

Chemistry for the IB Diploma

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CAMBRIDGE UNIVERSITY PRESS

Cambridge, New York, Melbourne, Madrid, Cape Town, Singapore, São Paulo, Delhi, Mexico City

Cambridge University Press

The Edinburgh Building, Cambridge CB2 8RU, UK

www.cambridge.org

Information on this title: www.cambridge.org/9780521182942

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First published 2011 Reprinted 2012

Printed in Poland by Opolgraf

A catalogue record for this publication is available from the British Library

ISBN 978-0-521-18294-2 Paperback with CD-ROM for Windows and Mac

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The publisher would like to thank the following teachers for reviewing the content:

Aidan Hayes, King's College School, London

Ronald F. Owens, Kinston High School, North Carolina

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Introduction

This book is designed as a complete guide to the IB Chemistry courses at both SL and HL. The book contains all the material required for the main part of the SL and HL courses and the CD-ROM contains the full text of the book in PDF format as well as the Options material (required for Paper 3). Also included on the CD-ROM are a comprehensive guide to Internal Assessment (writing up practical work) and a revision checklist.

Chemistry is about understanding and not just recalling facts, and the emphasis throughout the book and CD-ROM is on explaining the concepts involved in the course. At this level Chemistry should make sense and, hopefully, as you work your way through each chapter you will feel confident that you have fully grasped all the material.

Each chapter is divided into sections which include assessment statements as starting and reference points. Short-answer questions appear throughout the text so you can check your progress and make sure that you have fully understood what has been discussed. There are also links to interactive questions on the CD-ROM, which you can use to further test yourself, as well as animations and simulations that will help you gain a deeper understanding of the concepts. You can link straight through to these features by clicking on the CD icons in the PDF version of the book.

Examination style questions appear at the end of each chapter; these could be used either when you have finished studying a chapter or towards the end of the course when you are preparing for the exams. Overall in the book and the CD-ROM there are well over 1000 questions, so there should be plenty of opportunities to practise all aspects of the course. Answers to all questions are given on the CD-ROM.

How to use this book

Sections that cover material from the Higher Level syllabus only are marked with an 'HL' bar:



As you read this book you will see that certain features are shown in different coloured boxes.

At the start of each section you will find a list of learning objectives, detailing what you will be expected to know after studying the section. The learning objectives are derived from the assessment statements in the syllabus.

Ions are charged particles, which are formed when atoms lose or gain electrons. Throughout the text, key fact boxes (left) inform you of key definitions and other facts that you should memorise, while info bars (right) give additional information on various subjects related to the text.

Theory of Knowledge (TOK) boxes are also found throughout the book. These provide food for thought and support the TOK you will studying in your IB Diploma programme.

Learning objectives

- Understand what is meant by hybridisation
- Predict the hybridisation of an atom in a molecule

Again, a consideration of the formal charges on each atom would regard this structure as less likely.

There are various theories of acids and bases. We have encountered the Brønsted–Lowry and Lewis theories.

As you read, you will also see 'test yourself' questions at various points in the text, usually at the end of a section. These will allow you to keep a check on your progress as you work through each chapter.

Test yourself

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

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

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

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

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

Throughout the text there are boxes that give information about the applications of chemistry, historical references, internationalism or interesting facts related to the topic under consideration.

It was originally thought that all acids contain oxygen, and the names of this element in English, german (Sauerstoff) and several other languages reflect this mistaken assumption.

The CD symbol indicates extra features that are included on the CD accompanying this book. These include animations, extra sets of questions, simulations and so forth.



Moles 1

1.1 Relative masses

Quantitative chemistry

Most chemical reactions involve two or more substances reacting with each other. Chemical 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 present in a specific amount of that substance. However, the mass of an individual atom or molecule is so small, and the number of particles that make up even a very small mass is so large, that a more convenient method of working out and discussing 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 an atom of **carbon-12**, which is assigned a mass of exactly **12.00**. As these quantities are **relative**, they have **no units**.

The $A_{\rm r}$ of silver is 107.87. A naturally occurring sample of silver contains the isotopes ¹⁰⁷Ag and ¹⁰⁹Ag. 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)

The $M_{\rm r}$ is the sum of the relative atomic masses for the individual atoms making up a molecule.

Examples

The relative molecular mass of methane (CH₄) 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 (CH₃COOH) is:

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

If the 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.

Learning objectives

• Define relative atomic mass and relative molecular mass

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

The A_r of C is not 12.00, because carbon contains isotopes other than carbon-12 (see page **56**).

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.

If the compound contains ions, the **relative formula mass** is the mass of the formula unit relative to the mass of $\frac{1}{12}$ of an atom of carbon-12.



Self-test 1

Test yourself

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

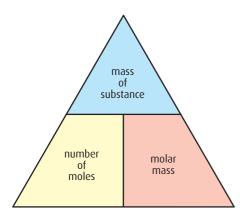
 SO_2 NH_3 C_2H_5OH $MgCl_2$ $Ca(NO_3)_2$ $CH_3(CH_2)_5CH_3$ PCl_5 $Mg_3(PO_4)_2$ $Na_2S_2O_3$ $CH_3CH_2CH_2COOCH_2CH_3$

Learning objectives

- 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 and the mass of a molecule

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

Note: when calculating the number of moles present in a mass of substance, the mass must be in grams.



1.2 The mole and Avogadro's constant

Moles

A 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** and has the value $6.02 \times 10^{23} \,\mathrm{mol}^{-1}$. It is sometimes given the symbol L (or N_{A}).

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

Thus $12.00 \,\mathrm{g}$ 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 $(6.02 \times 10^{23} \text{ atoms})$ or a mole of molecules $(6.02 \times 10^{23} \text{ molecules})$, but we could also have, for instance, a mole of ping-pong balls $(6.02 \times 10^{23} \text{ ping-pong balls})$.

The $A_{\rm r}$ of oxygen is 16.00, which means that, on average, each O atom is $\frac{16}{12}$ times as heavy as a carbon-12 atom. Therefore 16 g of O atoms must contain the same number of atoms as 12 g of carbon-12, i.e. 1 mole, or 6.02×10^{23} atoms. Similarly, a magnesium atom is on average $\frac{24.31}{12}$ times as heavy as a carbon-12 atom and, therefore 24.31 g of Mg atoms contains $6.02\times10^{23}\,{\rm Mg}$ atoms.

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

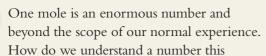
no. moles (n) =
$$\frac{\text{mass of substance}}{\text{molar mass}}$$

This triangle 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:

mass of substance = number of moles × molar mass

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

$$molar mass = \frac{mass of substance}{no. moles}$$



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 often 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 (1 light year is the distance that light travels in 1 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

Calculate the number of moles of Mg atoms in 10.0 g of Mg.

no. moles (n) =
$$\frac{\text{mass of substance}}{\text{molar mass}}$$

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

10.0 g of Mg is 0.411 mol.

Note: the unit for moles is mol.

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

Calculate the mass of 0.3800 mol CH₃COOH.

mass of substance = number of moles × molar mass

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

The mass of 0.3800 mol CH₃COOH is 22.82 g.

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



Self-test 2

Test yourself

2 Copy and complete the table. The first one has been done for you.

Compound	Molar mass/g mol ⁻¹	Mass/g	Number of moles / mol
H ₂ 0	18.02	9.01	0.500
CO ₂		5.00	
H ₂ S			0.100
NH ₃			3.50
Q		1.00	0.0350
Z		0.0578	1.12×10 ⁻³
Mg(NO ₃) ₂		1.75	
C ₃ H ₇ OH		2500	
Fe ₂ O ₃			5.68×10 ⁻⁵





The mass of a molecule

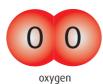
The mass of one mole of water is $18.02\,\mathrm{g}$. This contains 6.02×10^{23} molecules of water. The mass of one molecule of water can therefore be worked out by dividing the mass of one mole (18.02 g) by the number of molecules it contains (6.02×10^{23}):

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

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

Examiner's 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.



