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- Option D Medicinal chemistry

Self-test questions

Assessment guidance

Model exam papers

Nature of Science

Answers to exam-style questions

Answers to Options questions

Introduction

This second edition of *Chemistry for the IB Diploma* is fully updated to cover the content of the IB Chemistry Diploma syllabus that will be examined in the years 2016–2022.

Chemistry may be studied at Standard Level (SL) or Higher Level (HL). Both share a common core, and at HL the core is extended with additional HL material. In addition, at both levels, students then choose one Option to complete their studies. Each Option consists of common core and additional HL material. All common core and additional HL material is covered in this print book. The Options are included in the free online material that is accessible via education.cambridge.org/ibsciences

The content is arranged in topics that match the syllabus topics, with core and additional HL material on each topic combined in the book topics. The HL content is identified by 'HL' included in relevant section titles, and by a yellow page border.

Each section in the book begins with learning objectives as starting and reference points. Test yourself questions appear throughout the text so students can check their progress and become familiar with the style and command terms used, and exam-style questions appear at the end of each topic. Many worked examples appear throughout the text to help students understand how to tackle different types of questions.

Theory of Knowledge (TOK) provides a cross-curricular link between different subjects. It stimulates thought about critical thinking and how we can say we know what we claim to know. Throughout this book, TOK features highlight concepts in Chemistry that can be considered from a TOK perspective. These are indicated by the 'TOK' logo, shown here.

Science is a truly international endeavour, being practised across all continents, frequently in international or even global partnerships. Many problems that science aims to solve are international, and will require globally implemented solutions. Throughout this book, International-Mindedness features highlight international concerns in Chemistry. These are indicated by the 'International-Mindedness' logo, shown here.

Nature of Science is an overarching theme of the Chemistry course. The theme examines the processes and concepts that are central to scientific endeavour, and how science serves and connects with the wider community. Throughout the book, there are 'Nature of Science' paragraphs that discuss particular concepts or discoveries from the point of view of one or more aspects of Nature of Science. A chapter giving a general introduction to the Nature of Science theme is available in the free online material.



Free online material

Additional material to support the IB Chemistry Diploma course is available online. Visit education.cambridge.org/ibsciences and register to access these resources using:

Username: camib

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Besides the Options and Nature of Science chapter, you will find a collection of resources to help with revision and exam preparation. This includes guidance on the assessments, interactive self-test questions and model exam papers. Additionally, answers to the exam-style questions in this book and to all the questions in the Options are available.

Stoichiometric relationships 1

1.1 Introduction to the particulate nature of matter and chemical change

1.1.1 The particulate nature of matter

The three states of **matter** are solid, liquid and gas and these differ in terms of the arrangement and movement of particles. The particles making up a substance may be individual atoms or molecules or ions. Simple diagrams of the three states of matter are shown in Figure 1.1 in which the individual particles are represented by spheres.

Sublimation is the change of state when a substance goes directly from the solid state to the gaseous state, without going through the liquid state. Both iodine and solid carbon dioxide (dry ice) sublime at atmospheric pressure. The reverse process (gas \rightarrow solid) is often called *deposition* (or sometimes *desublimation*, *reverse sublimation* or occasionally just sublimation).

The properties of the three states of matter are summarised in Table 1.1.

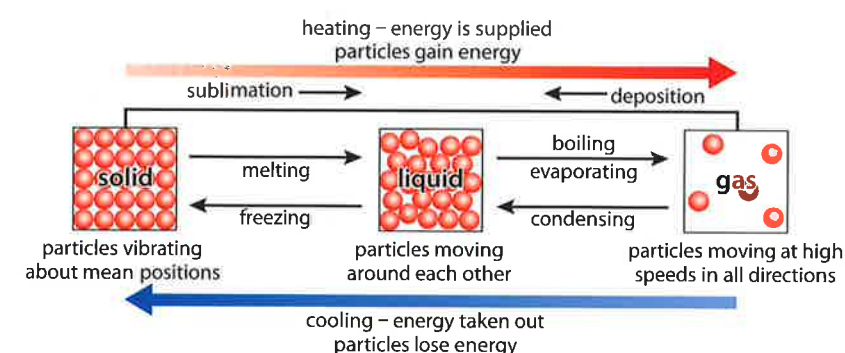


Figure 1.1 The arrangement of particles in solids, liquids and gases and the names of the changes of state. Note that evaporation can occur at any temperature – boiling occurs at a fixed temperature.

	Solids	Liquids	Gases
Distance between particles	close together	close but further apart than in solids	particles far apart
Arrangement	regular	random	random
Shape	fixed shape	no fixed shape – take up the shape of the container	no fixed shape – fill the container
Volume	fixed	fixed	not fixed
Movement	vibrate	move around each other	move around in all directions
Speed of movement	slowest	faster	fastest
Energy	lowest	higher	highest
Forces of attraction	strongest	weaker	weakest

Table 1.1 The properties of the three states of matter.

Learning objectives

- Describe the three states of matter
- Understand the changes involved when there is a change in state

If a pure substance is heated slowly, from below its melting point to above its **boiling point**, a graph of temperature against time can be obtained (Figure 1.2).

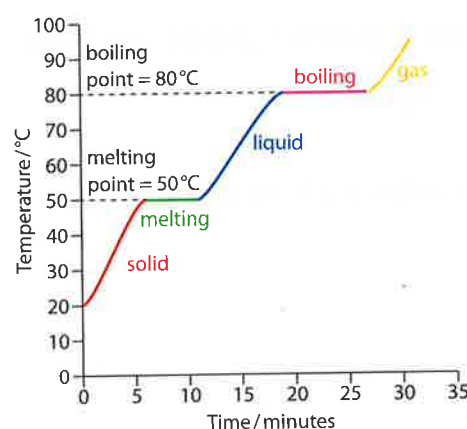


Figure 1.2 A heating curve showing changes of state.

As a solid is heated, its particles vibrate more violently – they gain **kinetic energy** and the temperature of the solid rises. At 50°C, the solid in Figure 1.2 begins to melt – at this stage there is solid and liquid present together and the temperature remains constant until all the solid has melted. All the **heat energy** being supplied is used to partially overcome the forces of attraction between particles so that they can move around each other. When all the solid has melted, the continued supply of heat energy causes the kinetic energy of the particles to increase so that the particles in the liquid move around each other more quickly. The kinetic energy of the particles increases until the boiling point of the liquid is reached. At this point (80°C) the continued supply of heat energy is used to overcome the forces of attraction between the particles completely and the temperature of the substance remains constant until all the liquid has been converted to gas. The continued supply of heat energy increases the kinetic energy of the particles of the gas so they move around faster and faster as the temperature of the gas increases.



Both refrigeration and air-conditioning involve changes of state of liquids and gases. In a refrigerator, heat energy is absorbed from the inside of the refrigerator and is used to convert a liquid coolant to a gas – the heat energy is given out to the surrounding as the gas is compressed back to a liquid. Refrigeration is essential in warm countries to preserve food and without it the food would go ‘off’ much more quickly and be wasted – but how essential is air-conditioning? CFCs (which cause destruction of the ozone layer) have been used as a refrigerant and in making the insulation for refrigerators. In many countries the disposal of old refrigerators is controlled carefully. More environmentally friendly refrigerators are being manufactured using alternatives to CFCs – they also use less electricity.

1.1.2 Chemical change

Elements and compounds

Chemistry is partly a study of how chemical elements combine to make the world and the Universe around us.

Gold is an **element** and all samples of pure gold contain only gold atoms.

An element is a pure substance that contains only one type of atom (but see *isotopes* in Topic 2).

An atom is the smallest part of an element that can still be recognised as that element.

The physical and chemical properties of a compound are very different to those of the elements from which it is formed.

Sodium and chlorine are elements – when they are mixed and heated they combine chemically to form a compound called sodium chloride. Sodium is a grey, reactive metal with a low melting point and chlorine is a yellow-green poisonous gas – but sodium chloride (common salt) is a non-toxic, colourless compound with a high melting point.

Similarly, when iron (a magnetic metal) is heated with sulfur (a non-magnetic yellow solid) a grey, non-metallic solid called iron sulfide is formed (Figure 1.3).

Chemical properties dictate how something reacts in a chemical reaction.

Physical properties are basically all the other properties of a substance – such as melting point, density, hardness, electrical conductivity etc.

The meaning of chemical equations

When elements combine to form compounds, they always combine in **fixed ratios** depending on the numbers of atoms required. When sodium and chlorine combine, they do so in the mass ratio 22.99 : 35.45 so that 22.99 g of sodium reacts exactly with 35.45 g of chlorine. Similarly, when hydrogen (an explosive gas) combines with oxygen (a highly reactive gas) to form water (liquid at room temperature), 1 g of hydrogen combines with 8 g of oxygen, or 2 g of hydrogen reacts with 16 g of oxygen (using rounded relative atomic masses) – that is, they always combine in a mass ratio of 1 : 8.

Learning objectives

- Understand that compounds have different properties to the elements they are made from
- Understand how to balance chemical equations
- Understand how to use state symbols in chemical equations
- Describe the differences between elements, compounds and mixtures
- Understand the differences between homogeneous and heterogeneous mixtures

A compound is a pure substance formed when two or more elements combine chemically.



Figure 1.3 Iron (left) combines with sulfur (centre) to form iron sulfide (right).

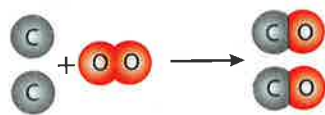


Figure 1.4 Two carbon atoms react with one oxygen molecule to form two molecules of carbon monoxide.

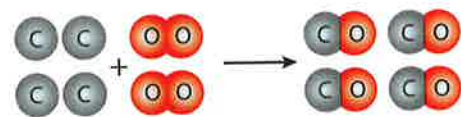


Figure 1.5 Four carbon atoms react with two oxygen molecules to form four molecules of carbon monoxide.

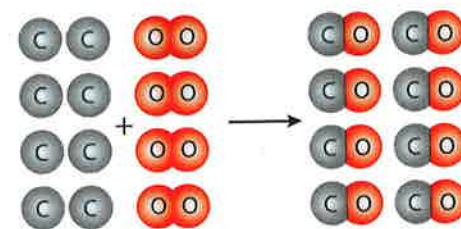


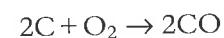
Figure 1.6 Eight carbon atoms react with four oxygen molecules to form eight molecules of carbon monoxide.

Mass is conserved in all chemical reactions.

Elements always combine in the same mass ratios because their atoms always combine in the same ratios, and each type of atom has a fixed mass.

Consider the reaction between carbon and oxygen to form carbon monoxide. This is shown diagrammatically in Figure 1.4. In this reaction, two carbon atoms combine with one oxygen molecule to form two molecules of carbon monoxide. Now look at Figure 1.5. If we started with four carbon atoms, they will react with two oxygen molecules to form four molecules of carbon monoxide.

The ratio in which the species combine is fixed in these equations. The number of molecules of oxygen is always half the number of carbon atoms, and the number of carbon monoxide molecules produced is the same as the number of carbon atoms (see Figures 1.4–1.6). So, we can construct the equation:



which tells us that two carbon atoms react with one oxygen molecule to form two carbon monoxide molecules, and that this ratio is constant however many carbon atoms react.

Balancing equations

If a reaction involves 5.00 g of one substance reacting with 10.00 g of another substance in a closed container (nothing can be added or can escape), then at the end of the reaction there will still be exactly 15.00 g of substance present. This 15.00 g may be made up of one or more products and some reactants that have not fully reacted, but the key point is that there will no more and no less than 15.00 g present.

A chemical reaction involves atoms joining together in different ways and electrons redistributing themselves between the atoms, but it is not possible for the reaction to involve atoms or electrons being created or destroyed.

When a chemical reaction is represented by a chemical equation, there must be exactly the same number and type of atoms on either side of the equation, representing the same number of atoms before and after this reaction:

	$\text{C}_3\text{H}_8 + 5\text{O}_2$	\rightarrow	$3\text{CO}_2 + 4\text{H}_2\text{O}$
	reactants		products
atoms	C 3		C 3
	H 8		H 8
	O 10		O 10

So this equation is balanced. It is important to realise that only coefficients (large numbers in front of the substances) may be added to balance a chemical equation. The chemical formula for water is H_2O , and this cannot be changed in any way when balancing an equation. If, for instance, the formula is changed to H_2O_2 then it represents a completely different chemical substance – hydrogen peroxide.

State symbols are often used to indicate the physical state of substances involved in a reaction:

(s) = solid

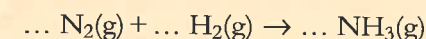
(l) = liquid

(g) = gas

(aq) = aqueous (dissolved in water)

Worked examples

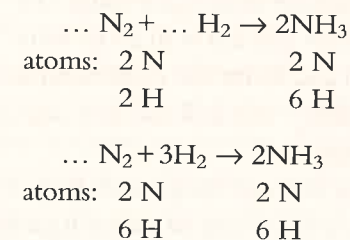
1.1 Balance the following equation



and work out the sum of the coefficients in the equation.

In the unbalanced equation, there are two N atoms and two H atoms on the left-hand side of the equation but one N atom and three H atoms on the right-hand side. It is not possible for two N atoms to react with two H atoms to produce one N atom and three H atoms; therefore, this equation is not balanced.

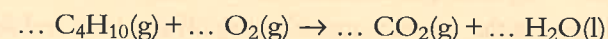
It can be balanced in two stages, as follows:



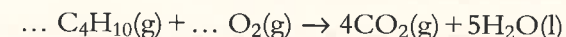
This equation is now balanced because there is the same number of each type of atom on both sides of the equation.

The sum of the coefficients in this equation is $1 + 3 + 2 = 6$. The coefficient of N_2 is 1, although we do not usually write this in an equation.

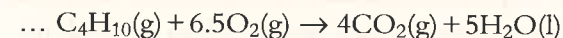
1.2 Balance the following equation:



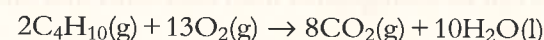
Compounds are balanced first, then elements:



There are two oxygen atoms on the left-hand side of the equation, and O_2 needs to be multiplied by 6.5 to give 13 oxygen atoms, which is the number of oxygen atoms on the other side $[(4 \times 2) + (5 \times 1)]$:

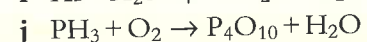
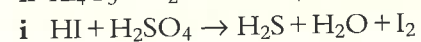
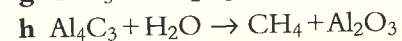
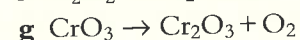
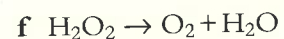
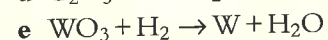
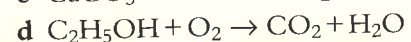
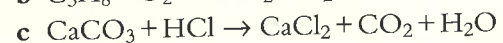
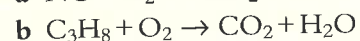
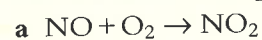


The equation is balanced as shown, but it looks much neater when balanced with whole numbers. To achieve this, all the coefficients are multiplied by 2:



? Test yourself

1 Balance the following equations:



Mixtures

Elements and compounds are pure substances but most things around us are not pure substances but mixtures. We breathe in air, which is a mixture; all the foods we eat are mixtures; oxygen is carried around our body by blood, another mixture.

A mixture contains two or more substances mixed together.

The components of a mixture can be elements or compounds – or mixtures! Air is a mixture of mostly elements (nitrogen, oxygen, argon) with smaller amounts of compounds (carbon dioxide, water vapour etc.).

The components of a mixture are not chemically bonded together and so retain their individual properties. In a mixture of iron and sulfur, the iron is shiny and magnetic; the sulfur is yellow and burns in air to form sulfur dioxide. When the mixture is heated and forms the compound iron sulfide, this is not shiny or magnetic or yellow – it is dull and grey and has completely different properties to its elements.

As you saw earlier, when atoms combine to form compounds they do so in fixed ratios, but the components of a mixture can be mixed together in any proportion. For example, ethanol and water can be mixed together in any ratio. Solutions are mixtures and a solution of sodium chloride could be made by dissolving 1 g of sodium chloride in 100 cm³ of water or 2 g of sodium chloride in 100 cm³ water or 10 g of sodium chloride in 100 cm³ of water or many other amounts.

The components of a mixture can be separated from each other by physical means – for example a mixture of sand and salt could be separated by dissolving the salt in water, filtering off the sand and then heating the salt solution to drive off the water.

A homogeneous mixture has the same (uniform) composition throughout the mixture and consists of only one phase.

A heterogeneous mixture does not have uniform composition and consists of separate phases. Heterogeneous mixtures can be separated by mechanical means.

Homogeneous and heterogeneous mixtures

One example of a **homogeneous mixture** is a solution. No individual particles can be seen in the solution and its concentration is the same throughout. If several 1 cm³ samples of a solution of sodium chloride are taken from a beaker and evaporated separately to dryness, the same mass of sodium chloride will be formed by each sample. Clean air (with no particulates) is also a homogeneous mixture.

One example of a **heterogeneous mixture** is sand in a beaker of water. The sand and water can be distinguished from each other and can also be separated by filtering.

Mixtures of different solids are also heterogeneous. For example, even though a mixture of iron and sulfur may have been made very carefully so that there are the same masses of iron and sulfur in each cubic centimetre, the composition is not uniform because there are distinct particles of iron and sulfur and each particle of iron and sulfur represents a different phase. The components of the mixture could be separated from each other using a magnet – or even a pair of tweezers to pick out each individual piece of iron and sulfur.



Sea water is a mixture and the process of obtaining fresh water from sea water is called desalination. Desalination is very important in some parts of the world where sufficient fresh water is not available from other sources (for example, in the Middle East). Fresh water obtained by desalination can be used for human consumption, agriculture or in industry.

Nature of science

Data collection is essential in science. The discussion above has used both quantitative (regarding reacting masses) and qualitative data (about the properties of substances). Accurate quantitative data are essential for the advancement of science and scientists analyse such data to make hypotheses and to develop theories. The law of definite proportions governing how elements combine may seem obvious nowadays in the light of the atomic theory but in the seventeenth and eighteenth centuries it was the subject of much debate.

? Test yourself

2 Classify each of the following as an element, a compound or a mixture:

- a water; b oxygen; c potassium iodide; d orange juice; e crude oil; f vanadium; g ammonia; h air; i hydrogen chloride; j magnesium oxide.

