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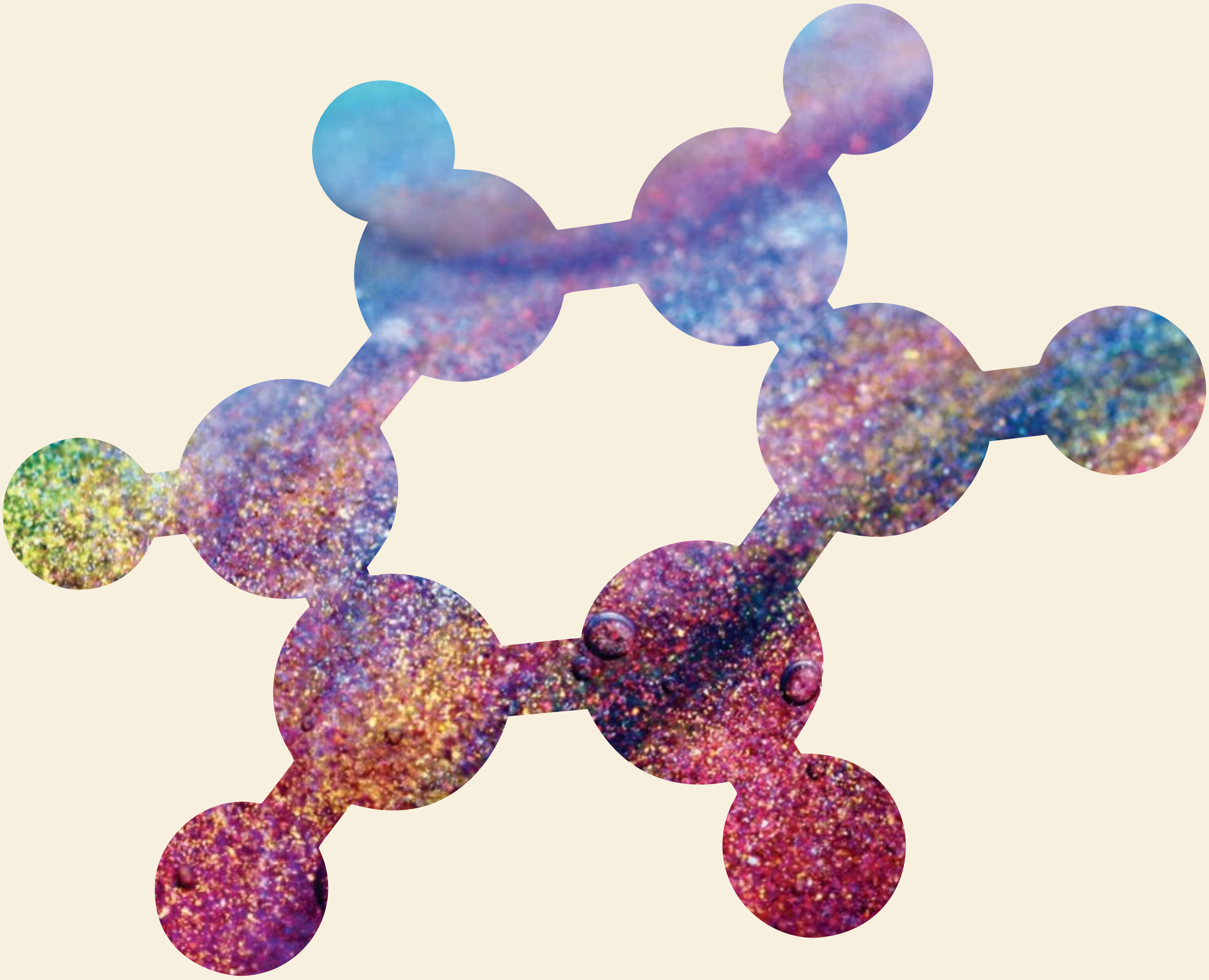

INTERACTIVE
TEXTBOOK
INCLUDED

Cambridge Senior Science

Chemistry

Brett **Drummond**
Simon **Maaser**
Lauren **Angley**
Scott **Fraser**
Trent **Lucas**
Zhen **Wang**

ISBN 978-1-009-22984-5 Drummond et al

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Please be aware that this publication may contain images of Aboriginal and Torres Strait Islander people who are now deceased. Several variations of Aboriginal and Torres Strait Islander terms and spellings may also appear; no disrespect is intended. Please note that the terms 'Indigenous Australians' and 'Aboriginal and Torres Strait Islander peoples' may be used interchangeably in this publication.