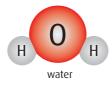
The number of particles When we write 1 mol O₂, it means

When we write 1 mol O_2 , it means one mole of O_2 molecules: that is, $6.02 \times 10^{23} O_2$ molecules. Each O_2 molecule contains two oxygen atoms; therefore, one mole of O_2 molecules contains $2 \times 6.02 \times 10^{23}$ = 1.204×10^{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 H atoms and one O atom. The total number of H atoms in 0.1 mol H_2O is $2 \times 6.02 \times 10^{22}$; i.e. 1.204×10^{23} H atoms; i.e. 0.2 mol H 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; i.e. 0.3 mol of atoms.

If we look at Table 1.1 we can see the connection between the number of moles of molecules and the number of moles of a particular atom in that molecule. Figure 1.1 illustrates the relationship between number of particles, number of moles and Avogadro's constant.



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
0 ₃	0.5	1.5
CH₃COOH	0.2	0.4

Table 1.1 The relationship between the number of moles of molecules and the number of moles of particular atoms.

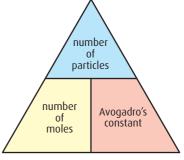


Figure 1.1 The relationship between the number of moles and the number of particles.

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 $0.25 \, \text{mol H}_2 \text{SO}_4$ there are 4×0.25 (i.e. $1.0 \, \text{mol}$) O atoms.

Examiner's tip

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



Self-test 3

Test yourself

- **3** Work out the mass of a molecule of each of the following:
 - a H₂O
 - **b** NH₃
 - \mathbf{c} CO₂
- **4** Work out the total number of hydrogen atoms in each of the following:
 - **a** 1.00 mol H₂
 - **b** 0.200 mol CH₄
 - c 0.0500 mol NH₃

- **5** Calculate the total number of atoms in each of the following:
 - **a** 0.0100 mol NH₃
 - **b** 0.200 mol C₂H₆
 - c 0.0400 mol C₂H₅OH
- **6** Calculate the number of moles of oxygen atoms in each of the following:
 - a 0.2 mol H₂SO₄
 - **b** 0.1 mol Cl₂O₇
 - c 0.03 mol XeO₄

1.3 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 following formula.

% by mass of an element = no. atoms of the element × relative atomic mass relative molecular mass

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

Worked examples

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

The relative molecular mass of $C_6H_5NO_2$ 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.

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

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

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

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

Calculate the mass of O present in 2.20 g of CO₂.

The relative molecular mass of CO_2 is 44.01. Of this, the amount contributed by the two oxygen atoms is $2 \times 16.00 = 32.00$

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

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:

$$\frac{63.02}{48.00}$$
 × 2.00 = 2.63 g

Alternative method

The percentage of O 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

$$\frac{100}{76.2}$$
 × 2.00 = 2.63 g

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



Self-test 4

Test yourself

- 7 Calculate the percentage by mass of oxygen in each of the following compounds:
 - a C₂H₅OH
 - **b** CH₃CH₂COOH
 - \mathbf{c} Cl₂O₇
- **8** Calculate the mass of oxygen in each of the following samples:
 - **a** $6.00 \,\mathrm{g}$ of $\mathrm{C_3H_7OH}$
 - **b** 5.00 g of SO₂
 - c 10.0 g of P_4O_{10}

- **9** For each of the following compounds work out the mass of substance that will contain 1.00 g of oxygen.
 - a CH₃OH
 - $b SO_3$
 - **c** P₄O₆

Empirical and molecular formulas

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.)

The 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 $(CH_2)_n$ i.e. C_2H_4 or C_3H_6 or C_4H_8 , etc.

Worked examples

If the formulas of two compounds are

- a C₄H₁₀O₂
- b Re₃Cl₉

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 2, and so the empirical formula is C_2H_5O .
- **b** In this case each subscript is divisible by 3, and so the empirical formula is ReCl₃.

The empirical formula of benzene is CH. Given that the molar mass is 78.12 g mol⁻¹, work out the 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 $(CH)_6$, 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

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.

	С	Н	0
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
no. 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 $C_5H_{12}O$.

b The empirical formula mass of the compound is 88.17. This is the same as the relative molecular mass, and thus the molecular formula is the same as the empirical formula $(C_5H_{12}O)$.

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

A uranium fluoride contains only uranium and fluorine.

% 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 $100\,\mathrm{g}$.

	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
no. 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 UF₆.

The experimental set-up shown in Figure 1.2 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.

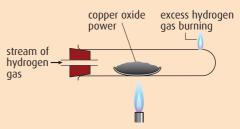


Figure 1.2 Hydrogen gas is passed over the heated copper oxide until all the copper oxide is reduced to copper.

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

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

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

mass of oxygen in copper oxide =
$$5.54 - 4.42 = 1.12 g$$

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

no. moles of copper =
$$\frac{4.42}{63.55}$$
 = 0.0696 mol

no. moles of oxygen =
$$\frac{1.12}{16.00}$$
 = 0.0700 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 thus 1:1, and the empirical formula is CuO.

The equation for the reaction is: $CuO + H_2 \rightarrow Cu + H_2O$

Composition by mass from combustion data

Worked examples

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: $C_xH_y + (x + \frac{y}{4})O_2 \rightarrow xCO_2 + \frac{y}{2}H_2O$

All the C in the CO_2 comes from the hydrocarbon ${\bf A}$.

no. moles of
$$CO_2 = \frac{8.08}{44.01} = 0.184 \,\text{mol}$$

Each CO₂ molecule contains one C atom. Therefore the number of moles of C in 2.50 g of the hydrocarbon is 0.184 mol.

All the H in the water comes from the hydrocarbon A.

no. moles of
$$H_2O = \frac{2.64}{18.02} = 0.147 \,\text{mol}$$

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

	С	Н
no. 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 5. Therefore the empirical formula is C_5H_8 .

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 some of the oxygen in the CO_2 and H_2O comes from the O in **B** (the rest comes from the oxygen in which it is burnt).

mass of C in 2.79 g of
$$CO_2 = \frac{12.01}{44.01} \times 2.79 = 0.76$$
 g

mass of H in 1.71 g of H₂O =
$$\frac{2.02}{18.02}$$
 × 1.71 = 0.19 g

mass of O in 1.46 g of **B** is
$$(1.46 - 0.76 - 0.19) = 0.51$$
 g

The empirical formula can now be calculated.

	С	Н	0
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 C_2H_6O .

b The empirical formula mass is 46.08.

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

Therefore, the molecular formula is $(C_2H_6O)_2$, i.e. $C_4H_{12}O_2$.



Self-test 5

Test yourself

10 Which of the following represent empirical formulas?

 $\begin{array}{cccccc} C_2H_4 & CO_2 & CH & HO & C_3H_8 \\ C_4H_{10} & H_2O & H_2O_2 & N_2H_4 & PCl_5 \\ CH_3COOH & C_6H_5CH_3 & & & \end{array}$

11 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
НО	34.02	
ClO ₃	166.90	
CH ₂	84.18	
BNH ₂	80.52	

12 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.
- **13** If an oxide of chlorine contains 81.6% chlorine, calculate its empirical formula.