3 Classify each of the diagrams below using as many words as appropriate from the list:

element compound mixture
solid liquid gas



a



b



c



d

Learning objectives

- Define relative atomic mass and relative molecular mass
- Understand what is meant by one mole of a substance
- Calculate the mass of one mole of a substance
- Calculate the number of moles present in a specified mass of a substance
- Work out the number of particles in a specified mass of a substance and also the mass of one molecule

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

The A_r of carbon is not 12.00, because carbon contains isotopes other than carbon-12 (see page 58).

The relative molecular mass (M_r) of a compound is the mass of a molecule of that compound relative to the mass of $\frac{1}{12}$ of an atom of carbon-12.

The relative formula mass is the mass of one formula unit relative to the mass of $\frac{1}{12}$ of an atom of carbon-12.

1.2 The mole concept

1.2.1 Relative masses

Most chemical reactions involve two or more substances reacting with each other. Substances react with each other in certain ratios, and stoichiometry is the study of the ratios in which chemical substances combine. In order to know the exact quantity of each substance that is required to react we need to know the number of atoms, molecules or ions in a specific amount of that substance. However, the mass of an individual ion atom or molecule is so small, and the number of particles that make up even a very small mass so large, that a more convenient method of working out reacting quantities had to be developed.

Relative atomic mass (A_r)

The mass of a hydrogen atom is approximately 1.7×10^{-24} g. Such small numbers are not convenient to use in everyday life, so we use scales of relative mass. These compare the masses of atoms and molecules etc. to the mass of one atom of carbon-12, which is assigned a mass of exactly 12.00. As these quantities are relative, they have no units.

The **relative atomic mass (A_r)** of silver is 107.87. A naturally occurring sample of silver contains the isotopes ^{107}Ag and ^{109}Ag . The 107 isotope is slightly more abundant than the 109 isotope. Taking into account the amount of each isotope present in a sample (the weighted mean) it is found that, on average, the mass of a silver atom is 107.87 times the mass of $\frac{1}{12}$ of a carbon-12 atom. No silver atoms actually exist with the mass of 107.87; this is just the average relative atomic mass of silver.

Relative molecular mass (M_r)

An **relative molecular mass (M_r)** is the sum of the relative atomic masses of the individual atoms making up a molecule. The relative molecular mass of methane (CH_4) is:

$$12.01(A_r \text{ of C}) + 4 \times 1.01(A_r \text{ of H}) = 16.05$$

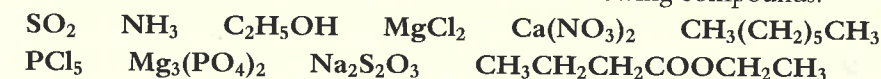
The relative molecular mass of ethanoic acid (CH_3COOH) is:

$$12.01 + (3 \times 1.01) + 12.01 + (2 \times 16.00) + 1.01 = 60.06$$

If a compound is made up of ions, and therefore does not contain discrete molecules, we should really talk about **relative formula mass**. However, relative molecular mass is usually used to refer to the mass of the formula unit of an ionic compound as well.

? Test yourself

4 Work out the relative molecular masses of the following compounds:



Moles

One mole is the amount of substance that contains the same number of particles (atoms, ions, molecules, etc.) as there are carbon atoms in 12 g of carbon-12. This number is called **Avogadro's constant**, has symbol L (or N_A), and has the value $6.02 \times 10^{23} \text{ mol}^{-1}$. So, 12.00 g of carbon-12 contains 6.02×10^{23} carbon atoms.

You can have a mole of absolutely anything. We usually consider a mole of atoms (6.02×10^{23} atoms) or a mole of molecules (6.02×10^{23} molecules), but we could also have, for instance, a mole of ping-pong balls (6.02×10^{23} ping-pong balls).

The A_r of oxygen is 16.00, which means that, on average, each oxygen atom is $\frac{16}{12}$ times as heavy as a carbon-12 atom. Therefore 16 g of oxygen atoms must contain the same number of atoms as 12 g of carbon-12, i.e. one mole, or 6.02×10^{23} atoms. Similarly, one magnesium atom is on average $\frac{24.31}{12}$ times as heavy as a carbon-12 atom and, therefore, 24.31 g of magnesium atoms contains 6.02×10^{23} magnesium atoms.

The number of moles present in a certain mass of substance can be worked out using the equation:

$$\text{number of moles } (n) = \frac{\text{mass of substance}}{\text{molar mass}}$$

The triangle in Figure 1.7 is a useful shortcut for working out all the quantities involved in the equation. If any one of the sections of the triangle is covered up, the relationship between the other two quantities to give the covered quantity is revealed. For example, if 'mass of substance' is covered, we are left with number of moles multiplied by molar mass:

$$\text{mass of substance} = \text{number of moles} \times \text{molar mass}$$

If 'molar mass' is covered, we are left with mass of substance divided by number of moles:

$$\text{molar mass} = \frac{\text{mass of substance}}{\text{number of moles}}$$

The molar mass (M) of a substance is its A_r or M_r in grams. The units of molar mass are g mol^{-1} . For example, the A_r of silicon is 28.09, and the molar mass of silicon is 28.09 g mol^{-1} . This means that 28.09 g of silicon contains 6.02×10^{23} silicon atoms.

When calculating the number of moles present in a certain mass of a substance, the mass must be in grams.

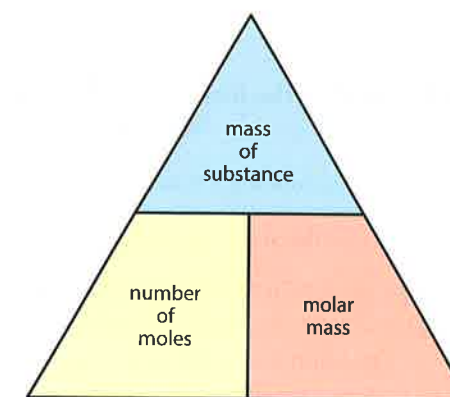


Figure 1.7 The relationship between the mass of a substance, the number of moles and molar mass.



One mole is an enormous number and beyond the scope of our normal experience. How do we understand a number this large?

One way is to describe the number in terms of things we are familiar with from everyday life. For instance, one mole of ping-pong balls would cover the surface of the Earth to about 800 times the height of Mount Everest! We know what a ping-pong ball looks like and we may have a rough idea of the height of Mount Everest, so perhaps this description gives us a context in which we can understand 6.02×10^{23} . Another description sometimes used is in terms of a mole of computer paper: one mole of computer printer paper sheets, if stacked one on top of each other, would

stretch over 6000 light years (one light year is the distance that light travels in one year)—this is over twice the thickness of our galaxy! Is this description better or worse than the previous one? It certainly sounds more impressive, but does it suffer from the fact that we have no real concept of the size of our galaxy? Can you think of any other ways of describing this number in terms of things you are familiar with from everyday life?

This is an example of a wider idea that we tend to understand things that are beyond our normal experience by reference to things with which we are more familiar.

Worked examples

1.3 Calculate the number of moles of magnesium atoms in 10.0 g of magnesium.

$$\text{number of moles } (n) = \frac{\text{mass of substance}}{\text{molar mass}}$$

$$n = \frac{10.0}{24.31} = 0.411 \text{ mol}$$

10.0 g of magnesium is 0.411 mol.

Note: the unit for moles is mol.

The answer is given to three significant figures, because the mass of substance is given to three significant figures.

1.4 Calculate the mass of 0.3800 mol CH_3COOH .

$$\text{mass of substance} = \text{number of moles} \times \text{molar mass}$$

$$\text{mass of substance} = 0.3800 \times 60.06 = 22.82 \text{ g}$$

The mass of 0.3800 mol CH_3COOH is 22.82 g.

The answer is given to four significant figures, because the number of moles and the molar mass are given to four significant figures.

? Test yourself

5 Copy and complete the table. The first row has been done for you.

Compound	Molar mass / g mol^{-1}	Mass / g	Number of moles / mol
H_2O	18.02	9.01	0.500
CO_2		5.00	
H_2S			0.100
NH_3			3.50
Q		1.00	0.0350
Z		0.0578	1.12×10^{-3}
$\text{Mg}(\text{NO}_3)_2$		1.75	
$\text{C}_3\text{H}_7\text{OH}$		2500	
Fe_2O_3			5.68×10^{-5}

The mass of a molecule

The mass of one mole of water is 18.02 g. This contains 6.02×10^{23} molecules of water. The mass of one molecule of water can be worked out by dividing the mass of one mole (18.02 g) by the number of molecules it contains (6.02×10^{23}):

$$\text{mass of one molecule} = \frac{18.02}{6.02 \times 10^{23}} = 2.99 \times 10^{-23} \text{ g}$$

$$\text{mass of one molecule} = \frac{\text{molar mass}}{\text{Avogadro's constant}}$$

Exam tip

Remember – the mass of a molecule is a very small number. Do not confuse the mass of a single molecule with the mass of one mole of a substance, which is a number greater than 1.

The number of particles

When we write '1 mol O_2 ', it means one mole of O_2 molecules: that is, 6.02×10^{23} O_2 molecules. Each O_2 molecule contains two oxygen atoms; therefore, one mole of O_2 molecules contains $2 \times 6.02 \times 10^{23} = 1.204 \times 10^{24}$ atoms. That is, one mole of O_2 **molecules** is made up of two moles of oxygen **atoms**.

When we talk about '0.1 mol H_2O ', we mean 0.1 mol H_2O molecules; i.e. $0.1 \times 6.02 \times 10^{23}$ H_2O molecules; i.e. 6.02×10^{22} H_2O molecules. Each H_2O molecule contains two hydrogen atoms and one oxygen atom. The total number of hydrogen atoms in 0.1 mol H_2O is $2 \times 6.02 \times 10^{22}$; i.e. 1.204×10^{23} hydrogen atoms; i.e. 0.2 mol hydrogen atoms.

Each H_2O molecule contains three atoms. Therefore, the total number of atoms in 0.1 mol H_2O is $3 \times 6.02 \times 10^{22}$; i.e. 1.806×10^{23} atoms; or 0.3 mol atoms.

If you look at Table 1.2 you can see the connection between the number of moles of molecules and the number of moles of a particular atom in that molecule. Figure 1.8 illustrates the relationship between number of particles, number of moles and Avogadro's constant.



oxygen



water

Exam tip

You must be clear which type of particle you are considering. Do you have one mole of atoms, molecules or ions?

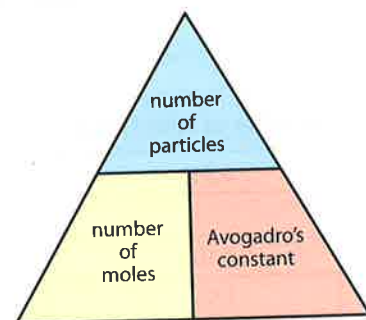


Figure 1.8 The relationship between the number of moles and the number of particles.

Compound	Moles of molecules	Moles of O atoms
H ₂ O	0.1	0.1
SO ₂	0.1	0.2
SO ₃	0.1	0.3
H ₃ PO ₄	0.1	0.4
O ₃	0.5	1.5
CH ₃ COOH	0.2	0.4

Table 1.2 The relationship between the number of moles of molecules and the number of moles of particular atoms.

If we multiply the number of moles of molecules by the number of a particular type of atom in a molecule (i.e. by the subscript of the atom), we get the number of moles of that type of atom. Thus, in 0.25 mol H₂SO₄ there are 4 × 0.25 (i.e. 1.0) mol oxygen atoms.

? Test yourself

- Work out the mass of one molecule of each of the following:
 - H₂O
 - NH₃
 - CO₂
- Work out the total number of hydrogen atoms in each of the following:
 - 1.00 mol H₂
 - 0.200 mol CH₄
 - 0.0500 mol NH₃
- Calculate the total number of atoms in each of the following:
 - 0.0100 mol NH₃
 - 0.200 mol C₂H₆
 - 0.0400 mol C₂H₅OH
- Calculate the number of moles of oxygen atoms in each of the following:
 - 0.2 mol H₂SO₄
 - 0.1 mol Cl₂O₇
 - 0.03 mol XeO₄

Learning objectives

- Determine the percentage composition by mass of a substance
- Understand what is meant by empirical and molecular formulas
- Calculate empirical and molecular formulas

1.2.2 Empirical and molecular formulas

Percentage composition of a compound

The percentage by mass of each element present in a compound can be worked out using the formula:

$$\% \text{ by mass of an element} = \frac{\text{number of atoms of the element} \times \text{relative atomic mass}}{\text{relative molecular mass}}$$

Worked examples

1.5 Find the percentage by mass of each element present in C₆H₅NO₂.

The relative molecular mass of C₆H₅NO₂ is 123.12.

Percentage of carbon: the relative atomic mass of carbon is 12.01, and there are six carbon atoms present, so the total mass of the carbon atoms is 6 × 12.01, i.e. 72.06.

$$\% \text{ carbon} = \frac{72.06}{123.12} \times 100 = 58.53\%$$

Percentage of the other elements present:

$$\% \text{ hydrogen} = \frac{5 \times 1.01}{123.12} \times 100 = 4.10\%$$

$$\% \text{ nitrogen} = \frac{14.01}{123.12} \times 100 = 11.38\%$$

$$\% \text{ oxygen} = \frac{2 \times 16.00}{123.12} \times 100 = 25.99\%$$

1.6 Calculate the mass of oxygen present in 2.20 g of CO₂.

The relative molecular mass of CO₂ is 44.01. Of this, the amount contributed by the two oxygen atoms is 2 × 16.00 = 32.00.

So the fraction of the mass of this compound that is contributed by oxygen is $\frac{32.00}{44.01}$

Therefore, in 2.20 g of CO₂, the amount of oxygen is $\frac{32.00}{44.01} \times 2.20 = 1.60$ g

1.7 What mass of HNO₃ contains 2.00 g of oxygen?

The relative molecular mass of HNO₃ is 63.02. Each molecule contains three oxygen atoms with a total mass of 3 × 16.00, i.e. 48.00.

The oxygen and the HNO₃ are in the ratio 48.00 : 63.02.

Therefore the mass of HNO₃ containing 2.00 g of oxygen is:

$$\frac{63.02}{48.00} \times 2.00 = 2.63 \text{ g}$$

Alternative method

The percentage of oxygen in HNO₃ is $\frac{3 \times 16.00}{63.02} \times 100 = 76.2\%$

So 76.2% of this sample is oxygen and has a mass of 2.00 g.

We need, therefore, to find the mass of 100%, which is given by

$$\frac{2.00}{76.2} \times 100 = 2.63 \text{ g}$$

Note: in order to obtain this answer, more figures were carried through on the calculator.

? Test yourself

- 10 Calculate the percentage by mass of oxygen in each of the following compounds:
a $\text{C}_2\text{H}_5\text{OH}$
b $\text{CH}_3\text{CH}_2\text{COOH}$
c Cl_2O_7
- 11 Calculate the mass of oxygen in each of the following samples:
a 6.00 g of $\text{C}_3\text{H}_7\text{OH}$
b 5.00 g of SO_2
c 10.0 g of P_4O_{10}
- 12 For each of the following compounds work out the mass of substance that will contain 1.00 g of oxygen.
a CH_3OH
b SO_3
c P_4O_6

Empirical and molecular formulas

A molecular formula is a whole number multiple of the empirical formula. Therefore, if the empirical formula of a compound is CH_2 , the molecular formula is $(\text{CH}_2)_n$ i.e. C_2H_4 or C_3H_6 or C_4H_8 , etc.

Empirical formula: the simplest whole number ratio of the elements present in a compound.

Molecular formula: the total number of atoms of each element present in a molecule of the compound. (The molecular formula is a multiple of the empirical formula.)

Worked examples

1.8 If the molecular formulas of two compounds are:

- a $\text{C}_4\text{H}_{10}\text{O}_2$ b Re_3Cl_9
what are the empirical formulas?

- a We need to find the simplest ratio of the elements present and therefore need to find the highest number that divides exactly into the subscript of each element. In this case, each subscript can be divided by two, and so the empirical formula is $\text{C}_2\text{H}_5\text{O}$.
- b In this case each subscript is divisible by three, and so the empirical formula is ReCl_3 .

1.9 The empirical formula of benzene is CH . Given that the molar mass is 78.12 g mol^{-1} , work out its molecular formula.

The mass of the empirical formula unit (CH) is $12.01 + 1.01 = 13.02$. The number of times that the empirical formula unit occurs in the actual molecule (n) is given by:

$$n = \frac{\text{relative molecular mass}}{\text{empirical formula mass}} = \frac{78.12}{13.02} = 6$$

Therefore the molecular formula is $(\text{CH})_6$, which is more commonly written as C_6H_6 .

Chemical analysis of a substance can provide the composition by mass of the compound. The empirical formula can then be calculated from these data. In order to work out the molecular formula, the relative molecular mass of the compound is also required.

Worked examples

1.10 A compound has the following composition by mass: C, 0.681 g; H, 0.137 g; O, 0.181 g.

- a Calculate the empirical formula of the compound.
b If the relative molecular mass of the compound is 88.17, calculate the molecular formula.

a This is most easily done by laying everything out in a table.

	C	H	O
mass/g	0.681	0.137	0.181
divide by relative atomic mass to give number of moles	$0.681/12.01$	$0.137/1.01$	$0.181/16.00$
number of moles/mol	0.0567	0.136	0.0113
divide by smallest to get ratio	$0.0567/0.0113$	$0.136/0.0113$	$0.0113/0.0113$
ratio	5	12	1

Therefore the empirical formula is $\text{C}_5\text{H}_{12}\text{O}$.

- b The empirical formula mass of the compound is 88.17. This is the same as the relative molecular mass, and so the molecular formula is the same as the empirical formula ($\text{C}_5\text{H}_{12}\text{O}$).

1.11 If a fluoride of uranium contains 67.62% uranium by mass, what is its empirical formula?

A uranium fluoride contains only uranium and fluorine.

$$\% \text{ fluorine} = 100.00 - 67.62 = 32.38\%$$

It makes no difference here that the percentage composition is given instead of the mass of each element present, as the percentage is the same as the mass present in 100 g.

