charged material, as in Figure 2.

Thomson measured the deflection of the negative particles in cathode rays very accurately and calculated their mass. The cathode ray tubes he used were the forerunners of the cathode ray tubes used in televisions and monitors (Figure 3) before the advent of flat screens.

Thomson's model of the atom became known as the 'plum pudding' model.

1871–1937, Ernest Rutherford

From work carried out in Manchester with his research students Hans Geiger and Ernst Marsden, Ernest Rutherford put forward the idea that the mass of the atom is not evenly spread. It is concentrated in a minute central region called the **nucleus**. Rutherford calculated the diameter of the nucleus to be 10^{-14} m.

All the positive charge of the atom is contained in the nucleus.

The electrons circulate in the rest of the atom, being kept apart by the repulsion of their negative charges.

These findings came from the interpretation of the results that are given in Figure 4.

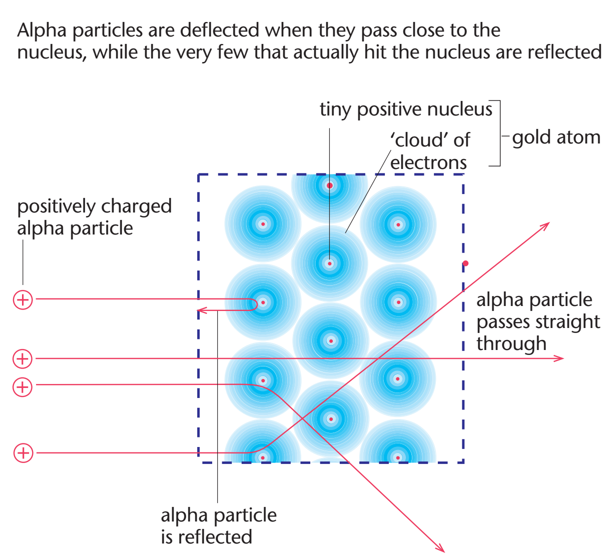

Figure 4 *Deflection of alpha particles by gold foil*

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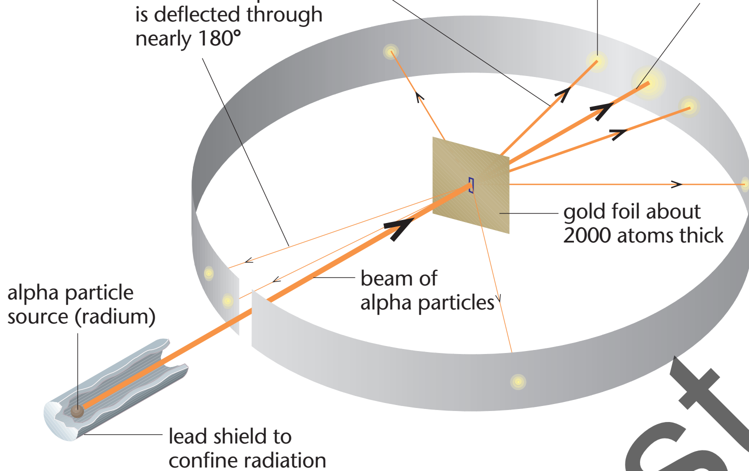

Figure 5 *Rutherford's experiment: the deflection of alpha particles through gold foil*

1888–1915, Henry Moseley and Ernest Rutherford

Moseley and Rutherford's idea was that the nucleus contained positively charged particles called **protons**. The number of protons (the atomic number) corresponds to the element's position in the Periodic Table. Protons make up about half the mass of the nucleus.

Moseley studied X-ray spectra of elements. Mathematically, he related the frequency of the X-rays to a number he called the **atomic number**. This corresponded to the element's position in the Periodic Table. Sadly, Moseley was killed in action at Gallipoli in World War 1. Rutherford's further calculations showed the charge on the nucleus, the positive charge. In 1919, he fired alpha particles at hydrogen gas and produced positive particles, which he called protons. His calculations also showed that the mass of the protons only accounted for half the mass of the nucleus.

1891–1974, James Chadwick

Chadwick identified the **neutron**. Neutrons have no charge. They have the same mass as a proton.

He bombarded a beryllium plate with alpha particles and produced uncharged radiation on the other side of the plate. He placed a paraffin wax disc (which contains many hydrogen atoms) in the path of the radiation and showed that the radiation caused protons to be knocked out of the wax (Figure 6).

1885–1962, Niels Bohr

Bohr's scientific idea was that electrons orbit the nucleus in energy levels. Energy levels have fixed energy values – they are **quantised**. Electrons can only occupy these set energy levels.

Bohr studied emission spectra and produced explanations that incorporated the ideas of Einstein and Planck. Electrons orbited the nucleus in energy levels, where each energy level has a fixed energy value.

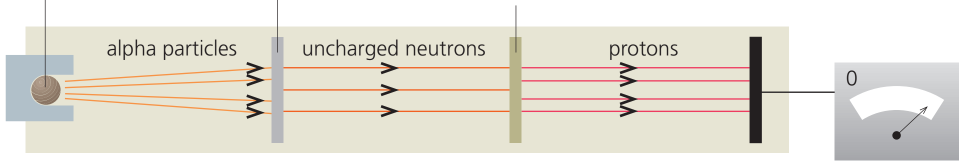

Figure 6 *Chadwick's experiment*

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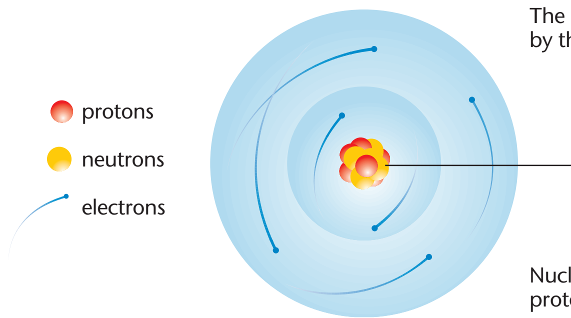

Figure 7 *This diagram summarises the model of the atom that scientists often use nowadays.*

QUESTION

1. Aristotle's theory of earth, fire, air and water lasted for about 2000 years and was a major setback to ideas about atomic structure. Why did it last so long?
2. What evidence led to the discovery of:
   a. the electron
   b. the nucleus
   c. the proton
   d. the neutron?
3. Why was the neutron the last major subatomic particle to be discovered?

Stretch and challenge

4. Describe how ideas about atomic structure changed from 1897 to 1932.

1.2 RELATIVE MASS AND RELATIVE CHARGE OF SUBATOMIC PARTICLES

Further experiments established the masses and charges of protons, electrons and neutrons. These are summarised in Table 1.

Because the values for mass are so small, the idea of **relative mass** is used. The relative mass of a proton is 1 and that of a neutron is 1. The relative mass of the electron is 5.45×10^{-4} or $\frac{1}{1837}$.

Charges on subatomic particles are also given relative to one another. A proton has a relative charge of $+1$ and an electron has a relative charge of -1. A neutron has no charge. The protons and neutrons together are called **nucleons**. Protons in the nucleus do not repel each other because a strong nuclear force acts over the small size of the nucleus and binds all the nucleons together.

Since atoms of any element are neutral, the number of protons (positive charge) must equal the number of electrons (negative charge). The atoms of all elements, except hydrogen, contain these three fundamental particles.

KEY IDEAS

- All matter is composed of atoms.
- The nucleus of an atom contains positive protons, with a relative mass of 1 and relative charge of $+1$, and neutral neutrons (except hydrogen), with a relative mass of 1 and no charge.
- Electrons orbit the nucleus in energy levels (shells). An electron has a very small mass and relative charge of -1.
- The number of electrons in an atom equals the number of protons, to give a neutral atom.

Particle	Mass/kg	Charge/C	Relative mass	Relative charge
Electron	9.109×10^{-31}	1.602×10^{-19}	5.45×10^{-4}	-1
Proton	1.672×10^{-27}	1.602×10^{-19}	1	$+1$
Neutron	1.674×10^{-27}	0	1	0

Note: The mass of the electron is so small compared to the mass of the proton and neutron that chemists often take it to be zero.

Table 1 *The fundamental atomic particles, their mass and charge*

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1.3 WORKING WITH VERY SMALL AND VERY LARGE NUMBERS

Working with very small numbers can be confusing. To help avoid this, scientists use standard form and standard prefixes when communicating their numerical work.

Standard form

Numbers with many zeros are difficult to follow, so scientists tend to express these in **standard form**. Standard form is a number between one and 10. So, how is the number 769 000 expressed in standard form?

- Locate the decimal point: 769 000.0
- Move the decimal point to give a number between 1 and 10: 7.69000
- Multiply the number by ten raised to the power x where x is the number of figures the decimal point was moved: 7.69×10^5

Sometimes the decimal point may move the other way. Take the mass of the electron (0.000 545 units) as an example.

- Find the decimal point and move it. This time it goes to the right: 00005.45
- Multiply the number by ten raised to the power x, where x is the number of figures the decimal point was moved. But, this time, the index will be negative: 5.45×10^{-4}

Calculations using standard form

Standard form makes multiplication and division of even the most complex numbers much easier to handle. When you multiply two numbers in standard form, you multiply the numbers and add the indices. For example:

$(3 \times 10^2) \times (2 \times 10^3) = 6 \times 10^5$

If you **divide** numbers in standard form, you divide the standard number and subtract the indices. For example:

$$\frac{8 \times 10^4}{4 \times 10^2} = 2 \times 10^2$$

Units and standard prefixes

Science is based on observations and measurements. When making measurements it is essential to use the correct units.

Again, to make numbers more manageable, scientists use prefixes that usually have intervals of a thousand. For example, attaching preferred prefixes to the unit metre, you have kilometre, millimetre and nanometre. But other intervals can be used if they are convenient for the task in hand.

A system of prefixes is used to modify units. Prefixes that are commonly used are listed in Table 2.

Prefix	Symbol	Multiplier	Meaning
mega	M	10^6	1 000 000
kilo	K	10^3	1000
deci	d	10^{-1}	0.1
centi	c	10^{-2}	0.01
milli	m	10^{-3}	0.001
micro	μ	10^{-6}	0.000 001
nano	n	10^{-9}	0.000 000 001
pico	p	10^{-12}	0.000 000 000 001

Table 2 *Standard prefixes*

Significant figures

When carrying out calculations based on measurements made, you must be confident that the answers you give are as precise as the measurements allow. This is done by counting the number of significant figures (sig figs) in the number given for a measurement. So, for example, a measured mass of:

3.4 g (two sig figs) means you are confident to the nearest 0.1 g

3.40 g (three sig figs) means you are confident to the nearest 0.01 g

3.400 g (four sig figs) means you are confident to the nearest 0.001 g.

Worked example 1

Using data from Table 1, calculate how many electrons have the same mass as a nucleus containing one proton and one neutron.

mass of nucleus $= (1.672 \times 10^{-27}) + (1.674 \times 10^{-27})$

number of electrons with the same mass

$$= \frac{(1.672 \times 10^{-27}) + (1.674 \times 10^{-27})}{9.109 \times 10^{-31}}$$

answer given on calculator = 3673.290153

Since the mass of each particle is given to four significant figures, the answer must contain no more than four significant figures. The answer must be rounded up or down. The answer is 3673 electrons.

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Remember:

- Do not round calculations up or down until you reach the final answer because errors can be carried through.
- The answer to a chemical calculation must not have more significant figures than the number used in the calculation with the fewest significant figures.

(Maths Skills 0.0, 0.1, 0.2, 0.4, 1.1)

Fact	Example
all non-zero digits are significant	275 has three sig figs
zero between non-zero digits is significant	205 has three sig figs
zero to the left of the first non-zero digit is not significant	301 has three sig figs, 0.31 has two sig figs
numbers ending in zero to the right of the decimal point: the zero is significant	2.9 has two sig figs, 2.90 has three sig figs
numbers ending in zero to the left of the decimal point: the zero may or may not be significant	a mass of 840 g has two sig figs if the balance is accurate to ± 10 g, and three sig figs if the balance is accurate to ± 1 g

Table 3 *Significant figures*

MATHS ASSIGNMENT 1: SIZE, SCALE AND SIGNIFICANT FIGURES

(MS 0.0, 0.1, 0.2; PS 1.1, 1.2, 3.2)

A single carbon atom measures about one ten-billionth of a metre across, a dimension so small that it is impossible to imagine. The nucleus is a thousand times smaller again, and the electron a hundred thousand times smaller than that!

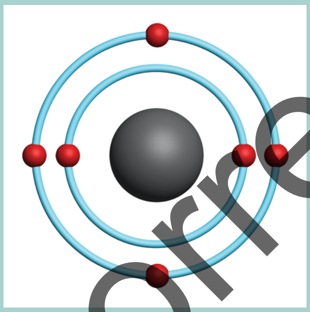

Figure A1 *A single carbon atom measures about one ten-billionth of a metre across.*

Because the numbers are so unimaginably small, scientists do not use grams and metres to describe atoms and subatomic particles. They use a different set of units.

You have already come across the idea of relative masses. Protons and neutrons both have a relative mass of one. We say these have a mass of one relative mass unit. The electron is a mere 0.000 545 relative mass units. Clearly, even with relative masses you have some awkward numbers.

Questions

Give your answers to the appropriate number of significant figures, and in standard form where appropriate.

A1. **a.** An atom of hydrogen contains only a proton and an electron. Calculate the mass of the hydrogen atom in kilograms.

b. A molecule of hydrogen contains two atoms. Calculate the mass of a hydrogen molecule in grams.

c. How many electrons have the same mass as a single neutron?

A2. Convert these quantities into measurements in grams expressed in standard form:

a. The mass of a neutron

b. 200 million electrons

c. 10 gold coins weighing a total of 0.311 kg

A3. A uranium atom contains 92 electrons. Calculate the mass in kilograms of protons in the atom.

A4. How many times heavier is the nucleus of a helium atom (two protons and two neutrons) than its electrons?

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1.4 ATOMIC NUMBER, MASS NUMBER AND ISOTOPES

Different elements have different numbers of electrons, protons and neutrons in their atoms. It is the number of protons in the nucleus of an atom that identifies the element. Remember that if an atom forms an ion by gain or transfer of electrons, it is still an ion of the same element. An atom can also have one or two more or fewer neutrons can also lose or gain one or two neutrons and still remain the same element. Using this information, you can define an element using two numbers: the atomic number and the mass number (Figure 9).

Atomic (proton) number (*Z*). The atomic number of an element is the number of protons in the nucleus of the atom. It has the symbol *Z* and is also known as the proton number. Its value is placed below the line in front of the element's symbol. Since atoms are neutral, the number of protons equals the number of electrons orbiting the nucleus. All atoms of the same element have the same atomic number.

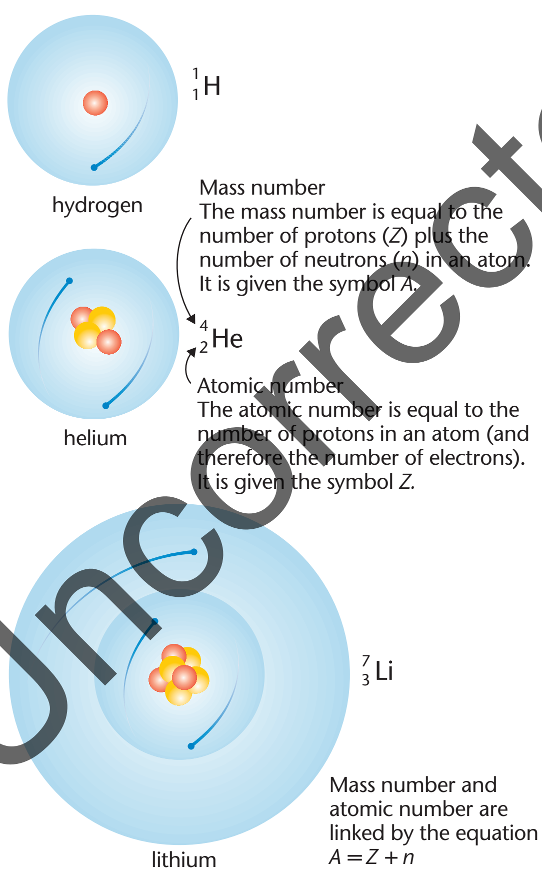

Figure 8 *Mass number and atomic number*

Mass number (*A*). The mass number of an element is the total number of protons and neutrons in the nucleus of an atom. It is a measure of its mass compared with other types of atom. Even in heavy atoms, the electron's mass is so small that it makes little difference to the overall mass of the atom. Protons and neutrons both have a mass of 1, so:

mass number (*A*) = number of protons (*Z*) + number of neutrons (*n*)

$$A = Z + n$$

The symbol for the mass number is *A*, and its value goes above the atomic number in front of the element's symbol.

You can calculate the number of neutrons in the nucleus using:

number of neutrons (*n*) = mass number (*A*) – atomic number (*Z*).

QUESTION

5. How many protons, neutrons and electrons do the following atoms and ions have?
   a. An element with mass number 19 and atomic number 9.
   b. An element with mass number 210 and atomic number 85.
   c. An ion with one positive charge, a mass number of 23 and atomic number 11.
   d. An ion with three negative charges, a mass number of 31 and atomic number 15.
   e. An ion with three positive charges, a mass number 52 and atomic number 24.

Isotopes

All atoms of the same element have the same number of protons and the same atomic number, *Z*. However, they may have a different number of neutrons and so a different mass number, *A*. Atoms of the same element with different mass numbers are called **isotopes**. Nitrogen has two isotopes, $^{14}_{7}N$ and $^{15}_{7}N$. Both isotopes have seven protons, but $^{14}_{7}N$ has seven neutrons and $^{15}_{7}N$ has eight neutrons. The notation for an isotope shows the mass number and the atomic number:

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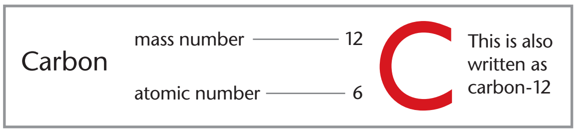


The isotopes of carbon and their sub-atomic particles are summarised in Table 4.

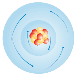
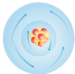
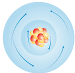
Name		No. of protons	No. of neutrons	No. of electrons	Relative abundance %
carbon-12		6	6	6	98.93
carbon-13		6	7	6	1.07
carbon-14		6	8	6	10^{-10}

Table 4 *Isotopes of carbon*

Properties of isotopes

The chemical properties of an element depend on the number and arrangement of the electrons in its atoms. Since all the isotopes of an element have the same number and arrangement of electrons, they also all have the same chemical properties. However, because of the difference in mass, isotopes differ slightly in their physical properties, such as in the rate of diffusion (which depends on mass), and their nuclear properties, such as radioactivity.

Isotopes that are not radioactive, such as chlorine-35 and chlorine-37, are called **stable isotopes**. Data books give you the relative abundance of each isotope present in such stable, naturally occurring elements.

Relative abundance of isotopes

The percentage of each isotope that naturally occurs on Earth is referred to as its **relative isotopic abundance**. Most elements have isotopes. Chlorine has two isotopes, $^{35}_{17}Cl$ and $^{35}_{17}Cl$. Any sample of naturally occurring chlorine will contain 75.53% of chlorine-35 and 24.47% of chlorine-37.

Hydrogen has three isotopes: $^{1}_{1}H$, $^{2}_{1}H$ (called deuterium) and $^{3}_{1}H$ (called tritium). Elements that occur in space may contain different percentages of isotopes. These percentages are called its **isotope signature**.

KEY IDEAS

- The atomic (proton) number *Z* is equal to the number of protons in the nucleus.
- The mass number *A* is equal to the number of protons plus the number of neutrons in the nucleus.
- Isotopes of an element have the same number of protons but different numbers of neutrons.

PRACTICAL ASSIGNMENT 2: ISOTOPE DETECTIVE

(MS 0.0, 0.1; PS 1.1, 1.2, 3.2)

Human beings have long been obsessed with the idea that life might exist or have existed on Mars, one of the closest planets to Earth. In 2003 the European Mars Express detected methane gas, CH_4. We use methane to heat our homes and for cooking food. On Earth, 90% of all methane comes from living things, such as the decay of organic material. This is how the gas in our homes originated. The remaining 10% was produced from geological activity.

The big question is: 'What is the origin of the methane gas on Mars?'. Perhaps it was formed by the decay of organic material billions of years ago. Or maybe it is being given off by present-day microbes that exist under the surface in areas heated by volcanic activity. Alternatively, was the

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Figure A2 *Nili Fossae, one of the regions on Mars emitting methane. Are the plumes of methane gas evidence for life on Mars?*

methane gas a result of geological processes? The answer may be found in isotopes.

Carbon has three isotopes: carbon-12, carbon-13 and carbon-14. Their abundances on Earth are given in Table A1.

Hydrogen has two naturally occurring isotopes: hydrogen-1, which has a 99.9885 % abundance on Earth and hydrogen-2, which has a 0.01115% abundance. (The other hydrogen isotope, hydrogen-3, is not naturally occuring. It is produced in nuclear reactors.)

Chemical reactions involve electrons and the presence of extra neutrons in isotopes does not affect these reactions. So, methane molecules may contain a mixture of these different isotopes. The three most common methane molecules are formed when one carbon-12 combines with four hydrogen-1 atoms, one atom of carbon-13 combines with four hydrogen-1 atoms, and when one atom of carbon-12 combines with three hydrogen-1 atoms and one hydrogen-2 atom. These can be written as: $^{12}CH_4$, $^{13}CH_4$ and $^{12}CH_3D$ respectively. (D stands for deuterium, which is the name given to hydrogen-2.)

Methane formula	Natural percentage abundance on Earth
$^{12}CH_4$	0.99827
$^{13}CH_4$	0.01110
$^{12}CH_3D$	0.00062

Table A1 *The isotopic signature of naturally occurring methane on Earth*

When scientists determine the isotopic signature of Martian methane, they can compare it with that on Earth. They may be a step nearer to deciding its origin.