- **14** A compound contains 76.0% iodine and 24.0% oxygen. Calculate the empirical formula of the compound.
- 15 A compound, **X**, contains 64.8% carbon and 13.6% hydrogen. If the only other element present is oxygen and a single molecule of the compound contains four carbon atoms, calculate the molecular formula of **X**.
- 16 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.
- 17 When 1.76 g of a hydrocarbon, **Q**, is burnt in excess oxygen, 5.27 g of carbon dioxide and 2.88 g of water are produced. What is the empirical formula of **Q**?
- 18 When 2.38 g of a hydrocarbon, **Z**, is burnt in excess oxygen, 7.21 g of carbon dioxide is produced. What is the empirical formula of **Z**?
- 19 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**?

1.4 Chemical equations

Balancing equations

If a reaction involves $5.00\,\mathrm{g}$ of one substance reacting with $10.00\,\mathrm{g}$ of another substance in a closed container (nothing can be added or escape), then at the end of the reaction there will still be exactly $15.00\,\mathrm{g}$ of substance present. This $15.00\,\mathrm{g}$ 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 $15.00\,\mathrm{g}$ 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.

Learning objectives

- Understand how to balance chemical equations
- Understand how to use state symbols in chemical equations

Mass is conserved in a chemical reaction.

Only whole numbers (coefficients) may be added in order to balance a chemical equation.

The chemical formula for water is H_2O , and this formula 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.

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 the reaction.

	C_3H_8	$C_3H_8 + 5O_2 \qquad \rightarrow \qquad$		$3CO_2 + 4H_2C$		
reactants			prod	lucts		
atoms	С	3		С	3	
	Н	8		Н	8	
	O	10		O	10	

This equation is balanced.

State symbols are often used to indicate the physical state of an element or compound. These may be written as either subscripts after the chemical formula or in normal type.

- (s) = solid
- (1) = liquid
- (g) = gas
- (aq) = aqueous (dissolved in water)

Worked examples

Balance the following equation

...
$$N_2(g) + ... H_2(g) \rightarrow ... NH_3(g)$$

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

At the moment 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:

atoms
$$2 N$$
 $2 N$
 $2 H$ $6 H$
... $N_2 + 3H_2 \rightarrow 2NH_3$
atoms $2 N$ $2 N$
 $6 H$ $6 H$

This equation is now balanced, as 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.

Balance the following equation:

...
$$C_4H_{10}(g) + ... O_2(g) \rightarrow ... CO_2(g) + ... H_2O(l)$$

Compounds are balanced first, then elements. The oxygen here does not depend on any other element.

...
$$C_4H_{10}(g) + ... O_2(g) \rightarrow 4CO_2(g) + 5H_2O(l)$$

There were two oxygen atoms on the left-hand side of the equation, and 2 needs to be multiplied by 6.5 to give 13, the number of oxygen atoms on the other side.

...
$$C_4H_{10}(g) + 6.5O_2(g) \rightarrow 4CO_2(g) + 5H_2O(l)$$

The equation is balanced as shown, but it looks much neater if balanced with whole numbers. To achieve this, all the coefficients are multiplied by 2 to get rid of the .5.

$$2C_4H_{10}(g) + 13O_2(g) \rightarrow 8CO_2(g) + 10H_2O(l)$$



Self-test 6

Test yourself

20 Balance the following equations:

a
$$NO + O_2 \rightarrow NO_2$$

b
$$C_3H_8+O_2 \rightarrow CO_2+H_2O$$

c
$$CaCO_3 + HCl \rightarrow CaCl_2 + CO_2 + H_2O$$

$$d C_2H_5OH + O_2 \rightarrow CO_2 + H_2O$$

e
$$WO_3 + H_2 \rightarrow W + H_2O$$

$$f H_2O_2 \rightarrow O_2 + H_2O$$

$$\mathbf{g} \operatorname{CrO}_3 \to \operatorname{Cr}_2\operatorname{O}_3 + \operatorname{O}_2$$

$$\mathbf{h} \ \mathrm{Al_4C_3} + \mathrm{H_2O} \rightarrow \mathrm{CH_4} + \mathrm{Al_2O_3}$$

i
$$HI + H_2SO_4 \rightarrow H_2S + H_2O + I_2$$

$$i PH_3 + O_2 \rightarrow P_4O_{10} + H_2O$$

Conservation of charge

Charge – that is, the number of electrons (and protons) – must also balance in a chemical equation. Ionic equations will be considered further in another chapter, but for the moment here is an example of an ionic equation that is not balanced, although there is the same number of atoms on both sides.

$$Cr_2O_7^{2-} + Fe^{2+} + 14H^+ \rightarrow 2Cr^{3+} + 7H_2O + Fe^{3+}$$

The total charge on the left-hand side of this equation is 14+, whereas the total charge on the right-hand side is 9+, so the equation is not balanced (there is a different number of electrons at the end of the reaction from at the beginning). The balanced ionic equation for this reaction is:

$$Cr_2O_7^{2-} + 6Fe^{2+} + 14H^+ \rightarrow 2Cr^{3+} + 7H_2O + 6Fe^{3+}$$

We will consider how to balance these equations on pages 381–386.

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:

$$Fe(s) + S(s) \rightarrow FeS(s)$$

Worked example

Consider the combustion of butane:

$$2C_4H_{10}(g) + 13O_2(g) \rightarrow 8CO_2(g) + 10H_2O(l)$$

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 = $10.00 + 35.78 = 45.78 \,\mathrm{g}$.

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

Therefore the mass of water = $45.78 - 30.28 = 15.50 \,\mathrm{g}$.

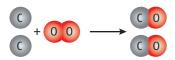


Figure 1.3 Two carbon atoms combine with one oxygen molecule to form two molecules of carbon monoxide.

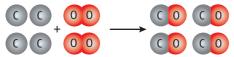


Figure 1.4 Four carbon atoms combine with two oxygen molecules to form four molecules of carbon monoxide.

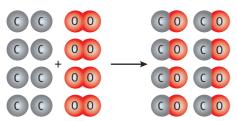


Figure 1.5 In this reaction, the ratio in which the species combine is fixed. So here we have eight carbon atoms combining with four oxygen molecules to form eight molecules of carbon monoxide.

The meaning of chemical equations

Consider the following chemical equation:

$$2C + O_2 \rightarrow 2CO$$

This is shown diagrammatically in Figure 1.3.

In this reaction, two C atoms combine with one O_2 molecule to form two molecules of CO.

Look at Figure **1.4**. If we started with four C atoms: four C atoms react with two O₂ molecules to form four molecules of CO.

The ratio in which the species combine is fixed in this equation. The number of molecules of oxygen is always half the number of C atoms, and the number of CO molecules produced is the same as the number of C atoms (see Figure 1.5).

Thus, if we imagine a very large number of C atoms, e.g. 6.02×10^{23} , we know that in this reaction they will combine with half as many molecules of O_2 , i.e. 3.01×10^{23} molecules. The number of molecules of CO produced will be the same as the number of C atoms, i.e. 6.02×10^{23} molecules of CO. However, 6.02×10^{23} is one mole, so we can also interpret the equation as one mole of C atoms reacting with half a mole of O_2 molecules to form one mole of CO molecules, or:

$$C + \frac{1}{2}O_2 \rightarrow CO$$
 i.e. $2C + O_2 \rightarrow 2CO$

This equation tells us that $2 \mod C$ atoms react with $1 \mod O_2$ molecules to form $2 \mod CO$ molecules.

1.5 Calculations involving moles and masses

Using moles

Very often we wish 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 to doing 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.