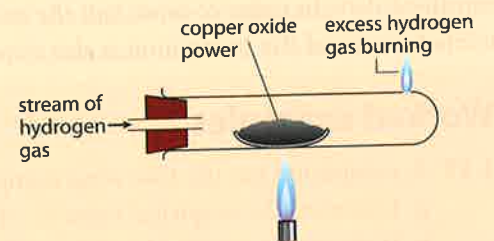
	U	F
percentage	67.62	32.38
mass in 100 g/g	67.62	32.38
divide by relative atomic mass to give number of moles	$67.62/238.03$	$32.38/19.00$
number of moles	0.2841	1.704
divide by smallest to get ratio	$0.2841/0.2841$	$1.704/0.2841$
ratio	1	6

There are therefore six fluorine atoms for every uranium atom, and the empirical formula is UF_6 .

1.12 The experimental set-up shown in the figure can be used to determine the empirical formula of copper oxide. The following experimental results were obtained.

Mass of empty dish / g	24.58
Mass of dish + copper oxide / g	30.12
Mass of dish + copper at end of experiment / g	29.00

Calculate the empirical formula of the copper oxide and write an equation for the reaction.



Hydrogen gas is passed over the heated copper oxide until all the copper oxide is reduced to copper.

$$\text{mass of copper oxide at start} = 30.12 - 24.58 = 5.54 \text{ g}$$

$$\text{mass of copper at end} = 29.00 - 24.58 = 4.42 \text{ g}$$

The difference in mass is due to the oxygen from the copper oxide combining with the hydrogen.

$$\text{mass of oxygen in copper oxide} = 5.54 - 4.42 = 1.12 \text{ g}$$

From now on, the question is a straightforward empirical formula question:

$$\text{number of moles of copper} = \frac{4.42}{63.55} = 0.0696 \text{ mol}$$

$$\text{number of moles of oxygen} = \frac{1.12}{16.00} = 0.0700 \text{ mol}$$

If each number of moles is divided by the smaller number (0.0696):

Cu	O
$\frac{0.0696}{0.0696} = 1$	$\frac{0.0700}{0.0696} = 1.01$

the ratio of copper to oxygen is 1:1, and the empirical formula is CuO.

The equation for the reaction is: $\text{CuO} + \text{H}_2 \rightarrow \text{Cu} + \text{H}_2\text{O}$

Composition by mass from combustion data

Worked examples

1.13 An organic compound, **A**, contains only carbon and hydrogen. When 2.50 g of **A** burns in excess oxygen, 8.08 g of carbon dioxide and 2.64 g of water are formed. Calculate the empirical formula.

The equation for the reaction is of the form: $\text{C}_x\text{H}_y + (x + \frac{y}{4})\text{O}_2 \rightarrow x\text{CO}_2 + \frac{y}{2}\text{H}_2\text{O}$

All the C in the CO_2 comes from the hydrocarbon **A**.

$$\text{number of moles of CO}_2 = \frac{8.08}{44.01} = 0.184 \text{ mol}$$

Each CO_2 molecule contains one carbon atom. Therefore the number of moles of carbon in 2.50 g of the hydrocarbon is 0.184 mol.

All the hydrogen in the water comes from the hydrocarbon **A**.

$$\text{number of moles of H}_2\text{O} = \frac{2.64}{18.02} = 0.147 \text{ mol}$$

Each H_2O molecule contains two hydrogen atoms, so the number of moles of hydrogen in 2.64 g of H_2O is $2 \times 0.147 = 0.293 \text{ mol}$. Therefore, the number of moles of hydrogen in 2.50 g of the hydrocarbon is 0.293 mol. The empirical formula and molecular formula can now be calculated.

	C	H
number of moles	0.184	0.293
divide by smaller	$0.184/0.184$	$0.293/0.184$
ratio	1.00	1.60

The empirical formula must be a ratio of whole numbers, and this can be obtained by multiplying each number by five. Therefore the empirical formula is C_5H_8 .

1.14 An organic compound, **B**, contains only carbon, hydrogen and oxygen. When 1.46 g of **B** burns in excess oxygen, 2.79 g of carbon dioxide and 1.71 g of water are formed.

a What is the empirical formula of **B**?

b If the relative molecular mass is 92.16, what is the molecular formula of **B**?

a The difficulty here is that the mass of oxygen in **B** cannot be worked out in the same way as the previous example, as only some of the oxygen in the CO_2 and H_2O comes from the oxygen in **B** (the rest comes from the oxygen in which it is burnt).

$$\text{mass of carbon in 2.79 g of CO}_2 = \frac{12.01}{44.01} \times 2.79 = 0.76 \text{ g}$$

$$\text{mass of hydrogen in 1.71 g of H}_2\text{O} = \frac{2.02}{18.02} \times 1.71 = 0.19 \text{ g}$$

$$\text{mass of oxygen in 1.46 g of B is } (1.46 - 0.76 - 0.19) = 0.51 \text{ g}$$

The empirical formula can now be calculated.

	C	H	O
mass/g	0.76	0.19	0.51
moles/mol	0.063	0.19	0.032
ratio	2	6	1

Therefore the empirical formula is $\text{C}_2\text{H}_6\text{O}$.

b The empirical formula mass is 46.08.

$$\frac{92.16}{46.08} = 2$$

Therefore, the molecular formula is $(\text{C}_2\text{H}_6\text{O})_2$, i.e. $\text{C}_4\text{H}_{12}\text{O}_2$.

More significant figures are carried through in subsequent calculations.

Note: 2.02 as there are 2 H atoms in a water molecule

? Test yourself

- 13 Which of the following represent empirical formulas?
- | | | |
|----------|------------|--------------|
| C_2H_4 | CO_2 | CH |
| HO | C_3H_8 | C_4H_{10} |
| H_2O | H_2O_2 | N_2H_4 |
| PCl_5 | CH_3COOH | $C_6H_5CH_3$ |
- 14 Copy the table below and complete it with the molecular formulas of the compounds, given the empirical formulas and relative molecular masses.

Empirical formula	Relative molecular mass	Molecular formula
HO	34.02	
ClO_3	166.90	
CH_2	84.18	
BNH_2	80.52	

- 15 Analysis of a sample of an organic compound produced the following composition:
C: 0.399 g H: 0.101 g
 a Calculate the empirical formula.
 b Given that the relative molecular mass is 30.08, determine the molecular formula.

- 16 If an oxide of chlorine contains 81.6% chlorine, calculate its empirical formula.
- 17 A compound contains 76.0% iodine and 24.0% oxygen. Calculate the empirical formula of the compound.
- 18 When 4.76 g of an organic compound, **D**, which contains only carbon, hydrogen and oxygen, is burnt in excess oxygen, 10.46 g of carbon dioxide and 5.71 g of water are produced. What is the empirical formula of **D**?
- 19 When 5.60 g of an iron oxide is heated with carbon, 3.92 g of iron is produced. Calculate the empirical formula of the iron oxide.

Learning objectives

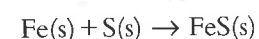
- Solve problems involving masses of substances
- Calculate the theoretical and percentage yield in a reaction
- Understand the terms *limiting reactant* and *reactant in excess* and solve problems involving these

1.3 Reacting masses and volumes

1.3.1 Calculations involving moles and masses

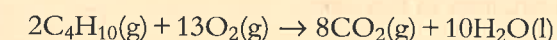
Conservation of mass

The fact that mass is conserved in a chemical reaction can sometimes be used to work out the mass of product formed. For example, if 55.85 g of iron reacts *exactly* and *completely* with 32.06 g of sulfur, 87.91 g of iron sulfide is formed:



Worked example

1.15 Consider the combustion of butane:



10.00 g of butane reacts exactly with 35.78 g of oxygen to produce 30.28 g of carbon dioxide. What mass of water was produced?

The masses given represent an exact chemical reaction, so we assume that all the reactants are converted to products.

The total mass of the reactants = $10.00 + 35.78 = 45.78$ g.

The total mass of the products must also be 45.78 g.

Therefore the mass of water = $45.78 - 30.28 = 15.50$ g.

Using moles

We often want to work out the mass of one reactant that reacts exactly with a certain mass of another reactant – or how much product is formed when certain masses of reactants react. This can be done by calculating the numbers of each molecule or atom present in a particular mass or, much more simply, by using the mole concept.

As we have seen, one mole of any substance always contains the same number of particles, so if we know the number of moles present in a certain mass of reactant we also know the number of particles and can therefore work out what mass of another reactant it reacts with and how much product is formed.

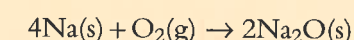
There are three main steps in a moles calculation.

- 1 Work out the number of moles of anything you can.
- 2 Use the chemical (stoichiometric) equation to work out the number of moles of the quantity you require.
- 3 Convert moles to the required quantity – volume, mass etc.

Questions involving masses of substances

Worked examples

1.16 Consider the reaction of sodium with oxygen:

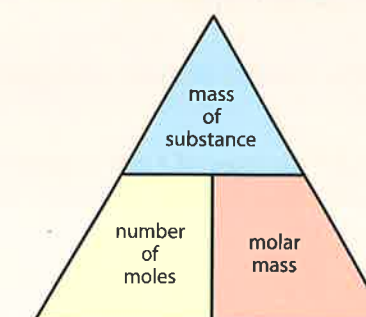


- How much sodium reacts exactly with 3.20 g of oxygen?
- What mass of Na_2O is produced?

- a Step 1 – the mass of oxygen is given, so the number of moles of oxygen can be worked out (you could use the triangle shown here).

$$\text{number of moles of oxygen} = \frac{3.20}{32.00} = 0.100 \text{ mol}$$

Note: the mass of oxygen was given to three significant figures, so all subsequent answers are also given to three significant figures.



Step 2 – the coefficients in the chemical (stoichiometric) equation tell us that 1 mol O₂ reacts with 4 mol sodium. Therefore 0.100 mol O₂ reacts with 4 × 0.100 mol sodium, i.e. 0.400 mol sodium.

Step 3 – convert the number of moles to the required quantity, mass in this case:

$$\text{mass of sodium} = 0.400 \times 22.99 = 9.20 \text{ g}$$

Note: the mass of sodium is worked out by multiplying the mass of one mole by the number of moles – the number of moles is *not* multiplied by the mass of four sodium atoms – the four was already taken into account when 0.100 mol was multiplied by 4 to give the number of moles of sodium.

b From the coefficients in the equation we know that 1 mol O₂ reacts with 4 mol sodium to produce 2 mol Na₂O. Therefore 0.100 mol O₂ reacts with 0.400 mol sodium to give 2 × 0.100 mol Na₂O, i.e. 0.200 mol Na₂O.

$$\begin{aligned}\text{The molar mass of Na}_2\text{O} &= 61.98 \text{ g mol}^{-1} \\ \text{So mass of Na}_2\text{O} &= 0.200 \times 61.98 = 12.4 \text{ g}\end{aligned}$$

Alternatively, the mass of Na₂O can be worked out using the idea of conservation of mass, i.e.:

$$\text{mass of Na}_2\text{O} = \text{mass of O}_2 + \text{mass of Na}.$$

Exam tip

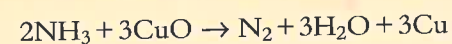
Masses may also be given in kilograms or tonnes.

$$1 \text{ kg} = 1000 \text{ g}$$

$$1 \text{ tonne} = 1 \times 10^6 \text{ g}$$

Before working out the number of moles, you must convert the mass to grams. To convert kilograms to grams, multiply by 1000; to convert tonnes to grams, multiply the mass by 1 × 10⁶.

1.17 Consider the following equation:



If 2.56 g of ammonia (NH₃) is reacted with excess CuO, calculate the mass of copper produced.

The CuO is in excess so there is more than enough to react with all the NH₃. This means that we do not need to worry about the number of moles of CuO.

Step 1 – the number of moles of NH₃ can be calculated:

$$\frac{2.56}{17.04} = 0.150 \text{ mol NH}_3$$

Step 2 – two moles of NH₃ produce three moles of copper, so 0.150 mol NH₃ produces 0.150 × $\frac{3}{2}$ mol copper, i.e. 0.225 mol copper.

The number of moles of copper is therefore 1.5 times the number of moles of NH₃.

Step 3 – the mass of 1 mol copper = 63.55 g, so the mass of copper produced = 0.225 × 63.55 = 14.3 g.

Formula for solving moles questions involving masses

An alternative way of doing these questions is to use a formula.

$$\frac{m_1}{n_1 M_1} = \frac{m_2}{n_2 M_2}$$

where

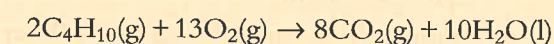
m_1 = mass of first substance

n_1 = coefficient of first substance (number in front in the chemical equation)

M_1 = molar mass of first substance

Worked example

1.18 The following equation represents the combustion of butane:



If 10.00 g of butane is used, calculate the mass of oxygen required for an exact reaction.

We will call butane substance 1 and oxygen substance 2 (it doesn't matter which you call what, but you have to be consistent).

$$m_1 = 10.00 \text{ g}$$

$$m_2 = ?$$

$$n_1 = 2$$

$$n_2 = 13$$

$$M_1 = 58.14 \text{ g mol}^{-1}$$

$$M_2 = 32.00 \text{ g mol}^{-1}$$

$$\frac{m_1}{n_1 M_1} = \frac{m_2}{n_2 M_2}$$

$$\frac{10.00}{2 \times 58.14} = \frac{m_2}{13 \times 32.00}$$

The equation can be rearranged:

$$m_2 = \frac{10.00 \times 13 \times 32.00}{2 \times 58.14} = 35.78$$

Therefore the mass of oxygen required for an exact reaction is 35.78 g.

? Test yourself

- 20 a How many moles of hydrogen gas are produced when 0.4 mol sodium react with excess water?
 $2\text{Na} + 2\text{H}_2\text{O} \rightarrow 2\text{NaOH} + \text{H}_2$
- b How many moles of O_2 react with 0.01 mol C_3H_8 ?
 $\text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O}$
- c How many moles of H_2S are formed when 0.02 mol HCl react with excess Sb_2S_3 ?
 $\text{Sb}_2\text{S}_3 + 6\text{HCl} \rightarrow 2\text{SbCl}_3 + 3\text{H}_2\text{S}$
- d How many moles of oxygen are formed when 0.6 mol KClO_3 react?
 $2\text{KClO}_3(\text{s}) \rightarrow 2\text{KCl}(\text{s}) + 3\text{O}_2(\text{g})$
- e How many moles of iron are formed when 0.9 mol CO react with excess iron oxide?
 $\text{Fe}_2\text{O}_3 + 3\text{CO} \rightarrow 2\text{Fe} + 3\text{CO}_2$
- f How many moles of hydrogen would be required to make 2.4×10^{-3} mol NH_3 ?
 $\text{N}_2 + 3\text{H}_2 \rightarrow 2\text{NH}_3$
- 21 a Calculate the mass of arsenic(III) chloride produced when 0.150 g of arsenic reacts with excess chlorine according to the equation:
 $2\text{As} + 3\text{Cl}_2 \rightarrow 2\text{AsCl}_3$
- b What mass of sulfur is produced when 5.78 g of iron(III) sulfide is reacted with excess oxygen?
 $2\text{Fe}_2\text{S}_3 + 3\text{O}_2 \rightarrow 2\text{Fe}_2\text{O}_3 + 6\text{S}$
- c Calculate the mass of iodine that must be reacted with excess phosphorus to produce 5.00 g of phosphorus(III) iodide according to the equation below.
 $2\text{P} + 3\text{I}_2 \rightarrow 2\text{PI}_3$
- d Consider the reaction shown below. What mass of SbCl_2 must be reacted with excess NaF to produce 2.25 g of NaCl ?
 $3\text{SbCl}_2 + 4\text{NaF} \rightarrow \text{Sb}_2\text{Cl}_2 + \text{SF}_4 + 4\text{NaCl}$



The fact that a theory can explain experimental observations does not necessarily make it correct. The explanations presented in this book fit in with experimental observations, but this does not mean that they are 'true' – they just represent our interpretation of the data at this stage in time. Each generation of scientists believes that they are presenting a true description of reality, but is it possible for more than one explanation to fit the facts? You, or indeed I, may not be able to think of a better explanation to fit many of the experimental observations in modern science, but that does not mean that there isn't one. Consider the following trivial example.

Experimentally, when 100 kg of calcium carbonate (CaCO_3) is heated, 44 kg of carbon dioxide (CO_2) is obtained. The following calculation can be carried out to explain this.

The equation for the reaction is:

$$\text{CaCO}_3 \rightarrow \text{CaO} + \text{CO}_2$$

$$\text{number of moles of CaCO}_3 = \frac{100}{(20 + 6 + (3 \times 8))} = 2 \text{ mol}$$

Two moles of CaCO_3 produces two moles of CO_2 .

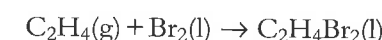
The mass of two moles of CO_2 is
 $2 \times (6 + (2 \times 8)) = 44 \text{ kg}$.

Hopefully you can see some mistakes in this calculation, but the result is what we got experimentally. It is also interesting to note that if, in your IB examination, you had just written down the final answer, you would probably have got full marks!

Calculating the yield of a chemical reaction

In any commercial process it is very important to know the **yield** (the amount of desired product) of a chemical reaction. For instance, if a particular process for the preparation of a drug involves four separate steps and the yield of each step is 95%, it is probably quite a promising synthetic route to the drug. If, however, the yield of each step is only 60% then it is likely that the company would look for a more efficient synthetic process.

The yield of a chemical reaction is usually quoted as a percentage – this gives more information than just quoting the yield of the product as a mass. Consider the preparation of 1,2-dibromoethane ($\text{C}_2\text{H}_4\text{Br}_2$):



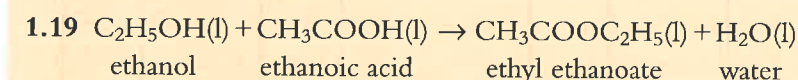
10.00 g of ethene (C_2H_4) will react exactly with 56.95 g of bromine.

The **theoretical yield** for this reaction is 66.95 g – this is the maximum possible yield that can be obtained. The **actual yield** of $\text{C}_2\text{H}_4\text{Br}_2$ may be 50.00 g.

$$\% \text{ yield} = \frac{50.00}{66.95} \times 100 = 74.68\%$$

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

Worked example



If the yield of ethyl ethanoate obtained when 20.00 g of ethanol is reacted with excess ethanoic acid is 30.27 g, calculate the percentage yield.