Cambridge University Press acknowledges the Australian Aboriginal and Torres Strait Islander peoples of this nation. We acknowledge the traditional custodians of the lands on which our company is located and where we conduct our business. We pay our respects to ancestors and Elders, past and present. Cambridge University Press is committed to honouring Australian Aboriginal and Torres Strait Islander peoples' unique cultural and spiritual relationships to the land, waters and seas and their rich contribution to society.

About the authors

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Scott Fraser has a wide-ranging set of experiences starting with a biomedical science undergraduate degree, followed by a Grad. Dip. Chemistry and PhD in chemistry. He has taught chemistry and biochemistry subjects across all levels of study and also has his own private teaching company that helps guide and support students towards medical careers.

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Contents

UNIT 3

How can design and innovation help to optimise chemical processes?

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UNIT 4

How are carbon-based compounds designed for purpose?

Answers are available in the Interactive Textbook and the Teacher Resources.

Overview: How to use this resource

This overview guides you through all the components of the **print and PDF textbooks**, the **Interactive Textbook (ITB)** and the teacher resources in the **Online Teaching Suite (OTS)**. Users of the award-winning *Cambridge Science 7–10 for the Victorian Curriculum* will recognise some similarities with this senior science resource, including the hosting of the digital material on the Edjin platform, which was developed by *Cambridge HOTmaths* and is already being used successfully by thousands of teachers and students across Victoria.

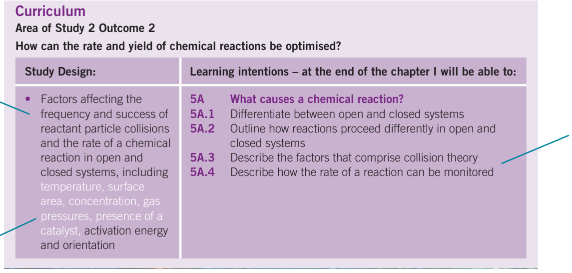
Print book features

Learning intentions

In the Curriculum table at the start of each chapter, the Study Design dot points are translated into Learning Intentions, describing what students should be able to do by the end of the chapter.

Black text indicates the portion of the dot point covered by the section shown in the second column

White text indicates the portion of the dot point covered by other sections



Curriculum
Area of Study 2 Outcome 2
How can the rate and yield of chemical reactions be optimised?

Study Design:		Learning intentions – at the end of the chapter I will be able to:
• Factors affecting the frequency and success of reactant particle collisions and the rate of a chemical reaction in open and closed systems, including temperature, surface area, concentration, gas pressures, presence of a catalyst, activation energy and orientation	**5A**	**What causes a chemical reaction?**
	5A.1	Differentiate between open and closed systems
	5A.2	Outline how reactions proceed differently in open and closed systems
	5A.3	Describe the factors that comprise collision theory
	5A.4	Describe how the rate of a reaction can be monitored

Learning intentions are turned into Success Criteria (achievement standards) at the end of the chapter and are assessed in the Chapter review and tracked in the Checklists

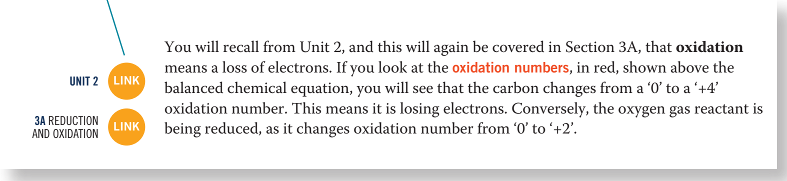
Relevant Study Design dot points are repeated at the start of each section in the chapter, and an overall curriculum grid is provided in the teacher resources.

Concept maps

Concept maps display each chapter's structure with annotations emphasising interconnectedness, providing a great memory aid. The versions in the ITB are hyperlinked and offer an alternative way of navigating through the course. An overall look at all concept maps of Units 3 & 4 is also provided after this overview.