Learning objectives

- Solve problems involving masses of substances
- Calculate the theoretical and percentage yield in a reaction
- Understand the term limiting reactant and solve problems involving this

Questions involving masses of substances

Worked examples

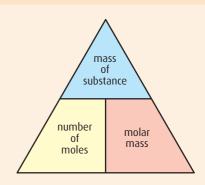
Consider the reaction of sodium with oxygen:

$$4Na(s) + O_2(g) \rightarrow 2Na_2O(s)$$

- a How much sodium reacts exactly with 3.20 g of oxygen?
- **b** What mass of Na₂O 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).

no. moles of oxygen =
$$\frac{3.20}{32.00}$$
 = 0.100 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 $1 \, \text{mol } O_2$ reacts with $4 \, \text{mol } Na$. Therefore $0.100 \, \text{mol } O_2$ reacts with $4 \times 0.100 \, \text{mol } Na$, i.e. $0.400 \, \text{mol } Na$.

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

mass of Na =
$$0.400 \times 22.99 = 9.20 \,\mathrm{g}$$

Note: the mass of Na 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 4Na – the four was already taken into account when 0.100 mol was multiplied by 4 to give the number of moles of Na.

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

molar mass of
$$Na_2O = 61.98 \,\mathrm{g}\,\mathrm{mol}^{-1}$$

mass of $Na_2O = 0.200 \times 61.98 = 12.4 \,\mathrm{g}$

Alternatively, the mass of Na_2O can be worked out using the idea of conservation of mass, i.e. the mass of Na_2O = mass of O_2 + mass of Na.

Examiner's 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 1×10^6 .

Consider the following equation.

$$2NH_3 + 3CuO \rightarrow N_2 + 3H_2O + 3Cu$$

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

CuO is in excess: i.e. more than enough is present 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 ammonia can be calculated:

$$\frac{2.56}{17.04}$$
 = 0.150 mol of ammonia

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

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

Step 3 – the mass of 1 mol Cu = 63.55 g. The mass of CuO that reacts = $0.225 \times 63.55 = 14.3$ 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

 M_1 = molar mass of first substance

Worked example

The following equation represents the combustion of butane:

$$2C_4H_{10}(g) + 13O_2(g) \rightarrow 8CO_2(g) + 10H_2O(l)$$

If 10.00 g of butane is used, calculate:

- a the mass of oxygen required for the exact reaction
- **b** the mass of carbon dioxide produced.
- **a** We will call butane substance 1 and oxygen substance 2 (this is arbitrary).

$$m_1 = 10.00 \,\mathrm{g}$$

$$m_2 = \frac{1}{2}$$

$$n_1 = 2$$

$$n_2 = 13$$

$$M_1 = 58.14 \,\mathrm{g}\,\mathrm{mol}^{-1}$$
 $M_2 = 32.00 \,\mathrm{g}\,\mathrm{mol}^{-1}$

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

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

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

The equation can be rearranged:

$$m_2 = \frac{10.00 \times 13 \times 32.00}{2 \times 58.14}$$
 i.e. $m_2 = 35.78$ g

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

b We will call butane substance 1 and carbon dioxide substance 2.

$$m_1 = 10.00 \,\mathrm{g}$$

$$n_1 = 2$$

$$n_2 = 8$$

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

$$M_1 = 58.14 \,\mathrm{g}\,\mathrm{mol}^{-1}$$
 $M_2 = 44.01 \,\mathrm{g}\,\mathrm{mol}^{-1}$

$$\frac{10.00}{2 \times 58.14} = \frac{m_2}{8 \times 44.01}$$

The equation can be rearranged:

$$m_2 = \frac{10.00 \times 8 \times 44.01}{2 \times 58.14}$$
 i.e. $m_2 = 30.28$ g

Therefore 30.28 g of carbon dioxide is produced.

D-**O**

Self-test 7



Test yourself

21 a How many moles of hydrogen gas are produced when 0.4 moles of sodium react with excess water?

$$2Na + 2H_2O \rightarrow 2NaOH + H_2$$

b How many moles of O_2 react with 0.01 mol C_3H_8 ?

$$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2O$$

- **c** How many moles of H_2S are formed when 0.02 mol of HCl react with excess Sb_2S_3 ? $Sb_2S_3 + 6HCl \rightarrow 2SbCl_3 + 3H_2S$
- **d** How many moles of oxygen are formed when $0.6 \,\text{mol}$ of KClO₃ react? $2 \,\text{KClO}_3(s) \rightarrow 2 \,\text{KCl}(s) + 3 \,\text{O}_2(g)$
- e How many moles of iron are formed when 0.9 mol CO react with excess iron oxide? Fe₂O₃ + 3CO \rightarrow 2Fe + 3CO₂
- **f** How many moles of hydrogen would be required to make 2.4×10^{-3} mol NH₃? $N_2 + 3H_2 \rightarrow 2NH_3$

- 22 a Calculate the mass of arsenic(III) chloride produced when $0.150\,\mathrm{g}$ of arsenic reacts with excess chlorine according to the equation: $2\mathrm{As} + 3\mathrm{Cl}_2 \rightarrow 2\mathrm{AsCl}_3$
 - **b** What mass of sulfur is produced when 5.78 g iron(III) sulfide is reacted with excess oxygen? $2Fe_2S_3+3O_2 \rightarrow 2Fe_2O_3+6S$
 - 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.

$$2P + 3I_2 \rightarrow 2PI_3$$

d Consider the reaction shown below. What mass of SCl₂ must be reacted with excess NaF to produce 2.25 g of NaCl?

$$3SCl_2 + 4NaF \rightarrow S_2Cl_2 + SF_4 + 4NaCl$$

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 a lot of the experimental observations in modern science, but that does not mean that there isn't one. Consider the

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

following trivial example.

The equation for the reaction is:

CaCO₃
$$\rightarrow$$
 CaO + CO₂
no. moles of calcium carbonate = $\frac{100}{(20+6+(3\times8))}$
= 2 moles

Two moles of calcium carbonate produces two moles of carbon dioxide.

The mass of two moles of carbon dioxide 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!



In any commercial process it is very important to know the yield 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%, it is likely that the company would seek a more efficient synthetic process.

The yield of a chemical reaction is usually quoted as a percentage, as that gives more information than just quoting the yield of the product as a mass. Consider the preparation of 1,2-dibromoethane:

$$C_2H_4(g) + Br_2(l) \rightarrow C_2H_4Br_2(l)$$

10.00 g of ethene 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 1,2-dibromoethane may be 50.00 g.

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

The yield of a chemical reaction is the amount of product obtained.

7

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

Worked example

$$C_2H_5OH(l) + CH_3COOH(l) \rightarrow CH_3COOC_2H_5(l) + H_2O(l)$$

ethanol ethanoic acid ethyl ethanoate water

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:

molar mass of ethanol =
$$46.08 \,\mathrm{g}\,\mathrm{mol}^{-1}$$

no. moles of ethanol = $\frac{20.00}{46.08} = 0.4340 \,\mathrm{mol}$

Ethanoic acid is in excess, i.e. more than enough is present to react with all the ethanol. This means that we do not need to worry about the number of moles of ethanoic acid.

The chemical equation tells us that 1 mol ethanol produces 1 mol ethyl ethanoate. Therefore, 0.4340 mol ethanol produces 0.4340 mol ethyl ethanoate.

The molar mass of ethyl ethanoate = $88.12 \,\mathrm{g} \,\mathrm{mol}^{-1}$.

The mass of ethyl ethanoate produced = $0.4340 \times 88.12 = 38.24$ g.

Thus, the theoretical yield is $38.24\,\mathrm{g}$, and the actual yield is $30.27\,\mathrm{g}$.

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

Therefore the percentage yield of ethyl ethanoate is 79.15%.