Questions

A1. What are the atomic numbers and mass numbers of:

a. the isotopes of carbon

b. the isotopes of hydrogen?

A2. Why is carbon-14 ignored in possible methane formulae?

A3. What is the difference in mass between $^{12}CH_4$ and $^{13}CH_4$?

A4. What is the difference in mass between $^{12}CH_4$ and $^{12}CH_3D$?

A5. Which form of methane is most common and why?

A6. Suggest a formula for an extremely rare type of methane.

A7. When scientists compare the isotopic signature of Martian methane with that on Earth, what assumptions are they making?

Figure 9 *Athletes undergo drugs tests during training and competition. Any found using performance enhancing drugs face bans from the sport.*

Performance enhancing drugs are illegal in most sports and most organisations use drug tests to ensure the competition is fair. An athlete may be asked to produce a urine sample and, sometimes, a blood sample. This is sent to a testing facility. The drug tests detect the presence of compounds that are produced by chemical reactions in the body as it processes the drug. **Mass spectrometers** are used to help analyse the sample.

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There are several different types of mass spectrometer. They can be used to identify the mass of an element, an isotope or a molecule. Knowing the mass of a particle helps scientists identify the particle. One type of spectrometer is called a **time-of-flight mass spectrometer**.

Time-of-flight mass spectrometer

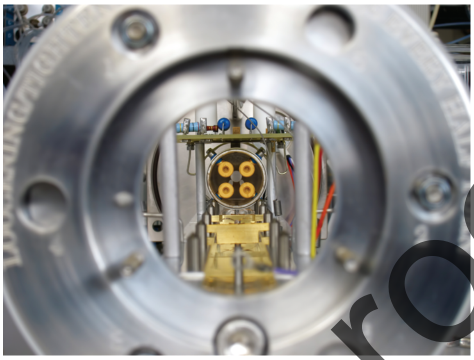


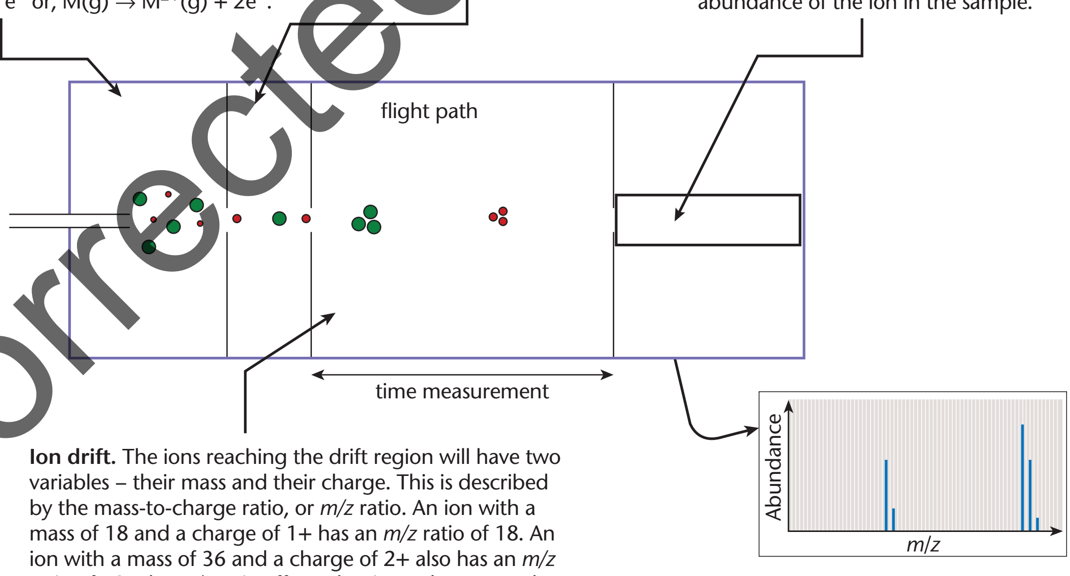
Figure 10 *Inside the flight tube of a triple quadrupole mass spectrometer*

Electrospray ionisation. The sample being tested is vaporised and injected into the spectrometer. A beam of electrons is fired at the sample and knocks out electrons to produce ions. A technique called electrospray ionisation is used because this reduces the number of molecules that break up or fragment. Most atoms or molecules lose just one electron, but a few lose two. Positively charged ions are produced. Only the most energetic electrons can knock out two electrons, so most ions have a single positive charge. If M is a molecule of the sample, then:

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

Acceleration. The electric field has a fixed strength – the potential difference is constant. It accelerates the ions so that all the ions with the same charge have the same kinetic energy – they are travelling at the same speed.

Ion detector. The ions are distinguished by different flight times at the ion detector. The electronic signal is used by computer software to produce a mass spectrum. The position of the peaks on the mass spectrum relate to the *m/z* charge of the ions. Since most ions have a 1+ charge, this will be the same as the mass of the ion. The size of the peak is proportional to the abundance of the ion in the sample.



Ion drift. The ions reaching the drift region will have two variables – their mass and their charge. This is described by the mass-to-charge ratio, or *m/z* ratio. An ion with a mass of 18 and a charge of 1+ has an *m/z* ratio of 18. An ion with a mass of 36 and a charge of 2+ also has an *m/z* ratio of 18. The *m/z* ratio affects the time taken to reach the detector. There is no accelerating field in this region – ions are 'free-wheeling'. Heavier ions move slower than lighter ions and singularly charged ions move slower than ions with two or more charges. The time taken to reach the ion detector is called the 'flight time'. For example, if the flight path is 0.6 m long and an ion has a mass of 26 atomic units, the flight time will be 6×10^{-6} seconds.

Figure 11 *The basic principles of a time-of-flight mass spectrometer*

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The mass spectrum of magnesium

The chart produced by a mass spectrometer is called a mass spectrum (plural: mass spectra).

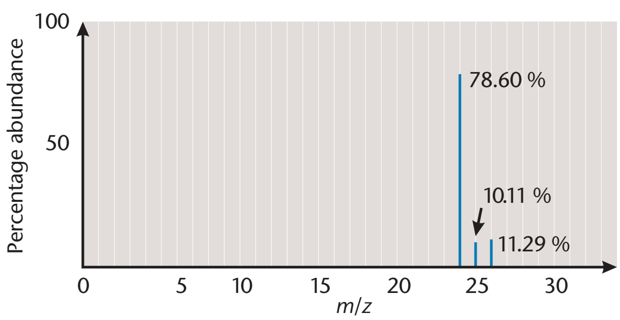

Figure 12 *Mass spectrum of magnesium*

When samples of magnesium vapour are fed into the mass spectrometer, they are bombarded by high energy electrons in the **ionisation region**. These fast-moving, energetic electrons knock electrons off the magnesium atoms to produce positively charged magnesium ions, Mg^+.

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

If bombarded with very high energy electrons, some magnesium ions lose a second electron:

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

These positively charged magnesium ions pass through the spectrometer and are accelerated by an electric field to give all ions with the same charge the same kinetic energy. Magnesium has three isotopes: magnesium-24, magnesium-25 and magnesium-26. The sample then passes into the drift region. If ions of all isotopes have the same charge, then the lighter magnesium-24 will take a shorter time to reach the ion detector than the heavier ions. The flight time will be less.

A mass spectrum is produced. The *y*-axis is the percentage abundance. The *x*-axis is the mass/charge (or *m*/*z*) ratio (Figure 12).

The spectrum of magnesium has three lines. These correspond to the three isotopes of magnesium. The heights of the lines are proportional to the amounts of each isotope present. The sample in Figure 12 contains 78.60% of magnesium-24, 10.11% of magnesium-25 and 11.29% of magnesium-26.

The mass spectrum of an element shows:

- the mass number of each isotope present (since mass numbers are masses compared to carbon-12, this number is called the relative isotopic mass)
- the relative abundance of each isotope.

Calculating the relative atomic mass from isotopic abundance

You can use information from mass spectra to calculate the **relative atomic mass**, A_r, of an element (see Section 1.5).

For magnesium, the isotopes ^{24}Mg, ^{25}Mg and ^{26}Mg are present in the ratio 78.60 : 10.11 : 11.29. This means that the mass of 100 magnesium atoms will be:

$$(78.60 \times 24) + (10.11 \times 25) + (11.29 \times 26)$$

The average mass of one magnesium atom will be:

$$\frac{(78.60 \times 24) + (10.11 \times 25) + (11.29 \times 26)}{100}$$

$$= 24.31 \text{ (to four significant figures)}$$

This is the relative atomic mass of magnesium. The A_r value for magnesium in your data book is 24.3.

Note that atoms of magnesium with this actual mass do not exist. This is the *average* mass of all the naturally occurring isotopes of magnesium, taking abundance into account.

The mass spectrum of lead

The mass spectrum of lead (Figure 13) shows that lead has four isotopes with mass numbers of 204, 206, 207 and 208. The heights of the lines show these are in the ratio of 1.50 : 23.6 : 22.6 : 52.3. These are percentage abundances and add up to 100.

To calculate the relative atomic mass of lead:

mass of 100 atoms

$$= (1.40 \times 204) + (23.6 \times 206) + (22.6 \times 207)$$

$$+ (52.3 \times 208)$$

relative atomic mass

$$= \frac{(1.40 \times 204) \times (23.6 \times 206)}{100}$$

$$\frac{+ (22.6 \times 207) + (52.3 \times 208)}{100}$$

$$= 207.24$$

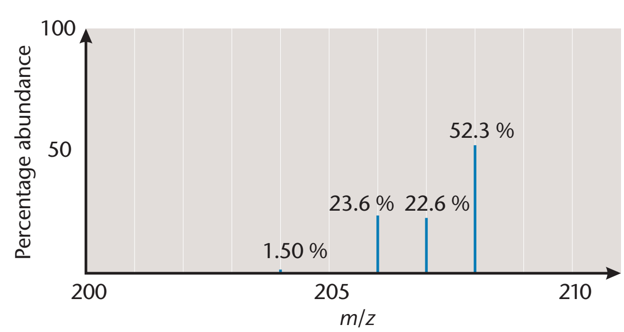

Figure 13 *Mass spectrum of lead*

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QUESTIONS

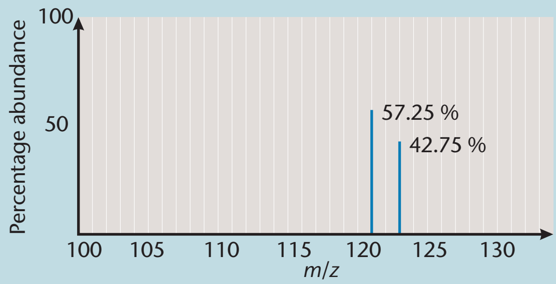

Figure 14 *Mass spectrum of antimony*

6. Look at the mass spectrum of a sample of antimony (Figure 14).
   a. How many isotopes does antimony have?
   b. What are their mass numbers?
   c. What is the percentage abundance of each isotope?
   d. Calculate the relative atomic mass of antimony from this spectrum.
7. Find the relative atomic mass of naturally occurring uranium that contains 0.006% uranium-234, 0.72% uranium-235 and 99.2% uranium-238.
8. Silver has two isotopes, silver-107 and silver-109. These are present in the ratio of 51.35:48.65 in naturally occurring silver. Calculate the relative atomic mass of silver.

MATHS ASSIGNMENT 3: ANALYSING HAIR

(MS 1.1, 1.2; PS 1.1, 1.2, 3.2)

Figure A3 *Scientists analyse hair to provide forensic evidence.*

Hair grows at a fairly uniform rate. Its composition depends partly on diet and the water you drink. The ratios of different isotopes in the water supply vary with your location and the rocks the water percolates through. For example, the isotopes of strontium (^{87}Sr and ^{88}Sr) and the isotopes of oxygen (^{16}O, ^{17}O and ^{18}O) vary all over the world. As your hair grows, the isotope ratios from your environment are set in your hair.

For the forensic scientist, analysing the isotopes in a sample of your hair can tell where you are from and where you have been. This is a very useful tool in cases such as deciding whether a terrorist suspect has been to a particular location.

Questions

A1. Strontium has an atomic number of 38. How many protons, neutrons and electrons are in one atom of strontium-87 and in one atom of strontium-88?

A2. Naturally occurring strontium has four isotopes with these percentage abundances:

Strontium isotope	Percentage abundance
strontium-84	0.56
strontium-86	9.86
strontium-87	7.00
strontium-88	82.58

Table A2

a. Sketch strontium's mass spectrum.

b. Calculate the relative atomic mass of strontium.

A3. The data given in Table A2 for strontium isotopes are average figures for all naturally occurring strontium isotopes on Earth. What information do forensic scientists need when using hair analysis to track people?

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1.5 RELATIVE ATOMIC MASS, A_r

Atoms have very small masses, between 10^{-24} g and 10^{-22} g. Instead of using these masses, scientists use **relative atomic mass** (symbol A_r). Relative here means the mass of one atom compared with another. Originally, the mass of each atom was compared to the mass of a hydrogen atom, where hydrogen had a mass of one. As mass spectroscopy developed and gave more accurate values for the masses of atoms, it was discovered that hydrogen's mass was slightly more than one.

Relative atomic mass is now defined as the average mass of an atom compared with $\frac{1}{12}$ the mass of a carbon-12 atom.

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

Relative atomic masses have no units because they show the number of times heavier one atom is compared with another. Books give different numbers of decimal places for these values. The A_r for magnesium is given as 24 in most GCSE Periodic Tables. You will now need to use the more precise value of 24.3 for most calculations.

Remember, this is the average mass of all isotopes of an element, taking relative abundance into consideration. These values can be found using mass spectroscopy and the calculations you did earlier.

1.6 RELATIVE MOLECULAR MASS, M_r

In chemistry, you also need to know the mass of molecules. The same relative atomic mass scale is used. The **relative molecular mass** is the mass of a molecule compared with $\frac{1}{12}$ the mass of a carbon-12 atom.

$$\text{relative molecular mass, } M_r = \frac{\text{average mass of one molecule}}{\frac{1}{12}\text{ the mass of one carbon-12 atom}}$$

Finding M_r values

The mass spectrometer can also be used to find relative molecular mass values. This is dealt with in more detail in Chapter 16. If a sample of vaporised molecules is introduced into the mass spectrometer, the bombarding electrons can knock an electron off a molecule in the same way as they did with a sample of atoms. This produces a positively charged ion called the **molecular ion, M^+**.

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

Most of these molecular ions are now split into fragments by the bombarding electrons, but some remain intact.

The line produced by these molecular ions on the mass spectrum represents the relative molecular mass of the sample – if the atoms in the molecule have isotopes, there will be more than one molecular ion peak. The mass spectrum of methane (Figure 15) shows the molecular ion peak at $m/z = 16$ and another at $m/z = 17$. The one at 16 is due to $^{12}CH_4{}^+$ and the much smaller one at 17 is due to $^{13}CH_4{}^+$. These can be used to calculate the relative molecular mass of methane.

You will find more information about relative atomic mass and relative molecular mass in Chapter 2.

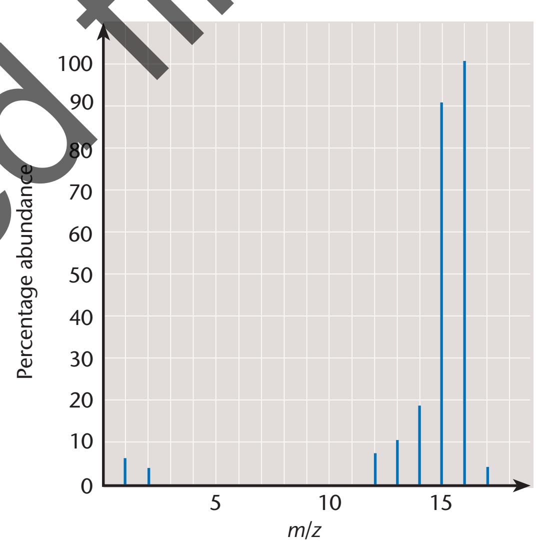

Figure 15 *The mass spectrum of methane, CH_4*

KEY IDEAS

- In a time-of-flight spectrometer, samples are ionised, accelerated to constant kinetic energy, allowed to drift and detected.
- A mass spectrum can be used to find the relative isotopic mass and abundance of isotopes of an element.

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- The mass spectrum of a compound can be used to find its M_r and provides clues about its structure.
- Relative atomic mass is the average mass of an atom compared with $\frac{1}{12}$ the mass of a carbon-12 atom.
- Relative molecular mass is the average mass of one molecule compared with $\frac{1}{12}$ the mass of a carbon-12 atom.

1.7 DESCRIBING ELECTRONS

Main shell	Sub-shell	Max no. electron pairs in sub-shell	Max no. electrons in sub-shell	Max. no. electrons in main shell
1	s	1	2	2
2	s	1	2	8
	p	3	6	
3	s	1	2	18
	p	3	6	
	d	5	10	
4	s	1	2	32
	p	3	6	
	d	5	10	
	f	7	14	

Figure 16 *Shells, sub-shells and number of electrons*

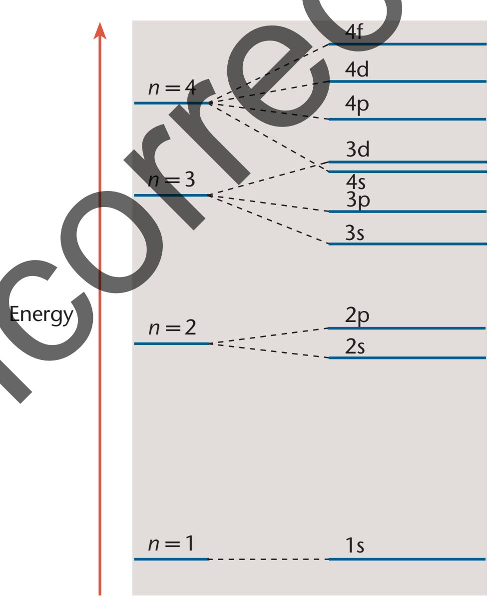

Figure 17 *The energies of the sub-shells in an atom with many electrons*

Electrons are arranged in **electron shells** around the nucleus. Each electron shell has a particular energy value. Electrons can be described as being in a particular shell. Within each shell, there are sub-shells (or orbitals). The number of sub-shells in each shell is shown in Figure 16. The sub-shells are given the letters s, p, d and f. This sequence of sub-shells corresponds to an increase in energy. The letters come from words used to describe emission spectral lines (this is discussed further a little later in this chapter). Each additional electron goes into the sub-shell with the next lowest energy. Figure 16 shows that the first shell has a maximum of two electrons and they are both in sub-shell s. The second electron shell has a maximum of eight electrons, two of which are in sub-shell s and six in sub-shell p. The order of filling is the same as the order of the elements in the Periodic Table.

Electron orbitals

Electrons are constantly moving, and it is impossible to know the exact position of an electron at any given time. However, measurements of the density of electrons as they move round the nucleus show that there are regions where it is highly probable to find an electron. These regions of high probability are called **orbitals**. Each s, p, d and f sub-shell corresponds to a differently shaped orbital.

The shapes of s and p orbitals are shown in Figure 18. Each orbital can hold two electrons, which spin in opposite directions. Table 5 shows the numbers of electrons and orbitals in the sub-shells.

Emission spectra and electrons

When an electrical voltage is applied to a gas at low pressure in a discharge tube, radiation in the visible part of the spectrum is emitted. This light can be split into its component colours using a spectroscope, an instrument designed by Robert Bunsen (the same Bunsen as in Bunsen burner).

One theory of light considers it to consist of particles, called photons, that move in a wave-like motion. Each photon has its own amount of energy, depending on the wavelength of the photon. The shorter the wavelength, the more energetic the photon and the higher the energy. Ultraviolet (UV) radiation has a shorter wavelength than infrared (IR) radiation, so a photon of UV radiation has more energy than a photon of IR radiation.

Many advertising signs are gas-discharge tubes often filled with neon. When neon absorbs electrical energy, electrons become excited to higher energy levels. As the

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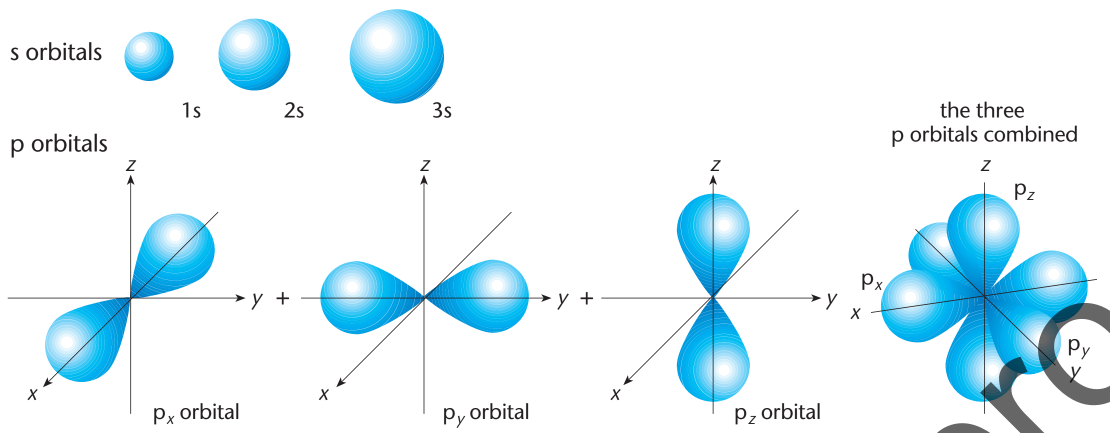

Figure 18 *The three-dimensional (3D) shape of the s and p orbitals*

Sub-level	s	p	d	f
Number of orbitals in sub-shell	1	3	5	7
Maximum number of electrons	2	6	10	14

Table 5 *Number of orbitals and maximum number of electrons per sub-shell*

electrons fall back, radiation in the yellow part of the visible spectrum is emitted. Other colours are usually obtained by using tinted glass.