The first step is to calculate the maximum possible yield, i.e. the theoretical yield:

$$\text{molar mass of C}_2\text{H}_5\text{OH} = 46.08 \text{ g mol}^{-1}$$

$$\text{number of moles of C}_2\text{H}_5\text{OH} = \frac{20.00}{46.08} = 0.4340 \text{ mol}$$

The chemical equation tells us that 1 mol $\text{C}_2\text{H}_5\text{OH}$ produces 1 mol $\text{CH}_3\text{COOC}_2\text{H}_5$. Therefore, 0.4340 mol $\text{C}_2\text{H}_5\text{OH}$ produces 0.4340 mol $\text{CH}_3\text{COOC}_2\text{H}_5$.

$$\text{The molar mass of CH}_3\text{COOC}_2\text{H}_5 = 88.12 \text{ g mol}^{-1}.$$

$$\text{The mass of ethyl ethanoate CH}_3\text{COOC}_2\text{H}_5 = 0.4340 \times 88.12 = 38.24 \text{ g}.$$

So, the theoretical yield is 38.24 g. The actual yield is 30.27 g (given in the question).

$$\% \text{ yield} = \frac{30.27}{38.24} \times 100 = 79.15\%$$

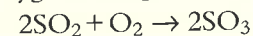
The percentage yield of $\text{CH}_3\text{COOC}_2\text{H}_5$ is 79.15%.

The CH_3COOH is in excess, i.e. more than enough is present to react with all the $\text{C}_2\text{H}_5\text{OH}$. This means that we do not need to worry about the number of moles of CH_3COOH .

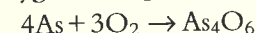
? Test yourself

22 Calculate the percentage yield in each of the following reactions.

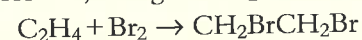
a When 2.50 g of SO_2 is heated with excess oxygen, 2.50 g of SO_3 is obtained.



b When 10.0 g of arsenic is heated in excess oxygen, 12.5 g of As_4O_6 is produced.



c When 1.20 g of C_2H_4 reacts with excess bromine, 5.23 g of $\text{CH}_2\text{BrCH}_2\text{Br}$ is produced.



Limiting reactant

Very often we do not use exact quantities in a chemical reaction, but rather we use an excess of one or more reactants. One reactant is therefore used up before the others and is called the **limiting reactant**. When the limiting reactant is completely used up, the reaction stops.

Figure 1.9 illustrates the idea of a limiting reactant and shows how the products of the reaction depend on which reactant is limiting.

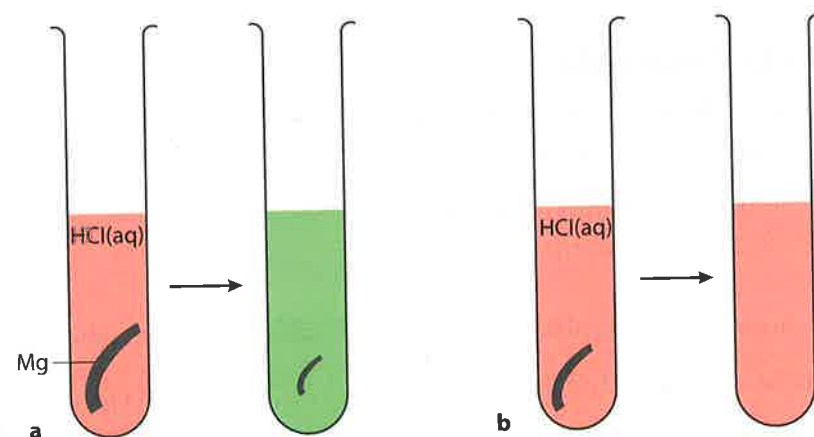
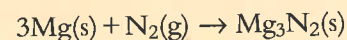


Figure 1.9 The reaction between magnesium and hydrochloric acid. In each test tube a small amount of universal indicator has been added. **a** In this test tube, the magnesium is in excess and the reaction finishes when the hydrochloric acid runs out. There is still magnesium left over at the end, and the solution is no longer acidic. **b** In this test tube, the hydrochloric acid is in excess. The magnesium is the limiting reactant, and the reaction stops when the magnesium has been used up. The solution is still acidic at the end.

Worked examples

1.20 Consider the reaction between magnesium and nitrogen:



10.00 g of magnesium is reacted with 5.00 g of nitrogen. Which is the limiting reactant?

$$\text{number of moles of magnesium} = \frac{10.00}{24.31} = 0.4114 \text{ mol}$$

$$\text{number of moles of N}_2 = \frac{5.00}{28.02} = 0.178 \text{ mol}$$

The equation tells us that 3 mol magnesium reacts with 1 mol N_2 . So 0.4114 mol magnesium reacts with $\frac{0.4114}{3}$ mol N_2 , i.e. 0.1371 mol N_2 .

Therefore, for an exact reaction, 0.1371 mol N_2 are required to react with 0.4114 mol magnesium. However, 0.178 mol N_2 are used, which is more than enough to react. This means that N_2 is in excess because there is more than enough to react with all the magnesium present. Magnesium is therefore the limiting reactant.

This can also be seen from working with the number of moles of N_2 – 0.178 mol N_2 was used in this reaction. This number of moles of N_2 would require 3×0.178 mol magnesium for an exact reaction, i.e. 0.534 mol magnesium. However, only 0.4114 mol magnesium are present; therefore, the magnesium will run out before all the N_2 has reacted.

Exam tip

If the number of moles of each reactant is divided by its coefficient in the stoichiometric equation, the smallest number indicates the limiting reactant.

1.21 Consider the reaction between sulfur and fluorine: $\text{S(s)} + 3\text{F}_2\text{(g)} \rightarrow \text{SF}_6\text{(g)}$

10.00 g of sulfur reacts with 10.00 g of fluorine.

- Which is the limiting reactant?
- What mass of sulfur(VI) fluoride is formed?
- What mass of the reactant in excess is left at the end?

$$\text{a number of moles of sulfur} = \frac{10.00}{32.07} = 0.3118 \text{ mol} \quad \text{number of moles of F}_2 = \frac{10.00}{38.00} = 0.2632 \text{ mol}$$

The coefficient of sulfur in the equation is 1 and that of F_2 is 3.

$0.3118 / 1 = 0.3118$ and $0.2632 / 3 = 0.08773$, therefore sulfur is in excess (larger number) and F_2 is the limiting reactant (smaller number).

Alternatively we can reason from the chemical equation that 0.2632 mol F_2 should react with 0.08773 mol sulfur (i.e. 0.2632 mol divided by three). There is more than 0.08773 mol sulfur present, so sulfur is present in excess and F_2 is the limiting reactant.

For the rest of the question we must work with the limiting reactant.

b When the limiting reactant is used up completely, the reaction stops. This means that the amount of product formed is determined by the amount of the limiting reactant we started with.

From the chemical equation, 0.2632 mol F_2 produces 0.08773 mol SF_6 (i.e. 0.2632 mol divided by three).

$$\text{molar mass of SF}_6 = 146.07 \text{ g mol}^{-1}$$

$$\text{mass of SF}_6 \text{ formed} = 0.08773 \times 146.07 = 12.81 \text{ g}$$

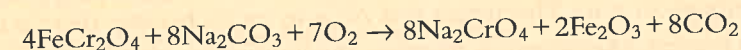
c From the chemical equation, 0.2632 mol F_2 reacts with 0.08773 mol sulfur (i.e. 0.2632 mol sulfur divided by three). Originally there were 0.3118 mol sulfur present; therefore the number of moles of sulfur left at the end of the reaction is $0.3118 - 0.08773 = 0.2241$.

The mass of sulfur left at the end of the reaction is $0.2241 \times 32.07 = 7.187 \text{ g}$.

Exam tip

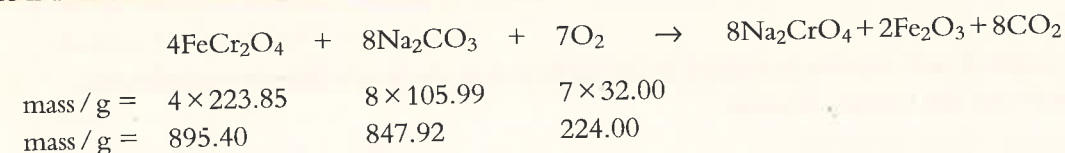
To do a moles question you need to know the mass of just one of the reactants. If you are given the masses of more than one reactant, you must consider that one of these reactants will be the limiting reactant and you must use this one for all calculations.

1.22 For the reaction:



there are 100.0 g of each reactant available. Which is the limiting reactant?

This question could be done by working out the number of moles of each reactant and then comparing them, but there is a shortcut – to work out the masses of each substance if molar quantities reacted:



These are the masses that are required for the exact reaction. Because the highest mass required is that of FeCr_2O_4 , if the same mass of each substance is taken, the FeCr_2O_4 will run out first and must be the limiting reactant.

Nature of science

Science is a constantly changing body of knowledge. Scientists take existing knowledge and try to build on it to improve theories so that they are more widely applicable and have better explanatory power. The concept of the mole developed from the concept of equivalent weight.

? Test yourself

23 What is the limiting reactant in each of the following reactions?

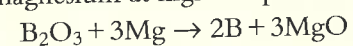
a 0.1 mol Sb_4O_6 react with 0.5 mol H_2SO_4
 $\text{Sb}_4\text{O}_6 + 6\text{H}_2\text{SO}_4 \rightarrow 2\text{Sb}_2(\text{SO}_4)_3 + 6\text{H}_2\text{O}$

b 0.20 mol AsCl_3 react with 0.25 mol H_2O
 $4\text{AsCl}_3 + 6\text{H}_2\text{O} \rightarrow \text{As}_4\text{O}_6 + 12\text{HCl}$

c 0.25 mol copper react with 0.50 mol dilute HNO_3 according to the equation:
 $3\text{Cu} + 8\text{HNO}_3 \rightarrow 3\text{Cu}(\text{NO}_3)_2 + 4\text{H}_2\text{O} + 2\text{NO}$

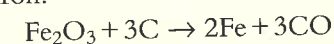
d 0.10 mol NaCl react with 0.15 mol MnO_2 and 0.20 mol H_2SO_4
 $2\text{NaCl} + \text{MnO}_2 + 2\text{H}_2\text{SO}_4 \rightarrow \text{Na}_2\text{SO}_4 + \text{MnSO}_4 + 2\text{H}_2\text{O} + \text{Cl}_2$

24 Boron can be prepared by reacting B_2O_3 with magnesium at high temperatures:



What mass of boron is obtained if 0.75 g B_2O_3 are reacted with 0.50 g magnesium?

25 Iron(III) oxide reacts with carbon to produce iron:



What mass of iron is obtained if 10.0 tonnes of Fe_2O_3 are reacted with 1.00 tonne of carbon?

1.3.2 Calculations involving volumes of gases

Real gases and ideal gases

An 'ideal gas' is a concept invented by scientists to approximate (model) the behaviour of real gases. Under normal conditions (around 100 kPa [approximately 1 atmosphere] pressure and 0°C) real gases such as hydrogen behave pretty much like ideal gases and the approximations work very well.

Two assumptions we make when defining the **ideal gas** are that the molecules themselves have no volume (they are point masses) and that no forces exist between them (except when they collide). If we imagine compressing a real gas to a very high pressure then the particles will be much closer together and, under these conditions, the forces between molecules and the volumes occupied by the molecules will be significant. This means that we can no longer ignore these factors and the behaviour of the gas will deviate significantly from our ideal gas model. This will also be the case at very low temperatures when the molecules are moving more slowly. Under conditions of very low temperature and very high pressure a gas is approaching the liquid state and will be least like our predictions for an ideal gas.

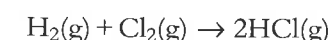
The idea that the volumes of the individual gas molecules are zero (so it makes no difference if the gas is H_2 or NH_3) and that there are no forces between the molecules (again no difference between NH_3 and H_2) means that all ideal gases must behave in the same way. This means that the volume occupied by a gas at a certain temperature and pressure depends only on the number of molecules present and not on the nature of the gas. In other words, at a certain temperature and pressure, the volume of a gas is proportional to the number of moles of the gas.

Using volumes of gases

Avogadro's law: equal volumes of ideal gases measured at the same temperature and pressure contain the same number of molecules.

In other words 100 cm^3 of H_2 contains the same number of molecules at 25°C and 100 kPa as 100 cm^3 of NH_3 , if we assume that they both behave as ideal gases. Under the same conditions, 50 cm^3 of CO_2 would contain half as many molecules.

This means that volumes can be used directly (instead of moles) in equations involving gases:



The above equation tells us that one mole of H_2 reacts with one mole of Cl_2 to give two moles of HCl . Or one volume of H_2 reacts with one volume of Cl_2 to give two volumes of HCl ; i.e. 50 cm^3 of H_2 reacts with 50 cm^3 of Cl_2 to give 100 cm^3 of HCl .

Learning objectives

- Understand Avogadro's law and use it to calculate reacting volumes of gases
- Use the molar volume of a gas in calculations at standard temperature and pressure
- Understand the relationships between pressure, volume and temperature for an ideal gas
- Solve problems using the equation
$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$
- Solve problems using the ideal gas equation

Gases deviate most from ideal behaviour at high pressure and low temperature.

Volume of gas \propto number of moles of the gas

1 cm^3 is the same as 1 ml.

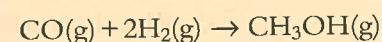


The ideal gas concept is an approximation which is used to model the behaviour of real gases. Why do we learn about ideal gases when they do not exist? What implications does the ideal gas concept have on the limits of knowledge gained from this course?

Worked examples

In both of these worked examples, assume that all gases behave as ideal gases and that all measurements are made under the same conditions of temperature and pressure.

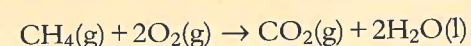
1.23 Consider the following reaction for the synthesis of methanol:



- What volume of H_2 reacts exactly with 2.50 dm^3 of CO ?
- What volume of CH_3OH is produced?

- From the equation we know that 1 mol CO reacts with 2 mol H_2 . Therefore, one volume of CO reacts with two volumes of H_2 – 2.50 dm^3 of CO reacts with 2×2.50 , i.e. 5.00 dm^3 , of H_2 .
- One volume of CO produces one volume of CH_3OH . Therefore, the volume of CH_3OH produced is 2.50 dm^3 .

1.24 If 100 cm^3 of oxygen reacts with 30 cm^3 of methane in the following reaction, how much oxygen will be left at the end of the reaction?



From the equation, we know that 1 mol CH_4 reacts with 2 mol O_2 . Therefore, one volume of CH_4 reacts with two volumes of O_2 – so 30 cm^3 of CH_4 reacts with 2×30 , i.e. 60 cm^3 of O_2 .

The original volume of O_2 was 100 cm^3 ; therefore, if 60 cm^3 reacted, the volume of oxygen gas left over at the end of the reaction would be $100 - 60 = 40 \text{ cm}^3$.

STP = standard temperature and pressure = 273 K, 100 kPa (1 bar)

$$100 \text{ kPa} = 1.00 \times 10^5 \text{ Pa}$$

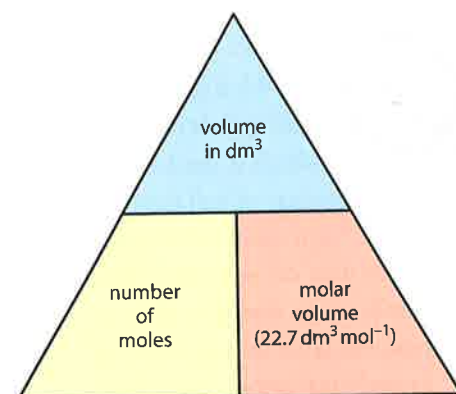


Figure 1.10 The relationship between the number of moles of a gas and its volume.

Converting volumes of gases to number of moles

Because the volume occupied by an ideal gas depends only on the number of particles present (assuming that pressure and temperature are constant) and not on the nature of the particles, the volume occupied by one mole of any ideal gas under a certain set of conditions will always be the same. The volume occupied by one mole of a gas under certain conditions is called the **molar volume**.

molar volume of an ideal gas at STP = $22.7 \text{ dm}^3 \text{ mol}^{-1}$ or $2.27 \times 10^{-2} \text{ m}^3 \text{ mol}^{-1}$

This means that under the same set of conditions, the volume occupied by one mole of NH_3 is the same as the volume occupied by one mole of CO_2 and one mole of H_2 , and this volume is 22.7 dm^3 at STP.

The relationship between the number of moles of a gas and its volume is:

$$\text{number of moles} = \frac{\text{volume}}{\text{molar volume}}$$

This is summarised in Figure 1.10.

The absolute, or Kelvin, scale of temperature starts at absolute zero, which is the lowest temperature possible. It is the temperature at which everything would be in its lowest energy state. **Absolute zero** corresponds to 0 K or -273.15°C (usually taken as -273°C) and is also the temperature at which the volume of an ideal gas would be zero. It is not possible to actually reach absolute zero, but scientists have managed to get very close – about 1 nanokelvin!

A change of 1°C is the same as a change of 1 K , and 0°C is equivalent to 273 K

To convert $^\circ\text{C}$ to K add 273:

e.g. 25°C is equivalent to $25 + 273$, i.e. 298 K

To convert K to $^\circ\text{C}$ subtract 273:

e.g. 350 K is equivalent to $350 - 273$, i.e. 77°C

Volumes of gases are often given in cm^3 and so it is important to know how to convert between cm^3 and dm^3 .

Because 1 dm^3 (1 litre) is equivalent to 1000 cm^3 to convert cm^3 to dm^3 we divide by 1000 (to go from $1000 (\text{cm}^3)$ to $1 (\text{dm}^3)$). The conversion is shown in Figure 1.11.



In different countries around the world's different scales of temperature are used – e.g. the Celsius and Fahrenheit scales. The Celsius and Fahrenheit scales are both artificial scales, but the Kelvin scale is an absolute scale. What is the advantage to scientists of using an absolute scale? Why has the **absolute scale of temperature** not been adopted in everyday life?



The Kelvin scale of temperature is named in honour of William Thompson, Lord Kelvin (1824–1907), a Scottish mathematician and physicist, who first suggested the idea of an absolute scale of temperature. Despite making many important contributions to the advancement of science, Kelvin had doubts about the existence of atoms, believed that the Earth could not be older than 100 million years and is often quoted as saying that 'heavier-than-air flying machines are impossible'.