Self-test 8

Test yourself

- 23 Calculate the percentage yield in each of the following reactions.
 - **a** When $2.50 \,\mathrm{g}$ of SO_2 is heated with excess oxygen, 2.50 g of SO₃ is obtained. $2SO_2 + O_2 \rightarrow 2SO_3$
 - **b** When 10.0 g of arsenic is heated in excess oxygen, 12.5 g of As₄O₆ is produced. $4As + 3O_2 \rightarrow As_4O_6$
- **c** When 1.20 g ethene reacts with excess bromine, 5.23 g of 1,2-dibromoethane is produced.

$$C_2H_4 + Br_2 \rightarrow CH_2BrCH_2Br$$

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

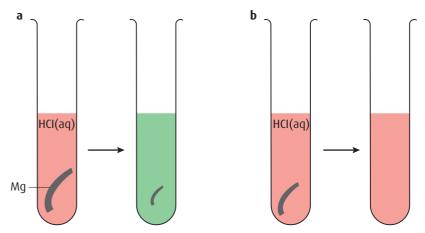


Figure 1.6 The reaction between magnesium and hydrochloric acid. In each test tube a small amount of universal indicator has been added. (a) In this test tube, the magnesium is in excess and the reaction finishes when the hydrochloric acid runs out. There is still magnesium left over at the end, and 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

Consider the reaction between magnesium and nitrogen:

$$3Mg(s) + N_2(g) \rightarrow Mg_3N_2(s)$$

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

no. moles of Mg =
$$\frac{10.00}{24.31}$$
 = 0.4114 mol no. moles of N₂ = $\frac{5.00}{28.02}$ = 0.178 mol

no. moles of
$$N_2 = \frac{5.00}{28.02} = 0.178 \,\text{mol}$$

The equation tells us that 3 mol Mg reacts with 1 mol N₂. So 0.4114 mol Mg reacts with 0.4114 mol N₂ divided by 3, i.e. $0.1371 \, \text{mol N}_2$.

Therefore, for an exact reaction, 0.1371 mol of N₂ are required to react with 0.4114 mol Mg. However, 0.178 mol of N_2 are used, which is more than enough to react. This means that N_2 is in excess, as there is more than enough to react with all the Mg present. Magnesium is therefore the limiting reactant.

This can also be seen from working with the number of moles of N_2 : $0.178 \,\mathrm{mol}\,\,\mathrm{N}_2$ was used in this reaction. This number of moles of N_2 would require 3×0.178 mol Mg for an exact reaction, i.e. 0.534 mol Mg. However, only 0.4114 mol Mg are present; therefore, the Mg will run out before all the N_2 has reacted.

Alternatively: divide the number of moles of each reactant by its coefficient in the stoichiometric equation, and the smallest number indicates the limiting reactant.

Consider the reaction between sulfur and fluorine: $S(s) + 3F_2(g) \rightarrow SF_6(g)$

10.00 g of sulfur reacts with 10.00 g of fluorine.

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

a no. moles of
$$S = \frac{10.00}{32.06} = 0.3119 \text{ mol}$$
 no. moles of $F_2 = \frac{10.00}{38.00} = 0.2632 \text{ mol}$

no. moles of
$$F_2 = \frac{10.00}{38.00} = 0.2632 \,\text{mol}$$

The coefficient of S in the equation is 1 and that of F_2 is 3. 0.3119/1 = 0.3119 and 0.2632/3 = 0.08773, therefore S is in excess and F_2 is the limiting reactant.

Alternatively, we can reason from the chemical equation, 0.2632 mol F₂ should react with 0.08773 mol S (i.e. 0.2632 mol S divided by 3). There is more than 0.08773 mol S present, so S is present in excess and F₂ 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 F₂ produces 0.08773 mol SF₆ (i.e. 0.2632 mol SF₆ divided by 3).

molar mass of
$$SF_6 = 146.06 \,\mathrm{g}\,\mathrm{mol}^{-1}$$

mass of
$$SF_6$$
 formed = $0.08773 \times 146.06 = 12.81 g$

c From the chemical equation, 0.2632 mol F₂ reacts with 0.08773 mol S (i.e. 0.2632 mol S divided by 3). Originally there were 0.3119 mol S present; therefore the number of moles of sulfur left at the end of the reaction is 0.3119 - 0.08773 = 0.2242.

The mass of sulfur left at the end of the reaction is $0.2242 \times 32.06 = 7.188 \,\mathrm{g}$.

Examiner's 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 use this one for all subsequent calculations.

For the reaction

$$4Fe_2Cr_2O_4 + 8Na_2CO_3 + 7O_2 \rightarrow 8Na_2CrO_4 + 2Fe_2O_3 + 8CO_2$$

there is 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:

$$4Fe_2Cr_2O_4 + 8Na_2CO_3 + 7O_2 \rightarrow 8Na_2CrO_4 + 2Fe_2O_3 + 8CO_2$$

$$mass / g = 4 \times 279.70 \qquad 8 \times 105.99 \qquad 7 \times 32.00$$

$$mass / g = 1118.80 \qquad 847.92 \qquad 224.00$$

These are the masses that are required for the exact reaction. As the greatest mass required is that of Fe₂Cr₂O₄, if the same mass of each substance is taken, the Fe₂Cr₂O₄ will run out first and must be the limiting reactant.



Self-test 9

Test yourself

- 24 What is the limiting reactant in each of the following reactions?
 - **a** $0.1 \,\text{mol Sb}_4\text{O}_6$ reacts with $0.5 \,\text{mol H}_2\text{SO}_4$ $Sb_4O_6 + 6H_2SO_4 \rightarrow 2Sb_2(SO_4)_3 + 6H_2O$
 - **b** 0.20 mol AsCl₃ reacts with 0.25 mol H₂O $4AsCl_3 + 6H_2O \rightarrow As_4O_6 + 12HCl$
 - c 0.25 mol Cu react with 0.50 mol dilute HNO₃ according to the equation:

$$3Cu + 8HNO_3$$

$$\rightarrow$$
 3Cu(NO₃)₂ + 4H₂O + 2NO

d 0.10 mol NaCl reacts with 0.15 mol MnO₂ and 0.20 mol H₂SO₄

$$2NaCl + MnO_2 + 2H_2SO_4$$

$$\rightarrow$$
 Na₂SO₄ + MnSO₄ + 2H₂O + Cl₂

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

$$B_2O_3 + 3Mg \rightarrow 2B + 3MgO$$

What mass of B is obtained if $0.75 \text{ g B}_2\text{O}_3$ is reacted with 0.50 g Mg?

26 Iron(III) oxide reacts with carbon to produce

$$Fe_2O_3 + 3C \rightarrow 2Fe + 3CO$$

What mass of Fe is obtained if 10.0 tonnes of Fe₂O₃ is reacted with 1.00 tonne of C?

1.6 Calculations involving volumes of gases

An ideal gas is a concept invented by scientists to approximate (model) the behaviour of real gases. Under normal conditions (around 1 atm pressure and 0 $^{\circ}$ C) real gases such as H₂ behave fairly much like ideal gases, and the approximations used here work very well.

Two postulates we use when defining an ideal gas are to say that the molecules themselves have no volume (they are point masses) and that no forces exist between them (except when they collide). This means that the volume occupied by a gas at a certain temperature and pressure depends only on the number of particles 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 present.

volume ∝ no. moles

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

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 $100\,\mathrm{cm}^3$ of $\mathrm{H_2}$ contains the same number of molecules at $25\,\mathrm{^{\circ}C}$ and $1\,\mathrm{atm}$ pressure as $100\,\mathrm{cm}^3$ of $\mathrm{NH_3}$, if we assume that they both behave as ideal gases. Under the same conditions, $50\,\mathrm{cm}^3$ of $\mathrm{CO_2}$ would contain half as many molecules.