The electrons in the atoms of gas in the discharge tube absorb electrical energy. This excites the electrons and they move into a higher energy level. This is not a stable arrangement and the electrons fall back to their original position, called the ground state, in one or more steps. You can see this in Figure 19. As the electron returns to a lower energy level (or shell), energy is emitted as radiation. If this radiation is in the visible range, you see it as coloured light. A spectroscope will split this radiation into lines of a particular colour. The energy gaps between the energy levels in the atom determine the wavelength of the radiation emitted. All the lines for an element make up its emission spectrum.

If the energies of electrons were not fixed, the **emission spectra** would be continuous, with no lines.

It was Niels Bohr who suggested that electrons could only exist at fixed energies. He gave each energy level (shell) the symbol n and numbered them 1, 2, 3, and so on, so that $n = 1$ is the first energy level (shell) and the ground state for hydrogen's 1 electron (see Figure 19).

Each line in hydrogen's emission spectrum represents the difference between the energy of the level to which the electron becomes excited and the level to which it falls back.

This is the basis of the **quantum theory**. Whereas Rutherford thought the electron moved smoothly, Bohr showed that it moved in small jumps, or quanta.

Emission spectra provide evidence for electrons in shells. You will read about other evidence later in this chapter.

QUESTION

Stretch and challenge

9. Why did Bohr suggest that electrons have fixed amounts of energy?

10. Draw a hydrogen atom with seven energy levels (shells). Show hydrogen's electron in the first shell. Annotate your diagram to show what happens when the electron absorbs energy and moves to $n = 3$ before falling back to the ground state. Label your diagram to show the outcome.

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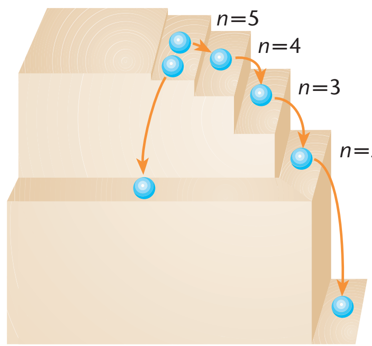


The staircase model for the levels of the energies emitted by the hydrogen electron. As shown, energy jumps can be down one step or more than one step.

Figure 19 *The staircase model for the energy levels in a hydrogen atom*

Electron configuration of atoms

The arrangement of electrons in an atom can be written as symbols in an **electron configuration**. The electron configuration includes sub-shells as well as shells, and shows the number of electrons in each:

- Hydrogen has one electron in shell 1, sub-shell s. Its electron configuration is 1s.
- Helium has two electrons with opposite spin. Its electron configuration is $1s^2$.
- Lithium has two electrons in 1s and one in 2s. Its electron configuration is $1s^2\ 2s^1$.

You can also draw a **spin diagram** for each sub-shell which shows the direction of spin of all the electrons. So, you can represent the 12 electrons in the shells/sub-shells of magnesium in two ways, electron configuration or a spin diagram.

Shells/sub-shells	1s	2s	2p	3s
Electron configuration	$1s^2$	$2s^2$	$2p^6$	$3s^2$
Spin diagram	↑↓	↑↓	↑↓ ↑↓ ↑↓	↑↓

Between hydrogen and argon, electrons of increasing energy are added, one per element, in sub-shell order 1s, 2s, 2p, 3s, 3p. Then, for potassium, the next electron skips sub-shell 3d and goes into 4s. Though shell three energies are lower overall than shell four energies, the 3d sub-shell has a higher energy than the 4s sub-shell as shown in Table 6 (and Figure 17). The order of filling is the order of elements in the Periodic Table and 4s is filled before 3d. Later, you will see that the chemical properties of elements reflect the energy levels of electrons.

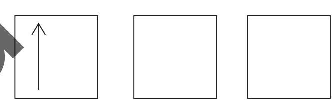
Filling orbitals

You have seen that the arrows in electron spin diagrams indicate their direction of spin and whether there are one or two electrons per orbital. The electrons fill the orbitals in a set order.

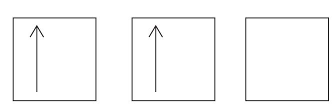
Electrons organise themselves so that they remain unpaired and fill the maximum number of sub-shells possible.

As you have seen, for the p sub-shells, this means that electrons first occupy empty orbitals and are parallel spinned. When these orbitals each have one electron, additional electrons are spin-paired; the second electron in an orbital will spin in the opposite direction.

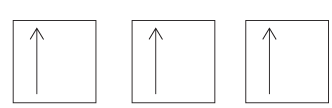
Electron $2p^1$ in boron is:



Electrons $2p^2$ in carbon are:

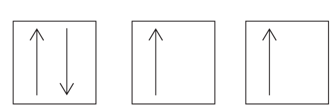


Electrons $2p^3$ in nitrogen are:



There is now one electron in each orbital. The next electron goes into the first orbital and spins in the opposite direction, so that:

Electrons $2p^4$ in oxygen are:



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Z	Element	Electron configuration	1s	2s	2p	3s	3p	3d	4s	4p
1	H	$1s^1$	[↑]							
2	He	$1s^2$	[↑↓]							
3	Li	$1s^22s^1$	[↑↓]	[↑]						
4	Be	$1s^22s^2$	[↑↓]	[↑↓]						
5	B	$1s^22s^22p^1$	[↑↓]	[↑↓]	[↑][ ][ ]					
6	C	$1s^22s^22p^2$	[↑↓]	[↑↓]	[↑][↑][ ]					
7	N	$1s^22s^22p^3$	[↑↓]	[↑↓]	[↑][↑][↑]					
8	O	$1s^22s^22p^4$	[↑↓]	[↑↓]	[↑↓][↑][↑]					
9	F	$1s^22s^22p^5$	[↑↓]	[↑↓]	[↑↓][↑↓][↑]					
10	Ne	$1s^22s^22p^6$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]					
11	Na	$1s^22s^22p^63s^1$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑]				
12	Mg	$1s^22s^22p^63s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]				
13	Al	$1s^22s^22p^63s^23p^1$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑][ ][ ]			
14	Si	$1s^22s^22p^63s^23p^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑][↑][ ]			
15	P	$1s^22s^22p^63s^23p^3$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑][↑][↑]			
16	S	$1s^22s^22p^63s^23p^4$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑][↑]			
17	Cl	$1s^22s^22p^63s^23p^5$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑]			
18	Ar	$1s^22s^22p^63s^23p^6$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]			
19	K	$1s^22s^22p^63s^23p^64s^1$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[ ][ ][ ][ ][ ]	[↑]	
20	Ca	$1s^22s^22p^63s^23p^64s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[ ][ ][ ][ ][ ]	[↑↓]	
21	Sc	$1s^22s^22p^63s^23p^63d^14s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑][ ][ ][ ][ ]	[↑↓]	
22	Ti	$1s^22s^22p^63s^23p^63d^24s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑][↑][ ][ ][ ]	[↑↓]	
23	V	$1s^22s^22p^63s^23p^63d^34s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑][↑][↑][ ][ ]	[↑↓]	
24	Cr	$1s^22s^22p^63s^23p^63d^54s^1$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑][↑][↑][↑][↑]	[↑]	
25	Mn	$1s^22s^22p^63s^23p^63d^54s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑][↑][↑][↑][↑]	[↑↓]	
26	Fe	$1s^22s^22p^63s^23p^63d^64s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑][↑][↑][↑]	[↑↓]	
27	Co	$1s^22s^22p^63s^23p^63d^74s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑][↑][↑]	[↑↓]	
28	Ni	$1s^22s^22p^63s^23p^63d^84s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓][↑][↑]	[↑↓]	
29	Cu	$1s^22s^22p^63s^23p^63d^{10}4s^1$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑]	
30	Zn	$1s^22s^22p^63s^23p^63d^{10}4s^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓]	
31	Ga	$1s^22s^22p^63s^23p^63d^{10}4s^24p^1$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓]	[↑][ ][ ]
32	Ge	$1s^22s^22p^63s^23p^63d^{10}4s^24p^2$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓]	[↑][↑][ ]
33	As	$1s^22s^22p^63s^23p^63d^{10}4s^24p^3$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓]	[↑][↑][↑]
34	Se	$1s^22s^22p^63s^23p^63d^{10}4s^24p^4$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑][↑]
35	Br	$1s^22s^22p^63s^23p^63d^{10}4s^24p^5$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑]
36	Kr	$1s^22s^22p^63s^23p^63d^{10}4s^24p^6$	[↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]	[↑↓][↑↓][↑↓][↑↓][↑↓]	[↑↓]	[↑↓][↑↓][↑↓]

Table 6 *Electron configurations and spin diagrams for the first 30 elements*

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Electrons $2p^5$ in fluorine are:

↑↓	↑↓	↑

Electrons $2p^6$ in neon are:

↑↓	↑↓	↑↓

In Table 6, shell one in helium is filled. The next element with a filled level is neon with the electron configuration $1s^2\ 2s^2\ 2p^6$.

Since the outermost shell is complete, these elements are very stable and are known as the noble gases. Noble gas configurations are used to write abbreviated electron configurations. For example, the full electron configuration for potassium is $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$. The abbreviated form is [Ar] $4s^1$.

Similarly, the abbreviated electron configuration for phosphorus is [Ne] $3s^2\ 3p^3$.

QUESTION

11. Use Table 6 to help you write abbreviated electron configurations for:
    a. sulfur
    b. aluminium
    c. calcium
    d. scandium
    e. silicon
    f. iron
    g. strontium
    h. copper.

Electron configuration of ions

An ion is an atom in which either:

- one or more electrons have been removed, producing a positively charged ion, or
- one or more electrons have been added, producing a negatively charged ion.

Worked example 2

What is the electron configuration of the sodium ion, Na^+?

The electron configuration of the sodium atom is $1s^2\ 2s^2\ 2p^6\ 3s^1$.

In Na^+ the outermost electron, $3s^1$, has been removed.

This is the electron of highest energy in sodium, and so takes the least energy to remove. The electron configuration of Na^+ is $1s^2\ 2s^2\ 2p^6$. Inner electron shells have the effect of shielding outermost electrons from the positive charge of the nucleus. A full shell has a strong shielding effect on a single outermost electron, which is then easy to remove, as in the case of Na^+.

QUESTION

12. Explain the meaning of 2, p and 6 in $2p^6$.
13. Write the electron configuration for:
    a. Ca^{2+}
    b. Cl^-
    c. Al^{3+}
    d. Br^-
    e. N^{3-}

KEY IDEAS

- Electrons in an atom are arranged in shells, with the first shell closest to the nucleus and with least energy.
- Electrons in a shell are usually located in orbitals. Different orbitals are called s, p, d and f orbitals and are referred to as sub-shells.
- An orbital contains a maximum of two electrons spinning in opposite directions.
- The electron configuration of an atom specifies the number of electrons in each shell and sub-shell.

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1.8 IONISATION ENERGIES

The energy required to remove an electron from an atom in its gaseous state is called the **ionisation energy**. The energy required to remove the first electron is called the **first ionisation energy** and can be written as:

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

The energy required to remove the second electron from an atom is called the second ionisation energy and can be written as:

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

Ionisation energy values for removing the second and subsequent electrons are called **successive ionisation energies**.

The ionisation energy for one atom is so small that, for convenience, ionisation energies are measured per mole of atoms, in kJ mol^{-1}.

QUESTION

14. Write equations using M to show the third and fourth ionisation energies.

The first ionisation energy is the enthalpy change (energy change) when one mole of gaseous atoms forms one mole of gaseous ions with a single positive charge.

Ionisation energies have been worked out for all but a few of the very heavy elements in the Periodic Table. Figure 20 shows the first ionisation energies for the elements from hydrogen to caesium.

1.9 EVIDENCE FOR SHELLS AND SUB-SHELLS

Patterns in first ionisation energies provide evidence for the existence of electron shells and sub-shells. You can see this if you look at the first ionisation energies down Group 2 and across Period 3. Successive ionisation energies of an element provide further evidence.

First ionisation energies of Group 2 elements

The Group 2 elements, beryllium to barium, are reactive metals. They are also known as the alkaline earth metals because they react with water to form an alkaline solution. The outer sub-shells of these elements contain a pair of electrons in an s orbital. The first ionisation energy measures how much energy is needed to remove one mole of these electrons from a mole of atoms.

Figure 21 shows how the first ionisation energies decrease down Group 2. That means the first electron becomes easier to remove. This is because:

- the number of electron shells between the outer electron and the nucleus is increasing and the electron shells shield the outer electron from the attraction of the nucleus, and
- the radius of the atoms are also increasing as you go down Group 2; the distance between the outer electron and the nucleus is increasing.

So, the outer electrons are easier to remove and the first ionisation energies decease. This is evidence for the existence of electron shells.

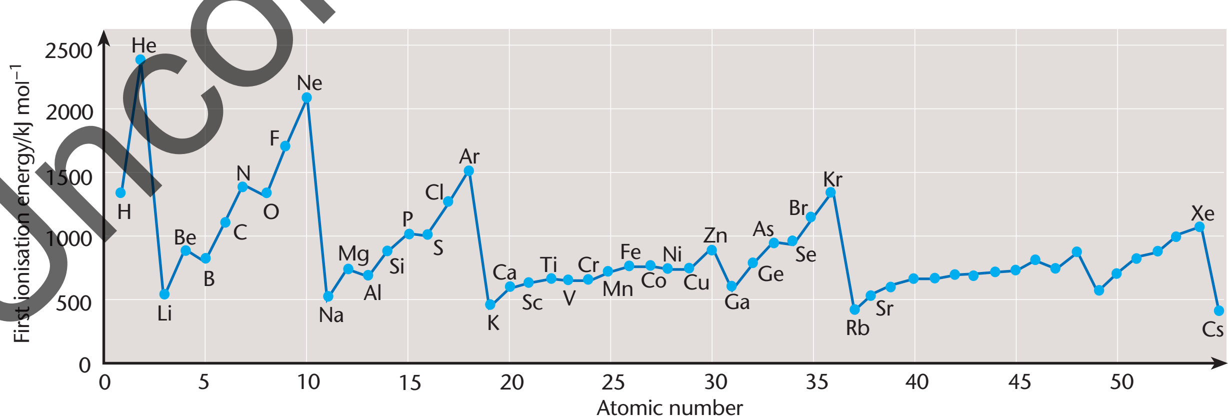

Figure 20 First ionisation energies of the elements to caesium

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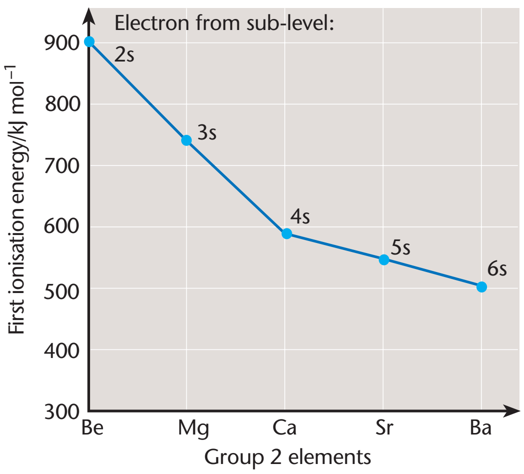

Figure 21 *First ionisation energies of Group 2 elements, beryllium to barium*

First ionisation energies of Period 3 elements

As an electron is added to each successive atom across Period 3, it fills the first available empty orbital. The electron for sodium fills the 3s orbital. The electrons in the first and second shells shield the 3s electron from the positive charge of the nucleus and it is relatively easy to remove.

Magnesium's electron completes the 3s orbital and spins in the opposite direction. Magnesium also has an extra proton, so the positive charge on the nucleus has increased. More energy is needed to remove magnesium's first electron. Magnesium's first ionisation energy is higher than sodium's.

Aluminium's electron is the first to fill a 3p orbital. p orbitals have higher energy than the s orbitals and aluminium's first electron is easier to remove than the 3s electron of magnesium. The first ionisation energy drops.

The electrons for silicon and phosphorus fill the remaining empty 3p orbitals. At the same time, the positive charge on the nucleus is increasing and more energy is needed to remove these electrons. The first ionisation energies increase from aluminium to phosphorus.

Sulfur's first electron enters a 3p orbital already containing one electron. These spin in opposite directions and repel each other. It takes less energy to remove sulfur's first electron than phosphorus's; the first ionisation energy is lower.

The electrons for chlorine and argon fill the remaining 3p orbitals. The positive charge on the nucleus continues to increase and the first ionisation energy increases as more energy is needed to remove an electron.

The general trends for first ionisation energy are:

- A sharp fall in ionisation energy between neon and sodium and between argon and potassium as electrons enter a new shell. This is evidence that the outer electron is on its own in a new shell and shielded from the charge on the nucleus by electrons in the inner shells.

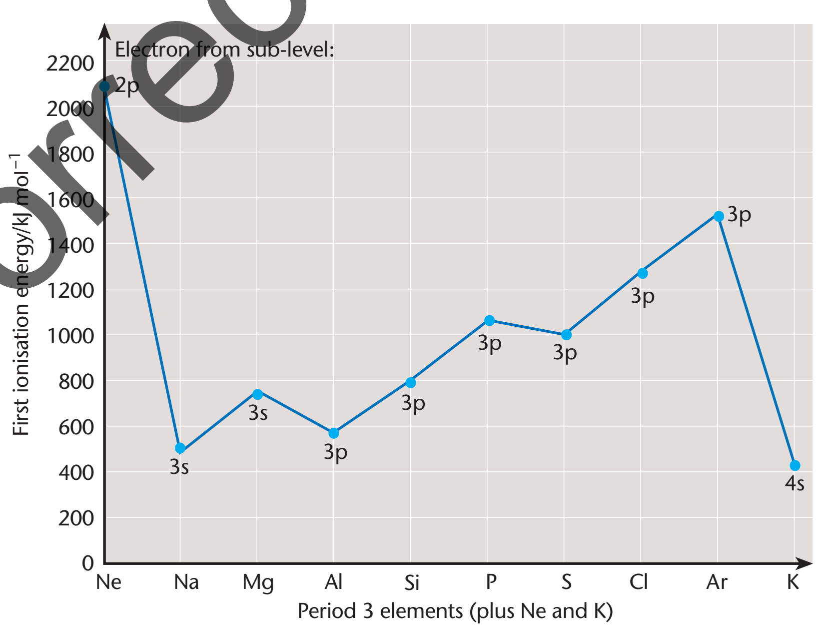

Figure 22 *First ionisation energies of Period 3 elements from sodium to argon*

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- An overall increase in the first ionisation energy across period 3 as the positive charge on the nucleus increases and electrons are attracted more strongly.
- An increase for each sub-shell as the charge on the nucleus increases and electrons are attracted more strongly.
- A fall in ionisation energy between magnesium and aluminium as electrons start to fill a new sub-shell, 3p. This is evidence that a new sub-shell is being filled.
- A fall in ionisation energy between phosphorus and sulfur as electrons start to pair up in the 3p sub-shells. This is evidence that electrons are pairing up in sub-shells.

Successive ionisation energies

Magnesium has the electron configuration 2,8,2. Its first three successive ionisation energies are:

$$Mg(g) \rightarrow Mg^{+}(g) + e^{-}$$
first ionisation energy and = +738 kJ mol^{-1}

$$Mg^{+}(g) \rightarrow Mg^{2+}(g) + e^{-}$$
second ionisation energy and = +1451 kJ mol^{-1}

$$Mg^{2+}(g) \rightarrow Mg^{3+}(g) + e^{-}$$
third ionisation energy and = +7733 kJ mol^{-1}

Figure 23 shows a graph of the $\log_{10}$ (ionisation energy) against the number of electrons removed for magnesium. We use $\log_{10}$ to make the numbers easier to handle.

The first two electrons are removed from the third or outer shell. The increase between the second and third electron is because the third electron is taken from the second shell. The gradual increase from the third to the tenth electron is electrons being removed from the second shell. The large increase between the tenth electron and eleventh electron is because the eleventh electron is taken from the first shell.

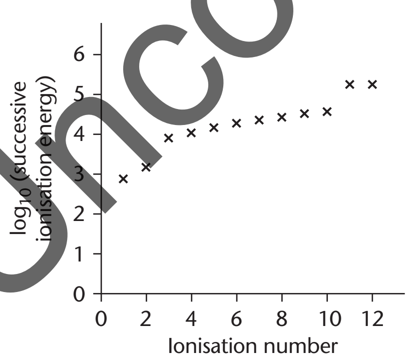

Figure 23 *The trend in the successive ionisation energies of magnesium*

Ionisation	Ionisation energy/ kJ mol^{-1}
1	738
2	1451
3	7733
4	10 543
5	13 630
6	18 020
7	21 711
8	25 661
9	31 653
10	35 458
11	169 988
12	189 368

Table 7 *The successive ionisation energies for magnesium*

QUESTION

Stretch and challenge

15. Plot a graph of successive ionisation energy divided by the charge on the remaining ion against the number of electrons removed, using Use Table 7 and the successive ionisation energies for magnesium.

16. Using your knowledge of shell and sub-shells, explain the shape of the graph you obtained.

17. These are the first five successive ionisation energies for elements X, Y and Z:

X	578, 1817, 2745, 11578, 14831
Y	496, 4563, 6913, 9544, 13352
Z	738, 1451, 7733, 10541, 13629

In which group of the Periodic Table are these elements found?

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MATHS ASSIGNMENT 4: WHY DO SCIENTISTS THINK ELECTRONS ARE ARRANGED IN SHELLS AND SUB-SHELLS?