Links

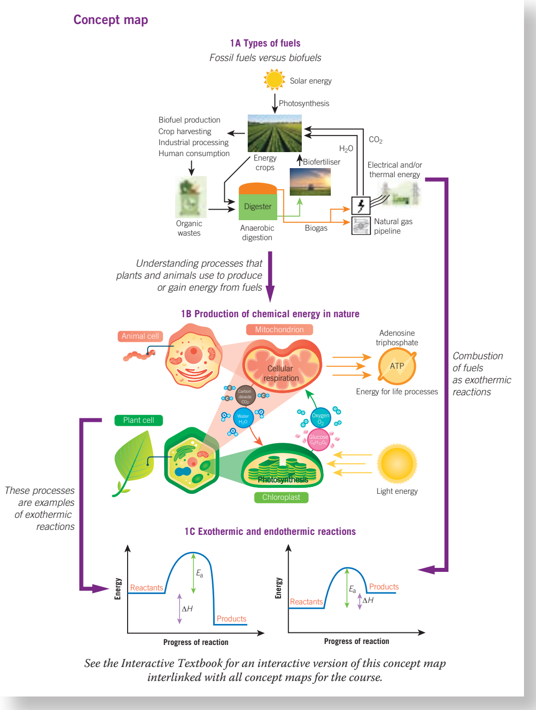
The interconnectedness of topics in VCE Chemistry is demonstrated through links between sections, displayed in the margins. In the ITB, these are hyperlinks that provide an alternative way of navigating through the course.



UNIT 2 LINK

3A REDUCTION AND OXIDATION LINK

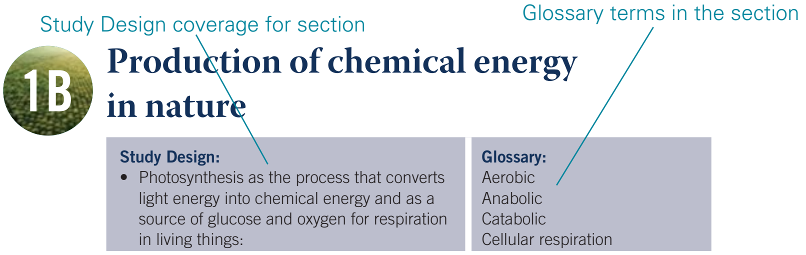
You will recall from Unit 2, and this will again be covered in Section 3A, that **oxidation** means a loss of electrons. If you look at the oxidation numbers, in red, shown above the balanced chemical equation, you will see that the carbon changes from a '0' to a '+4' oxidation number. This means it is losing electrons. Conversely, the oxygen gas reactant is being reduced, as it changes oxidation number from '0' to '+2'.



See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter sections

Chapters are divided into numbered sections, each with a consistent set of features.



Study Design coverage for section

Glossary terms in the section

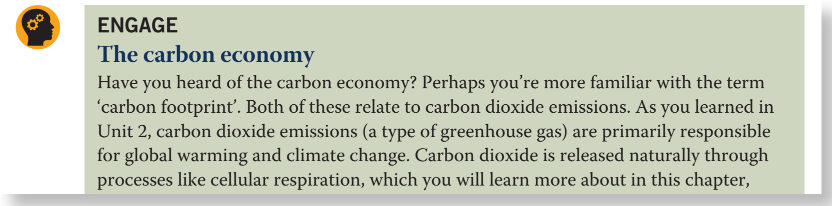
1B Production of chemical energy in nature

Study Design:
- Photosynthesis as the process that converts light energy into chemical energy and as a source of glucose and oxygen for respiration in living things:

Glossary:
Aerobic
Anabolic
Catabolic
Cellular respiration

Engage

At the start of each section, these boxes provide points of interest for the topic, emphasising its place in chemistry. This material, though not assessable, can be used as examples of applications.



ENGAGE

The carbon economy

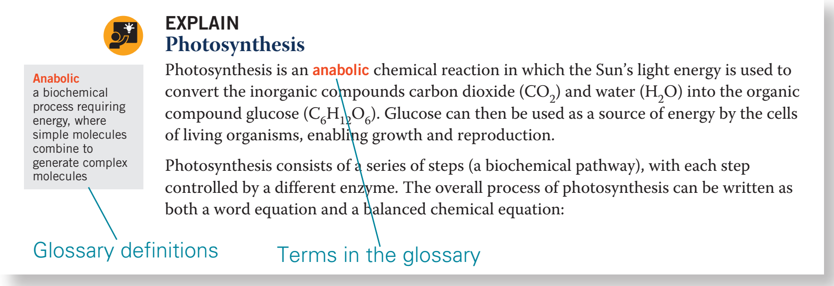
Have you heard of the carbon economy? Perhaps you're more familiar with the term 'carbon footprint'. Both of these relate to carbon dioxide emissions. As you learned in Unit 2, carbon dioxide emissions (a type of greenhouse gas) are primarily responsible for global warming and climate change. Carbon dioxide is released naturally through processes like cellular respiration, which you will learn more about in this chapter,

Explain

This icon marks the start of essential content that is assessed.