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

$$H_2(g) + Cl_2(g) \rightarrow 2HCl(g)$$

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. $50 \, \text{cm}^3$ of H_2 reacts with $50 \, \text{cm}^3$ of Cl_2 to give $100 \, \text{cm}^3$ of HCl.

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.

Consider the following reaction for the synthesis of methanol:

$$CO(g) + 2H_2(g) \rightarrow CH_3OH(g)$$

- a What volume of H₂ reacts exactly with 2.50 dm³ of CO?
- **b** What volume of CH₃OH is produced?
- **a** 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 dm³ of CO reacts with 2 × 2.50, i.e. 5.00 dm³, of H_2 .
- **b** One volume of CO produces one volume of CH₃OH. Therefore the volume of CH₃OH produced is 2.50 dm³.

If 100 cm³ of oxygen reacts with 30 cm³ of methane in the following reaction, how much oxygen will be left at the end of the reaction?

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

From the equation we know that 1 mol CH₄ reacts with 2 mol O_2 . Therefore one volume of CH₄ reacts with two volumes of O_2 , i.e. $30 \, \text{cm}^3$ of CH₄ reacts with 2×30 , i.e. $60 \, \text{cm}^3$ of O_2 .

The original volume of O_2 was $100 \, \text{cm}^3$; therefore, if $60 \, \text{cm}^3$ 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, 1 atm $(1.01 \times 10^5 \text{ Pa})$

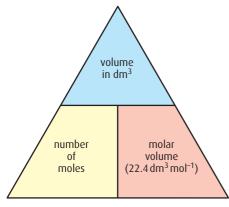


Figure 1.7 The relationship between the number of moles of a gas and its volume.

Converting volumes of gases to number of moles

As the volume occupied by an ideal gas is dependent only on the number of particles present (assuming 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 = $22.4 \,\mathrm{dm^3 \,mol^{-1}}$ or $2.24 \times 10^{-2} \,\mathrm{m^3 \,mol^{-1}}$

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 $22.4 \,\mathrm{dm}^3$ at STP.

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

no. moles =
$$\frac{\text{volume}}{\text{molar volume}}$$

This is summarised in Figure 1.7.

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!

1°C is the same as 1K, and so 0°C is equivalent to 273K

To convert °C to K add 273: e.g. 25 °C is equivalent to 25 + 273, i.e. 298 K To convert K to °C subtract 273: e.g. 350 K is equivalent to 350 – 273, i.e. 77 °C

Volumes of gases are often given in dm³ (litres) and so it is important to know how to convert between cm³ and dm³.

As 1 dm³ (1 litre) is equivalent to 1000 cm³ (1 cm³ is the same as 1 ml), to convert cm³ to dm³ we divide by 1000 (to go from **1000 cm³** to **1 dm³**). The conversion is shown in Figure **1.8**.

In different countries around the world 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 mathematican 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'.

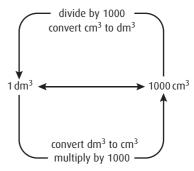


Figure 1.8 Converting between cm³ and dm³.

Worked examples

- a Calculate the number of moles in $250 \, \text{cm}^3$ of O_2 at STP.
- **b** Calculate the volume of 0.135 mol of CO₂ at STP.

a no. moles =
$$\frac{\text{volume in dm}^3}{22.4}$$

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

no. moles =
$$\frac{0.250}{22.4}$$
 = 0.0112 mol

b volume = no. moles \times 22.4 = 0.135 \times 22.4 = 3.02 dm³

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

mass of substance

> molar mass

number

moles

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

Step 1 – work out the number of moles of calcium carbonate:

no. moles of calcium carbonate =
$$\frac{10.01}{100.09}$$
 = 0.1000 mol

Step 2 – the chemical equation tells us that 1 mol CaCO₃ decomposes to give 1 mol CO₂.

Therefore 0.1000 mol CaCO₃ decomposes to give 0.1000 mol CO₂.

Step 3 – convert the number of moles to volume.

1 mol of CO₂ occupies 22.4 dm³ at STP

volume of CO_2 = no. moles × volume of 1 mole (22.4 dm³)

volume of
$$CO_2 = 0.1000 \times 22.4 = 2.24 \,\text{dm}^3$$

Therefore the volume of CO₂ produced is 2.24 dm³.

Potassium chlorate(V) decomposes when heated:

$$2KClO_3(s) \rightarrow 2KCl(s) + 3O_2(g)$$

What mass of potassium chlorate(V) decomposes to produce 100.0 cm³ 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 dm³:

volume of
$$O_2$$
 in $dm^3 = \frac{100.0}{1000} = 0.1000 dm^3$

no. moles of
$$O_2 = \frac{0.1000}{22.4} = 4.464 \times 10^{-3} \text{ mol}$$

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

$$\frac{2}{3} \times 4.464 \times 10^{-3} = 2.976 \times 10^{-3} \,\text{mol}$$

Step 3 – convert the number of moles of KClO₃ to mass.

molar mass of
$$KClO_3 = 122.55 \,\mathrm{g}\,\mathrm{mol}^{-1}$$

mass of KClO₃ =
$$122.55 \times 2.976 \times 10^{-3} = 0.3647$$
 g

Therefore the mass of KClO₃ required is 0.3647 g.

Formula for solving moles questions involving volumes of gases

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

$$\frac{m_1}{n_1 M_1} = \frac{V_2}{n_2 M_{\rm v}}$$

where:

 $m_1 = \text{mass of first substance (in g)}$

 n_1 = coefficient of first substance

 M_1 = molar mass of first substance

 V_2 = volume (in dm³) of second substance if it is a gas

 n_2 = coefficient of second substance

 $M_{\rm v}$ = molar volume of a gas = 22.4 dm³ at STP

This equation 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 already described.

Note – this is very similar to the equation that was used earlier with masses.

There is no need to convert units of volume to dm³ with this equation $-V_2$ will have the same units as V_1 .

Worked example

Consider the following equation:

$$2As_2S_3 + 9O_2 \rightarrow 2As_2O_3 + 6SO_2$$

What volume of SO₂ is obtained (measured at STP) when 1.000 kg of As₂S₃ is heated in oxygen?

Let As_2S_3 be substance 1 and SO_2 be substance 2:

$$m_1 = 1.000 \,\mathrm{kg} = 1000 \,\mathrm{g}$$

$$n_1 = 2$$

$$M_1 = 246.02 \,\mathrm{g}\,\mathrm{mol}^{-1}$$

$$V_2 = ?$$

$$n_2 = 6$$

$$M_{\rm v} = 22.4 \, \mathrm{dm}^3$$
 at STP

$$\frac{1000}{2 \times 246.02} = \frac{V_2}{6 \times 22.4}$$

Rearranging the equation:
$$V_2 = \frac{1000 \times 6 \times 22.4}{2 \times 246.02} = 273 \,\text{dm}^3$$

Mass in g must be used.