One piece of evidence for this theory came from patterns from ionisation energy plots. These are the first ionisation energies for Period 2:

Element	Li	Be	B	C	N	O	F	Ne
First ionisation energy/ kJ mol^{-1}	520	899	801	1087	1402	1313	1681	2080

Questions

A1. Plot a graph of first ionisation energy against atomic number, *Z*.

A2. Why is there an overall increase across Period 2 from lithium to neon?

A3. Why is the first ionisation energy of beryllium higher than that of lithium?

A4. Why are there dips in the pattern at boron and oxygen?

A5. Why is there an increase in the first ionisation energy between:

a. boron and nitrogen

b. oxygen and neon?

A6. If there was a regular increase in the first ionisation energy across Period 2, what might scientists conclude about the existence of sub-shells?

A7. What is the evidence for the existence of:

a. electron shells

b. electron sub-shells?

A8. How does lithium's first ionisation energy help to predict its reactivity?

A9. How does neon's first ionisation energy help to predict its stability and/or lack of reactivity?

KEY IDEAS

- The first ionisation energies decrease down Group 2 because the outermost electrons are increasingly shielded from the attraction of the nucleus.
- There is an overall increase in the first ionisation energy across a period because of the increasing nuclear charge.
- The first ionisation energies provide evidence for the existence of shells and sub-shells.

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EXAM PRACTICE QUESTIONS

1. The element rubidium exists as the isotopes ^{85}Rb and ^{87}Rb.
   a. State the number of protons and the number of neutrons in an atom of the isotope ^{85}Rb
   b. i. Explain how the gaseous atoms of rubidium are ionised in a mass spectrometer.
      ii. Write an equation, including state symbols, to show the process that occurs when the first ionisation energy of rubidium is measured.
   c. Table Q1 shows the first ionisation energies of rubidium and some other elements in the same group.

Element	Sodium	Potassium	Rubidium
First ionisation energy/ kJ mol^{-1}	494	418	402

Table Q1

State one reason why the first ionisation energy of rubidium is lower than the first ionisation energy of sodium.

   d. i. State the block of elements in the Periodic Table that contains rubidium.
      ii. Deduce the full electron configuration of a rubidium atom.
   e. A sample of rubidium contains the isotopes ^{85}Rb and ^{87}Rb only. The isotope ^{85}Rb has an abundance 2.5 times greater than that of ^{87}Rb. Calculate the relative atomic mass of rubidium in this sample. Give your answer to one decimal place.
   f. By reference to the relevant part of the mass spectrometer, explain how the abundance of an isotope in a sample of rubidium is determined.

AQA June 2012 Unit 1 Question 1

2. The element nitrogen forms compounds with metals and non-metals.
   a. Nitrogen forms a nitride ion with the electron configuration $1s^2\ 2s^2\ 2p^6$. Write the formula of the nitride ion.
   b. An element forms an ion Q with a single negative charge that has the same electron configuration as the nitride ion. Identify the ion Q.
   c. Use the Periodic Table and your knowledge of electron arrangement to write the formula of lithium nitride.

AQA Jan 2012 Unit 1 Question 5a, b

3. Mass spectrometry can be used to identify isotopes of elements.
   a. i. In terms of fundamental particles, state the difference between isotopes of an element.
      ii. State why isotopes of an element have the same chemical properties.
   b. Give the meaning of the term relative atomic mass.
   c. The mass spectrum of element X has four peaks. Table Q2 gives the relative abundance of each isotope in a sample of element X.

m/z	64	66	67	68
Relative abundance	12	8	1	6

Table Q2

      i. Calculate the relative atomic mass of element X. Give your answer to one decimal place.
      ii. Use the Periodic Table to identify the species responsible for the peak at $m/z = 64$.
   d. Explain how the detector in a mass spectrometer enables the abundance of an isotope to be measured.

AQA June 2011 Unit 1 Question 1

4. Indium is in Group 3(13) in the Periodic Table and exists as a mixture of the isotopes ^{113}In and ^{115}In.
   a. Use your understanding of the Periodic Table to complete the electron configuration of indium.
      $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^6$ ______

Uncorrected first proofs

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b. A sample of indium must be ionised before it can be analysed in a mass spectrometer.
   i. State what is used to ionise a sample of indium in a mass spectrometer.
   ii. Write an equation, including state symbols, for the ionisation of indium that requires the minimum energy.
   iii. State why more than the minimum energy is not used to ionise the sample of indium.
   iv. Give two reasons why the sample of indium must be ionised.

c. A mass spectrum of a sample of indium showed two peaks at *m*/*z* = 113 and *m*/*z* = 115. The relative atomic mass of this sample of indium is 114.5
   i. Give the meaning of the term relative atomic mass.
   ii. Use these data to calculate the ratio of the relative abundances of the two isotopes.

d. State and explain the difference, if any, between the chemical properties of the isotopes ^{113}In and ^{115}In.

AQA Jan 2011 Unit 1 Question 2

5. a. Copy and complete Table Q3.

	Relative mass	Relative charge
Proton		
Electron		

Table Q3

b. An atom has twice as many protons and twice as many neutrons as an atom of ^{19}F. Deduce the symbol, including the mass number, of this atom.

c. The Al^{3+} ion and the Na^{+} ion have the same electron arrangement.
   i. Give the electron arrangement of these ions in terms of s and p electrons.
   ii. Explain why more energy is needed to remove an electron from the Al^{3+} ion than from the Na^{+} ion.

d. The first ionisation energies of a group of elements provides evidence for the existence of electron shells.
   i. Describe the trend in first ionisation energies down Group 2.
   ii. Explain how the trend you have described in d.i. provides evidence for the existence of electron shells.

e. First ionisation energies across a period provide evidence for the existence of electrons in sub-shells.
   i. Describe the trend in first ionisation energies in Period 3.
   ii. Explain how the trend you have described in e.i. provides evidence for the existence of electron sub-shells.

AQA January 2007 2 Unit 1 Question 1

6. a. Copy and complete Table Q4.

	Relative mass	Relative charge
Proton		
Electron		

Table Q4

b. An atom of element Q contains the same number of neutrons as are found in an atom of ^{27}Al. An atom of Q also contains 14 protons.
   i. Give the number of protons in an atom of ^{27}Al.
   ii. Deduce the symbol, including mass number and atomic number, for this atom of element Q.

c. Define the term *relative atomic mass* of an element.

d. Table Q5 gives the relative abundance of each isotope in a mass spectrum of a sample of magnesium.

m/*z*	24	25	26
Relative abundance	73.5	10.1	16.4

Table Q5

(Continued)

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Calculate the relative atomic mass of this sample of magnesium, using the data in Table Q5. Give your answer to one decimal place.

e. State how the relative molecular mass of a covalent compound is obtained from its mass spectrum.

AQA June 2004 Unit 1 Question 1

7. 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 time-of-flight (TOF) mass spectrometer. In the mass spectrometer, the sample is first vaporised and then ionised.

i. State what is meant by the term *isotopes*.

ii. Give an equation to show a gaseous iron atom producing one electron and an iron ion in the ionisation area.

iii. State the two variables that determine the time taken for an ion to move across the drift area.

iv. Explain why it is difficult to distinguish between an $^{56}Fe^{+}$ ion and a $^{112}Cd^{2+}$ ion in a mass spectrometer.

b. i. Define the term relative atomic mass of an element.

ii. The relative abundances of the isotopes in this sample of iron are shown in Table Q6.

m/z	54	56	57
Relative abundance	5.8	91.6	2.6

Table Q6

Calculate the relative atomic mass of iron in this sample, using the data in Table Q6. Give your answer to one decimal place.

AQA June 2005 Unit 1 Question 1

8. a. Titanium is a d block element in Period 4

i. State what is meant by a d block element.

ii. Write the full electron configuration for titanium in terms of s, p and d electrons.

b. Titanium has five stable isotopes, with ^{48}Ti being the most abundant.

i. State one difference and two similarities between the stable isotopes if titanium.

ii. Explain why stable isotopes of titanium have the same chemical properties.

c. Mass spectroscopy can be used to determine the relative abundance of titanium isotopes. Why is it difficult to distinguish between $^{48}Ti^{2+}$ and $^{24}Mg^{+}$ ions on a mass spectrum?

Stretch and challenge

9. Scandium is a d block element and is used on alloys to make sporting equipment such as golf clubs and fishing rods.

a. Give the electron configuration for scandium.

b. When d block elements form ions, the s electrons are lost first, then d electrons. Most d block elements form ions with more than one charge, but the scandium ions has a +3 charge in most of its compounds.

i. Give the electron configuration for the Sc^{3+} ion.

ii. Suggest why most d block elements have ions with a +2 charge.

c. Like scandium, zinc only forms ions with a +2 charge. Give the electron configuration for a Zn^{2+} ion.

d. Iron forms ions with a +2 charge and with a +3 charge. Give the electron configuration for the Fe^{3+} ion.

Multiple choice

10. Which element has an isotope with an atomic number of 35 and a mass number of 79?

A. Chlorine

B. Gold

C. Bromine

D. Selenium

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11. How many neutrons are present in an atom of $^{27}_{13}Al$?

A. 13

B. 27

C. 14

D. 40

12. What is 0.00859 in standard form?

A. 8.59×10^{-1}

B. 8.59×10^{-2}

C. 8.59×10^{-3}

D. 8.59×10^{-4}

13. What determines the flight time of ions in the drift region of a time-of-flight spectrometer?

A. Mass only

B. Charge only

C. *m*/*z* ratio

D. The number of electrons removed by electrospray ionisation only.

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2 AMOUNT OF SUBSTANCE

PRIOR KNOWLEDGE

You read in Chapter 1 that we use relative atomic mass and relative molecular mass to compare the masses of atoms and molecules. You may already know how to use a chemical equation to describe a chemical reaction. You may have also learned how chemists use moles to count particles and you have possibly carried out some calculations using moles.

LEARNING OBJECTIVES

In this chapter on amounts of substance you will build on these ideas and learn how amounts of chemical substances in solids, liquids, gases and solutions can be measured in moles.

(3.1.2.1, 3.1.2.2, 3.1.2.3, 3.1.2.4, 3.1.2.5)

Ibuprofen is an anti-inflammatory medicine that was first patented in the 1960s. It is now available without prescription ('over-the-counter'), and is sold under several different brand names, such as Nurofen and Ibuleve. The early manufacture of ibuprofen involved a series of six different chemical reactions, but each stage generated unwanted products. This meant that there was a lot of waste, which was associated with expense and the potential for environmental harm. The process also resulted in only 40.1% of all the atoms in the reactants ending up in the ibuprofen molecules. During the 1990s, Boots™ developed an alternative process for the manufacture of ibuprofen that involved only three stages. Less waste was produced and 77.4% of atoms in the reactants ended up in the ibuprofen molecules. Scientists use the idea of atom economy to calculate percentages of waste products. You will find out more about atom economy in this chapter.

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2.1 RELATIVE MASSES

Relative atomic mass, A_r

Relative atomic mass values for elements can be found on your Periodic Table.

The masses of atoms vary from 1×10^{-24} g for hydrogen to 1×10^{-22} g for the heavier elements. These are very small masses that are impossible to imagine. Small numbers like these also complicate calculations.

As described in Chapter 1, you can use the idea of relative atomic mass, A_r, with the mass of a carbon-12 atom as the standard, to deal with the mass of atoms.

Relative atomic mass is the average mass of an atom of an element compared to one-twelfth of the mass of an atom of carbon-12.

For an element,

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

You use the average mass of an element because most elements have more than one isotope. Therefore, not all the element's atoms have the same mass.

For example, chlorine has two naturally occurring isotopes: chlorine-35 and chlorine-37. Any sample of chlorine contains 75.53% of ${}^{35}_{17}\mathrm{Cl}$ and 24.47% of ${}^{37}_{17}\mathrm{Cl}$. This gives a relative atomic mass of 35.453, which is usually rounded up to 35.5.

Relative molecular mass, M_r

For molecules rather than atoms, you use relative molecular mass, symbol M_r. As with A_r, M_r has no units.

Relative molecular mass (M_r) is the sum of the relative atomic masses of all the atoms in a molecule.

You can also define relative molecular mass as:

$$M_r = \frac{\text{average mass of one molecule of an element or compound}}{\frac{1}{12}\text{ the mass of one atom of carbon-12}}$$

Worked example 1

To calculate the relative molecular mass of ammonia, NH_3:

Step 1 Look up the relative atomic mass values for each atom in the formula: nitrogen = 14; hydrogen = 1.

Step 2 Add up the masses of all the atoms in the molecule:

nitrogen: $1 \times 14 = 14$ hydrogen: $3 \times 1 = 3$

M_r of ammonia = 17.

QUESTION

1. Calculate the relative molecular mass of:
   a. sulfur dioxide, SO_2
   b. ethane, C_2H_6
   c. ethanol, C_2H_5OH
   d. phosphorus(V) chloride, PCl_5
   e. glucose, $C_6H_{12}O_6$

   (A_r: H 1; C 12; O 16; P 31; S 32; Cl 35.5)

Relative formula mass, M_f

Relative molecular mass applies to molecules, which are covalently bonded. Many of the formulae that you meet in this course have giant structures with ionic or covalent bonding. Sodium chloride has ionic bonding and consists of a large number of sodium ions and an equally large number of chloride ions held together in a lattice by electrostatic charges. The formula NaCl is called the **formula unit** and shows the ratio of each type of atom in the lattice. Silicon dioxide, SiO_2, has covalent bonding and a macromolecular structure (a giant covalent structure). The formula SiO_2 is the formula unit. The mass of the formula unit is called the relative formula mass. It has the symbol M_f, though you may find that M_r is still used. It is calculated in the same way as the relative molecular mass. Many ionic and molecular compounds have brackets in their formulae.

You can also define relative formula mass as:

$$M_f = \frac{\text{average mass of one formula unit of an element or compound}}{\frac{1}{12}\text{ the mass of one atom of carbon-12}}$$

Worked example 2

To find the relative formula mass of ammonium sulfate, $(NH_4)_2SO_4$:

Step 1 Look up the relative atomic mass value for each atom in the formula: nitrogen = 14; hydrogen = 1; sulfur = 32;
oxygen = 16

Step 2 Add up the masses of the atoms in the formula: nitrogen: $2 \times 14 = 28$; hydrogen: $8 \times 1 = 8$; sulfur: $1 \times 32 = 32$; oxygen: $4 \times 16 = 64$. Total: 132

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The relative formula mass of ammonium sulfate is 132.

Remember, atoms (or ions) inside a bracket are multiplied by the subscript number after the bracket.

QUESTION

2. Calculate *Mf* for the following:
   a. $MgBr_2$
   b. $Ca(OH)_2$
   c. $Al(NO_3)_3$
   d. $Al_2(SO_4)_3$
   e. $(CH_3COO)_2Ca$

   (*Ar*: H 1; C 12; N 14; O 16; Mg 24; Al 27; S 32; Ca 40; Br 80)

KEY IDEAS

- Relative atomic mass is the average mass of an atom of an element compared to 1/12 the mass of one atom of carbon-12.
- Relative molecular mass is the sum of the relative atomic masses of all the atoms in a molecule.
- Relative formula mass is the sum of the atoms that make a formula unit of a compound with a giant structure.

2.2 THE MOLE AND THE AVOGADRO CONSTANT

When ammonia is manufactured, the amount of product that can be generated is calculated from the amounts of reactants (nitrogen and hydrogen) that are used.

From the equation for the reaction you know that three hydrogen molecules react with one nitrogen molecule:

$$3H_2(g) + N_2(g) \rightarrow 2NH_3(g)$$

However, you cannot count out molecules to get reactants in the right proportion. Chemists count the number of particles in moles, for which we use the symbol mol. A mole of particles contains 1.205×10^{24} particles. For ammonia manufacturers, a mole of hydrogen refers to 1.205×10^{24} molecules of hydrogen and a mole of nitrogen refers to 1.205×10^{24} molecules of nitrogen.

But a mole can be 1.205×10^{24} particles of anything – atoms, molecules, ions, electrons. It is important to state the type of particles, for example, a mole of chlorine atoms, Cl, or a mole of chlorine molecules, Cl_2. A mole of chlorine molecules has twice the mass of a mole of chlorine atoms.

Since atoms have different masses, moles of atoms will have different masses. The mass of a mole of atoms of an element, in grams, is the relative atomic mass in grams.

The standard for relative atomic masses is the carbon-12 isotope of carbon. It is assigned the value 12.000 and all other atoms are measured relative to this.

One mole of carbon-12 atoms $(6.023 \times 10^{23}$ atoms$)$ has a mass of 12.000 g.

Two moles of carbon-12 atoms $(1.205 \times 10^{24}$ atoms$)$ have a mass of 24.000 g.

And so on.

The number 1.205×10^{24} is the Avogadro constant (symbol L). It was named after Amedeo Avogadro, a 19th-century Italian lawyer who was interested in mathematics and physics. He hypothesised that, at the same temperature and pressure, equal volumes of different gases contain the same numbers of particles. However, he did not calculate the number of particles in a mole. The first person to do this was an Austrian school teacher called Josef Loschmidt, in 1825.

Moles and relative mass

The relative atomic mass of carbon-12 is 12 and the relative atomic mass of magnesium-24 is 24. Therefore:

- one magnesium-24 atom has twice the mass of one carbon-12 atom
- 1.205×10^{24} magnesium atoms have twice the mass of 1.205×10^{24} carbon atoms
- 1 mole of magnesium-24 atoms has twice the mass of 1 mole of carbon-12 atoms
- 1 mole of carbon-12 atoms weighs 12 grams, 1 mole of magnesium-24 atoms weighs 24 grams.

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The mass of a mole of molecules, in grams, is the relative molecular mass in grams, and the mass of a mole of formula units in grams is the relative formula mass in grams.

Earlier you learned that relative atomic mass is the average mass of an atom of an element compared with one-twelfth of the mass of an atom of carbon-12. Chlorine, for example, has two isotopes: chlorine-35 and chlorine-37. Taking into account their relative abundances, the relative atomic mass for chlorine is 35.5. It is these average values that we use in calculations. So, we can say that:

- 1 mole of carbon dioxide, CO_2, molecules has a mass of $12 + (2 \times 16) = 44$ g
- 0.1 mole of carbon dioxide molecules has a mass of 4.4 g
- 1 mole of sodium chloride, NaCl, has a mass of $23 + 35.5 = 58.5$ g
- 5 moles of sodium chloride has a mass of $58.5 \times 5 = 292.5$ g

Calculations involving the Avogadro constant

We can use the Avogadro constant to find the number of atoms or molecules in an amount of moles.

Worked example 3

Helium is a monatomic gas, He. How many atoms are in 0.200 mol helium gas?

Step 1 1 mol helium contains 6.023×10^{23} atoms

Step 2 0.200 mol helium contains $0.2 \times 6.023 \times 10^{23}$ $= 1.205 \times 10^{23}$ atc

Carbon dioxide exists as molecules, CO_2. How many molecules are in 0.125 mol carbon dioxide?

Step 1 1 mol carbon dioxide contains 1.205×10^{24} molecules

Step 2 0.125 mol carbon dioxide contains $0.125 \times 6.023 \times 10^{23} = 7.529 \times 10^{22}$ molecules

(Maths Skill 0.1)

QUESTION

3. How many atoms are there in:
   - **a.** 3.000 mol aluminium
   - **b.** 0.0100 mol argon
   - **c.** 0.2750 mol chromium
   - d. 1.750 mol lithium
   - **e.** 0.007 mol calcium?
4. How many molecules are there in:
   - **a.** 5.00 mol water
   - **b.** 0.725 mol sulfur dioxide
   - **c.** 20 mol oxygen
   - **d.** 0.025 mol ammonia
   - **e.** 0.001 mol hydrogen chloride?

Converting mass to moles

You will need to be able to convert the mass of a substance into the number of moles and vice versa.

To convert the mass of an element (consisting of atoms) to moles, you can use the formula:

mass $= A_r \times$ number of moles

To convert the mass of a substance consisting of molecules to moles, simply substitute M_r for A_r.

You may find the triangle in Figure 1 useful, where mass = moles $\times M_r$, moles = mass/M_r and M_r = mass/mol

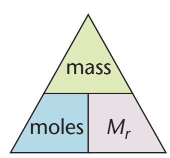

Figure 1 *This relationship triangle can help you to calculate the mass and the number of moles of substances.*

Worked example 4

How many moles are there in 414 g of lead?

Step 1 A_r lead = 207

Step 2 moles $= \dfrac{414}{207}$

$= 2$ mol

How many moles are there in 1 kg of glucose, $C_6H_{12}O_6$?

Step 1
M_r glucose $= (6 \times 12) + (12 \times 1) + (6 \times 16) = 180$

1 kg = 1000 g

Step 2 moles $= \dfrac{1000}{180}$

$= 5.56$ mol

(Maths Skills 2.1 and 2.2)

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Converting moles to mass

For elements consisting of atoms:

mass (g) = moles × relative atomic mass (A_r)

For substances consisting of molecules or formula units:

mass (g) =

moles × relative molecular or formula mass (M_r)

Worked example 5

What is the mass in grams of 2 moles of argon gas? (A_r: Ar 40)

$$\text{mass (g)} = 2 \times 40$$
$$= 80 \text{ g}$$

What is the mass in grams of 2.5 moles of ethanol, C_2H_5OH?