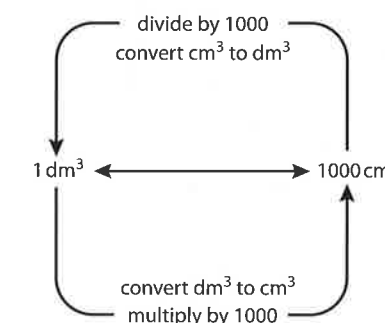


Figure 1.11 Converting between cm^3 and dm^3 .

Worked examples

- Calculate the number of moles in 250 cm^3 of O_2 at STP.
- Calculate the volume of 0.135 mol CO_2 at STP.

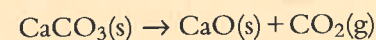
$$\text{a number of moles} = \frac{\text{volume in dm}^3}{22.7}$$

$$250 \text{ cm}^3 = \frac{250}{1000} \text{ dm}^3 = 0.250 \text{ dm}^3$$

$$\text{number of moles} = \frac{0.250}{22.7} = 0.0110 \text{ mol}$$

$$\text{b volume} = \text{number of moles} \times 22.7 = 0.135 \times 22.7 = 3.06 \text{ dm}^3$$

1.26 Calculate the volume of carbon dioxide (collected at STP) produced when 10.01 g of calcium carbonate decomposes according to the equation:



Step 1 – work out the number of moles of CaCO_3 :

$$\text{number of moles of CaCO}_3 = \frac{10.01}{100.09} = 0.1000 \text{ mol}$$

Step 2 – the chemical equation tells us that 1 mol CaCO_3 decomposes to give 1 mol CO_2 .

Therefore 0.1000 mol CaCO_3 decomposes to give 0.1000 mol CO_2 .

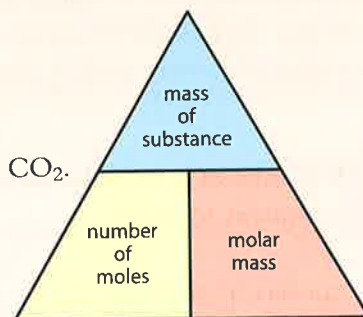
Step 3 – convert the number of moles to volume:

1 mol CO_2 occupies 22.7 dm^3 at STP

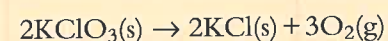
volume of CO_2 = number of moles \times volume of 1 mole (22.7 dm^3)

$$\text{volume of CO}_2 = 0.1000 \times 22.7 = 2.27 \text{ dm}^3$$

The volume of CO_2 produced is 2.27 dm^3 .



1.27 Potassium chlorate(V) decomposes when heated:



What mass of potassium chlorate(V) decomposes to produce 100.0 cm^3 of oxygen gas measured at STP?

Step 1 – work out the number of moles of O_2 . The volume of O_2 must first be converted to dm^3 :

$$\text{volume of O}_2 \text{ in dm}^3 = \frac{100.0}{1000} = 0.1000 \text{ dm}^3$$

$$\text{number of moles of O}_2 = \frac{0.1000}{22.7} = 4.405 \times 10^{-3} \text{ mol}$$

Step 2 – the chemical equation tells us that 3 mol O_2 are produced from 2 mol KClO_3 . Therefore the number of moles of KClO_3 is two-thirds of the number of moles of O_2 :

$$\frac{2}{3} \times 4.405 \times 10^{-3} = 2.937 \times 10^{-3} \text{ mol}$$

Step 3 – convert the number of moles of KClO_3 to mass:

$$\text{molar mass of KClO}_3 = 122.55 \text{ g mol}^{-1}$$

$$\text{mass of KClO}_3 = 122.55 \times 2.937 \times 10^{-3} = 0.3599 \text{ g}$$

The mass of KClO_3 required is 0.3599 g.

Formula for solving moles questions involving volumes of gases

An alternative way of doing these questions is to use a formula.

$$\frac{m_1}{n_1 M_1} = \frac{V_2}{n_2 M_v}$$

where:

m_1 = mass of first substance (in g)

n_1 = coefficient of first substance

M_1 = molar mass of first substance

V_2 = volume (in dm^3) of second substance if it is a gas

n_2 = coefficient of second substance

M_v = molar volume of a gas = 22.7 dm^3 at STP

This formula can be used if the mass of one substance is given and the volume of another substance is required, or vice versa.

If a volume is given and a volume is required, then an alternative form of this equation is:

$$\frac{V_1}{n_1} = \frac{V_2}{n_2}$$

where:

V_1 = volume of first substance if it is a gas

V_2 = volume of second substance

However, with questions involving just gases it is usually easier to work them out using Avogadro's law, as described earlier.

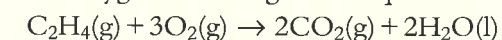
Note: this is very similar to the formula that was used earlier with masses.

There is no need to convert units of volume to dm^3 with this equation – but V_2 must have the same units as V_1 .

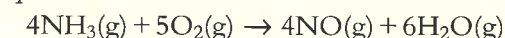
? Test yourself

Assume that all gases behave as ideal gases and that all measurements are made under the same conditions of temperature and pressure.

26 a Calculate the volume of carbon dioxide produced when 100 cm^3 of ethene burns in excess oxygen according to the equation:



b Calculate the volume of nitric oxide (NO) produced when 2.0 dm^3 of oxygen is reacted with excess ammonia according to the equation:



27 Determine the number of moles present in each of the following at standard temperature and pressure:

- | | |
|--|--|
| a 0.240 dm^3 of O_2 | d 400.0 cm^3 of N_2 |
| b 2.00 dm^3 of CH_4 | e 250.0 cm^3 of CO_2 |
| c 0.100 dm^3 of SO_2 | |

28 Work out the volume of each of the following at standard temperature and pressure:

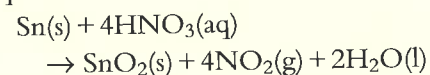
- | | |
|--|------------------------------------|
| a $0.100 \text{ mol C}_3\text{H}_8$ | d 0.8500 mol NH_3 |
| b 100.0 mol SO_3 | e 0.600 mol O_2 |
| c 0.270 mol N_2 | |

- 29 Sodium nitrate(V) decomposes according to the equation:



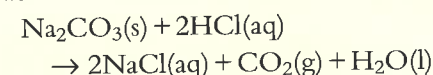
Calculate the volume (in cm^3) of oxygen produced (measured at STP) when 0.850 g of sodium nitrate(V) decompose.

- 30 Tin reacts with nitric acid according to the equation:

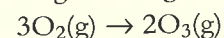


If 2.50 g of tin are reacted with excess nitric acid what volume of nitrogen dioxide (in cm^3) is produced at STP?

- 31 Calculate the mass of sodium carbonate that must be reacted with excess hydrochloric acid to produce 100.0 cm^3 of carbon dioxide at STP.

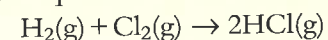


- 32 a Oxygen can be converted to ozone (O_3) by passing it through a silent electric discharge:



If 300 cm^3 of oxygen are used and 10% of the oxygen is converted to ozone, calculate the total volume of gas present at the end of the experiment.

- b Hydrogen reacts with chlorine according to the equation:



What is the total volume of gas present in the container at the end of the experiment if 100 cm^3 of hydrogen are reacted with 200 cm^3 of chlorine?

Macroscopic properties of ideal gases

So far, all the questions we have dealt with have involved working out volumes of gases at STP. In order to work out volumes of gases under other conditions we must understand a little more about the properties of gases.

The relationship between pressure and volume (Boyle's law)

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

This means that if the pressure of a gas is doubled at constant temperature, then the volume will be halved, and vice versa. This relationship is illustrated in Figure 1.12.

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

The relationship can also be written as:

$$P = \frac{k}{V}$$

where k is a constant.

This can be rearranged to give

$$PV = k$$

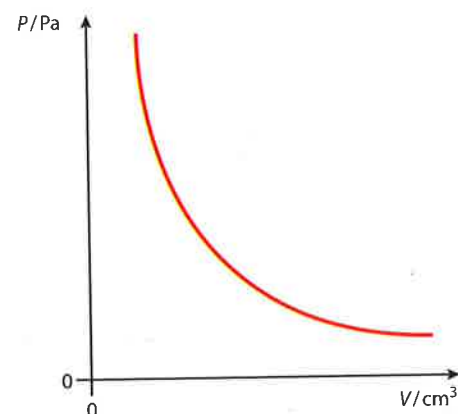


Figure 1.12 The relationship between pressure and volume of a fixed mass of an ideal gas at constant temperature.

This means that the product of the pressure and volume of an ideal gas at a particular temperature is a constant and does not change as the pressure and the volume change.

Other graphs can also be drawn to illustrate this relationship (see Figures 1.13 and 1.14).

Because pressure is proportional to $\frac{1}{\text{volume}}$, a graph of pressure against $\frac{1}{\text{volume}}$ would be a straight-line graph that would pass through the origin (although this graph will never actually pass through the origin – the gas would have to have infinite volume at zero pressure). This is shown in Figure 1.13.

Because $PV = k$, where k is a constant, a graph of PV against pressure (or volume) will be a straight, horizontal line. This is shown in Figure 1.14.

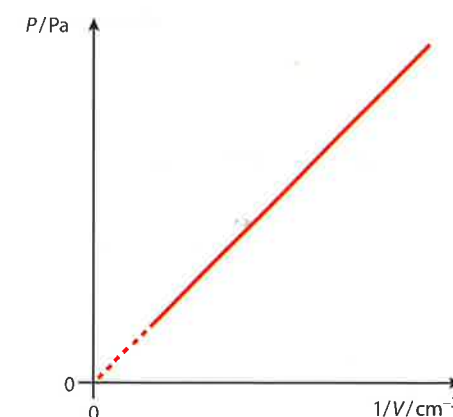


Figure 1.13 The relationship between the pressure and $\frac{1}{\text{volume}}$ of a fixed mass of an ideal gas at constant temperature.

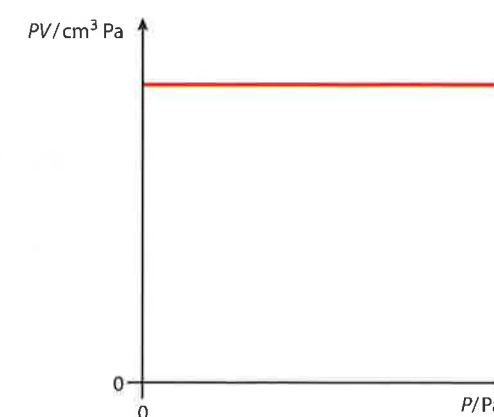


Figure 1.14 The relationship between PV and P for a fixed mass of an ideal gas at constant temperature.

The relationship between volume and temperature (Charles' law)

If the temperature is in kelvin, the following relationship exists between the volume and the temperature:

The volume of a fixed mass of an ideal gas at constant pressure is directly proportional to its kelvin temperature.

$$V \propto T$$

Therefore, if the kelvin temperature is doubled and the pressure remains constant, the volume of the gas is doubled, and vice versa. This means that if an ideal gas has a volume of 200 cm^3 at 120 K, it will have a volume of 400 cm^3 at 240 K if the pressure remains constant. This is illustrated in Figure 1.15.

This relationship does not work for temperatures in $^{\circ}\text{C}$ (Figure 1.16). For instance, if the volume of an ideal gas at 25°C is 500 cm^3 , the volume it will occupy at 50°C will be about 560 cm^3 .

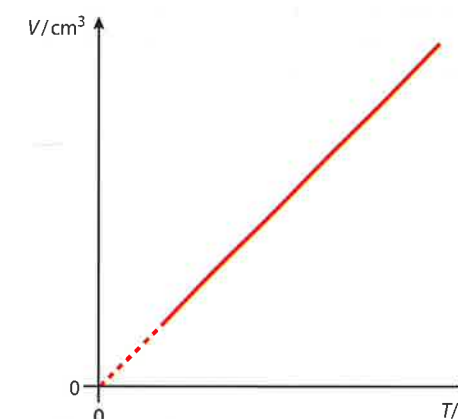


Figure 1.15 The relationship between the volume and temperature (in kelvin) of a fixed mass of an ideal gas at constant pressure.

An ideal gas can never liquefy because there are no forces between the molecules.

This is a linear relationship but not a proportional one because the graph does not pass through the origin.

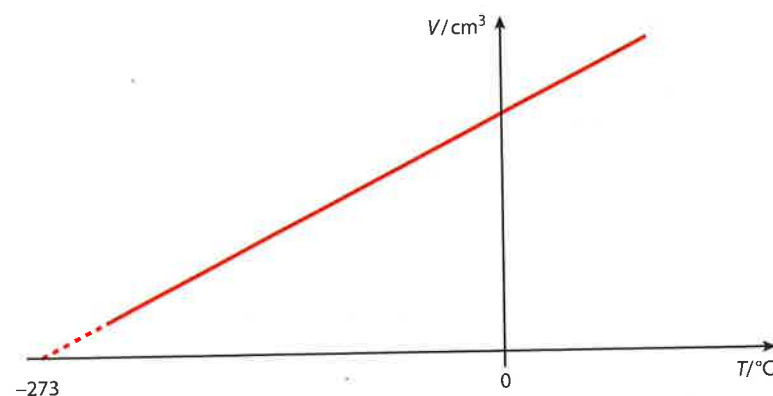


Figure 1.16 The relationship between the volume and temperature (in °C) of a fixed mass of an ideal gas at constant pressure. As can be seen, the temperature at which the volume of an ideal gas is zero will be -273°C . This temperature is **absolute zero**.

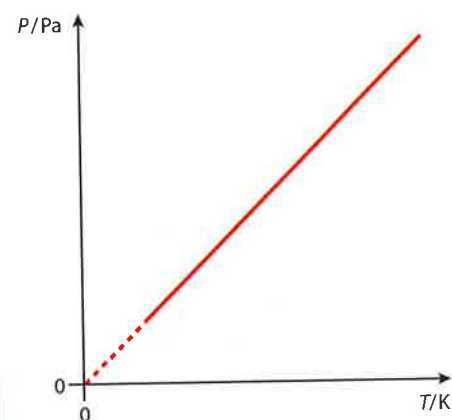


Figure 1.17 The relationship between the pressure and temperature (kelvin) of a fixed mass of an ideal gas at constant volume.

The relationship between pressure and temperature

For a fixed mass of an ideal gas at constant volume, the pressure is directly proportional to its absolute temperature: $P \propto T$

If the temperature (in **kelvin**) of a fixed volume of an ideal gas is doubled, the pressure will also double (Figure 1.17).

The overall gas law equation

An ideal gas is one that obeys all of the above laws exactly.

The three relationships above can be combined to produce the following equation:

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

Note: any units may be used for P and V , so long as they are consistent on both sides of the equation.

The temperature must be kelvin.

Worked examples

1.28 If the volume of an ideal gas collected at 0°C and 100 kPa, i.e. at STP, is 50.0 cm^3 , what would be the volume at 60°C and 108 kPa?

$$P_1 = 100\text{ kPa}$$

$$V_1 = 50.0\text{ cm}^3$$

$$P_2 = 108\text{ kPa}$$

$$V_2 = ?$$

The units of P_1 and P_2 are consistent with each other.

$$T_1 = 0^{\circ}\text{C} = 273\text{ K}$$

$$T_2 = 60^{\circ}\text{C} = 60 + 273\text{ K} = 333\text{ K}$$

Temperature must be in K.

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

$$\frac{100 \times 50.0}{273} = \frac{108 \times V_2}{333}$$

Rearranging the equation:

$$V_2 = \frac{100 \times 50.0 \times 333}{273 \times 108} = 56.5\text{ cm}^3$$

The units of V_2 are the same as those of V_1 .

Therefore, the volume occupied by the gas at 60°C and 108 kPa is 56.5 cm^3 .

1.29 What temperature (in °C) is required to cause an ideal gas to occupy 1.34 dm^3 at a pressure of 200 kPa if it occupies 756 cm^3 at STP?

$$P_1 = 200\text{ kPa}$$

$$P_2 = 100\text{ kPa}$$

$$V_1 = 1.34\text{ dm}^3$$

$$V_2 = 756\text{ cm}^3, \text{ i.e. } \frac{756}{1000}\text{ dm}^3 \text{ or } 0.756\text{ dm}^3$$

The units of P_1 are the same as those of P_2 .

$$T_1 = ?$$

$$T_2 = 273\text{ K}$$

$$\frac{200 \times 1.34}{T_1} = \frac{100 \times 0.756}{273}$$

The units of V_1 and V_2 were made consistent with each other. We could have also changed V_1 to cm^3 .

Rearranging the equation:

$$200 \times 1.34 \times 273 = 100 \times 0.756 \times T_1$$

$$T_1 = \frac{200 \times 1.34 \times 273}{100 \times 0.756} = 968\text{ K}$$

This must now be converted to $^{\circ}\text{C}$ by subtracting 273.

$$\text{Temperature} = 968 - 273 = 695^{\circ}\text{C}$$

The temperature must be 695°C for the gas to occupy a volume of 1.34 dm^3 .

The ideal gas equation

If the relationships between P , V and T are combined with Avogadro's law, the ideal gas equation is obtained:

$$PV = nRT$$

Where R is the **gas constant** and n is the number of moles. Although R is a universal constant, it can be quoted with various units and its value depends on these units. The SI units for the gas constant are $\text{J K}^{-1} \text{mol}^{-1}$, and this requires the following set of units:

$R = 8.31 \text{ J K}^{-1} \text{mol}^{-1}$
Pressure: N m^{-2} or Pa
Volume: m^3
Temperature: K

A consistent set of units must be used.

Exam tip

A set of units that is equivalent to this uses volume in dm^3 and pressure in kPa – if you use these units you can avoid the problem of converting volumes into m^3 .



SI stands for *Système International d'Unités* and refers to the internationally accepted system of units used in science.

$$1\,000\,000 \text{ cm}^3 \Leftrightarrow 1 \text{ m}^3$$

$$1000 \text{ dm}^3 \Leftrightarrow 1 \text{ m}^3$$

To convert m^3 to cm^3 multiply by 1 000 000.
 To convert cm^3 to m^3 divide by 1 000 000.
 To convert m^3 to dm^3 multiply by 1000.
 To convert dm^3 to m^3 divide by 1000.