Glossary

Scientific terms are highlighted in the text; definitions are given in the margin of the print and PDF textbooks, or on mouseover in the ITB; and the terms are listed at the start of each chapter and section.



EXPLAIN

Photosynthesis

Anabolic a biochemical process requiring energy, where simple molecules combine to generate complex molecules

Photosynthesis is an **anabolic** chemical reaction in which the Sun's light energy is used to convert the inorganic compounds carbon dioxide (CO_2) and water (H_2O) into the organic compound glucose ($C_6H_{12}O_6$). Glucose can then be used as a source of energy by the cells of living organisms, enabling growth and reproduction.

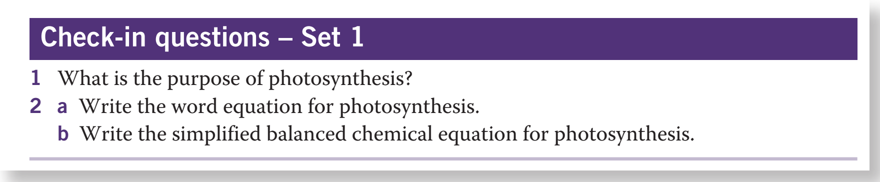
Photosynthesis consists of a series of steps (a biochemical pathway), with each step controlled by a different enzyme. The overall process of photosynthesis can be written as both a word equation and a balanced chemical equation:

Glossary definitions

Terms in the glossary

Check-in questions

Each section in the chapter has one or more sets of check-in questions, for formative assessment. Full answers are provided in the digital resources.



Check-in questions – Set 1

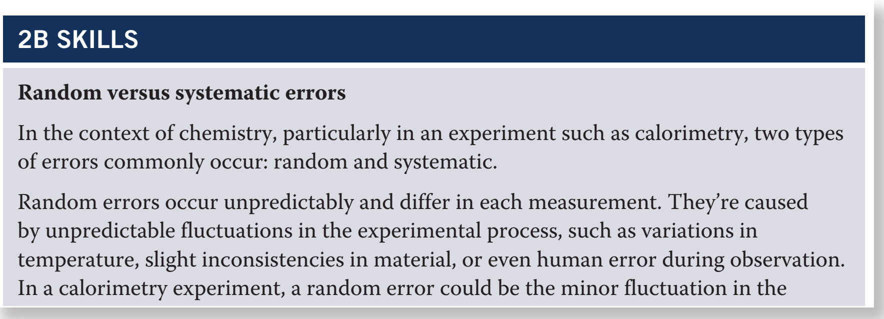
1 What is the purpose of photosynthesis?

2 a Write the word equation for photosynthesis.

b Write the simplified balanced chemical equation for photosynthesis.

Skills

Skills boxes in every section provide advice and guidance on how to answer and prepare for questions, especially in examinations. The ITB has guided video versions of these, which provide extra comments and an alternative medium of delivery.



2B SKILLS

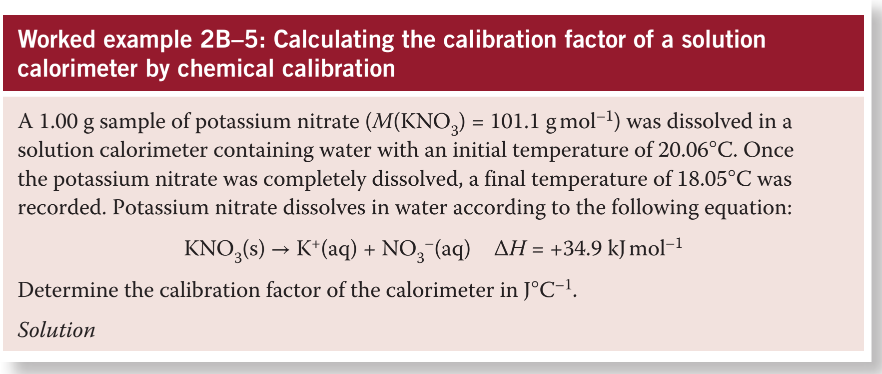
Random versus systematic errors

In the context of chemistry, particularly in an experiment such as calorimetry, two types of errors commonly occur: random and systematic.