Step 1 M_r ethanol $= (2 \times 12) + (5 \times 1) + 16 + 1 = 46$

Step 2 mass (g) $= 2.5 \times 46$

$= 115$ g

(Maths Skills 2.1 and 2.2)

Figure 2 *The photograph shows 1 mole of different compounds. They have different masses, but they each contain 6.023 × 10^{23} formula units.*

QUESTION

5. Calculate the number of moles of:
   a. atoms in 6.00 g magnesium
   b. formula units in 60.0 g calcium carbonate, $CaCO_3$
   c. molecules in 109.5 g hydrogen chloride, HCl
   d. formula units in 303 g potassium nitrate, KNO_3
   e. formula units in 26.5 g anhydrous sodium carbonate, Na_2CO_3
   f. molecules in 4.00 g hydrogen gas
   g. atoms in 4.00 g hydrogen gas
   h. atoms in 336 g iron
   i. atoms in 27.0 kg aluminium
   j. molecules in 9.80 g sulfuric acid, H_2SO_4
6. Calculate the mass in grams of:
   a. 0.500 mol chromium
   b. 0.200 mol bromine atoms
   c. 10.0 mol lead
   d. 0.100 mol zinc(II) chloride,$ZnCl_2$
   e. 0.500 mol potassium hydroxide, KOH
   f. 0.010 mol ethanol, C_2H_5OH
   g. 0.001 mol sulfuric acid
   h. 5.00 mol nitrogen atoms
   i. 5.00 mol nitrogen molecules
   j. 0.025 mol sodium hydroxide, NaOH

More calculations using the Avogadro constant

We can use the Avogadro constant to work out the number of atoms or molecules in the mass of a substance.

Worked example 6

How many atoms are in 19.70 g gold (Au)?

Step 1: convert the mass to moles. (A_r: Au 197)

$$19.70 \text{ g gold} = \frac{19.70}{197} \text{ mol gold}$$
$$= 0.10 \text{ mol}$$

Step 2: 0.10 mol contains $0.1 \times 6.023 \times 10^{23}$ atoms $= 6.023 \times 10^{22}$ atoms

How many molecules are in 3.910 g ammonia?

Step 1: convert mass to moles. (A_r: H 1; N 14)

M_r $NH_3 = 14 + (3 \times 1) = 17$

$$3.910 \text{g } NH_3 = \frac{3.910}{17} \text{ mol } NH_3$$
$$= 0.230 \text{ mol}$$

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Step 2: 0.23 mol contains 0.23×6.023 :

$\times 6.023 \times 10^{23}$ molecules $= 1.385 \times 10^{23}$ molecules

(Maths Skills 0.1, 2.1and 2.2)

You may find the diagram in Figure 3 useful when doing calculations involving the Avogadro constant.

Remember, if you are given a mass in kilograms, you will need to convert it to grams first.

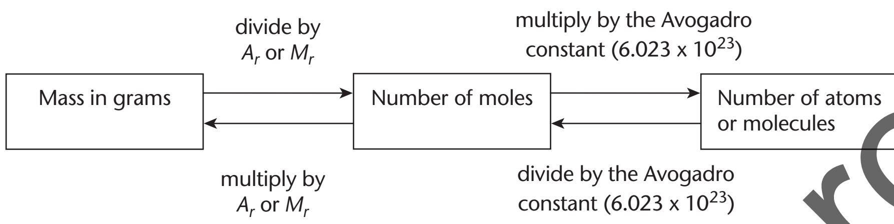

Figure 3 *This diagram shows the relationship between mass, moles and the number of atoms or molecules in an element or compound.*

QUESTION

7. How many atoms are there in:
   a. 0.040 g helium
   b. 2.30 g sodium
   c. 0.054 g aluminium
   d. 2.10 g lithium
   e. 0.238 g uranium

8. How many molecules are there in:
   a. 4.00 g oxygen gas
   b. 1.80 g water
   c. 0.014 g carbon monoxide
   d. 0.335 g chlorine gas
   e. 2.00 kg water

   (A_r: H 1; He 4; Li 6.9; C 12; O 16; Na 23.0; Al 27.0; Cl 35.5; U 238.0)

MATHS ASSIGNMENT 1: HOW MANY ATOMS ARE THERE IN THE WORLD?

MS 0.0, 0.1, 0.2, 0.4; PS 1.1, 1.2, 3.2

The world is made up of atoms too numerous to count, but you can estimate the number of atoms if you know the mass of the Earth. This is estimated to be 5 980 000 000 000 000 000 000 000 000 grams or, put in standard form, 5.98×10^{27} g.

All atoms are tiny (see Figure A1), but atoms of different elements have different masses. Table A1 gives the percentage abundance of the most common types of atom that make up the Earth. Most percentage abundance figures for elements in the Earth only include the amount of element found in the Earth's crust. So, as we do not know exactly what is in the centre of the Earth, a bit of estimating based on some good scientific theories is needed.

Table A1 also includes the mass of a **mole** of atoms of each element. This is the relative atomic mass of the element in grams. Moles are used to count particles. One mole contains 6.023×10^{23} particles.

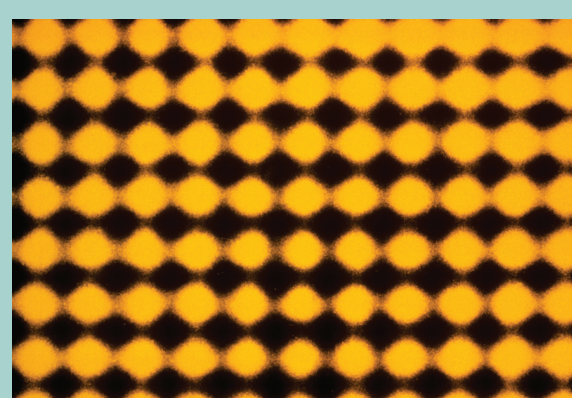

Figure A1 *An image of gold atoms obtained using scanning tunnelling microscopy. Gold atoms are about 0.1441 nm in diameter. That is 1.441×10^{-10} m.*

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Element	Mass of 1 mole/g	Percentage of the Earth/%	Mass in the Earth/g	Number of atoms
Iron	55.8	35	2.09×10^{27}	2.26×10^{49}
Oxygen	16.0	30	1.79×10^{27}	6.75×10^{49}
Silicon	16.0	15	8.97×10^{26}	1.92×10^{49}
Magnesium	24.3	13	7.77×10^{26}	1.93×10^{49}
Sulfur	32.1	2	1.20×10^{26}	2.24×10^{48}
Calcium	40.1	1	5.98×10^{25}	8.98×10^{47}
Aluminium	27.0	1	5.98×10^{25}	1.33×10^{48}

Table A1 *The abundance and estimated mass of the most common elements that make up the Earth*

Questions

A1. If Earth has a mass of 5.98×10^{27} g. , what is the mass of iron in the Earth?

A2. How many moles of iron are in the Earth? [A_r: Fe 55.8]

A3. If one mole of particles contains 6.02×10^{23} particles, how many iron atoms are there in the Earth?

Stretch and challenge

A4. Repeat the steps in questions A1, A2 and A3 for the other elements in the table and calculate the total number of atoms on Earth.

2.3 THE IDEAL GAS EQUATION

Measuring the mass of a gas is not easy. Gases are usually measured by volume, but the volume of a gas depends upon its temperature and pressure. So, to find the mass of a gas after measuring its volume, you need to understand the way that gases change in volume when temperature and pressure change. Each gas behaves very slightly differently compared with other gases but, for most practical purposes, the differences are small enough to assume that gases all behave like an imaginary 'ideal gas'.

An **ideal gas** has a number of assumed properties:

- It is made up of identical particles in continuous random motion.
- The particles can be thought of as point-like, with position but with zero volume (which means that the volume of the gas particles is taken to be zero).
- The particles do not react when they collide.
- Collisions between particles are perfectly elastic – the total kinetic energy (energy of motion) of the particles after a collision is the same as that before the collision.
- The particles have no intermolecular forces, meaning they do not attract or repel each other. (You will find out more about intermolecular forces in Chapter 3.)

As shown in Figure 4, no real gas follows this model exactly. In an ideal gas there are no intermolecular forces, so the particles are not attracted to each other. In a real gas, attractive intermolecular forces divert the paths of particles. These forces explain why, under the right conditions, gases can be liquefied.

Some gases do behave like an ideal gas over a limited range of temperatures and pressures. Hydrogen, nitrogen, oxygen and the inert (noble) gases behave most like ideal gases.

The effect of pressure

Robert Boyle was one of the first chemists to study the behaviour of gases under different conditions. He noticed that when he kept the number of moles of gas and the temperature constant, but increased the

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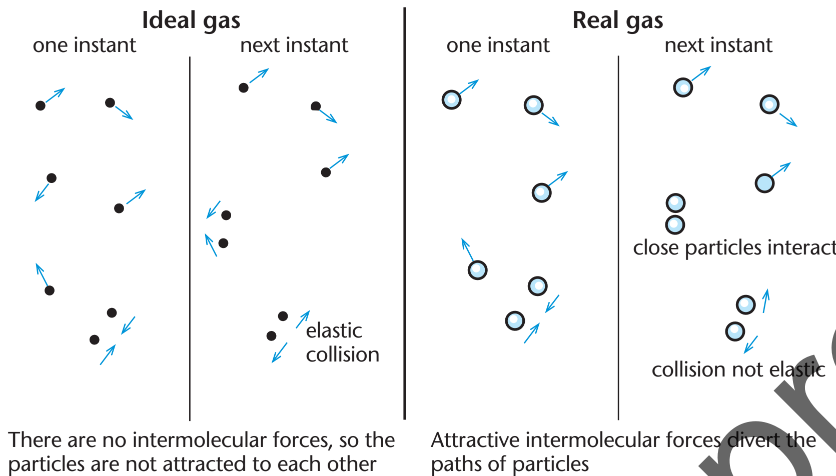

Figure 4 *Movement of particles in an ideal gas and a real gas*

pressure on the gas, then its volume became smaller. In 1662, based on this evidence, he stated:

At constant temperature *T*, the volume *V* of a fixed mass of gas is inversely proportional to the pressure *p* applied to it.

When this theory proved generally to be true, it became known as Boyle's law. You can write it mathematically as:

$$V \propto \frac{1}{p}$$

when *T* and the mass of gas are constant,

which is the same as:

$$p \times V = \text{constant}$$

when *T* and the mass of gas are constant.

The effect of temperature

About a hundred years after Robert Boyle made his conclusions, the Frenchman Jacques Charles was studying during a period when ballooning was all the rage in France. Balloons were initially filled with hydrogen. Since the density of hydrogen was less than that of air, balloons filled with enough hydrogen floated up from the ground. Disastrous fires, exemplified by the Hindeberg disaster (Figure 5), did put an end to the use of hydrogen, however. Ballons were subsequently filled with air that was heated to reduce its density. As soon as the total mass of the balloon, passengers and air in the balloon was less than that of the air displaced, the balloon could rise into the air. This is the method that is still used today (Figure 6).

Charles was looking at the effect of changing the temperature of gas and measuring the resulting

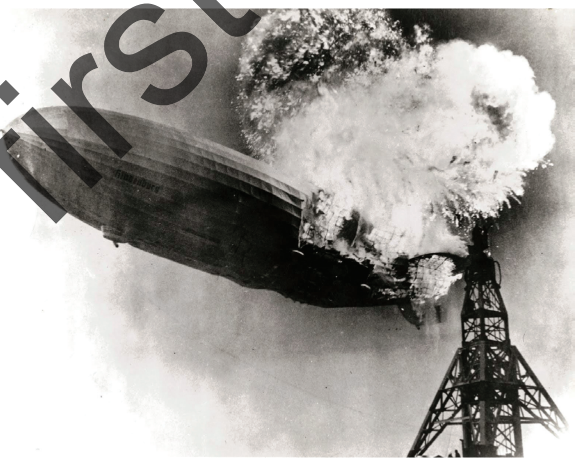

Figure 5 *The Hindeberg was the largest airship that used a hydrogen-filled balloon. In 1937, it burst into flames when trying to dock at the end of its first North American transatlantic journey. This marked the end of the airship era.*

changes in volume. As temperature was increased, the gases expanded because their molecules moved faster and were further apart, so their density decreased. As temperature was decreased, the gases became more dense as they contracted. The effect was the same for a wide range of gases and, in 1787, Charles published his law:

At constant pressure, the volume of a fixed mass of gas is proportional to its temperature.

$$V = \text{constant} \times T$$

when *p* and the mass of gas are constant.

The equation for Charles's law implies that at constant pressure, as the temperature goes down, the volume of any sample of gas decreases until, at a certain very

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Figure 6 *Balloon rides today use hot air and work on the principle that air expands and becomes less dense.*

low temperature, the volume becomes zero. Plotting the volumes of most gases against temperature and extrapolating (Figure 7) produces a surprising result – they would all reach zero volume at the same temperature, $-273.15\ °C$, which is known as the **absolute zero** temperature.

At this temperature the atoms or molecules are assumed to have no kinetic energy, to have ceased moving and colliding, and to be so close together as to occupy a negligible volume. Of course, at normal pressures, the gases would be solids at $-273.15\ °C$, which is why you have to 'extrapolate' to obtain the value (Figure 7). On the kelvin temperature scale, this temperature is 0 kelvin (0 K), at which an ideal gas is assumed to occupy zero volume. In your calculations using gas laws, always remember to use temperatures in kelvins, converting celsius to kelvin by adding 273.

Combining Boyle's law and Charles's law

Boyle's law and Charles's law can be combined into a single ideal gas equation, but one more piece of information is needed, which was discovered by the Italian Amedeo Avogadro. He found that:

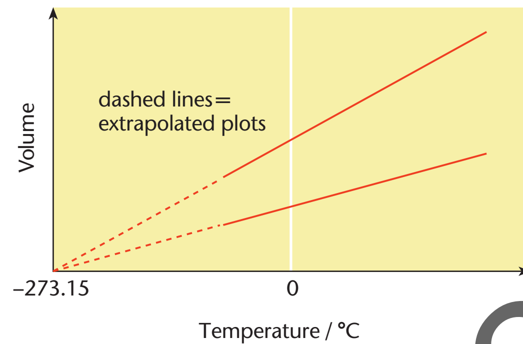

Figure 7 *The relationship between volume of a gas and temperature*

Equal volumes of all gases at the same pressure and temperature contain the same number of particles.

This means that the molar volume, which is the volume occupied by one mole of a gas, is the same for all gases at the same temperature and pressure. For example, Figure 8 shows that the volume of a mole of different gases at 298 K (25 °C) is 24 dm^3.

As a consequence, the volume of a gas is proportional to the number of moles of the gas present when the pressure and temperature are constant. Thus:

$$V = \text{constant} \times n$$

when p and T are constant and n is the number of moles of the gas.

The **ideal gas equation** combines all the equations above for gases into one equation:

$$pV = nRT$$

where:

p = pressure of the gas in pascals (Pa)

V = volume of the gas in m^3

n = number of moles of the gaseous particles

R = molar gas constant $(8.31\ JK^{-1}mol^{-1})$

T = temperature in kelvin (K)

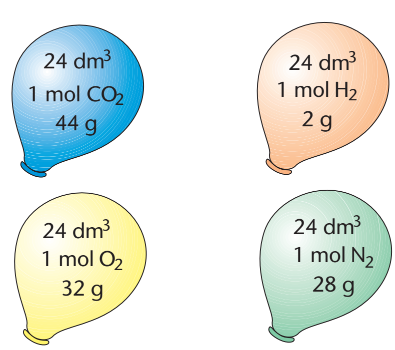

Figure 8 *The molar volume of gases at 298 K and 100 kPa*

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Determining the molar gas constant

A simple laboratory experiment can be carried out to calculate the value of the gas constant R. The equipment is shown in Figure 9. It includes a gas syringe with a friction-free plunger, which allows gas in the syringe to reach atmospheric pressure. The experiment gives values for all the quantities in the ideal gas equation that are needed to calculate R.

The syringe is filled several times from the cylinder. This gives a sum of volumes $= V$

The total mass of gas lost from the cylinder is recorded and the number of moles calculated $= n$

The temperature is recorded $= T$

The atmospheric pressure is recorded $= p$

Then the gas constant is calculated from:

$$R = \frac{pV}{nT}$$

You need to be able to use the ideal gas equation to carry out calculations in the practical and in the other examples.

Finding the M_r of a volatile liquid

The apparatus used for this is shown in Figure 10. A small syringe is used to inject a known mass of the volatile liquid into a large gas syringe. At the recorded temperature the liquid changes to a gas and its volume in the large syringe is measured.

Some sample results from an experiment to find the M_r of hexane are given. You can use these data to calculate the M_r of hexane.

volume of air $= 10\ \text{cm}^3$

volume of vapour + air $= 100\ \text{cm}^3$

mass of sample $= 2.59$ g

temperature $= 87\ °\text{C}$

pressure $= 100$ kPa [this is a pressure of 1 atmosphere (atm)]

First, convert the measurements to SI units (as in the gas equation):

$$\begin{aligned} \text{volume of sample} &= 100 - 10\ \text{cm}^3 \\ &= 90\ \text{cm}^3 \\ &= 90 \times 10^{-6}\ \text{m}^3 \\ \text{temperature} &= 87 + 273\ \text{K} \\ &= 360\ \text{K} \\ \text{pressure} &= 100\,000\ \text{Pa} \end{aligned}$$

Rearrange the ideal gas equation to give M_r as the subject:

$$\text{number of moles} = \frac{\text{mass (g)}}{M_r}$$

$$pV = \frac{mRT}{M_r}$$

$$M_r = \frac{mRT}{pV}$$

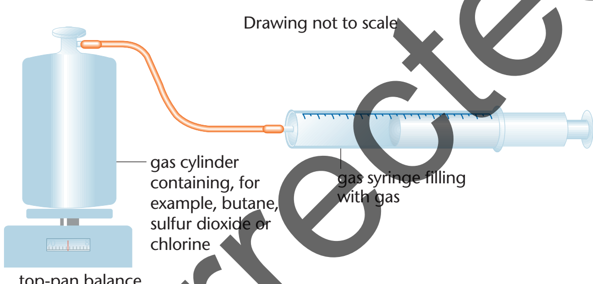

Figure 9 *This apparatus is used to calculate the molar gas constant, R, used in the ideal gas equation.*

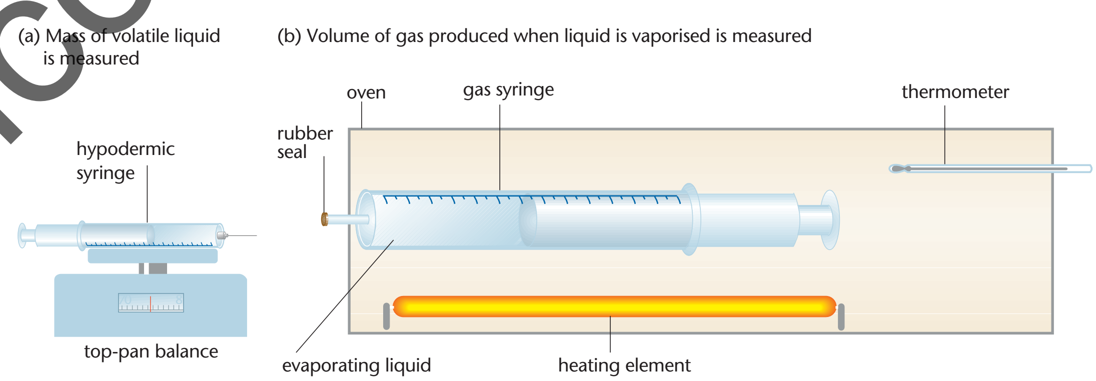

Figure 10 *Apparatus to find the M_r of a volatile liquid*

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Insert values into the ideal gas equation:

$$M_r = \frac{2.59 \times 8.31 \times 360}{100\,000 \times 90 \times 10^{-6}}$$

$$M_r = 86$$

Remember that the answer can only contain two significant figures because the volume of the sample is given as 90 cm^3. Do not round up or down until the end of the calculation because you may lose accuracy.

Calculating moles from gas volume

Worked example 7

How many moles of oxygen are there in 500 cm^3 of gas at 25 °C and 100 KPa?

Step 1 Convert the units to the units of the ideal gas equation:

$$p = 100 \text{ kPa} = 100\,000 \text{ Pa}$$

$$V = 500 \text{ cm}^3 = 500 \times 10^{-6} \text{m}^3$$

$$T = 25\text{ °C} = 298 \text{ K}$$

Step 2 Rewrite the ideal gas equation to make n the subject:

$$n = \frac{pV}{RT}$$

Step 3 Insert the values:

$$n = \frac{105 \times 500 \times 10^{-6}}{8.31 \times 298}$$

moles of oxygen = 0.0200 mol

(Maths Skills 2.1, 2.2, 2.3, and 2.4)

Calculating the volume of a reactant gas and the mass of a gas product

Worked example 8

Methane reacts with oxygen to produce carbon dioxide and water. Calculate the volume of oxygen needed to react with 20 dm^3 methane, and the mass of carbon dioxide produced at 120 kPa and 30 °C.

The equation for the reaction is:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l)$$

Step 1 The equation shows that one mole of methane reacts with two moles of oxygen to give one mole of carbon dioxide.

From Avogadro's rule, at constant temperature and pressure, 20 dm^3 of methane therefore requires 40 dm^3 oxygen for the reaction.

Similarly, the volume of carbon dioxide produced is 20 dm^3.

Step 2 To find the mass of 20 dm^3 CO_2, first use the ideal gas equation to find the number of moles. Using $n = pV/RT$, insert the values converted to the correct units:

$$n = \frac{120 \times 100 \times 20 \times 10^{-3}}{8.31 \times 303}$$

$$= 0.953 \text{ mol}$$

The reaction produces 0.95 mol of carbon dioxide.

Step 3 Convert mass (g) into moles:

$$\text{mass (g)} = \text{moles} \times M_r$$

$$= 0.953 \times 44$$

$$= 41.9 \text{ g}$$

The mass of carbon dioxide produced in the reaction = 41.9 g.

(Maths Skills 2.1, 2.2, 2.3, and 2.4)

Calculating the volume of gas produced in a reaction involving a non-gas reactant

Worked example 9

When potassium nitrate is heated, it gives off oxygen and becomes potassium nitrite. Calculate the volume in dm^3 of oxygen produced from 345 g potassium nitrate at 38 °C and 100 kPa.