Worked examples

1.30 An ideal gas occupies 590 cm^3 at 120°C and 202 kPa . What amount of gas (in moles) is present?

If we use the value of $8.31 \text{ J K}^{-1} \text{mol}^{-1}$ for the gas constant, all values must be converted to the appropriate set of units:

$$P = 202 \text{ kPa} = 2.02 \times 10^5 \text{ Pa}$$

$$V = 590 \text{ cm}^3 = \frac{590}{1\,000\,000} \text{ m}^3 = 5.90 \times 10^{-4} \text{ m}^3$$

$$n = ?$$

$$R = 8.31 \text{ J K}^{-1} \text{mol}^{-1}$$

$$T = 120^\circ\text{C} = 120 + 273 \text{ K} = 393 \text{ K}$$

$$PV = nRT$$

$$2.02 \times 10^5 \times 5.90 \times 10^{-4} = n \times 8.31 \times 393$$

Rearranging the equation:

$$n = \frac{2.02 \times 10^5 \times 5.90 \times 10^{-4}}{8.31 \times 393} = 0.0365 \text{ mol}$$

The number of moles is 0.0365 mol .

1.31 A gas has a density of 1.24 g dm^{-3} at 0°C and $1.00 \times 10^5 \text{ Pa}$. Calculate its molar mass.

$$\text{density} = \frac{\text{mass}}{\text{volume}}$$

We know the density, so we know the mass of 1 dm^3 of the gas. If we can find the number of moles in 1 dm^3 , we can work out the molar mass.

$$P = 1.00 \times 10^5 \text{ Pa}$$

$$V = 1.00 \text{ dm}^3 = \frac{1.00}{1000} \text{ m}^3 = 1.00 \times 10^{-3} \text{ m}^3$$

$$n = ?$$

$$R = 8.31 \text{ J K}^{-1} \text{mol}^{-1}$$

$$T = 0^\circ\text{C} = 273 \text{ K}$$

Using $PV = nRT$

$$n = \frac{1.00 \times 10^5 \times 1.00 \times 10^{-3}}{8.31 \times 273} = 0.0441 \text{ mol}$$

This number of moles has a mass of 1.24 g .

$$\text{molar mass} = \frac{\text{mass}}{\text{number of moles}}$$

$$\text{molar mass} = \frac{1.24}{0.0441} = 28.1 \text{ g mol}^{-1}$$

1.32 What is the molar volume of an ideal gas at 18°C and $1.10 \times 10^5 \text{ Pa}$? (Give your answer in $\text{m}^3 \text{mol}^{-1}$ and $\text{dm}^3 \text{mol}^{-1}$.)

The molar volume of a gas is the volume occupied by one mole of the gas. We are familiar with the value for the molar volume of a gas at STP, which is $22.7 \text{ dm}^3 \text{mol}^{-1}$.

$$P = 1.10 \times 10^5 \text{ Pa}$$

$$V = ?$$

$$n = 1.00 \text{ mol}$$

$$R = 8.31 \text{ J K}^{-1} \text{mol}^{-1}$$

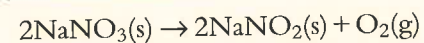
$$T = 18^\circ\text{C} = 18 + 273 \text{ K} = 291 \text{ K}$$

Using $PV = nRT$:

$$V = \frac{1.00 \times 8.31 \times 291}{1.10 \times 10^5} = 0.0220 \text{ m}^3$$

The molar volume is $0.0220 \text{ m}^3 \text{mol}^{-1}$ at 18°C and $1.10 \times 10^5 \text{ Pa}$. This must be multiplied by 1000 to convert to dm^3 i.e., $22.0 \text{ dm}^3 \text{mol}^{-1}$.

1.33 When sodium nitrate(V) (often just called sodium nitrate) is heated, it decomposes to give sodium nitrate(III) (also called sodium nitrite) and oxygen gas. When a certain mass of sodium nitrate(V) is heated, 241 cm³ of oxygen is obtained, measured at 97.0 kPa and 22 °C. Calculate the mass of sodium nitrate(III) formed.



We can use $PV = nRT$ to work out the number of moles of O₂:

$$P = 97.0 \text{ kPa} = 9.70 \times 10^4 \text{ Pa}$$

$$V = 241 \text{ cm}^3 = \frac{241}{1\,000\,000} \text{ m}^3 = 2.41 \times 10^{-4} \text{ m}^3$$

$$n = ?$$

$$R = 8.31 \text{ J K}^{-1} \text{ mol}^{-1}$$

$$T = 22^\circ\text{C} = 295 \text{ K}$$

$$\text{Using } PV = nRT: n = \frac{9.70 \times 10^4 \times 2.41 \times 10^{-4}}{8.31 \times 295} = 9.54 \times 10^{-3} \text{ mol}$$

This gives the number of moles of O₂.

From the chemical equation, the number of moles of O₂ is half the number of moles of NaNO₂. Therefore, the number of moles of NaNO₂ is $9.54 \times 10^{-3} \times 2 = 1.91 \times 10^{-2} \text{ mol}$.

The molar mass of NaNO₂ is 69.00 g mol⁻¹, so the mass of NaNO₂ is $69.00 \times 1.91 \times 10^{-2} = 1.32 \text{ g}$.



You would probably say that the room you are sitting in at the moment is full of air. If, however, you do a quick calculation (making a couple of approximations) you should be able to work out that the volume of the molecules of gas in the room is only about 0.01% of the volume of

the room – scientific reality is very different from our everyday reality. (There is actually a very small probability that all these molecules could at any one time all end up in the same corner of the room – our survival depends on the fact that this probability is very small!)

Nature of science

A scientific law is a general statement (often in mathematical form) based on observation/experiment of some aspect of the physical world. It will often involve the relationship between various quantities under specified conditions. For example, Boyle's law describes the relationship between the volume and pressure of a fixed mass of an ideal gas at constant temperature. A law does not explain anything – it is just a description of what happens.

A theory is a way of explaining scientific observations or laws. To be accepted, a theory will have been rigorously tested by experiments and observations – for example the particle theories and kinetic theory can be used to explain Boyle's law.

There is no progression from a theory to a law – they are different things.

Avogadro's original hypothesis was that equal volumes of different gases contain the same number of molecules. This was based on deductions from careful measurements and observations made by other scientists such as Gay-Lussac.

? Test yourself

In all questions, take the value of the ideal gas constant as $8.31 \text{ J K}^{-1} \text{ mol}^{-1}$.

- 33** If a certain mass of an ideal gas occupies 20.0 cm³ at 0 °C and $1.01 \times 10^5 \text{ Pa}$, what volume would it occupy at 38 °C and $1.06 \times 10^5 \text{ Pa}$?
- 34** A certain mass of an ideal gas occupies 250.0 cm³ at 20 °C and $9.89 \times 10^4 \text{ Pa}$. At what temperature (in °C) will it occupy 400.0 cm³ if the pressure remains the same?
- 35** How many moles of an ideal gas are present in a container if it occupies a volume of 1.50 dm³ at a pressure of $1.10 \times 10^5 \text{ Pa}$ and a temperature of 30 °C?
- 36** Calculate the molar mass of an ideal gas if 0.586 g of the gas occupies a volume of 282 cm³ at a pressure of $1.02 \times 10^5 \text{ Pa}$ and a temperature of -18 °C.
- 37** What is the molar volume of an ideal gas at $1.10 \times 10^5 \text{ Pa}$ and 100 °C?
- 38** Copper nitrate decomposes when heated according to the equation:

$$2\text{Cu}(\text{NO}_3)_2(\text{s}) \rightarrow 2\text{CuO}(\text{s}) + 4\text{NO}_2(\text{g}) + \text{O}_2(\text{g})$$
 If 1.80 g of copper nitrate is heated and the gases collected at a temperature of 22 °C and 105 kPa:
a what volume (in dm³) of oxygen is collected?
b what is the total volume of gas collected in cm³?
- 39** When a certain mass of manganese heptoxide (Mn₂O₇) decomposed, it produced 127.8 cm³ of oxygen measured at 18 °C and $1.00 \times 10^5 \text{ Pa}$. What mass of manganese heptoxide decomposed?

$$2\text{Mn}_2\text{O}_7(\text{aq}) \rightarrow 4\text{MnO}_2(\text{s}) + 3\text{O}_2(\text{g})$$

1.3.3 Calculations involving solutions

Solutions

Solute: a substance that is dissolved in another substance.

Solvent: a substance that dissolves another substance (the solute).

The solvent should be present in excess of the solute.

Solution: the substance that is formed when a solute dissolves in a solvent.

When a sodium chloride (NaCl) **solution** is prepared, NaCl solid (the **solute**) is dissolved in water (the **solvent**).

Note: when a solute is dissolved in a certain volume of water, say 100.0 cm³, the total volume of the solution is not simply 100.0 cm³ or the sum of the volumes occupied by the solute and the volume of the solvent. The total volume of solution produced depends on the forces of attraction between the solute particles and the solvent particles compared with the forces of attraction in the original solvent. This is why concentration is defined in terms of the volume of the solution rather than the volume of the solvent.

Learning objective

- Solve problems involving solutions

Solutions in water are given the symbol (aq) in chemical equations. *aq* stands for *aqueous*.



Reported values for the concentration of gold in seawater vary greatly. A value of about $2 \times 10^{-11} \text{ g dm}^{-3}$ or $1 \times 10^{-13} \text{ mol dm}^{-3}$ is probably a reasonable estimate. The volume of water in the oceans is estimated to be about $1.3 \times 10^{21} \text{ dm}^3$, so there is an awful lot of gold in the oceans. Many people (including Nobel Prize-winning scientist Fritz Haber) have tried to come up with ways to extract the gold. The problem is that the concentrations are so low.

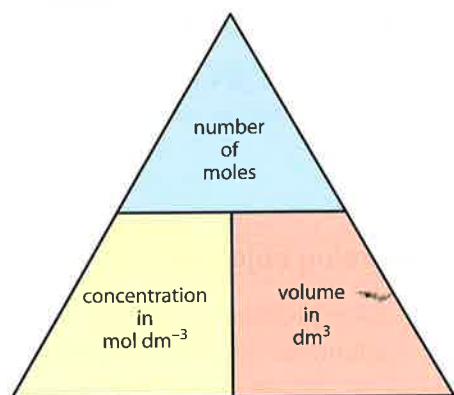


Figure 1.18 The relationship between concentration, number of moles and volume of solution.

Worked examples

1.34 If 10.00 g of sodium hydroxide (NaOH) is dissolved in water and the volume is made up to 200.0 cm^3 , calculate the concentration in mol dm^{-3} and g dm^{-3} .

Concentration (g dm^{-3})

$$\text{concentration in g dm}^{-3} = \frac{\text{mass}}{\text{volume in dm}^3}$$

$$\text{volume in dm}^3 = \frac{200.0}{1000} = 0.2000 \text{ dm}^3$$

$$\text{concentration} = \frac{10.00}{0.2000} = 50.00 \text{ g dm}^{-3}$$

The **concentration** of a solution is the amount of solute dissolved in a unit volume of **solution**. The volume that is usually taken is 1 dm^3 . The amount of solute may be expressed in g or mol therefore the units of concentration are g dm^{-3} or mol dm^{-3} .

Concentrations are sometimes written with the unit M, which means mol dm^{-3} but is described as 'molar'. Thus 2 M would refer to a '2 molar solution', i.e. a solution of concentration 2 mol dm^{-3} .

The relationship between concentration, number of moles and volume of solution is:

$$\text{concentration (mol dm}^{-3}\text{)} = \frac{\text{number of moles (mol)}}{\text{volume (dm}^3\text{)}}$$

This is summarised in Figure 1.18.

If the concentration is expressed in g dm^{-3} , the relationship is:

$$\text{concentration (g dm}^{-3}\text{)} = \frac{\text{mass (g)}}{\text{volume (dm}^3\text{)}}$$

Concentration (mol dm^{-3})

$$\text{molar mass of NaOH} = 40.00 \text{ g mol}^{-1}$$

$$\text{number of moles} = \frac{10.00}{40.00} = 0.2500 \text{ mol}$$

$$\text{concentration} = \frac{\text{number of moles}}{\text{volume in dm}^3}$$

$$\text{concentration} = \frac{0.2500}{0.2000} = 1.250 \text{ mol dm}^{-3}$$

Alternatively, once we have the concentration in g dm^{-3} we can simply divide by the molar mass to get the concentration in mol dm^{-3} :

$$\text{concentration} = \frac{50.00}{40.00} = 1.250 \text{ mol dm}^{-3}$$

1.35 Calculate the number of moles of hydrochloric acid (HCl) present in 50.0 cm^3 of 2.00 mol dm^{-3} hydrochloric acid.

$$\text{number of moles} = \text{concentration} \times \text{volume in dm}^3$$

$$\text{number of moles} = 2.00 \times \frac{50}{1000} = 0.100 \text{ mol}$$

Therefore the number of moles is 0.100 mol.

Square brackets are often used to denote concentrations in mol dm^{-3} . So $[\text{HCl}]$ indicates the molar concentration of hydrochloric acid and we could write $[\text{HCl}] = 2.00 \text{ mol dm}^{-3}$ in this worked example.

Concentrations of very dilute solutions

When dealing with very small concentrations, you will occasionally come across the unit *parts per million*, *ppm*. For instance, if 1 g of a solute is present in 1 million grams of a solution then the concentration is 1 ppm. So, in general, the concentration in ppm is given by:

$$\text{concentration in ppm} = \frac{\text{mass of solute} \times 10^6}{\text{mass of solution}}$$

The ppm notation is most often used when writing about pollution – e.g. *the concentration of arsenic in drinking water in the US should not exceed 0.010 ppm*.

The units of mass of solute and mass of solution must be the same so that they cancel.

Worked examples

1.36 If a sample of 252.10 g of water is found to contain 2.03 mg of cyanide, what is the cyanide concentration in ppm?

The mass in mg must first be converted to a mass in g by dividing by 1000:

$$\text{mass of cyanide} = 2.03 \times 10^{-3} \text{ g}$$

$$\text{concentration of cyanide in ppm} = \frac{2.03 \times 10^{-3} \times 10^6}{252.10} = 8.05 \text{ ppm}$$

Although the concentration in ppm is properly defined as above, it is often used in newspaper articles etc. in a slightly more convenient (but not completely correct) way as the mass of solute, in mg, per dm^3 (litre) of solution. This is a reasonable approximation because the mass of 1 dm^3 of water (which will make up most of the solution) is 1000 g – i.e. 1 000 000 mg. So if the copper concentration in a sample of tap water is 1.2 ppm, this is roughly equivalent to 1.2 mg of copper per dm^3 of water.



The companion units of parts per billion (ppb) and parts per trillion (ppt) are often used when discussing extremely low concentrations – these units can cause some confusion because the definitions of billion and trillion are different in different countries. It used to be that a billion in British English referred to 1×10^{12} but now the US definition of 1×10^9 is the commonly accepted value.

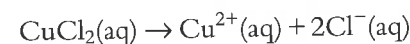
The ppm notation is also used when discussing the concentrations of various pollutant gases in air. In this case it is defined as:

$$\text{concentration in ppm} = \frac{\text{volume of gas} \times 10^6}{\text{volume of air}}$$

For instance, the carbon monoxide concentration in a sample of air might be 10 ppm. This indicates that there would be 10 dm³ of CO per 1 000 000 dm³ of air. At STP this would roughly convert to 12 g CO per million dm³ of air. So, in a classroom with dimensions of about 5 m × 4 m × 2 m, there would be approximately 0.5 g of carbon monoxide.

Working out the concentration of ions

When ionic substances (see page 119) dissolve in water, the substance breaks apart into its constituent ions. So, for instance, when copper(II) chloride (CuCl₂) dissolves in water, it splits apart into Cu²⁺ and Cl[−] ions:



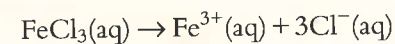
Therefore when 0.100 mol CuCl₂ dissolves in water, 2 × 0.100 mol (i.e. 0.200 mol) Cl[−] ions are produced. The concentration of the chloride ions is therefore twice the concentration of the CuCl₂.

Worked example

1.37 Calculate the number of moles of chloride ions present in 50.0 cm³ of a 0.0500 mol dm^{−3} solution of iron(III) chloride (FeCl₃) and the total concentration of all the ions present.

$$\text{number of moles} = \text{concentration} \times \text{volume in dm}^3$$

$$\text{number of moles of FeCl}_3 = \frac{50.0}{1000} \times 0.0500 = 2.50 \times 10^{-3} \text{ mol FeCl}_3$$



So dissolving 2.50×10^{-3} mol FeCl₃ produces $3 \times 2.50 \times 10^{-3}$ mol Cl[−](aq), i.e. 7.50×10^{-3} mol Cl[−](aq).

The number of moles of chloride ions present is 7.50×10^{-3} mol.

When one FeCl₃ unit dissolves in water, four ions are produced (Fe³⁺ + 3Cl[−])

So the total concentration of the ions present is four times the concentration of the FeCl₃, i.e. 4×0.0500 mol dm^{−3}.

The total concentration of ions present is 0.200 mol dm^{−3}.

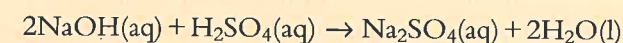
Titration

Titration is a technique for finding the volumes of solutions that react exactly with each other. One solution is added from a burette to the other solution in a conical flask (Figure 1.19). An indicator is often required to determine the end point of the titration.

In order for the technique to be used to determine the concentration of a particular solution, the concentration of one of the solutions it reacts with must be known accurately – this is a standard solution.

Worked example

1.38 Sulfuric acid (H₂SO₄) is titrated against 25.00 cm³ of 0.2000 mol dm^{−3} sodium hydroxide solution (NaOH). It is found that 23.20 cm³ of sulfuric acid is required for neutralisation. Calculate the concentration of the sulfuric acid.



Step 1 – work out the number of moles of NaOH:

$$\text{number of moles} = \text{concentration} \times \text{volume in dm}^3$$

$$\text{number of moles} = 0.2000 \times \frac{25.00}{1000} = 5.000 \times 10^{-3} \text{ mol}$$

Step 2 – the balanced equation tells us that 2 mol NaOH react with 1 mol H₂SO₄. Therefore 5.000×10^{-3} mol NaOH react with $\frac{5.000 \times 10^{-3}}{2}$ mol H₂SO₄, i.e. 2.500×10^{-3} mol H₂SO₄. This is the number of moles of H₂SO₄ in 23.20 cm³ of H₂SO₄.