Se

Self-test 10

Test yourself

- 27 Assume that all gases behave as ideal gases and that all measurements are made under the same conditions of temperature and pressure.
 - **a** Calculate the volume of CO₂ produced when $100\,\mathrm{cm}^3$ of ethene burns in excess oxygen according to the equation:

$$C_2H_4(g) + 3O_2(g) \rightarrow 2CO_2(g) + 2H_2O(l)$$

b Calculate the volume of NO produced when 2.0 dm³ of oxygen is reacted with excess ammonia according to the equation:

$$4NH_3(g) + 5O_2(g) \rightarrow 4NO(g) + 6H_2O(g)$$

- **28** Determine the number of moles present in each of the following at standard temperature and pressure:
 - **a** $0.240 \, \text{dm}^3 \text{ of } O_2$
- **d** $400.0 \, \text{cm}^3 \text{ of N}_2$
- **b** $2.00 \, \text{dm}^3 \text{ of CH}_4$
- **e** $250.0 \, \text{cm}^3 \text{ of CO}_2$
- **c** $0.100 \, \text{dm}^3 \text{ of SO}_2$
- **29** Work out the volume of each of the following at standard temperature and pressure:
 - **a** $0.100 \, mol \, C_3H_8$
- **d** 0.8500 mol NH₃
- **b** 100.0 mol SO₃
- **e** 0.600 mol O₂
- $c 0.270 \, mol \, N_2$
- **30** Sodium nitrate(V) decomposes according to the equation:

$$2\text{NaNO}_3(s) \rightarrow 2\text{NaNO}_2(s) + \text{O}_2(g)$$

Calculate the volume (in cm³) of oxygen
produced (measured at STP) when $0.820\,\text{g}$ of
sodium nitrate(V) decomposes.

31 Tin reacts with nitric acid according to the equation:

$$Sn(s) + 4HNO_3(aq)$$

$$\rightarrow$$
 SnO₂(s) + 4NO₂(g) + 2H₂O(l)

If 2.50 g of tin are reacted with excess nitric acid what volume of NO₂ (in cm³) is produced at STP?

32 Calculate the mass of sodium carbonate that must be reacted with excess hydrochloric acid to produce $100.0 \, \text{cm}^3$ of CO_2 at STP.

$$Na_2CO_3(s) + 2HCl(aq)$$

$$\rightarrow$$
 2NaCl(aq) + CO₂(g) + H₂O(l)

- 33 Assume that all gases behave as ideal gases and that all measurements are made under the same conditions of temperature and pressure.
 - **a** Oxygen (O₂) can be converted to ozone (O₃) by passing it through a silent electric discharge. $3O_2(g) \rightarrow 2O_3(g)$

If 300 cm³ of oxygen is 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:

$$H_2(g) + Cl_2(g) \rightarrow 2HCl(g)$$

What is the total volume of gas present in the container at the end of the experiment if $100 \, \mathrm{cm}^3$ of hydrogen is reacted with $200 \, \mathrm{cm}^3$ of chlorine?

'Macroscopic' means 'on a large scale'. The opposite is 'microscopic'. Microscopic properties of a gas are the properties of the particles that make up the gas.

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 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 1.9.

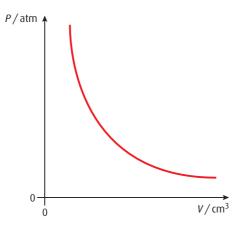


Figure 1.9 The relationship between pressure and volume of a fixed mass of an ideal gas at constant temperature

Other graphs can also be drawn to illustrate this relationship (see Figures 1.10 and 1.11).

As 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 1.10.

As 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 1.11.

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

The relationship can also be written as:

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

where k is a constant. This can be rearranged to give

$$PV = k$$

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.

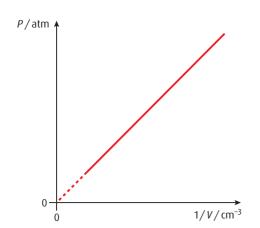


Figure 1.10 The relationship between the pressure and $\frac{1}{\text{volume}}$ of a fixed mass of an ideal gas at constant temperature.

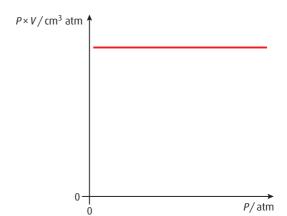


Figure 1.11 The relationship between *PV* and *P* for a fixed mass of an ideal gas at constant temperature.

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

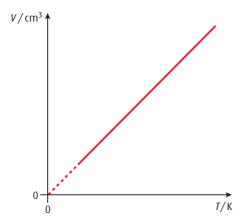


Figure 1.12 The relationship between the volume and temperature (in kelvin) of a fixed mass of an ideal gas at constant pressure.

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

The relationship between volume and temperature (Charles' law)

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

$$V \propto T$$

Therefore, if the temperature in **kelvin** 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 $200 \, \text{cm}^3$ at $120 \, \text{K}$, it will have a volume of $400 \, \text{cm}^3$ at $240 \, \text{K}$ if the pressure remains constant. This is illustrated in Figure **1.12**.

This relationship does not work for temperatures in °C (Figure 1.13). For instance, if the volume of an ideal gas at 25 °C is 500 cm³, the volume it will occupy at 50 °C will be about 560 cm³.

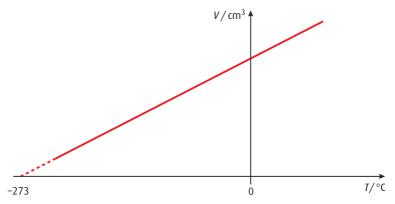


Figure 1.13 The relationship between the volume and temperature (in °C) of a fixed mass of an ideal gas at constant pressure. As can be seen from this graph, the temperature at which the volume of an ideal gas is zero will be −273 °C. This temperature is **absolute zero**.

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

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.

Therefore, if the temperature (in **kelvin**) of a fixed volume of an ideal gas is doubled, the pressure will also double (Figure **1.14**).

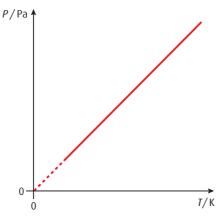


Figure 1.14 The relationship between the pressure and temperature (in kelvin) of a fixed mass of an ideal gas at constant volume.



The three relationships you have seen can be combined to produce the following equation:

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

$$P \propto T$$

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

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

Temperature must be in K.

Worked examples

If the volume of an ideal gas collected at $0\,^{\circ}$ C and 1.00 atmosphere pressure $(1.01\times10^{5}\,\text{Pa})$, i.e. at STP, is $50.0\,\text{cm}^{3}$, what would be the volume at $60\,^{\circ}$ C and $1.08\times10^{5}\,\text{Pa}$?

$$P_1 = 1.01 \times 10^5 \,\text{Pa}$$

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

$$P_2 = 1.08 \times 10^5 \,\text{Pa}$$

 $V_2 = ?$

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.

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

$$\frac{1.01 \times 10^5 \times 50.0}{273} = \frac{1.08 \times 10^5 \times V_2}{333}$$

Rearranging the equation:

$$V_2 = \frac{1.01 \times 10^5 \times 50.0 \times 333}{273 \times 1.08 \times 10^5} = 57.0 \,\mathrm{cm}^3$$

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

Therefore, the volume occupied by the gas at $60 \,^{\circ}\text{C}$ and $1.08 \times 10^{5} \,\text{Pa}$ is $57.0 \,\text{cm}^{3}$.

What temperature (in °C) is required to cause an ideal gas to occupy 1.34 dm³ at a pressure of 2.05 atm if it occupies 756 cm³ at STP?

$$P_1 = 2.05 \text{ atm}$$

$$P_1 = 2.05 \text{ atm}$$
 $P_2 = 1.00 \text{ atm}$

$$V_1 = 1.34$$

$$V_1 = 1.34$$
 $V_2 = 756 \text{ cm}^3, \text{ i.e. } \frac{756}{1000} \text{ dm}^3, \text{ i.e. } 0.756 \text{ dm}^3$

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

$$T_1 = ?$$

$$T_2 = 273 \,\mathrm{K}$$

$$\frac{2.05 \times 1.34}{T_1} = \frac{1.00 \times 0.756}{273}$$

The units of V_1 and V_2 must be made consistent with each other. We could have also changed V_1 to cm³.