Random errors occur unpredictably and differ in each measurement. They're caused by unpredictable fluctuations in the experimental process, such as variations in temperature, slight inconsistencies in material, or even human error during observation. In a calorimetry experiment, a random error could be the minor fluctuation in the

Worked examples

Worked examples are provided for questions requiring computation – for example, in stoichiometry.



Worked example 2B–5: Calculating the calibration factor of a solution calorimeter by chemical calibration

A 1.00 g sample of potassium nitrate ($M(KNO_3) = 101.1\ g\,mol^{-1}$) was dissolved in a solution calorimeter containing water with an initial temperature of 20.06°C. Once the potassium nitrate was completely dissolved, a final temperature of 18.05°C was recorded. Potassium nitrate dissolves in water according to the following equation:

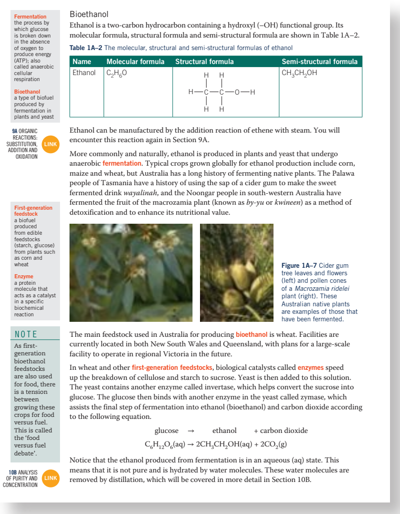
$$KNO_3(s) \rightarrow K^+(aq) + NO_3^-(aq) \quad \Delta H = +34.9\ kJ\,mol^{-1}$$

Determine the calibration factor of the calorimeter in J°C^{-1}.

Solution

Charts, diagrams and tables

Detailed charts integrating text and diagrams, and illustrated tables, feature throughout the print book.



Fermentation the process by which glucose is broken down in the absence of oxygen to produce energy (ATP); also called anaerobic cellular respiration

Bioethanol a type of biofuel produced by fermentation in plants and yeast

9A ORGANIC REACTIONS: SUBSTITUTION, ADDITION AND OXIDATION LINK

First-generation feedstock a biofuel produced from edible feedstocks (starch, glucose) from plants such as corn and wheat

Enzyme a protein molecule that acts as a catalyst in a specific biochemical reaction

NOTE

As first-generation bioethanol feedstocks are also used for food, there is a tension between growing these crops for food versus fuel. This is called the 'food versus fuel debate'.

10B ANALYSIS OF PURITY AND CONCENTRATION LINK

Bioethanol

Ethanol is a two-carbon hydrocarbon containing a hydroxyl (–OH) functional group. Its molecular formula, structural formula and semi-structural formula are shown in Table 1A–2.

Table 1A–2 The molecular, structural and semi-structural formulas of ethanol

Name	Molecular formula	Structural formula	Semi-structural formula
Ethanol	C_2H_6O		CH_3CH_2OH

Ethanol can be manufactured by the addition reaction of ethene with steam. You will encounter this reaction again in Section 9A.

More commonly and naturally, ethanol is produced in plants and yeast that undergo anaerobic **fermentation**. Typical crops grown globally for ethanol production include corn, maize and wheat, but Australia has a long history of fermenting native plants. The Palawa people of Tasmania have a history of using the sap of a cider gum to make the sweet fermented drink *wayalinah*, and the Noongar people in south-western Australia have fermented the fruit of the macrozamia plant (known as *by-yu* or *kwineen*) as a method of detoxification and to enhance its nutritional value.

Figure 1A–7 Cider gum tree leaves and flowers (left) and pollen cones of a *Macrozamia ridelei* plant (right). These Australian native plants are examples of those that have been fermented.

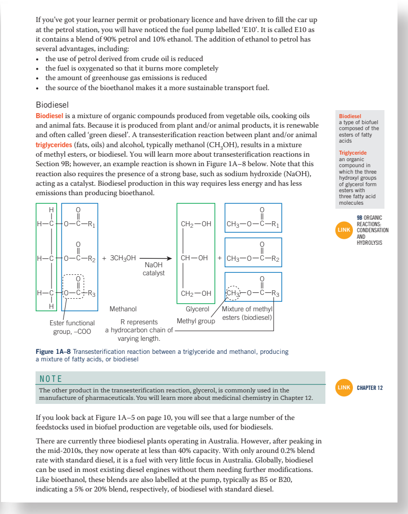
The main feedstock used in Australia for producing **bioethanol** is wheat. Facilities are currently located in both New South Wales and Queensland, with plans for a large-scale facility to operate in regional Victoria in the future.