The equation for the reaction is:

$$2KNO_3(s) \rightarrow 2KNO_2(s) + O_2(g)$$

Step 1 Work out the number of moles in 345 g of potassium nitrate:

$$M_r\, KNO_3 = 101 \qquad (A_r\text{: K 39; N 14; O 16})$$

$$\text{moles } KNO_3 = \frac{\text{mass}}{M_r}$$

$$= \frac{345}{101}$$

$$= 3.42$$

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Step 2 From the reaction equation, calculate the moles of O_2:

3.42 moles KNO_3 produces 0.5×3.42 moles $O_2 = 0.171$

Step 3 Work out the temperature in kelvin:

$T = 38 + 273 = 311$

Step 4 Write the ideal gas equation, making V the subject, and insert the values:

$$V = \frac{nRT}{p}$$

$$V = \frac{1.71 \times 8.31 \times 31}{100 \times 10^3}$$

$$= 0.0442\ m^3\ O_2$$

The volume of oxygen produced is $44\ dm^3$.

(Maths Skills 2.1, 2.2, 2.3, and 2.4)

QUESTION

9. a. Convert these temperatures into kelvin:
   i. 25 °C
   ii. 250 °C
   iii. −78 °C
   b. What is the volume in m^3 of 5 mol of oxygen gas at 25 °C and 100 kPa?
   c. What volume (dm^3) of hydrogen gas is produced when 19.5 g zinc metal dissolves in excess hydrochloric acid at 30 °C and 100 kPa?
   d. A fairground balloon is filled with 1000 cm^3 of helium gas. The temperature is 25 °C and the pressure 100 kPa. How many moles of gas does the balloon contain?

KEY IDEAS

- Theories and equations about the behaviour of gases assume that all gases are ideal gases.
- Ideal gases have point-like particles in random motion. The particles do not react on collision, are elastic and have no intermolecular forces.
- The ideal gas equation is $pV = nRT$, where p = pressure (Pa), V = volume (m^3), n = amount (mol), R = molar gas contant, T = temperature (K).

2.4 EMPIRICAL AND MOLECULAR FORMULAE

Remember that:

- the empirical formula is the simplest whole number ratio of atoms of each element that are in a compound
- the chemical formula (molecular formula or formula unit) is the actual number of atoms of each element used to make a molecule of formula unit.

When chemists need to find the composition of a compound, they measure the mass of each element in that compound. They use this information to work out the empirical formula of the compound. The empirical formula gives the simplest ratio of atoms of each element present in the compound. For example, the molecular formula of ethane is C_2H_6, but it has the empirical formula CH_3, because the simplest whole number ratio of carbon to hydrogen is 1:3.

As an example of calculating an empirical formula, consider a compound that was found to contain 40% by mass of calcium, 12% by mass of oxygen and 48% by mass of oxygen. From these figures, you can calculate that 100 g of the compound would contain 40 g calcium, 12 g carbon and 48 g oxygen. If you convert these masses to amounts in moles, you will know the ratio of each element (Table 1).

element	calcium		carbon		oxygen
mass/g	40		12		48
amount/mol	$\frac{40}{40}$		$\frac{12}{12}$		$\frac{48}{16}$
ratio of elements	1	:	1	:	3

Table 1

If the substance has a lattice structure (either bonded covalently or ionically), the **formula unit** shows the ratio of atoms of each element in the substance. For example, calcium carbonate, $CaCO_3$, consists of ions held in a giant structure, as shown in Figure 11. The formula unit is $CaCO_3$,

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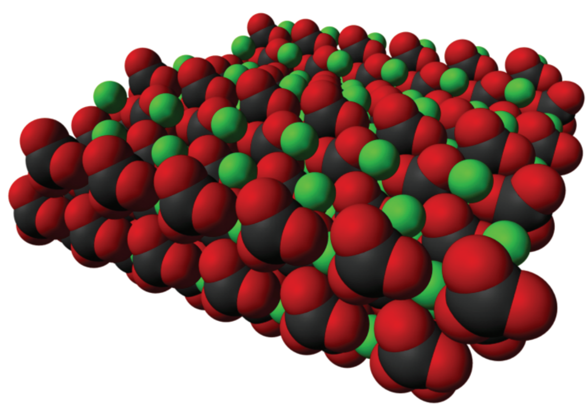

Figure 11 Calcium carbonate giant lattice. The green spheres represent calcium ions, Ca^{2+}, and the grey spheres each with three red spheres attached represent carbonate ions, CO_3^{2-} (grey for carbon and red for oxygen).

showing that it is made from one calcium atom, one carbon atom and three oxygen atoms.

The ratio of atoms in a chemical formula (molecular formula or formula unit) stays the same.

Therefore, one molecule of CO_2 is made from one atom of carbon and two atoms of oxygen, and 100 molecules of CO_2 are made from 100 atoms of carbon and 200 atoms of oxygen.

Since you can count the number of particles in moles:

one mole of CO_2 is made from one mole of carbon atoms and two moles of oxygen atoms.

Calculating a molecular formula

Worked example 10

An investigation to identify a carbohydrate found that it contained 0.34 g carbon, 0.057 g hydrogen and 0.46 g oxygen. Find its empirical formula.

Step 1 Note that the mass of each element is given in the question, rather than the percentage composition. Treat this in exactly the same way as described earlier. You may need some common sense to sort out the whole-number ratio (Table 2).

The empirical formula is CH_2O.

Step 2 To find the molecular formula, you need to know the relative molecular mass.

If the M_r of this carbohydrate is 180, then to calculate the molecular formula you first find the M_r of the empirical formula:

$$M_r\ CH_2O = 12 + (2 \times 1) + 16$$
$$= 30$$

element	carbon	hydrogen	oxygen
mass/g	0.34	0.057	0.46
amount/mol	$\frac{0.34}{12}$	$\frac{0.057}{1}$	$\frac{0.46}{16}$
=	0.028	0.057	0.029
ratio of elements (divide by the lowest)	$\frac{0.028}{0.028}$	$\frac{0.057}{0.028}$	$\frac{0.029}{0.029}$
=	1.0 :	2.0 :	1.0

Table 2

Step 3 Since the M_r of the carbohydrate is 180, if you divide 30 into 180, the answer will show how many times you need to multiply the empirical formula to give the molecular formula:

$$\frac{180}{30} = 6$$

The molecular formula is 6 × (empirical formula)

$$= 6 \times (CH_2O)$$
$$= C_6H_{12}O_6$$

(Maths Skill 0.2)

QUESTION

10. **a.** Find the empirical formula of a compound containing 84 g magnesium and 56 g oxygen.

b. 3.36 g of iron combine with 1.44 g of oxygen to form an oxide of iron. What is its empirical formula?

c. A compound contains, by mass, 20.14% iron, 11.51% sulfur, 63.31% oxygen and 5.04% hydrogen. Find its empirical formula.

d. A hydrocarbon contains 82.8% by mass of carbon. Find its empirical formula. (Hint: what types of atoms are hydrocarbons made from?)

e. Another hydrocarbon has a relative molecular mass of 28 and contains 85.7% by mass of carbon and 14.3% by mass of hydrogen. Calculate its empirical formula and its molecular formula.

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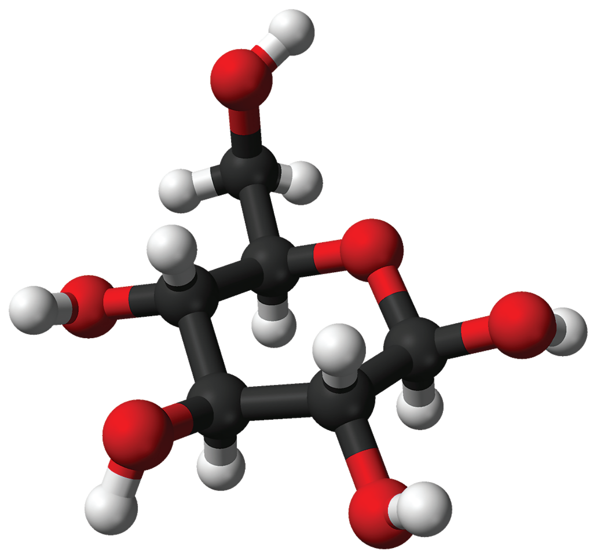

Figure 12 Model of a glucose molecule, which has the empirical formula CH_2O. The molecular formula $C_6H_{12}O_6$. The grey spheres represent carbon, the white are hydrogen and the red are oxygen atoms.

KEY IDEAS

- A mole contains 6.023×10^{23} particles.
- The empirical formula is the simplest whole number ratio of atoms of each element used to make a compound.
- The molecular formula is the actual number of atoms of each element used to make a molecule.
- The chemical formula of an element or a compound with a giant structure is the number of atoms of each element used to make a formula unit.

2.5 CHEMICAL EQUATIONS

Balancing chemical equations

A **chemical equation** is a shorthand way of writing a chemical reaction. The equation uses **chemical formulae** for the reactants and the products. Formulae use letter symbols to represent the elements and numbers to show how many atoms of each element are involved.

A chemical equation can also include the **state** of reactants and products:

(s) means the solid state

(l) means the liquid state

(g) means the gaseous state

(aq) means aqueous, that is, in aqueous (dissolved in water) solution

As an example, sulfur burns in oxygen to produce sulfur dioxide. This is how you write the reaction using chemical formulae:

reactants product

$$S(s) + O_2(g) \rightarrow SO_2(g)$$

A chemical equation must balance. This means there must be the same number of each type of atom on both sides of the arrow. In this example, there is one sulfur atom on the left and one sulfur atom on the right. There are two oxygen atoms on the left and two oxygen atoms on the right. So the equation is balanced and we call it a balanced equation.

Sulfur dioxide reacts with oxygen to produce sulfur trioxide. You could use chemical formulae to write the reaction like this:

$$SO_2(g) + O_2(g) \rightarrow SO_3(g)$$

Is this equation balanced? There is one sulfur atom on the left and one on the right. But there are four oxygen atoms on the left and only three on the right. So the equation needs to be altered so that it is balanced.

A SO_2 molecule is made from one S atom and two O atoms. A SO_3 molecule is made from one S atom and three O atoms. So one extra O atom is needed to make SO_3 rather than SO_2. One oxygen molecule is made from enough oxygen atoms to react with two molecules of sulfur dioxide and produce two molecules of sulfur trioxide. So we can now write a balanced equation:

$$2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)$$

Figure 13 The manufacture of sulfuric acid includes two oxidation reactions: $SO_2(g) + O_2(g) \rightarrow SO_3(g)$ and $2SO_2(g) + O_2(g) \rightarrow 2SO_3(g)t$.

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This is a very simple equation. Others are more complicated, but the basic procedure is the same. Take it step by step and you should have no problems. Balancing chemical equations is trial and error. With each step you take, you need to check whether you need more steps to rebalance the equation. Worked example 11 shows how to balance the equation for ammonia burning in oxygen.

Worked example 11

$NH_3 + O_2 \rightarrow NO_2 + H_2O$

Look at nitrogen. There is one atom on either side, so the nitrogen balances.

Look at hydrogen. There are three atoms on the left and two on the right. Use two ammonia molecules and three water molecules to give six hydrogen atoms on each side:

$2NH_3 + O_2 \rightarrow NO_2 + 3H_2O$

Now the nitrogen is unbalanced, so double the nitrogen dioxide [nitrogen(IV) oxide] on the right:

$2NH_3 + O_2 \rightarrow 2NO_2 + 3H_2O$

Now check on the oxygen. There are two atoms on the left and seven on the right. First of all, double both sides to get even numbers:

$4NH_3 + 2O_2 \rightarrow 4NO_2 + 6H_2O$

The nitrogen and hydrogen are still balanced. You have 14 oxygen atoms on the right, so you need seven oxygen molecules on the left:

$4NH_3 + 7O_2 \rightarrow 4NO_2 + 6H_2O$

Add state symbols:

$4NH_3(g) + 7O_2(g) \rightarrow 4NO_2(g) + 6H_2O(g)$

QUESTION

11. Balance the equations a–e:
    a. $C_2H_5OH(l) + O_2(g) \rightarrow CO_2(g) + H_2O(g)$
    b. $Al(s) + NaOH(aq) \rightarrow Na_3AlO_3(aq) + H_2(g)$
    c. $CO_2(g) + H_2O(l) \rightarrow C_6H_{12}O_6(aq) + O_2(g)$
    d. $C_3H_8(g) + O_2(g) \rightarrow CO_2(g) + H_2O(l)$
    e. $Al(s) + H_2SO_4(l) \rightarrow Al_2(SO_4)_3(aq) + SO_2(g) + H_2O(l)$

12. Write balanced symbol equations for the reactions a–e, and include state symbols.
    a. iron(III) chloride + ammonia in water $\rightarrow$ iron(III) iron(III) hydroxide + ammonia chloride
    b. copper(II) carbonate + hydrochloric acid $\rightarrow$ copper (II) chloride + carbon dioxide + water
    c. sodium hydroxide + phosphoric acid (H_3PO_4) $\rightarrow$ sodium phosphate + water (phosphate is PO_4^{3-})
    d. iron + chlorine $\rightarrow$ iron(III) chlor
    e. copper(II)) oxide + sulfuric acid $\rightarrow$ copper(II) sulfate + water

Using chemical equations and moles

Chemical equations enable you to calculate the masses of reactants and the masses of products formed in a chemical reaction.

Look at this reaction:

$$CaCO_3(s) + 2HCl(aq) \rightarrow CaCl_2(s) + CO_2(g) + H_2O(l)$$

To carry out the reaction without leaving a surplus of either reactant, one mole of $CaCO_3$ is needed for every two moles of HCl. So you can write the moles in the reaction as:

1 mol $CaCO_3$ reacts with 2 mol HCl to produce 1 mol $CaCl_2$ + 1 mol CO_2 + 1 mol H_2O

But since you can calculate the mass of a mole, you can take a given mass of calcium carbonate and work out exactly what mass of hydrochloric acid in solution reacts with it. You can also calculate the mass of each product that is made.

Calcium carbonate decomposes when it is heated in a furnace to make calcium oxide, sometimes called quicklime.The simple equation is:

$$CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$$

This is a reversible reaction, but if the carbon dioxide is allowed to escape, then all the calcium carbonate decomposes.

So, one mole of calcium carbonate breaks down to give one mole of calcium oxide and one mole of carbon dioxide.

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Calculating the mass of product formed

Worked example 12

How much calcium oxide could be obtained from 800 kg of calcium carbonate?

Step 1 Write a balanced equation:

$CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$

Step 2 Calculate the M_f for the calcium carbonate and calcium oxide:

(A_r: Ca 40; C 12; O 16)

M_f $CaCO_3 = 40 + 12 + 48 = 100$

M_f $CaO = 40 + 16 = 56$

Step 3 Calculate the moles of $CaCO_3$ used:

$$\text{moles} = \frac{\text{mass of } CaCO_3(s)}{M_f}$$

$$= \frac{800 \times 10^3}{100}$$

$$= 8000 \text{ mol}$$

Step 4 From the equation, find the moles of calcium oxide produced:

1 mol $CaCO_3$ produces 1 mol CaO

8000 mol $CaCO_3$ produces 8000 mol CaO

Step 5 Convert the moles of calcium oxide into mass (g)

$$\text{Mass (g)} = \text{moles} \times M_f$$

$$= 8000 \times 56$$

$$= 448\,000 \text{ g}$$

$$\text{Mass} = 448 \text{ kg}$$

(Maths Skills 2.1, 2.2, 2.3, and 2.4)

Calculating reacting masses

Worked example 13

Copper carbonate reacts with hydrochloric acid to produce copper chloride. What mass of copper chloride is made when 24.7 g copper carbonate react with excess acid?

Step 1 Write a balanced equation:

$CuCO_3(s) + 2HCl(aq) \rightarrow CuCl_2(aq) + H_2O(l) + CO_2(g)$

Step 2 Calculate the M_r for the substances involved in the question.

(A_r: Cu 63.5; C 12; O 16)

M_f $CuCO_3 = 63.5 + 12 + 48$

$= 123.5$

M_f $CuCl_2 = 63.5 + 71$

$= 134.5$

Step 3 Calculate the moles of $CuCO_3$ used:

$$\text{moles } CuCO_3 = \frac{\text{mass (g)}}{M_f}$$

$$= \frac{24.7}{123.5}$$

$$= 0.2 \text{ mol}$$

Step 4 Use the equation to find the moles of $CuCl_2$ produced:

1 mol $CuCO_3$ → 1 mol $CuCl_2$;

0.2 mol $CuCO_3$ → 0.2mol $CuCl_2$

(A_r: Cu 63.5; Cl 35.5)

M_f $CuCl_2 = 63.5 + (2 \times 35.5) = 134.5$

Step 5 Convert the moles of $CuCl_2$ into mass (g)

$$\text{mass (g)} = \text{moles} \times M_f$$

$$= 0.2 \times 134.5$$

$$= 26.8 \text{ g}$$

(Maths Skills 2.1, 2.2, 2.3, and 2.4)

Percentage yield

Example 2 showed that 800 kg of calcium carbonate could produce 448 kg of calcium oxide. This is called the theoretical yield. The reality is that although industries strive to achieve the maximum yield possible and make the maximum profit, it is never possible to achieve the theoretical yield. Calcium carbonate only decomposes when the temperature is over 1000 °C. The reaction is also reversible so complete decomposition depends on the carbon dioxide escaping. Some calcium oxide may be lost when transferring it from the kiln to the next stage.

The mass of product actually obtained is called the actual yield. It can only be found by actually doing the

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206093 AS Chemistry A-Level_Ch2.indd 43 4/1/15 12:39 AM

reaction. Percentage yield is used to express how close the actual yield is to the theoretical yield.

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

Worked example 14

If 800 kg of calcium carbonate produced 314 kg of calcium oxide in an actual process, calculate the percentage yield.

Step 1 Calculate the theoretical yield from the equation:

$$CaCO_3(s) \rightleftharpoons CaO(s) + CO_2(g)$$

800 kg calcium carbonate can produce a theoretical yield of 448 kg calcium oxide (from calculation in Worked example 12).

Step 2 $\text{percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$

$$= \frac{314}{448} \times 100\%$$

$$= 70.0\%$$

(Maths Skills 0.2, 2.1, 2.2, 2.3, and 2.4)

Percentage atom economy

Chemists have traditionally measured the efficiency of a reaction by its percentage yield. However, this is only half the story because many atoms in the reactants are not needed in the product. They make up the waste or side products.

Percentage atom economy is a way to compare the maximum mass of a product that can be obtained

Figure 14 *In the cement kiln, calcium oxide is heated with silicon dioxide and aluminium oxide at 1400 °C. Calcium sulfate is added to the produce from the kiln and the mixture is then ground to the fine grey powder you probably know as Portland cement. Cement manufacturers are actively researching ways to increase their percentage atom economy.*

with the mass of the reactants. It is calculated from the equation:

percentage atom economy

$$= \frac{\text{molecular mass of desired product}}{\text{sum of molecular masses for all reactants}} \times 100$$

Developing chemical processes with high atom economies can have economic, ethical and environmental benefits for industry and the society it serves.

Copper can be extracted by heating copper(II) oxide with carbon as in the equation:

$$2CuO(s) + C(s) \rightarrow 2Cu(s) + CO_2(g)$$

Two moles (159 g) of copper(II) oxide react with one mole (12 g) of carbon. The reactants need to be added in these reacting quantities. Theoretically, the reaction can produce 127 g of copper from 159 g of copper oxide and 12 g of carbon. So:

$$\text{percentage atom economy} = \frac{127}{171} \times 100$$

$$= 74\%$$

The reaction uses 74% of the mass of the reactants to give the product required. The remaining 26% ends up as waste or side products, assuming the percentage yield is 100%. The reality is that the yield will be lower because the percentage yield is unlikely to be 100%.

QUESTION

13. a. What theoretical yield of iron can be obtained from reacting 320 tonnes of iron(III) oxide with carbon monoxide in the blast furnace? The equation for the reaction is:

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

b. If the actual yield in 13a is 200 tonnes, what is the percentage yield?

c. What is the percentage atom economy of the reaction in 13a?

d. Sulfuric acid is reacted with calcium carbonate to produce calcium sulfate for use in making plaster. Calculate the theoretical mass of calcium sulfate that can be made from 490 tonnes of sulfuric acid.

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206093 AS Chemistry A-Level_Ch2.indd 44 4/1/15 12:39 AM

e. If the actual yield is 550 tonnes of calcium sulfate, calculate the percentage yield.

f. Calculate the percentage atom economy for the reaction in 13d.

g. A student is extracting copper metal by displacing it from copper(II) sulfate using zinc metal. She uses 23.93 g of copper sulfate and obtains 4.76 g of copper. What is the percentage yield?

Stretch and challenge

14. Cracking can be used to produce alkenes from alkanes. Decane can be cracked to give two products:

$$C_{10}H_{22} \rightarrow C_2H_4 + C_8H_{18}$$

a. If only the alkene can be sold, what is the percentage atom ecomony?

b. If both products can be sold, what is the percentage atom ecomony?

MATHS ASSIGNMENT 2: GREEN CHEMISTRY

MS 0.2; PS 1.1, 1.2, 3.2

The ethos of green chemistry is that the chemical industry must not adversely affect the environment so that the environment is protected both now, and for future generations. A key aim is to reduce the production of waste. Taking into account the percentage atom economy of industrial reactions represents an important step towards reducing waste from industrial processes. In fact, atom economy is the key idea behind green chemistry.

Phenol is the starting point for making many products. Its formula is C_6H_5OH . The traditional method for manufacturing phenol used benzene, C_6H_6 , sulfuric acid and sodium hydroxide. The overall equation for the reaction is:

$$C_6H_6\,(l) + H_2SO_4\,(aq) + 2NaOH(aq) \rightarrow C_6H_5OH(l) + Na_2SO_3\,(aq) + 2H_2O\,(l)$$

So, 1 mol of benzene (78 g) should yield 1 mol of phenol (94 g). In practice, 1 mol of benzene yields about 77 g of phenol, which is a good percentage yield.