Rearranging the equation:

$$2.05 \times 1.34 \times 273 = 1.00 \times 0.756 \times T_1$$

$$T_1 = \frac{2.05 \times 1.34 \times 273}{1.00 \times 0.756} = 992 \,\mathrm{K}$$

This must now be converted to °C by subtracting 273.

Temperature =
$$992 - 273 = 719$$
 °C

Therefore, the temperature must be 719 °C for the gas to occupy a volume of 1.34 dm³.

R is the gas constant (ideal gas constant).

$$n = \text{no. moles}$$

A consistent set of units must be used.

Examiner's tip

A set of units that is equivalent to this uses volume in dm³ and pressure in kPa - if you use these units you can avoid the problem of converting volumes into m^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:

$$PV = nRT$$

Although the gas constant 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 JK⁻¹ mol⁻¹, and this requires the following set of units:

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

Pressure: Nm⁻² or Pa

Volume: m³ Temperature: K

 $1000000 \, \mathrm{cm}^3 \Leftrightarrow 1 \, \mathrm{m}^3$ $1000\,\mathrm{dm}^3 \Leftrightarrow 1\,\mathrm{m}^3$

To convert m³ to cm³ multiply by 1 000 000.

To convert cm³ to m³ divide by 1 000 000.

To convert m³ to dm³ multiply by 1000.

To convert dm³ to m³ divide by 1000.

Worked examples

An ideal gas occupies 590 cm³ at 120 °C and 2.00 atm. 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:

To convert atm to Pa, multiply the pressure

in atm by 1.01×10^5 (1 atm in Pa).

$$P = 2.00 \text{ atm} = 1.01 \times 10^5 \times 2 \text{ Pa} = 2.02 \times 10^5 \text{ Pa}$$

$$V = 590 \,\mathrm{cm}^3 = \frac{590}{1000000} \,\mathrm{m}^3 = 5.90 \times 10^{-4} \,\mathrm{m}^3$$

$$n = 3$$

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

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

$$PV = nRT$$

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

Rearranging the equation:

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

Therefore the number of moles is 0.0365 mol.

An alternative value of the gas constant and set of units can be used:

$$R = 82.05 \,\mathrm{cm}^3 \,\mathrm{atm} \,\mathrm{K}^{-1} \,\mathrm{mol}^{-1}$$

The above example would have been much more straightforward with these units and value for the gas constant, but only $8.31\,\mathrm{J\,K}^{-1}\,\mathrm{mol}^{-1}$ is given in the IBO Chemistry Data booklet.

A gas has a density of $1.25\,\mathrm{g\,dm}^{-3}$ at $0\,^{\circ}\mathrm{C}$ and $1.01\times10^{5}\,\mathrm{Pa}$. Calculate its molar mass.

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

As we know the density, we know the mass of 1 dm³ of the gas. If we can find the number of moles in 1 dm³, we can work out the molar mass.

$$P = 1.01 \times 10^5 \,\mathrm{Pa}$$

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

$$n = 3$$

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

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

Using PV = nRT

$$n = \frac{1.01 \times 10^5 \times 1.00 \times 10^{-3}}{8.31 \times 273} = 0.0445 \,\text{mol}$$

This number of moles has a mass of 1.25 g.

$$molar mass = \frac{mass}{no. moles}$$

molar mass =
$$\frac{1.25}{0.0445}$$
 = 28.1 g mol⁻¹

What is the molar volume of an ideal gas at $18\,^{\circ}$ C and 1.01×10^{5} Pa? (Give your answer in m³ mol⁻¹ and dm³ 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 $22.4 \,\mathrm{dm}^3 \,\mathrm{mol}^{-1}$.

$$P = 1.01 \times 10^5 \, \text{Pa}$$

$$V = ?$$

$$n = 1.00$$

$$V = ?$$

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

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

Using PV = nRT:

$$V = \frac{1.00 \times 8.31 \times 291}{1.01 \times 10^5} = 0.0239 \,\mathrm{m}^3$$

Therefore the molar volume is $0.0239\,\mathrm{m^3\,mol^{-1}}$ at $18\,^{\circ}\mathrm{C}$ and $1.01\times10^5\,\mathrm{Pa}$. This must be multiplied by 1000 to convert to $\mathrm{dm^3}$: $23.9\,\mathrm{dm^3\,mol^{-1}}$.

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 0.973 atm and 22 °C. Calculate the mass of sodium nitrate(III) formed.

$$2NaNO_3(s) \rightarrow 2NaNO_2(s) + O_2(g)$$

One way of approaching the problem is to use the equation:

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

to correct the volume of oxygen given off to STP and then work out the number of moles of oxygen gas using the molar volume of a gas at STP (22.4 dm³ mol⁻¹).

Another, probably easier, way is to use PV = nRT to work out the number of moles of oxygen:

$$P = 0.973 \text{ atm} = 1.01 \times 10^5 \times 0.973 \text{ Pa} = 9.83 \times 10^4 \text{ Pa}$$

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

$$n = 2$$

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

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

Using PV = nRT:

$$n = \frac{9.83 \times 10^4 \times 2.41 \times 10^{-4}}{8.31 \times 295} = 9.66 \times 10^{-3} \,\text{mol}$$

This gives the number of moles of O_2 .

From the chemical equation, the number of moles of O_2 is half the number of moles of NaNO₂. Therefore, the number of moles of NaNO₂ is $9.66 \times 10^{-3} \times 2 = 1.93 \times 10^{-2}$ mol.

The molar mass of NaNO₂ is $69.00 \,\mathrm{g}\,\mathrm{mol}^{-1}$, therefore the mass of NaNO₂ is $69.00 \times 1.93 \times 10^{-2} = 1.33 \,\mathrm{g}$.

You would probably say that the room that 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!)



Self-test 11

Test yourself

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

- 34 If a certain mass of an ideal gas occupies $20.0\,\mathrm{cm^3}$ at $0\,^\circ\mathrm{C}$ and $1.01\times10^5\,\mathrm{Pa}$, what volume would it occupy at $38\,^\circ\mathrm{C}$ and $1.06\times10^5\,\mathrm{Pa}$?
- 35 A certain mass of an ideal gas occupies 250.0 cm³ at 20 °C and 9.89 × 10⁴ Pa. At what temperature (in °C) will it occupy 400.0 cm³ if the pressure remains the same?
- 36 How many moles of an ideal gas are present in a container if it occupies a volume of $1.50 \,\mathrm{dm}^3$ at a pressure of $1.10 \times 10^5 \,\mathrm{Pa}$ and a temperature of $30 \,^{\circ}\mathrm{C}$?
- 37 Calculate the molar mass of an ideal gas if $0.586 \,\mathrm{g}$ of the gas occupies a volume of $282 \,\mathrm{cm}^3$ at a pressure of $1.02 \times 10^5 \,\mathrm{Pa}$ and a temperature of $-18 \,\mathrm{^{\circ}C}$.

- 38 What is the molar volume of an ideal gas at 1.10×10^5 Pa and 100 °C?
- **39** Copper nitrate decomposes when heated according to the equation:

 $2Cu(NO_3)_2(s) \rightarrow 2CuO(s) + 4NO_2(g) + O_2(g)$ 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?
- **40** When a certain mass of Mn_2O_7 decomposed, it produced $127.8 \, cm^3$ of oxygen measured at $18 \, ^{\circ}C$ and $1.00 \times 10^5 \, Pa$. What mass of Mn_2O_7 decomposed?

$$2Mn_2O_7(aq) \rightarrow 4MnO_2(s) + 3O_2(g)$$