Step 3 – convert number of moles to concentration:

$$\text{concentration} = \frac{\text{number of moles}}{\text{volume in dm}^3}$$

$$23.20 \text{ cm}^3 = \frac{23.20}{1000} \text{ dm}^3 = 0.02320 \text{ dm}^3$$

$$[\text{H}_2\text{SO}_4] = \frac{2.500 \times 10^{-3}}{0.02320} = 0.1078 \text{ mol dm}^{-3}$$

The concentration of the H₂SO₄ is 0.1078 mol dm^{−3}.

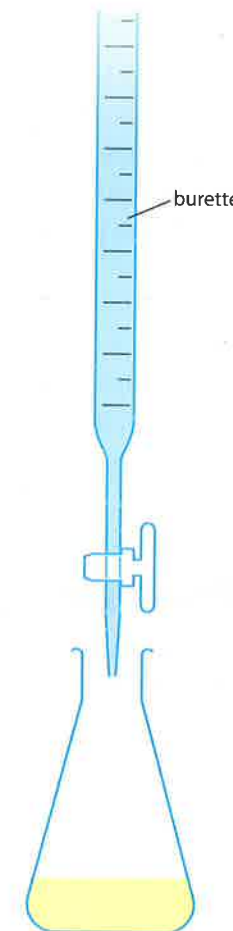


Figure 1.19 Titration set-up.

A standard solution can be made up from a solid (primary standard). A certain mass of the solute is weighed out accurately and then dissolved in a small amount of distilled water in a beaker. This solution is then transferred to a volumetric flask (washing out the beaker with several lots of distilled water to ensure that all the solute is transferred). Finally, water is added to make the solution up to the mark so that the total volume of the solution is known.

Alternatively, the concentration of a standard solution may be known because it has been titrated against another standard solution.

Exam tip

This equation is useful for solving titration problems in the multiple-choice paper.

Equation for solving moles questions involving solutions

The following equation may be used as an alternative method for solving problems:

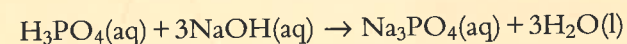
$$\frac{c_1 v_1}{n_1} = \frac{c_2 v_2}{n_2}$$

where:

- c_1 = concentration of first substance
- v_1 = volume of first substance
- n_1 = coefficient of first substance
- c_2 = concentration of second substance
- v_2 = volume of second substance
- n_2 = coefficient of second substance

Worked example

1.39 For neutralisation, 25.00 cm³ of phosphoric(V) acid (H₃PO₄) requires 28.70 cm³ of sodium hydroxide (NaOH) of concentration 0.1500 mol dm⁻³. What is the concentration of the phosphoric(V) acid?



Let H₃PO₄ be substance 1 and NaOH be substance 2.

$$\begin{array}{ll} c_1 = ? & c_2 = 0.1500 \text{ mol dm}^{-3} \\ v_1 = 25.00 \text{ cm}^3 & v_2 = 28.70 \text{ cm}^3 \\ n_1 = 1 & n_2 = 3 \end{array}$$

$$\frac{c_1 v_1}{n_1} = \frac{c_2 v_2}{n_2}$$

There is no need to convert the volume to dm³ when this equation is used so we can use the volume in cm³ directly.

$$\frac{c_1 \times 25.00}{1} = \frac{0.1500 \times 28.70}{3}$$

$$\text{Rearranging the equation: } c_1 = \frac{1 \times 0.1500 \times 28.70}{3 \times 25.00} = 0.05740 \text{ mol dm}^{-3}$$

The concentration of H₃PO₄ is 0.05740 mol dm⁻³.

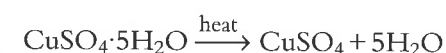
? Test yourself

- 40 a** What mass of sodium sulfate (Na₂SO₄) must be used to make up 250 cm³ of a 0.100 mol dm⁻³ solution?
- b** What is the concentration of sodium ions in the solution in **a**?
- 41** Work out the numbers of moles of solute present in the following solutions:
- a** 20.0 cm³ of 0.220 mol dm⁻³ NaOH(aq)
 - b** 27.8 cm³ of 0.0840 mol dm⁻³ HCl(aq)
 - c** 540 cm³ of 0.0200 mol dm⁻³ KMnO₄(aq)
- 42** If 29.70 cm³ of sulfuric acid of concentration 0.2000 mol dm⁻³ is required for neutralisation of 25.00 cm³ of potassium hydroxide solution, calculate the concentration of the potassium hydroxide solution.
- $$2\text{KOH}(\text{aq}) + \text{H}_2\text{SO}_4(\text{aq}) \rightarrow \text{K}_2\text{SO}_4(\text{aq}) + 2\text{H}_2\text{O}(\text{l})$$
- 43** Calcium carbonate is reacted with 50.0 cm³ of 0.500 mol dm⁻³ hydrochloric acid.
- $$\text{CaCO}_3(\text{s}) + 2\text{HCl}(\text{aq}) \rightarrow \text{CaCl}_2(\text{aq}) + \text{CO}_2(\text{g}) + \text{H}_2\text{O}(\text{l})$$
- a** What mass of calcium carbonate is required for an exact reaction?
 - b** What volume of carbon dioxide, measured at STP, will be produced?
- 44** What volume (in cm³) of 0.0100 mol dm⁻³ barium chloride must be reacted with excess sodium sulfate to produce 0.100 g of barium sulfate?
- $$\text{BaCl}_2(\text{aq}) + \text{Na}_2\text{SO}_4(\text{aq}) \rightarrow \text{BaSO}_4(\text{s}) + 2\text{NaCl}(\text{aq})$$
- 45** If 0.100 g of magnesium is reacted with 25.00 cm³ of 0.200 mol dm⁻³ hydrochloric acid, calculate the volume of hydrogen gas produced at STP.
- $$\text{Mg}(\text{s}) + 2\text{HCl}(\text{aq}) \rightarrow \text{MgCl}_2(\text{aq}) + \text{H}_2(\text{g})$$

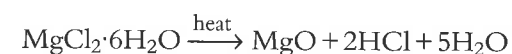
Water of crystallisation

Some substances crystallise with water as an integral part of the crystal lattice. Examples are hydrated copper sulfate (CuSO₄·5H₂O) and hydrated magnesium chloride (MgCl₂·6H₂O). The water is necessary for the formation of the crystals and is called **water of crystallisation**. Substances that contain water of crystallisation are described as hydrated, whereas those that have lost their water of crystallisation are described as anhydrous. So, we talk about 'hydrated copper sulfate' (CuSO₄·5H₂O) and 'anhydrous copper sulfate' (CuSO₄). Hydrated copper sulfate can be obtained as large blue crystals, but anhydrous copper sulfate is white and powdery.

In the case of CuSO₄·5H₂O, the water can be removed by heating:



However, this is not always the case. When MgCl₂·6H₂O is heated, magnesium oxide (MgO) is formed:



Worked examples

1.40 When 2.56 g of hydrated magnesium sulfate ($\text{MgSO}_4 \cdot x\text{H}_2\text{O}$) is heated, 1.25 g of anhydrous magnesium sulfate (MgSO_4) is formed. Determine the value of x in the formula.

mass of water given off = $2.56 - 1.25$, i.e. 1.31 g

mass of $\text{MgSO}_4 = 1.25$ g

This is now basically just an empirical formula question, and we need to find the ratio between the numbers of moles of MgSO_4 and H_2O .

molar mass of $\text{H}_2\text{O} = 18.02 \text{ g mol}^{-1}$

molar mass of $\text{MgSO}_4 = 120.38 \text{ g mol}^{-1}$

number of moles of $\text{H}_2\text{O} = \frac{1.31}{18.02} = 0.0727 \text{ mol}$

number of moles of $\text{MgSO}_4 = \frac{1.25}{120.38} = 0.0104 \text{ mol}$

Divide by the smaller number to get the ratio:

$$\frac{0.0727}{0.0104} = 7$$

The value of x is 7, and the formula of hydrated magnesium sulfate is $\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$.

1.41 a If 10.00 g of hydrated copper sulfate ($\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$) are dissolved in water and made up to a volume of 250.0 cm^3 , what is the concentration of the solution?

b What mass of anhydrous copper sulfate would be required to make 250.0 cm^3 of solution with the same concentration as in **a**?

a molar mass of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O} = 249.72 \text{ g mol}^{-1}$

number of moles $\text{CuSO}_4 \cdot 5\text{H}_2\text{O} = \frac{10.00}{249.72} = 0.04004 \text{ mol}$

concentration = $\frac{\text{number of moles}}{\text{volume in dm}^3} = \frac{0.04004}{0.2500} = 0.1602 \text{ mol dm}^{-3}$

So dissolving 10.00 g of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ in water and making up the solution to 250.0 cm^3 produces a CuSO_4 solution of concentration $0.1602 \text{ mol dm}^{-3}$.

b The number of moles of CuSO_4 present in 250.0 cm^3 solution will be exactly the same as above, i.e. 0.04004 mol because the concentration is the same.

molar mass of $\text{CuSO}_4 = 159.62 \text{ g mol}^{-1}$

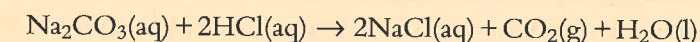
mass of $\text{CuSO}_4 = \text{molar mass} \times \text{number of moles} = 159.62 \times 0.04004 = 6.391 \text{ g}$

The mass of CuSO_4 required to make 250 cm^3 of a solution of concentration $0.1602 \text{ mol dm}^{-3}$ is 6.391 g, as opposed to 10.00 g of $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$. The two solutions will be identical.

When a hydrated salt is dissolved in water, the water of crystallisation just becomes part of the solvent, and the solution is the same as if the anhydrous salt were dissolved in water.

$0.04004 \text{ mol CuSO}_4 \cdot 5\text{H}_2\text{O}$
contains $0.04004 \text{ mol CuSO}_4$

1.42 A 3.92 g sample of hydrated sodium carbonate ($\text{Na}_2\text{CO}_3 \cdot x\text{H}_2\text{O}$) was dissolved in water and made up to a total volume of 250.0 cm^3 . Of this solution, 25.00 cm^3 was titrated against $0.100 \text{ mol dm}^{-3}$ hydrochloric acid, and 27.40 cm^3 of the acid was required for neutralisation. Calculate the value of x in $\text{Na}_2\text{CO}_3 \cdot x\text{H}_2\text{O}$.



Step 1 – work out the number of moles of HCl:

number of moles = concentration \times volume in dm^3

number of moles = $0.100 \times \frac{27.40}{1000} = 2.74 \times 10^{-3} \text{ mol}$

Step 2 – the balanced equation tells us that 2 mol HCl react with 1 mol Na_2CO_3 . Therefore $2.74 \times 10^{-3} \text{ mol HCl}$ react with $\frac{2.74 \times 10^{-3}}{2} = 1.37 \times 10^{-3} \text{ mol Na}_2\text{CO}_3$. This is the number of moles of Na_2CO_3 in 25.00 cm^3 .

The original mass of $\text{Na}_2\text{CO}_3 \cdot x\text{H}_2\text{O}$ was dissolved in a total volume of 250.0 cm^3 . Therefore the number of moles of Na_2CO_3 in 250.0 cm^3 of solution is $1.37 \times 10^{-3} \times 10$, i.e. $1.37 \times 10^{-2} \text{ mol}$.

Step 3 – convert number of moles to mass:

molar mass of $\text{Na}_2\text{CO}_3 = 105.99 \text{ g mol}^{-1}$

mass of $1.37 \times 10^{-2} \text{ mol Na}_2\text{CO}_3 = \text{number of moles} \times \text{molar mass}$

mass of $\text{Na}_2\text{CO}_3 = 1.37 \times 10^{-2} \times 105.99 = 1.45 \text{ g}$

The total mass of $\text{Na}_2\text{CO}_3 \cdot x\text{H}_2\text{O} = 3.92 \text{ g}$.

The mass of this that is due to the water of crystallisation = $3.92 - 1.45 = 2.47 \text{ g}$.

number of moles of water of crystallisation = $\frac{\text{mass}}{\text{molar mass}} = \frac{2.47}{18.02} = 0.137 \text{ mol}$

The ratio moles of water of crystallisation: moles of sodium carbonate can be worked out by dividing the number of moles of water by the number of moles of sodium carbonate:

ratio = $\frac{0.137}{1.37 \times 10^{-2}} = 10$

The value of x is 10, and the formula for the hydrated sodium carbonate is $\text{Na}_2\text{CO}_3 \cdot 10\text{H}_2\text{O}$.

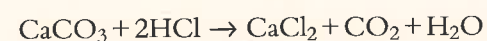
Back titration

This is a technique by which a known excess of a particular reagent, A, is added to another substance, X, so that they react. Then the excess A is titrated against another reagent to work out how much A reacted with the substance – and therefore how many moles of X were present. This is useful when X is an impure substance.

Worked example

1.43 Limestone is impure calcium carbonate (CaCO_3). 2.00 g of limestone is put into a beaker and 60.00 cm^3 of $3.000 \text{ mol dm}^{-3}$ hydrochloric acid (HCl) is added. They are left to react and then the impurities are filtered off and the solution is made up to a total volume of 100.0 cm^3 . Of this solution, 25.00 cm^3 require 35.50 cm^3 of $1.000 \text{ mol dm}^{-3}$ sodium hydroxide (NaOH) for neutralisation. Work out the percentage calcium carbonate in the limestone (assume that none of the impurities reacts with hydrochloric acid).

Let us consider the first part of the question: '2.00 g of limestone is put into a beaker and 60.00 cm³ of 3.000 mol dm⁻³ hydrochloric acid is added':



The limestone is impure, so we cannot work out the number of moles of CaCO_3 present, but we do have enough information to work out the number of moles of HCl :

number of moles of HCl = concentration \times volume in dm^3

$$\text{number of moles of HCl} = 3.000 \times \frac{60.00}{1000} = 0.1800 \text{ mol}$$

If the limestone were pure CaCO_3 , the number of moles present in 2.00 g would be 0.0200 mol, which would react with 0.0400 mol HCl.

This is excess HCl, and when the limestone is reacted with it there will be some HCl left over.

The second part of the question is: 'They are left to react and then . . . the solution is made up to a total volume of 100.0 cm³'.

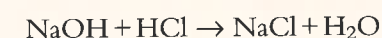
This 100.0 cm³ of solution now contains the HCl left over after the reaction with the CaCO₃.

In order to work out the number of moles of HCl that did not react, we must consider the third part of the question: 'Of this solution, 25.00 cm³ require 35.50 cm³ of 1.000 mol dm⁻³ sodium hydroxide for neutralisation':

number of moles of NaOH = concentration \times volume in dm^3

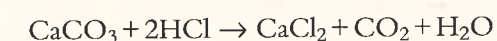
$$\text{number of moles of NaOH} = 1.000 \times \frac{35.50}{1000} = 0.03550 \text{ mol}$$

This reacts with HCl according to the equation:



Therefore 0.03550 mol NaOH react with 0.03550 mol HCl. This means that 25.00 cm³ of the HCl solution contained 0.03550 mol HCl. Therefore in 100.0 cm³ of this solution there were 4×0.03550 , i.e. 0.1420 mol HCl. This is the number of moles of HCl left over after it has reacted with the CaCO₃.

Because 0.1800 mol HCl was originally added to the limestone, the amount that reacted with the CaCO_3 was $0.1800 - 0.1420$, i.e. 0.0380 mol.



0.0380 mol HCl reacts with $\frac{0.0380}{2}$, i.e. 0.0190, mol CaCO_3

$$\text{molar mass of CaCO}_3 = 100.09 \text{ g mol}^{-1}$$

$$\text{mass of CaCO}_3 = \text{number of moles} \times \text{molar mass} = 100.09 \times 0.0190 = 1.90 \text{ g}$$

$$\% \text{CaCO}_3 \text{ in the limestone} = \frac{1.90}{2.00} \times 100 = 95.1\%$$

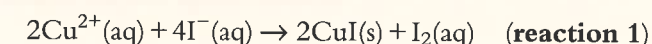
Linked reactions

Sometimes the product of one reaction becomes the reactant in a second reaction. A common example of this is the determination of the concentration of copper ions in solution using sodium thiosulfate.

Worked example

1.44 A 25.0 cm³ sample of a solution of copper(II) nitrate is added to 10.0 cm³ of 1 mol dm⁻³ potassium iodide. The iodine produced is titrated against 0.0200 mol dm⁻³ sodium thiosulfate solution using starch indicator near the end point. 22.50 cm³ of the sodium thiosulfate solution was required for the titration. Calculate the concentration of the copper(II) nitrate solution.

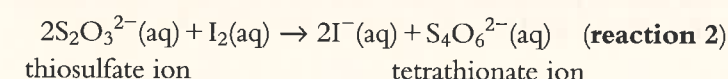
The initial reaction of copper(II) ions with iodide ions is:



This is a redox titration and these will be considered again in Topic 9.

A large excess of iodide ions is added to make sure that all the copper ions react. A precipitate of CuI is formed as well as the iodine. If we can determine the number of moles of iodine produced in the solution, we can also find the number of moles of copper ions.

The amount of iodine is determined by titration with sodium thiosulfate solution:



The number of moles of thiosulfate in 22.50 cm^3 of $0.0200 \text{ mol dm}^{-3}$ solution:

$$\text{number of moles} = \text{volume in dm}^3 \times \text{concentration} = \frac{22.50}{1000} \times 0.0200 = 4.50 \times 10^{-4} \text{ mol S}_2\text{O}_3^{2-}$$

From reaction 2 we can see that 2 mol $\text{S}_2\text{O}_3^{2-}$ react with 1 mol I_2 . Therefore 4.50×10^{-4} mol $\text{S}_2\text{O}_3^{2-}$ react with $\frac{4.50 \times 10^{-4}}{2}$ mol I_2 , i.e. 2.25×10^{-4} mol I_2 . This is the amount of iodine produced in reaction 1.

From reaction 1, 2 mol Cu^{2+} produce 1 mol I_2 , so the number of moles of Cu^{2+} is twice the number of moles of I_2 . Therefore the number of moles of Cu^{2+} is $2 \times 2.25 \times 10^{-4}$, i.e. 4.50×10^{-4} mol.