However, the reaction also produces 1 mol of sodium sulfite (Na_2SO_3) for every mole of phenol produced. At present we do not have any uses for sodium sulfite. It creates serious problems for waste disposal, which adds to the costs.

A better method is to manufacture phenol from benzene and propene, CH_3CHCH_2 . The reaction also uses oxygen and the overall equation is:

$$C_6H_6\,(l) + CH_3CHCH_2\,(l) + O_2(g) \rightarrow C_6H_5OH(l) + CH_3COCH_3\,(l)$$

CH_3COCH_3 is propanone, which is commonly called acetone. It has many uses, including as a component of nail polish removers. So, by manufacturing phenol using an alternative reaction it is possible to generate another product that is useful, which means there is no waste.

Figure A2 *Phenol is an important chemical. It is used to make plastics, detergents and many other products.*

Questions

A1. What is the percentage yield of phenol when it is manufactured from benzene, sulfuric acid and sodium hydroxide?

A2. Calculate the percentage atom economy for the production of phenol from benzene, sulfuric acid and sodium hydroxide.

A3. Calculate the percentage atom economy when phenol is manufactured using propene. Consider both products as desired.

A4. Explain why manufacturing phenol using benzene and propene may be a better method than using benzene, sulfuric acid and sodum hydroxide.

A5. How might percentage yield affect your answer to question A4?

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206093 AS Chemistry A-Level_Ch2.indd 45 4/1/15 12:39 AM

2.6 IONIC EQUATIONS

Ionic equations provide a shorthand way to show the essential chemistry involving the ions in a reaction. They enable you to make generalisations about a reaction and to pick out the species that have lost or gained electrons.

Working from a full equation to an ionic equation

Consider how to work out the ionic equation for the reaction between hydrochloric acid and sodium hydroxide that produces sodium chloride and water.

First write out the full equation:

$$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l)$$

Now write the equation as ions and cancel the ions that appear on both sides:

$$H^+(aq) + Cl^-(aq) + Na^+(aq) + OH^-(aq) \rightarrow$$
$$Na^+(aq) + Cl^-(aq) + H_2O(l)$$

Water molecules are covalently bonded, so they forms no ions.

The ionic equation is:

$$H^+(aq) + OH^-(aq) \rightarrow H_2O(l)$$

The ions that have cancelled out are called **spectator ions**. They are not written in the final ionic equation.

Worked example 15

Write the ionic equation for the reaction between zinc and hydrochloric acid.

Step 1 First write out the full equation:

$$Zn(s) + 2HCl(aq) \rightarrow ZnCl_2(aq) + H_2(g)$$

Step 2 Then write the equation as ions:

$$Zn(s) + 2H^+(aq) + 2Cl^-(aq) \rightarrow$$
$$Zn^{2+}(aq) + 2Cl^-(aq) + H_2(g)$$

Hydrogen molecules are covalently bonded, so they form no ions.

Step 3 Finally, cancel out ions that appear on both sides to give the ionic equation:

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

In this reaction the zinc has been **oxidised** (it has lost electrons) and the hydrochloric acid has been **reduced** (the hydrogen has tgained electrons).

QUESTION

15. Iron displaces silver from silver nitrate solution. The ionic equation is:

$$Fe(s) + 2Ag^+(aq) \rightarrow Fe^{2+}(aq) + 2Ag(s)$$

What is the maximum mass of silver that can be displaced using 9.52 g iron and excess silver nitrate solution? (Ar: Fe 55.8; Ag 107.9)

Calculations from ionic equations

You can also calculate amounts from ionic equations.

One mole of sodium chloride has a mass of 58.5 g. This is calculated as the mass of a mole of sodium atoms plus the mass of a mole of chlorine atoms $(23 + 35.5)$ g.

But sodium chloride consists of sodium ions, Na^+, and chloride ions, Cl^-.

Since the mass of the electrons lost or gained is negligible, the mass of 1 mol Na^+ is taken as the same as the mass of 1 mol sodium atoms. Similarly, the mass of 1 mol Cl^- is taken as the same as the mass of 1 mol of chlorine atoms.

Worked example 16

You can use an ionic equation to calculate an amount. Zinc metal reacts with copper sulfate solution to deposit copper metal. Calculate the mass of copper that can be obtained from 130 g of zinc, using excess copper sulfate.

Step 1 The chemical equation is:

$$Zn(s) + CuSO_4(aq) \rightarrow ZnSO_4(aq) + Cu(s)$$

Step 2 Write the equation as separate ions:

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

Step 3 Write the ionic equation:

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

Step 4 From the ionic equation:

1 mol zinc atoms $\rightarrow$ 1 mol copper atoms

so 65 g Zn $\rightarrow$ 63.5 g Cu

and, 130 g Zn $\rightarrow$ 128 g Cu

You will meet many ionic equations in this course. (Maths skill 0.2)

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206093 AS Chemistry A-Level_Ch2.indd 46 4/1/15 12:39 AM

2.7 REACTIONS IN SOLUTIONS

A solution contains a solute dissolved in a solvent. Water and ethanol are common solvents. The solute dissolved in the solvent can be solid, liquid or gas. Solutions in the home are commonplace. In fizzy drinks, for example, the solutes are carbon dioxide, which makes them fizzy, and other ingredients such as flavouring, colouring and sweeteners. The solvent is water. In shampoo the solutes are detergent, perfume, preservatives and other ingredients, which you can read on the label, and water as the solvent.

You will use solutions in most of the practical work that you do. You need to be able to do calculations that involve concentrations. Concentration is measured in mol dm^{-3}. Occasionally, you may be asked to calculate concentration in g dm^{-3}.

To calculate concentration, you need to know:

- the mass of solute
- the volume of the solution.

Then you can use this equation:

$$\text{concentration/mol dm}^{-3} = \frac{\text{moles of solute}}{\text{volume of solution/dm}^3}$$

You may find it useful to use Figure 16, where:

n = moles of solute

c = concentration (mol dm^{-3})

V = volume (dm^3)

Then:

$$n = c \times V$$

$$c = \frac{n}{V} \quad \text{and} \quad V = \frac{n}{c}$$

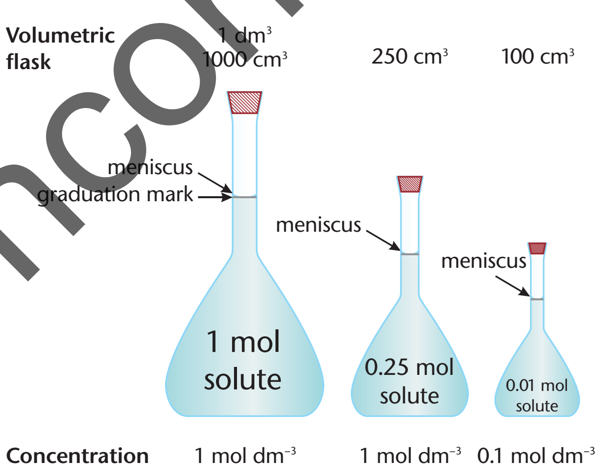

Figure 15 *Concentrations of solutions*

Worked example 17

4 g of sodium hydroxide is dissolved in 1 dm^3 of solution. Calculate its concentration in mol dm^{-3}.

M_r NaOH = 23 + 16 + 1 = 40

moles of NaOH in 4 g $= \frac{4}{40}$

$= 0.1$ mol

Since $c = \frac{n}{V}$

concentration (mol dm^{-3}) $= \frac{0.1}{1}$

$= 0.1$ mol dm^{-3}

(Maths Skills 2.1 and 2.2)

Worked example 18

4 g of sodium hydroxide is dissolved in 250 cm^3 solution. Find its concentration.

4 g NaOH = 0.1 mol (from Worked example 17)

250 cm^3 = 0.25 dm^3

concentration (mol dm^{-3}) $= \frac{0.1}{0.25}$

$= 0.025$ mol dm^{-3}

(Maths Skills 2.1 and 2.2)

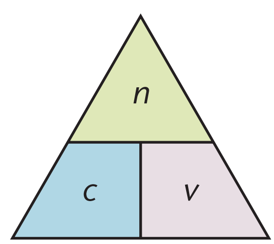

Figure 16 *The diagram can help to calculate the number of moles of a solute, the concentration of solution and its volume.*

QUESTION

16. Calculate the concentration of:

a. 0.98 g sulfuric acid dissolved in 1 dm^3 solution

b. 1.00 g sodium hydroxide dissolved in 1 dm^3 solution

c. 1.00 g sodium hydroxide dissolved in 2 dm^3 solution

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206093 AS Chemistry A-Level_Ch2.indd 47 4/1/15 12:39 AM

d. 49.0 g sulfuric acid dissolved in 2 dm^3 solution

e. 49.0 g sulfuric acid dissolved in 250 cm^3 solution

17. Calculate the number of moles of solute in:

a. 500 cm^3 of 0.50 mol dm^{-3} sodium hydroxide solution

b. 25 cm^3 of 0.10 mol dm^{-3} sodium hydroxide solution

c. 100 cm^3 of 0.25 mol dm^{-3} hydrochloric acid solution

d. 10 cm^3 of 2.00 mol dm^{-3} sulfuric acid solution

e. 2.00 cm^3 of 0.50 mol dm^{-3} potassium manganate(VII) solution

Making a volumetric solution

When chemists carry out practical work to determine unknown concentrations, they usually carry out a **titration**, sometimes called a **volumetric analysis**. They need to make a volumetric (or standard) solution. A volumetric solution is one in which the precise concentration is known. It involves dissolving a known mass of solute in a solvent and making the solution up to a known volume.

To make 1 dm^3 of a standard solution of sodium carbonate with a concentration of 0.1 mol dm^{-3}, you first need to calculate the relative formula mass, M_f, for Na_2CO_3

M_f Na_2CO_3 = (23 × 2) + 12 + (16 × 3) = 10

106 g is the mass of sodium carbonate we would need to dissolve in 1 dm of solution to produce a concentration of 0.1 mol dm.

To make 1 dm of 0.1 mol dm solution, you need 0.1 × 106 g of Na_2Co_3 or 10.

QUESTION

18. a. What mass of sodium carbonate would need to be dissolved in 250 cm^3 of solution to give a standard solution of concentration 0.100 mol dm^{-3}?

b. If the mass of sodium carbonate in 18a was dissolved in 100 cm^3 of solution, what would be its new concentration?

c. What mass of sodium carbonate would need to be dissolved in 1 dm^3 solution to produce a concentration of 0.01 mol dm^{-3}?

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206093 AS Chemistry A-Level_Ch2.indd 48 4/1/15 12:39 AM

REQUIRED PRACTICAL: APPARATUS AND TECHNIQUES (PART 1)

(Practicals Skill 4.1, Apparatus and Techniques a, d, e, k)

Make a volumetric solution

This is the first part of the required practical activity 'Make up a volumetric solution and carry out a simple acid–base titration'. It gives you the opportunity to show that you can:

- use appropriate apparatus to record (a) mass, (b) volume of liquids
- use a volumetric flask, including an accurate technique for making up a standard solution
- safely and carefully handle solids and liquids, including corrosive, irritant, flammable and toxic substances.

Apparatus

A volumetric flask, like the one shown in Figure P2, is used to make solutions of known concentration accurately. These solutions are called volumetric (or standard) solutions.

Technique

To prepare a volumetric solution a known number of moles of solute must be dissolved in deionised water and the solution made up to a known volume. Occasionally other solvents are used.

Preparation involves weighing a small container such as a weighing bottle or boat, and measuring the required mass of compound into it. The number of moles can be calculated from the mass and the relative molecular or formula mass of the compound.

The compound needs to be transferred quantitatively, meaning that the compound weighed out is all transferred. This is generally done by putting a small

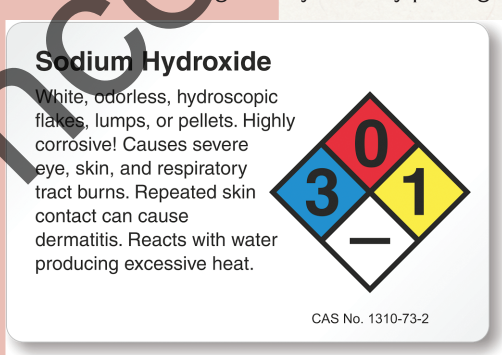

Figure P1 *Hazard cards give the information you need to complete a risk assessment.*

Figure P2 *Volumetric flasks come in a range of sizes. The graduation mark is on the neck of the flask. The temperature for which it is graduated is also shown on the flask.*

funnel in the neck of a volumetric flask. The compound is tipped or poured in and any remaining in the container is washed in using a wash bottle containing deionised water.

It is important to dissolve the compound completely before filling the flask to its graduation mark with water. Typically, the flask is filled to about one-third and the contents swirled until the compound dissolves. More deionised water is added, swirling the flask regularly to ensure thorough mixing, until the solution is about 1 cm below the flask's graduation mark. Deionised water is then added drop-by-drop until the bottom of the meniscus is just level with the graduation mark, as shown in Figure P3. With the stopper held in place, the flask is repeatedly turned up and down until the solution is thoroughly mixed.

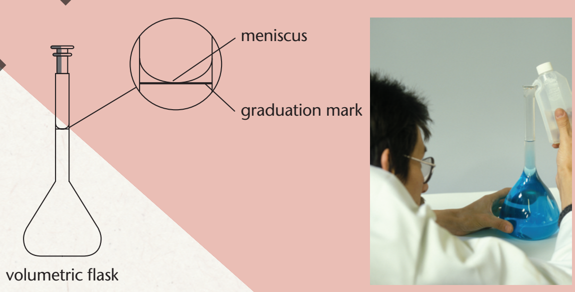

Figure P3 *The bottom of the meniscus must be level with the graduation mark.*

An alternative method is to dissolve the compound in water in a beaker then transfer the solution to the flask. This is better if the compound is difficult to dissolve and may need warming. If it is warmed to dissolve the compound, the solution must be allowed to cool to room temperature before transferring to the volumetric flask.

P1. Why can 100 cm^3 of a liquid be measured more accurately in a 100 cm^3 volumetric flask than in a 100 cm^3 measuring cylinder?

P2. Look at the design of a volumetric flask. Why is the graduation mark in the neck of the flask?

P3. A solid is added to a beaker containing water. The mixture is heated to dissolve the solid. Why must the solution be allowed to cool to room temperature before transferring it to a volumetric flask and making it up to volume?

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206093 AS Chemistry A-Level_Ch2.indd 49 4/1/15 12:39 AM

Finding concentrations and volumes of solutions

Sodium hydroxide reacts with hydrochloric acid in a neutralisation reaction:

$$NaOH(aq) + HCl(aq) \rightarrow NaCl(aq) + H_2O(l)$$

If you add the precise amount of hydrochloric acid required to neutralise the sodium hydroxide, the resulting solution will contain only sodium chloride and water and have pH 7. This procedure is called a **titration**.

If you are given $0.100\ \text{mol dm}^{-3}$ hydrochloric acid (the standard solution) you can carry out a titration to determine the concentration of a sample of sodium hydroxide solution.

A burette is filled with $0.100\ \text{mol dm}^{-3}$ hydrochloric acid. $25.0\ \text{cm}^3$ aliquots of the sodium hydroxide solution are titrated against the acid. The volume of acid required to neutralise each aliquot is called a **titre**. To improve reliability, a minimum of three titres within $0.1\ \text{cm}^3$ are usually obtained and an average titre calculated.

From the sample results in Table 1, you can now calculate the concentration of the hydrochloric acid.

Here is the calculation:

$25\ \text{cm}^3$ of sodium hydroxide solution is neutralised by $19.80\ \text{cm}^3$ $0.100\ \text{mol dm}^3$ hydrochloric acid. We now need to calculate the concentration of the alkali.

$19.80\ \text{cm}^3$ $0.100\ \text{mol dm}^{-3}$ hydrochloric acid contains

$$\frac{19.80}{1000} \times 0.100\ \text{mol HCl}$$

$$= 1.98 \times 10^3\ \text{mol HCl}$$

From the equation

$$HCl(aq) + NaOH(aq) \rightarrow NaCl(aq) + H_2O(l)$$

Titration	Rough	1	2	3
Final burette reading/cm^3	23.80	43.60	21.40	41.15
Initial burette reading/cm^3	3.60	23.80	1.55	21.40
Titre /cm^3	20.20	19.80	19.85	19.75
Used in mean	No	Yes	Yes	Yes
	Mean titre = $19.80\ \text{cm}^3$			

Table 1 *Sample results for the titration of $25\ \text{cm}^3$ sodium hydroxide solution against $0.100\ \text{mol dm}^{-3}$ hydrochloric acid*

1 mol HCl reacts with 1 mol NaOH

Therefore, there must be 1.98×10^{-3} mol NaOH in 25.0 cm of the sodium hydroxide solution.

If there are 1.98×10^{-3} mol NaOH in $25.0\ \text{cm}^3$, then the moles in $1\ \text{dm}^3$ are:

$$1.98 \times 10^{-3} \times \frac{1000}{25}$$

$$= 0.0792\ \text{mol NaOH}$$

Therefore, the concentration of sodium hydroxide solution $= 0.0792\ \text{mol dm}^{-3}$.

Worked example 19

Sodium carbonate is a soluble compound used as washing soda. Calculate the volume of $0.100\ \text{mol dm}^{-3}$ hydrochloric acid needed to react exactly with $25\ \text{cm}^3$ of $0.220\ \text{mol dm}^{-3}$ sodium carbonate solution.

Step 1 First work out how many moles of sodium carbonate is contained in the solution:

$25\ \text{cm}^3$ of $0.220\ \text{mol dm}^{-3}$ sodium carbonate solution contains

$$0.220 \times \frac{25}{1000}\ \text{mol } Na_2CO_3$$

$$= 5.5 \times 10^{-3}\ \text{mol } Na_2CO_3$$

Step 2 From the equation

$$2HCl(aq) + Na_2CO_3(aq) \rightarrow 2NaCl(aq) + CO_2(g) + H_2O(l)$$

1 mol sodium carbonate reacts with 2 mol hydrochloric acid.

Therefore, 5.5×10^{-3} mol Na_2CO_3 reacts with $2 \times 5.5 \times 10^{-3}$ mol HCl = 0.0110 mol HCl.

Step 3 To find the volume of $0.100\ \text{mol dm}^{-3}$ hydrochloric acid containing 0.0110 mol HCl:

0.100 mol HCl in $1\ \text{dm}^3$ $0.100\ \text{mol dm}^{-3}$ hydrochloric acid

1 mol HCl in $10\ \text{dm}^3$ of $0.100\ \text{mol dm}^{-3}$ hydrochloric acid

0.0110 mol HCl in $(10 \times 0.0110)\ \text{dm}^3$ of $0.100\ \text{mol dm}^{-3}$ hydrochloric acid

$= 0.110\ \text{dm}^3 = 110\ \text{cm}^3$

Therefore, 110 cm of 0.100 mol dm hydrochloric acid is needed to react with 25 cm of 0.220 mol dm sodium carbonate solution.

(Maths Skills 0.1, 0.1, 2.1, 2.2, 2.3 and 2.4)

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206093 AS Chemistry A-Level_Ch2.indd 50 4/1/15 12:39 AM

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REQUIRED PRACTICAL: APPARATUS AND TECHNIQUES (PART 2)

(Practicals Skill 4.1, Apparatus and Techniques a, d, e, k)

Carry out a simple acid–base titration

This is the second part of the required practical activity 'Make up a volumetric solution and carry out a simple acid–base titration'. It gives you the opportunity to show that you can:

- use appropriate apparatus to record the volume of liquids
- use laboratory apparatus for a titration, using burette and pipette
- safely and carefully handle solids and liquids, including corrosive, irritant, flammable and toxic substances.

Apparatus

A pipette (Figure P4) is used to transfer an accurately measured volume of liquid. A burette (Figure P5) is used measure accurately any volume with in its capacity.

Technique

Using a pipette:

- The pipette must be clean and dry and some of the solution to be analysed should be poured into a clean, dry beaker. This avoids possible contamination of the rest of the solution.
- A safety filler must be used to draw the solution into the pipette. Never suck it up by mouth. The tip of the pipette must be below the surface of the solution being pipetted at all times.

Figure P4 *Like a volumetric flask, a pipette is calibrated at a fixed temperature (usually 20 °C) and has a tolerance, e.g.* $25 \pm 0.06\ cm^3$.

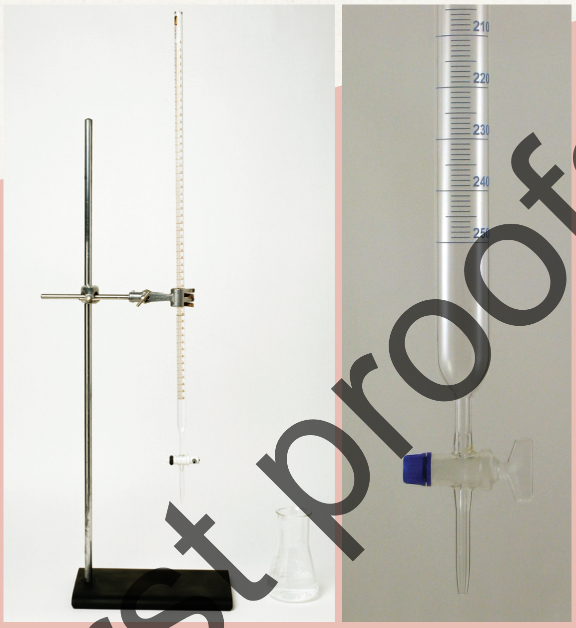

Figure P5 *A 25 cm^3 burette can measure between 0 and 25 cm^3 of liquid to an accuracy of about 0.02 cm^3. However, the reading is usually taken to the nearest 0.05 cm^3 by an experienced user or to the nearest 0.1 cm^3 by people who are less experienced.*

- The solution is drawn up to just above the graduation line, the pipette removed from the solution and the outside of the pipette wiped with a tissue.
- Controlling the release with the safety filler, the solution is drained out until the bottom of the meniscus is level with the graduation line on the pipette. The tip of the pipette is touched on a clean glass surface.
- To empty the solution and run it freely into the conical flask ready for titration, the filler is removed. When the solution has emptied, touch the tip of the pipette on the surface of the solution in the flask. The pipette is designed to deliver a known volume of solution and leave a small amount in its tip, so it is important not to blow out any solution remaining in the pipette.