In wheat and other **first-generation feedstocks**, biological catalysts called **enzymes** speed up the breakdown of cellulose and starch to sucrose. Yeast is then added to this solution. The yeast contains another enzyme called invertase, which helps convert the sucrose into glucose. The glucose then binds with another enzyme in the yeast called zymase, which assists the final step of fermentation into ethanol (bioethanol) and carbon dioxide according to the following equation.

$$\text{glucose} \rightarrow \text{ethanol} + \text{carbon dioxide}$$

$$C_6H_{12}O_6(aq) \rightarrow 2CH_3CH_2OH(aq) + 2CO_2(g)$$

Notice that the ethanol produced from fermentation is in an aqueous (aq) state. This means that it is not pure and is hydrated by water molecules. These water molecules are removed by distillation, which will be covered in more detail in Section 10B.



If you've got your learner permit or probationary licence and have driven to fill the car up at the petrol station, you will have noticed the fuel pump labelled 'E10'. It is called E10 as it contains a blend of 90% petrol and 10% ethanol. The addition of ethanol to petrol has several advantages, including:

- the use of petrol derived from crude oil is reduced
- the fuel is oxygenated so that it burns more completely
- the amount of greenhouse gas emissions is reduced
- the source of the bioethanol makes it a more sustainable transport fuel.

Biodiesel

Biodiesel is a mixture of organic compounds produced from vegetable oils, cooking oils and animal fats. Because it is produced from plant and/or animal products, it is renewable and often called 'green diesel'. A transesterification reaction between plant and/or animal **triglycerides** (fats, oils) and alcohol, typically methanol (CH_3OH), results in a mixture of methyl esters, or biodiesel. You will learn more about transesterification reactions in Section 9B; however, an example reaction is shown in Figure 1A–8 below. Note that this reaction also requires the presence of a strong base, such as sodium hydroxide (NaOH), acting as a catalyst. Biodiesel production in this way requires less energy and has less emissions than producing bioethanol.

Figure 1A–8 Transesterification reaction between a triglyceride and methanol, producing a mixture of fatty acids, or biodiesel

NOTE

The other product in the transesterification reaction, glycerol, is commonly used in the manufacture of pharmaceuticals. You will learn more about medicinal chemistry in Chapter 12.

If you look back at Figure 1A–5 on page 10, you will see that a large number of the feedstocks used in biofuel production are vegetable oils, used for biodiesels.

There are currently three biodiesel plants operating in Australia. However, after peaking in the mid-2010s, they now operate at less than 40% capacity. With only around 0.2% blend rate with standard diesel, it is a fuel with very little focus in Australia. Globally, biodiesel can be used in most existing diesel engines without them needing further modifications. Like bioethanol, these blends are also labelled at the pump, typically as B5 or B20, indicating a 5% or 20% blend, respectively, of biodiesel with standard diesel.

Biodiesel a type of biofuel composed of the esters of fatty acids

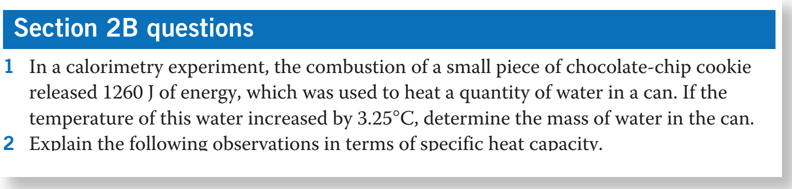
Triglyceride an organic compound in which the three hydroxyl groups of glycerol form esters with three fatty acid molecules

LINK 9B ORGANIC REACTIONS: CONDENSATION AND HYDROLYSIS

LINK CHAPTER 12

Section questions

Summative assessment is provided at the end of each section, again with full answers provided in the digital resources.



Section 2B questions

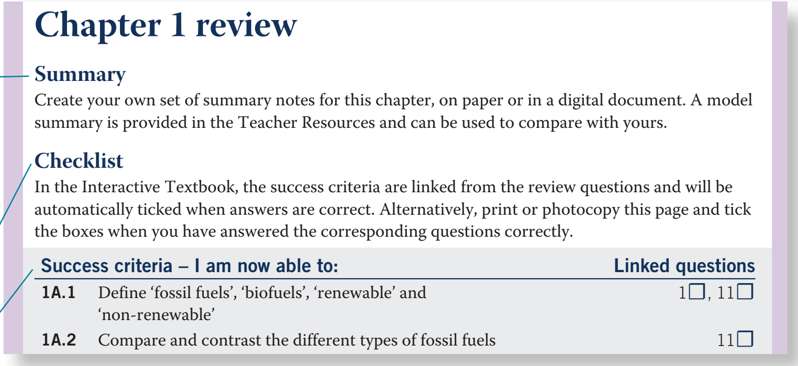
1 In a calorimetry experiment, the combustion of a small piece of chocolate-chip cookie released 1260 J of energy, which was used to heat a quantity of water in a can. If the temperature of this water increased by 3.25°C, determine the mass of water in the can.