From reaction 1, 2 mol Cu^{2+} react to form 1 mol I_2 . In reaction 2, 1 mol I_2 reacts with 2 mol $\text{S}_2\text{O}_3^{2-}$. Therefore, overall, the number of moles of Cu^{2+} is equivalent to the number of moles of $\text{S}_2\text{O}_3^{2-}$.

The volume of the solution containing Cu^{2+} ions was 25.0 cm^3 , and this allows us to work out the concentration:

$$\text{concentration} = \frac{\text{number of moles}}{\text{volume in dm}^3} = \frac{4.50 \times 10^{-4}}{0.0250} = 0.0180 \text{ mol dm}^{-3}$$

Therefore the concentration of the copper(II) nitrate solution was $0.0180 \text{ mol dm}^{-3}$.

More examples of question types

Some questions can look very difficult at first sight, but a good place to start is to work out the number of moles of whatever you can and see where you can go from there.

Worked examples

1.45 A solution of a chloride of formula MCl_x (concentration $0.0170 \text{ mol dm}^{-3}$) reacts with silver nitrate (AgNO_3) solution to precipitate silver chloride (AgCl). It is found that 25.0 cm^3 of $0.0110 \text{ mol dm}^{-3}$ silver nitrate solution reacts with 5.40 cm^3 of the chloride solution.

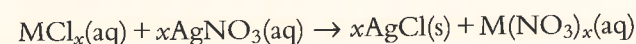
- Calculate the number of moles of silver nitrate.
- Calculate the number of moles of the chloride.
- Calculate the formula of the chloride.

a number of moles = concentration \times volume in dm^3

$$\text{number of moles of AgNO}_3 = \frac{25.0}{1000} \times 0.0110 = 2.75 \times 10^{-4} \text{ mol}$$

b number of moles of $\text{MCl}_x = \frac{5.40}{1000} \times 0.0170 = 9.18 \times 10^{-5} \text{ mol}$

c The general equation for the reaction is:

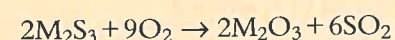


The silver ions in the solution react with the chloride ions to precipitate silver chloride. The ratio of the number of moles of AgNO_3 to the number of moles of MCl_x will give us the value of x .

$$\frac{\text{number of moles of AgNO}_3}{\text{number of moles of MCl}_x} = \frac{2.75 \times 10^{-4}}{9.18 \times 10^{-5}} = 3$$

Therefore the value of x is 3, and the formula of the chloride is MCl_3 .

1.46 One of the stages in the extraction of arsenic, antimony and bismuth from their ores involves the roasting of the sulfide in oxygen:



A certain mass of the sulfide reacted with 180.0 cm^3 of oxygen gas, measured at 15°C and 101 kPa pressure to produce 0.335 g of M_2O_3 . Determine the identity of the element M.

We can use $PV = nRT$ to work out the number of moles of oxygen. Substituting the values gives:

$$n = \frac{101000 \times 1.80 \times 10^{-4}}{8.31 \times 288} = 7.60 \times 10^{-3} \text{ mol}$$

We can now use the balanced chemical equation to work out the number of moles of M_2O_3 .

From the chemical equation, 9 mol O_2 react to form $2 \text{ mol M}_2\text{O}_3$. Therefore, the number of moles of M_2O_3 is two-ninths of the number of moles of O_2 :

$$\text{number of moles of M}_2\text{O}_3 = \frac{2}{9} \times 7.60 \times 10^{-3} = 1.69 \times 10^{-3} \text{ mol}$$

Now that we have the number of moles and the mass of M_2O_3 , we can work out the molar mass:

$$\text{molar mass} = \frac{\text{mass}}{\text{number of moles}} = \frac{0.335}{1.69 \times 10^{-3}} = 198 \text{ g mol}^{-1}$$

The formula of the compound is M_2O_3 , and its molar mass is 198 g mol^{-1} . The relative atomic mass of M can be worked out by taking away three times the relative atomic mass of O and then dividing the answer by two:

$$\text{mass of M}_2 = 198 - (3 \times 16) = 150$$

$$\text{relative atomic mass of M} = \frac{150}{2} = 75$$

This value is closest to the relative atomic mass of arsenic (74.92) therefore the element M is arsenic.

Exam-style questions

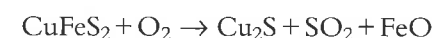
1 What is the total number of atoms in 1.80 g of water?

- A 6.02×10^{22} B 6.02×10^{23} C 1.80×10^{23} D 1.80×10^{24}

2 88 kg of carbon dioxide contains:

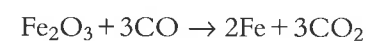
- A 2.0 mol B 2000 mol C 0.50 mol D 3872 mol

3 What is the sum of the coefficients when the following equation is balanced with the smallest possible whole numbers?



- A 7 B 8 C 11 D 12

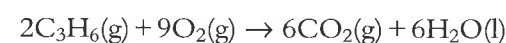
4 Iron(III) oxide reacts with carbon monoxide according to the equation:



How many moles of iron are produced when 180 mol carbon monoxide react with excess iron(III) oxide?

- A 120 mol B 180 mol C 270 mol D 360 mol

5 Propene undergoes complete combustion to produce carbon dioxide and water.



What volume of carbon dioxide is produced when 360 cm^3 of propene react with 360 cm^3 of oxygen at 273 K and 100 kPa pressure?

- A 120 cm^3 B 240 cm^3 C 540 cm^3 D 1080 cm^3

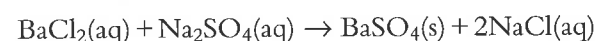
6 What mass of $\text{Na}_2\text{S}_2\text{O}_3 \cdot 5\text{H}_2\text{O}$ must be used to make up 200 cm^3 of a $0.100 \text{ mol dm}^{-3}$ solution?

- A 3.16 g B 4.96 g C 24.8 g D 31.6 g

- 7 20.00 cm³ of potassium hydroxide (KOH) is exactly neutralised by 26.80 cm³ of 0.100 mol dm⁻³ sulfuric acid (H₂SO₄). The concentration of the potassium hydroxide is:

A 0.0670 mol dm⁻³ C 0.268 mol dm⁻³
B 0.134 mol dm⁻³ D 1.34 mol dm⁻³

- 8 Barium chloride solution reacts with sodium sulfate solution according to the equation:



When excess barium chloride solution is reacted with 25.00 cm³ of sodium sulfate solution, 0.2334 g of barium sulfate (molar mass 233.40 g mol⁻¹) is precipitated.

The concentration of sodium ions in the sodium sulfate solution was:

A 0.08000 mol dm⁻³ C 0.001000 mol dm⁻³
B 0.04000 mol dm⁻³ D 0.002000 mol dm⁻³

- 9 When potassium chlorate(V) (molar mass 122.6 g mol⁻¹) is heated, oxygen gas (molar mass 32.0 g mol⁻¹) is produced:



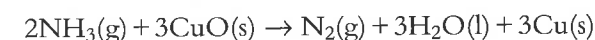
When 1.226 g of potassium chlorate(V) are heated, 0.320 g of oxygen gas are obtained. The percentage yield of oxygen is:

A 100% B 66.7% C 26.1% D 17.4%

- 10 Elemental analysis of a nitrogen oxide shows that it contains 2.8 g of nitrogen and 8.0 g of oxygen. The empirical formula of this oxide is:

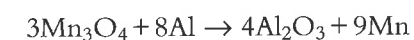
A NO B NO₂ C N₂O₃ D N₂O₅

- 11 Nitrogen can be prepared in the laboratory by the following reaction:



If 227 cm³ of ammonia, when reacted with excess copper oxide, produce 85 cm³ of nitrogen, calculate the percentage yield of nitrogen. All gas volumes are measured at STP. [3]

- 12 Manganese can be extracted from its ore, hausmannite, by heating with aluminium.



- a 100.0 kg of Mn₃O₄ are heated with 100.0 kg of aluminium. Work out the maximum mass of manganese that can be obtained from this reaction. [4]
b 1.23 tonnes of ore are processed and 200.0 kg of manganese obtained. Calculate the percentage by mass of Mn₃O₄ in the ore. [3]

- 13 A hydrocarbon contains 88.8% C. 0.201 g of the hydrocarbon occupied a volume of 98.9 cm³ at 320 K and 1.00 × 10⁵ Pa.

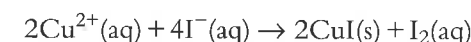
- a Determine the empirical formula of the hydrocarbon. [3]
b Determine the molecular formula of the hydrocarbon. [3]

- 14 Limestone is impure calcium carbonate. A 1.20 g sample of limestone is added to excess dilute hydrochloric acid and the gas collected; 258 cm³ of carbon dioxide were collected at a temperature of 27 °C and a pressure of 1.10 × 10⁵ Pa.



- a Calculate the number of moles of gas collected. [3]
b Calculate the percentage purity of the limestone (assume that none of the impurities in the limestone react with hydrochloric acid to produce gaseous products). [3]

- 15 25.0 cm³ of 0.100 mol dm⁻³ copper(II) nitrate solution is added to 15.0 cm³ of 0.500 mol dm⁻³ potassium iodide. The ionic equation for the reaction that occurs is:



- a Determine which reactant is present in excess. [3]
b Determine the mass of iodine produced. [3]

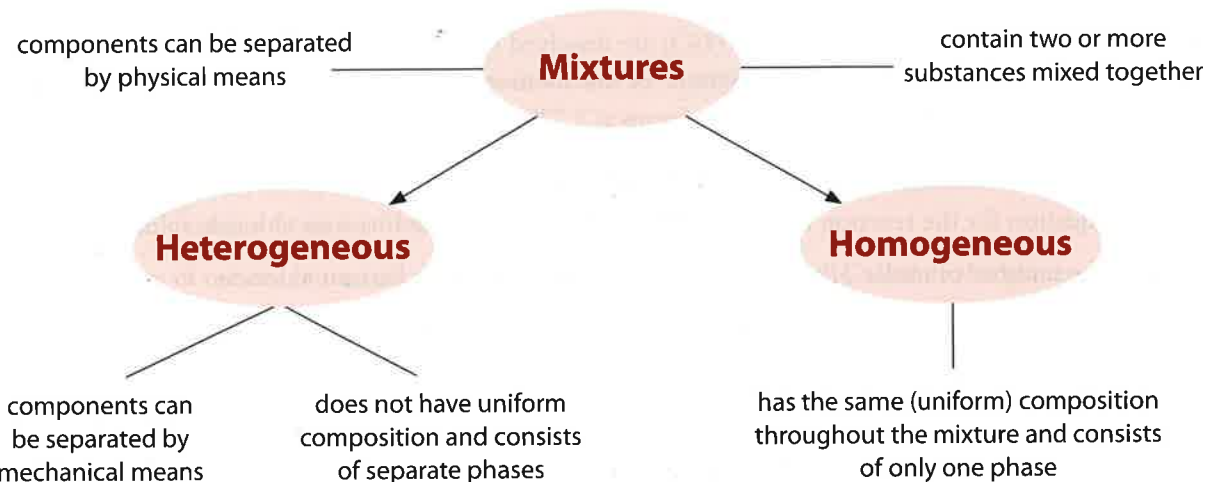
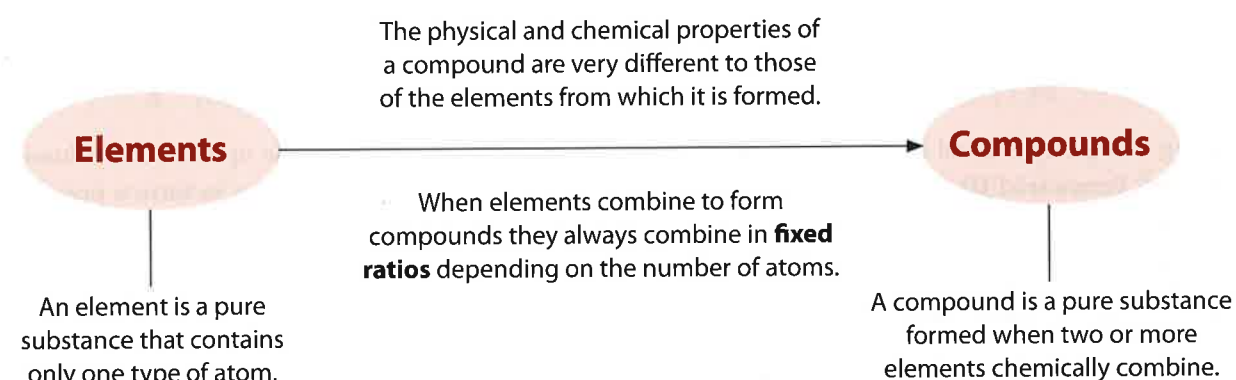
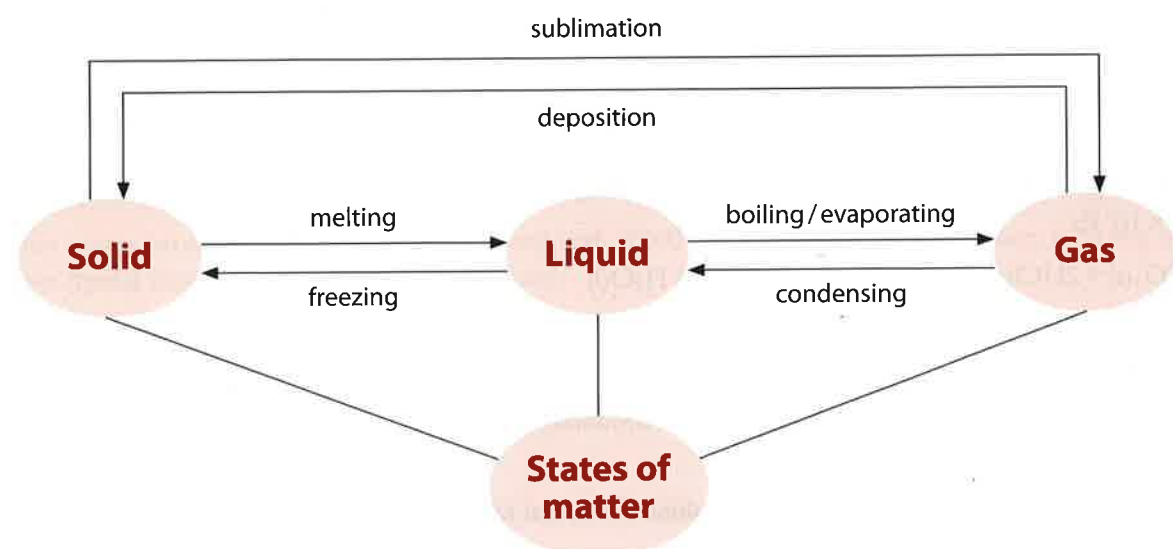
- 16 0.0810 g of a group 2 metal iodide, MI₂, was dissolved in water and the solution made up to a total volume of 25.00 cm³. Excess lead(II) nitrate solution (Pb(NO₃)₂(aq)) was added to the MI₂ solution to form a precipitate of lead(II) iodide (PbI₂). The precipitate was dried and weighed and it was found that 0.1270 g of precipitate was obtained.

- a Determine the number of moles of lead iodide formed. [2]
b Write an equation for the reaction that occurs. [1]
c Determine the number of moles of MI₂ that reacted. [1]
d Determine the identity of the metal, M. [3]

- 17 0.4000 g of hydrated copper sulfate (CuSO₄·xH₂O) are dissolved in the solution water and made up to a total volume of 100.0 cm³ with distilled water. 10.00 cm³ of this solution are reacted with excess barium chloride (BaCl₂) solution. The mass of barium sulfate that forms is 3.739 × 10⁻² g.

- a Calculate the number of moles of barium sulfate formed. [2]
b Write an equation for the reaction between copper sulfate solution and barium chloride solution. [1]
c Calculate the number of moles of copper sulfate that reacted with the barium chloride. [1]
d Calculate the number of moles of CuSO₄ in 0.4000 g of hydrated copper sulfate. [1]
e Determine the value of x. [3]

Summary



Real gases deviate most from ideal behaviour at low temperature and high pressure.

for ideal gases: $pV = nRT$ (T in kelvin)

$$\frac{P_1 V_1}{T_1} = \frac{P_2 V_2}{T_2}$$

molar volume of an ideal gas at STP = $22.7 \text{ dm}^3 \text{ mol}^{-1}$

$$\text{number of moles} = \frac{\text{volume}}{\text{molar volume}}$$

Avogadro's law: equal volumes of ideal gases at the same temperature and pressure contain the same number of molecules.

$$\frac{C_1 V_1}{n_1} = \frac{C_2 V_2}{n_2}$$

$$\text{concentration (mol dm}^{-3}\text{)} = \frac{\text{number of moles (mol)}}{\text{volume (dm}^3\text{)}}$$

$$\text{concentration (ppm)} = \frac{\text{mass of solute} \times 10^6}{\text{mass of solution}}$$

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

MOLES

Use the limiting reactant to determine the amount of products in a reaction.

To find the limiting reactant in a reaction, divide the number of moles of each reactant by its coefficient. The lowest number indicates the limiting reactant.

Moles calculations

- 1 Work out the number of moles of anything you can.
- 2 Use the chemical equation to work out the number of moles of the quantity you require.
- 3 Convert moles to the required quantity – volume, mass etc.

1 mol is the amount of substance which contains the same number of particles as there are carbon atoms in 12 g of ^{12}C .

Avogadro's constant (L) = $6.02 \times 10^{23} \text{ mol}^{-1}$

$$\text{number of moles} = \frac{\text{mass of substance}}{\text{molar mass}}$$

$$\text{molar mass} = M_r \text{ in g mol}^{-1}$$

$$\text{mass of 1 molecule} = \frac{\text{molar mass}}{\text{Avogadro's constant}}$$

Relative molecular mass (M_r): sum of all A_r values in a molecule.

Relative atomic mass (A_r): average of the masses of the isotopes in a naturally occurring sample of the element relative to $\frac{1}{12}$ mass of a ^{12}C atom.

Empirical formula: simplest whole number ratio of the elements present in a compound.

$$\% \text{ by mass of an element in a compound} = \frac{\text{number of atoms of the element} \times A_r}{M_r}$$

Molecular formula: total number of atoms of each element present in a molecule of the compound.