Using a burette:

- The burette must be clean and dry and clamped vertically. Before use it should be rinsed with three lots of about 10 cm^3 to 15 cm^3 of the volumetric solution.
- The volumetric solution is poured in through a funnel until it is 3 cm to 4 cm above the zero graduation.

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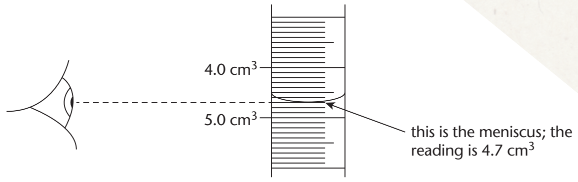

Figure P6 *A burette has graduation lines for each 1 cm^3 quantity. Each 1 cm^3 is subdivided into 0.1 cm^3 sections. Read the burette with your eye level with the bottom of the meniscus.*

- The solution is run out, making sure that there is no trapped air bubble below the tap, until the bottom of the meniscus is just level with the 0.00 cm^3 mark. If it falls below this mark it does not matter, but the burette reading must be recorded.
- To record a burette reading your eye should be level with the meniscus and the reading taken at the bottom of the meniscus (Figure P6). A piece of white card held behind it can make the meniscus easier to see.

Carrying out a titration:

- The volumetric solution is added from a burette in 1–2 cm^3 amounts, swirling the flask between additions. As the end point gets closer, the colour takes longer to change.
- The burette reading is recorded when the colour change is permanent (does not disappear when the flask is swirled). It does not matter if a little too much is added. This is a 'rough' titration.
- The titration is repeated, but this time the volumetric solution is added 1–2 cm^3 at a time, swirling the contents of the flask thoroughly after each addition, until it is within 2–3 cm^3 of the 'rough' titration. At this point the solution is added drop by drop until the end point is reached. This may be repeated again.

Figure P7 *Carrying out a titration accurately requires care and practice.*

Questions

P4. Which apparatus will measure 20 cm^3 with greater precision: a 20 cm^3 pipette or a 50 cm^3 burette?

P5. Explain why a 'rough titration' is carried out and why its value is usually ignored when taking an average of the repeated titration values.

Stretch and challenge

P6. You will often find that a 50 cm^3 burette is used for titrations and the concentration of the volumetric solution for routine analyses of similar samples is adjusted so that each titre is between 20 cm^3 and 25 cm^3. Why do you think this is?

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206093 AS Chemistry A-Level_Ch2.indd 52 4/1/15 12:40 AM

PRACTICAL ASSIGNMENT 3: HOW ACCURATE ARE YOUR TITRATION RESULTS?

MS1.1, 1.2, 1.3; PS 2.1, 2.3, 4.1

There are two sources of error in a titration experiment.

- **Procedural errors:** errors due to the way the experiment was carried out. These are errors that can be avoided with care and practice.
- **Apparatus errors:** errors due to the limitations of precision of the apparatus used. These limitations are due to the manufacturing of the apparatus and are usually printed on the side of glassware.

A top-pan balance may measure mass in grams to two decimal places (to the nearest 0.01 g). The second decimal place is an approximation of the third decimal place. So, a reading of 2.56 g may be anything between 2.555 g and 2.564 g. This means that the second decimal place is uncertain and has an error of ±0.005 g .

A 250 cm^3 volumetric flask has an error of ±0.3 cm^3 .

A 25 cm^3 pipette has an error of ±0.06 cm^3 .

One drop from a burette has a volume of 0.05 cm^3 . This is why all burette readings should include two decimal places and the second place should be 0 or 5.

Since measuring a volume from a burette involves two readings, the error on a volume measured from a burette is $\pm 2 \times 0.05 = \pm 0.10$ cm^3 .

Errors are often written as percentage errors:

$$\text{percentage error} = \frac{\text{error due to limitation of the apparatus's precision}}{\text{reading taken using the apparatus}} \times 100\ \%$$

For example, to calculate the percentage error on a balance reading of 3.69 g:

$$\%\ \text{error} = \frac{0.05}{3.69} \times 100$$

$$= 1.36\%$$

Figure A3 *This 250 cm^3 volumetric flask has an error of ±0.25 cm*

Questions

A1. Calculate the percentage error:

- **a.** on a 250 cm^3 volumetric flask
- **b.** on a 25 cm^3 pipette
- **c.** on a burette reading of 24.00 cm^3
- **d.** on a balance reading of 55.60 g
- **e.** on a balance reading of 5.56 g

A2. Which has the bigger percentage error, a larger or smaller balance reading?

A3. The overall percentage error for an experiment can be found by adding together all the percentage errors for the apparatus used. What is the overall percentage error for using a burette and a 25 cm^3 pipette to carry out a titration?

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206093 AS Chemistry A-Level_Ch2.indd 53 4/1/15 12:40 AM

PRACTICAL ASSIGNMENT 4: HOW MUCH ASPIRIN IS IN AN ASPIRIN TABLET?

MS1.1, 1.2, 1.3; PS 2.1, 2.3, 4.1

Figure A4 *Extracts from willow and similar plants have been used to reduce fever for hundreds of years. In the mid-nineteenth century, scientists started experimenting with the active ingredient in willow to find a related substitute. Today we use acetylsalicylic acid in aspirin tablets.*

Not all of an aspirin tablet is aspirin. It contains other ingredients. The ingredients list for a medicine tablet may include, amongst other substances, corn starch, cellulose and binders.

The active ingredient in an aspirin tablet is acetylsalicylic acid. The fact that it is an acid allows us to carry out an acid–base titration to find out how much is in the tablet.

The formula for acetylsalicylic acid is $CH_3COOC_6H_4COOH$.

The acid–base titration reaction is:

$$CH_3COOC_6H_4COOH + NaOH \rightarrow CH_3COOC_6H_4COONa + H_2O$$

A student carried out the following practical.

The tablet was ground up and added to a conical flask. It was then dissolved in 10.0 cm^3 ethanol (this is because aspirin does not dissolve in water easily).

The aspirin solution was titrated against 0.100 mol dm^{-3} sodium hydroxide, using phenolphthalein as the indicator.

The rough titre is an outlier (a measurement that lies outside the range of the others).

Questions

A1. From the results in Table A2, calculate the average titre.

Titration	Rough	1	2	3
Final burette reading/cm^3	16.35	31.05	45.70	40.80
Initial burette reading/cm^3	0.00	16.35	31.05	26.05
Titre/cm^3	16.35	14.70	14.65	14.75

Table A2 *Results of an acid–base titration to find the mass of aspirin in a tablet*

A2. How many moles of sodium hydroxide were used to neutralise the aspirin?

A3. From the equation above, how many moles of sodium hydroxide react with one mole of acetylsalicylic acid?

A4. How many moles of acetylsalicylic acid reacted with the sodium hydroxide in the titration?

A5. Calculate the relative molecuar mass, M_r, of acetylsalicylic acid.

A6. What is the mass of acetylsalicylic acid in the aspirin tablet? Note: decide on a suitable number of significant figures for your answer.

A7. Calculate the percentage errors for the apparatus C used and an overall percentage error.

KEY IDEAS

- Concentration is measured in mol dm^{-3}.
- Concentration $\left(\text{mol dm}^{-3}\right) = \dfrac{\text{moles of solute}}{\text{volume of solution}\left(\text{dm}^3\right)}$
- A volumetric solution is one in which the concentration is known.
- A titration is used to find an unknown volume or concentration of a reactant.

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206093 AS Chemistry A-Level_Ch2.indd 54 4/1/15 12:40 AM

EXAM PRACTICE QUESTIONS

1. The metal lead reacts with warm dilute nitric acid to produce lead(II) nitrate, nitrogen monoxide and water, according to the following equation:

$$3Pb(s) + 8HNO_3(aq) \rightarrow 3Pb(NO_3)_2(aq) + 2NO(g) + 4H_2O(l)$$

   a. In an experiment, an 8.14 g sample of lead reacted completely with a 2.00 mol dm^{-3} solution of nitric acid. Calculate the volume, in dm^3, of nitric acid required for the complete reaction. Give your answer to 3 significant figures.

   b. In a second experiment, the nitrogen monoxide gas produced in the reaction occupied 638 cm^3 at 101 kPa and 298 K. Calculate the amount, in moles, of NO gas produced. (The gas constant R = 8.31 J K^{-1} mol^{-1})

   c. When lead(II) nitrate is heated it decomposes to form lead(II) oxide, nitrogen dioxide and oxygen.

      i. Balance the following equation that shows this thermal decomposition.

      ....$Pb(NO_3)_2(s) \rightarrow$ ......$PbO(s)$ + ...$NO_2(g)$ + ...$O_2(g)$

      ii. Suggest one reason why the yield of nitrogen dioxide formed during this reaction is often less than expected.

      iii. Suggest one reason why it is difficult to obtain a pure sample of nitrogen dioxide from this reaction.

AQA Jan 2012 Unit 1 Q6

2. Norgessaltpeter was the first nitrogen fertiliser to be manufactured in Norway. It has the formula $Ca(NO_3)_2$.

   a. Norgessaltpeter can be made by the reaction of calcium carbonate with dilute nitric acid as shown by the following equation:

$$CaCO_3(s) + 2HNO_3(aq) \rightarrow Ca(NO_3)_2(aq) + CO_2(g) + H_2O(l)$$

   In an experiment, an excess of powdered calcium carbonate was added to 36.2 cm^3 of 0.586 mol dm^{-3} nitric acid.

      i. Calculate the amount, in moles, of HNO_3 in 36.2 cm^3 of 0.586 mol dm^{-3} nitric acid. Give your answer to 3 significant figures.

      ii. Calculate the amount, in moles, of $CaCO_3$ that reacted with the nitric acid. Give your answer to 3 significant figures.

      iii. Calculate the minimum mass of powdered $CaCO_3$ that should be added to react with all of the nitric acid. Give your answer to 3 significant figures.

      iv. State the type of reaction that occurs when calcium carbonate reacts with nitric acid.

   b. Norgessaltpeter decomposes on heating as shown by the following equation:

$$2Ca(NO_3)_2(s) \rightarrow 2CaO(s) + 4NO_2(g) + O_2(g)$$

   A sample of Norgessaltpeter was decomposed completely. The gases produced occupied a volume of 3.50×10^{-3} m^3 at a pressure of 100 kPa and a temperature of 31 °C. (The gas constant R = 8.31 J K^{-1} mol^{-1})

      i. Calculate the total amount, in moles, of gases produced.

      ii. Hence calculate the amount, in moles, of oxygen produced.

   c. Hydrated calcium nitrate can be represented by the formula $Ca(NO_3)_2.xH_2O$ where x is an integer. A 6.04 g sample of $Ca(NO_3)_2.xH_2O$ contains 1.84 g of water of crystallisation. Use this information to calculate a value for x. Show your working.

AQA Jun 2011 Unit 1 Q2

3. a. An unknown metal carbonate, M_2CO_3, reacts with hydrochloric acid according to the following equation:

$$M_2CO_3(aq) + 2HCl(aq) \rightarrow 2MCl(aq) + CO_2(g) + H_2O(l)$$

   A 3.44 g sample of M_2CO_3 was dissolved in distilled water to make 250 cm^3 of solution. A 25.0 cm^3 portion of this solution required

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33.2 cm^3 of 0.150 mol dm^{-3} hydrochloric acid for complete reaction.

i. Calculate the amount, in moles, of HCl in 33.2 cm^3 of 0.150 mol dm^{-3} hydrochloric acid. Give your answer to 3 significant figures.

ii. Calculate the amount, in moles, of M_2CO_3 that reacted with this amount of HCl. Give your answer to 3 significant figures.

iii. Calculate the amount, in moles, of M_2CO_3 in the 3.4 g sample. Give your answer to 3 significant figures.

iv. Calculate the relative formula mass, M_r, of M_2CO_3. Give your answer to 1 decimal place.

v. Hence determine the relative atomic mass, A_r, of the metal M and deduce its identity.

b. In another experiment, 0.658 mol of CO_2 was produced. This gas occupied a volume of 0.0220 m^3 at a pressure of 100 kPa. Calculate the temperature of this CO_2 and state the units. (The gas constant R = 8.31 J K^{-1} mol^{-1})

c. Suggest one possible danger when a metal carbonate is reacted with an acid in a sealed flask.

d. In a different experiment, 6.27 g of magnesium carbonate was added to an excess of sulfuric acid. The following reaction occurred:

$$MgCO_3 + H_2SO_4 \rightarrow MgSO_4 + CO_2 + H_2O$$

i. Calculate the amount, in moles, of $MgCO_3$ in 6.27 g of magnesium carbonate.

ii. Calculate the mass of $MgSO_4$ produced in this reaction assuming a 95% yield.

AQA Jan 2011 Unit 1 Q3

4. In this question give all your answers to 3 significant figures.

Magnesium nitrate decomposes on heating to form magnesium oxide, nitrogen dioxide and oxygen, as shown in the following equation:

$$2Mg(NO_3)_2(s) \rightarrow 2MgO(s) + 4NO_2(g) + O_2(g)$$

a. Thermal decomposition of a sample of magnesium nitrate produced 0.741 g of magnesium oxide.

i. Calculate the amount, in moles, of MgO in 0.741 g of magnesium oxide.

ii. Calculate the total amount, in moles, of gas produced from this sample of magnesium nitrate.

b. In another experiment, a different sample of magnesium nitrate decomposed to produce 0.402 mol of gas. Calculate the volume, in
dm^3, that this gas would occupy at 333 K and 1.00×10^5 Pa. (The gas constant $R = 8.31$ J K^{-1} mol^{-1})

c. A 0.0152 mol sample of magnesium oxide, produced from the decomposition of magnesium nitrate, was reacted with hydrochloric acid.

$$MgO + 2HCl \rightarrow MgCl_2 + H_2O$$

i. Calculate the amount, in moles, of HCl needed to react completely with the 0.0152 mol sample of magnesium oxide.

ii. This 0.0152 mol sample of magnesium oxide required 32.4 cm^3 of hydrochloric acid for complete reaction. Use this information and your answer to part c) i) to calculate the concentration, in mol dm^{-3}, of the hydrochloric acid.

AQA Jun 2010 Unit 1 Q3

5. a. An acid, H_2X, reacts with sodium hydroxide as shown in the following equation:

$$H_2X(aq) + 2NaOH(aq) \rightarrow 2Na^+(aq) + X^{2-}(aq) + 2H_2O(l)$$

A solution of this acid was prepared by dissolving 1.92 g of H_2X in water and making the volume up to 250 cm^3 in a volumetric flask.

A 25.0 cm^3 sample of this solution required 21.70 cm^3 of 0.150 mol dm^{-3} aqueous NaOH for complete reaction.

i. Calculate the number of moles of NaOH in 21.70 cm^3 of 0.150 mol dm^{-3} aqueous NaOH

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ii. Calculate the number of moles of H_2X which reacted with this amount of NaOH. Hence, deduce the number of moles of H_2X in the 1.92 g sample.

iii. Calculate the relative molecular mass, M_r, of H_2X.

b. Analysis of a compound, Y, showed that it contained 49.31% of carbon, 6.85% of hydrogen and 43.84% of oxygen by mass. (The M_r of Y is 146.0)

i. State what is meant by the term *empirical formula*.

ii. Use the above data to calculate the empirical formula and the molecular formula of Y.

c. Sodium hydrogencarbonate decomposes on heating as shown in the equation below:

$2NaHCO_3(s) \rightarrow$
$Na_2CO_3(s) + CO_2(g) + H_2O(g)$

A sample of $NaHCO_3$ was heated until completely decomposed. The CO_2 formed in the reaction occupied a volume of 352 cm^3 at 1.00×10^5 Pa and 298 K.

i. State the ideal gas equation and use it to calculate the number of moles of CO_2 formed in this decomposition. (The gas constant R = 8.31 J K^{-1} mol^{-1})

ii. Use your answer from part c) i) to calculate the mass of the $NaHCO_3$ that has decomposed. (If you have been unable to calculate the number of moles of CO_2 in part c) i), you should assume this to be 0.0230 mol. This is not the correct value.)

6. Nitroglycerine, $C_3H_5N_3O_9$, is an explosive that, on detonation, decomposes rapidly to form a large number of gaseous molecules. The equation for this decomposition is:

$4C_3H_5N_3O_9(l) \rightarrow$
$12CO_2(g) + 10H_2O(g) + 6N_2(g) + O_2(g)$

a. A sample of nitroglycerine was detonated and produced 0.350 g of oxygen gas.

i. State what is meant by the term *one mole* of molecules.

ii. Calculate the number of moles of oxygen gas produced in this reaction, and hence deduce the total number of moles of gas formed.

iii. Calculate the number of moles, and the mass, of nitroglycerine detonated.

b. A second sample of nitroglycerine was placed in a strong sealed container and detonated. The volume of this container was 1.00×10^{-3} m^3. The resulting decomposition produced a total of 0.873 mol of gaseous products at a temperature of 1100 K. State the ideal gas equation and use it to calculate the pressure in the container after detonation. (The gas constant R = 8.31 J K^{-1} mol^{-1})

7. Magnesium chloride is also know as E511 and is used in the preparation of tofu. Magnesium chloride can be prepared in the lab using the reaction:.

$MgCO_3(s) + 2HCl(aq) \rightarrow$
$MgCl_2(aq) + H_2O(l) + CO_2(g)$

a. What is the maximum yield of magnesium chloride that can be obtained from 8.4 g magnesium carbonate?

b. If the actual yield is 6.3 g, what is the percentage yield?

c. State one reason why the percentage yield is less than 100%.

d. What is the percentage atom ecomony for the reaction?

e. Give one advantage of using a reaction with a high atom ecomony in the chemical industry?

8. Students were determining the concentration of a sample of hydrochloric acid by titrating it against 0.100 mol dm^{-3} sodium hydroxide solution.

a. A pipette was used to transfer 25 cm^3 sodium hydroxide solution into a conical flask. Explain how the students could use phenolphthalein indicator and a burette to carry out the titration.

b. State the changes that they would need to make in the procedure if they used a pH probe instead of an indicator.

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Table Q1 shows their results using phenolphthalein indicator.

c. Calculate the titres for each titration and select the three best results to calculate an average titre.

d. Calculate the following:

i. the number of moles of 0.100 mol dm^{-3} sodium hydroxide in 25 cm^3 solution

ii. the numer of moles of hydrochloric acid this reacted with

iii. concentration of the hydrochloric acid to the appropriate number of significant figures.

e. The error on a burette reading is $\pm$0.05 cm^3. What is the error on a titre?

Multiple Choice

9. For which of the compounds **A–D** is relative formula mass used?

A sodium chloride

B water

C carbon dioxide

D glucose

	Titration 1	Titration 2	Titration 3	Titration 4
Final burette reading/cm^3	24.00	46.50	24.75	47.15
Initial burette reading/cm^3	0.00	24.00	2.15	24.75

Table Q1

10. Which of **A–D** is the number of atoms in one mole of atoms?

A 6.023 × 10

B 6.023×10^{-23}

C 6.023 × 1010

D 6.023×10^{23}

11. Which of ***A–D*** is the correct ideal gas equation?

A $nR = pVT$

B $pV = nRT$

C $nV = pRT$

D $pT = nRV$

12. Which of **A–D** represents the empirical formula of glucose, $C_6H_{12}O_6$?

A CH_2O

B $C_6H_{12}O_6$

C CHO

D CHO_2

Stretch and challenge

13. The acid in vinegar is ethanoic acid (its old-fashioned name was acetic acid). The concentration of ethanoic acid in vinegar can be determined by titration. Ethanoic acid reacts with sodium hydroxide to produce sodium ethanoate and water:

$$CH_3COOH(aq) + NaOH(aq) \rightarrow CH_3COONa(aq) + H_2O(l)$$

The graph in Figure Q1 shows the changes in pH when vinegar was titrated against sodium hydroxide solution.

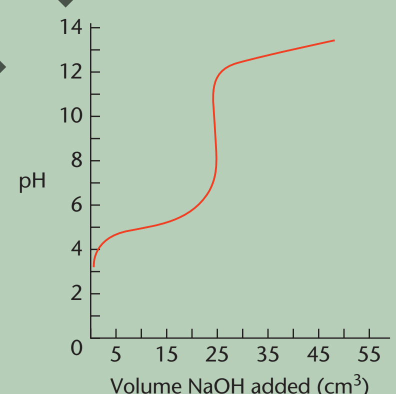

Figure Q1 *pH titration curve of weak acid (CH_3COOH) and strong base (NaOH)*

a. Assuming the pH of sodium ethanoate solution is 7, what volume of sodium hydroxide is needed to neutralise the vinegar?

b. What is present in the reaction mixture when:

i. 10 cm^3 sodium hydroxide solution has been added

ii. 35 cm^3 sodium hydroxide solution has been added?

c. Explain the changes in pH as the titration proceeds.

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d. A different brand of vinegar, X, was similarly tested. This brand was found to contain a higher concentration of ethanoic acid. Copy the pH titration curve in Figure Q1 and add a second curve to show the changes in pH when vinegar X was titrated against the same concentration of sodium hydroxide solution. Label the second curve 'Vinegar X'.

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