2 Explain the following observations in terms of specific heat capacity.

Chapter reviews

Summaries: Students are encouraged to make their own set of summary notes to help them assimilate the material. Model summaries are provided in the Teacher Resources and are to be given to students who need help. Creating summaries can also be turned into an assessment task, with the models serving as the answer.

Checklists and **Success criteria:** The learning intentions from the front of the chapter are listed again in the form of success criteria linked to the **multiple-choice** and **short-answer questions** that follow. The checklists can be printed from the ITB, and students can tick off their achievement manually. If they do the questions in the ITB, they are ticked automatically when the questions are marked.



Chapter 1 review

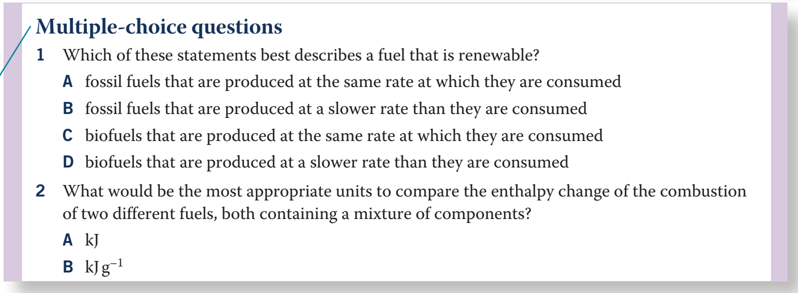
Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
1A.1	Define 'fossil fuels', 'biofuels', 'renewable' and 'non-renewable'	1☐, 11☐
1A.2	Compare and contrast the different types of fossil fuels	11☐



Multiple-choice questions

1 Which of these statements best describes a fuel that is renewable?

A fossil fuels that are produced at the same rate at which they are consumed

B fossil fuels that are produced at a slower rate than they are consumed

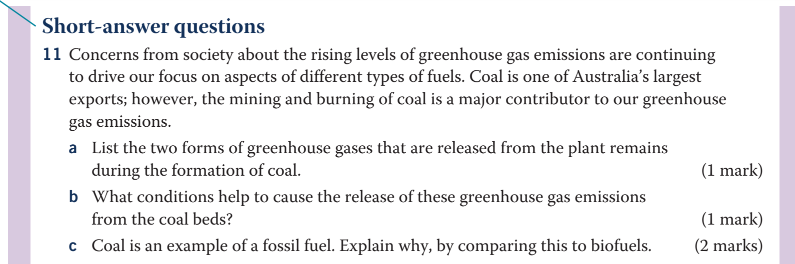
C biofuels that are produced at the same rate at which they are consumed

D biofuels that are produced at a slower rate than they are consumed

2 What would be the most appropriate units to compare the enthalpy change of the combustion of two different fuels, both containing a mixture of components?

A kJ

B $kJ\,g^{-1}$



Short-answer questions

11 Concerns from society about the rising levels of greenhouse gas emissions are continuing to drive our focus on aspects of different types of fuels. Coal is one of Australia's largest exports; however, the mining and burning of coal is a major contributor to our greenhouse gas emissions.

a List the two forms of greenhouse gases that are released from the plant remains during the formation of coal. (1 mark)

b What conditions help to cause the release of these greenhouse gas emissions from the coal beds? (1 mark)

c Coal is an example of a fossil fuel. Explain why, by comparing this to biofuels. (2 marks)

Unit revision exercises

Each Unit has a revision exercise in the print book, with both multiple-choice and short-answer questions.

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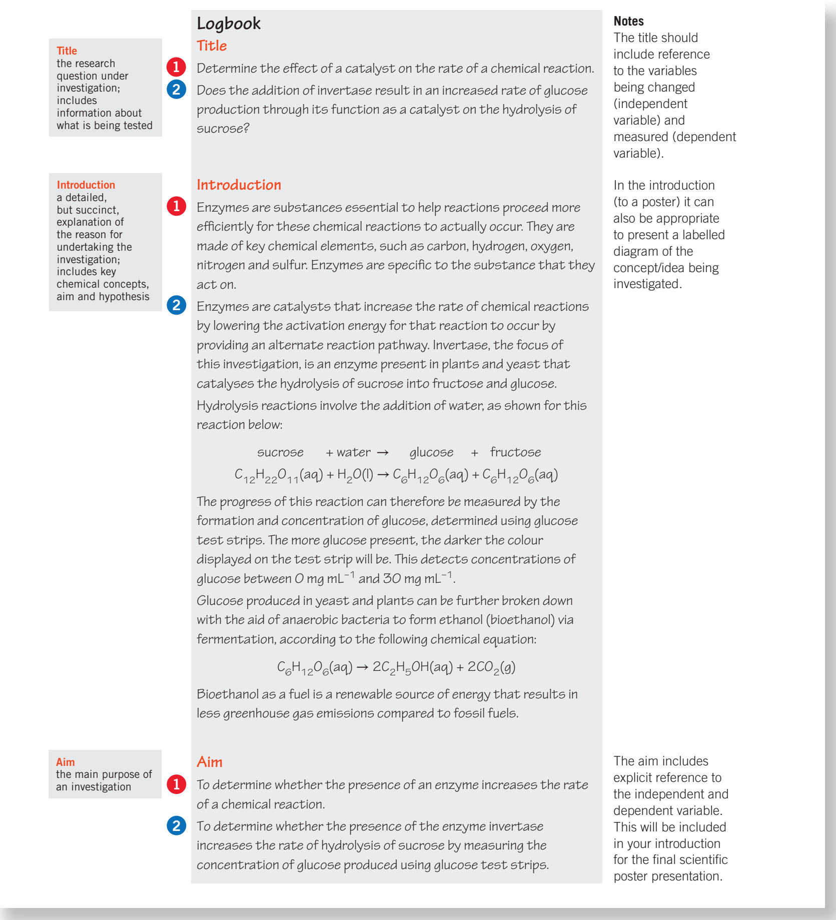
Special content

- **Chapter 13 Scientific investigations** includes the different ways scientific investigations may be undertaken by students. It features the modelling of logbook development for students' own practical investigations, with detailed examples. The digital textbook includes information on other investigation methodologies.



Title
the research question under investigation; includes information about what is being tested

Logbook

Title

① Determine the effect of a catalyst on the rate of a chemical reaction.

② Does the addition of invertase result in an increased rate of glucose production through its function as a catalyst on the hydrolysis of sucrose?

Notes
The title should include reference to the variables being changed (independent variable) and measured (dependent variable).

Introduction
a detailed, but succinct, explanation of the reason for undertaking the investigation; includes key chemical concepts, aim and hypothesis

Introduction

① Enzymes are substances essential to help reactions proceed more efficiently for these chemical reactions to actually occur. They are made of key chemical elements, such as carbon, hydrogen, oxygen, nitrogen and sulfur. Enzymes are specific to the substance that they act on.

② Enzymes are catalysts that increase the rate of chemical reactions by lowering the activation energy for that reaction to occur by providing an alternate reaction pathway. Invertase, the focus of this investigation, is an enzyme present in plants and yeast that catalyses the hydrolysis of sucrose into fructose and glucose.

Hydrolysis reactions involve the addition of water, as shown for this reaction below:

$$\text{sucrose} + \text{water} \rightarrow \text{glucose} + \text{fructose}$$

$$C_{12}H_{22}O_{11}(aq) + H_2O(l) \rightarrow C_6H_{12}O_6(aq) + C_6H_{12}O_6(aq)$$

The progress of this reaction can therefore be measured by the formation and concentration of glucose, determined using glucose test strips. The more glucose present, the darker the colour displayed on the test strip will be. This detects concentrations of glucose between 0 mg mL^{-1} and 30 mg mL^{-1}.

Glucose produced in yeast and plants can be further broken down with the aid of anaerobic bacteria to form ethanol (bioethanol) via fermentation, according to the following chemical equation:

$$C_6H_{12}O_6(aq) \rightarrow 2C_2H_5OH(aq) + 2CO_2(g)$$

Bioethanol as a fuel is a renewable source of energy that results in less greenhouse gas emissions compared to fossil fuels.

In the introduction (to a poster) it can also be appropriate to present a labelled diagram of the concept/idea being investigated.

Aim
the main purpose of an investigation

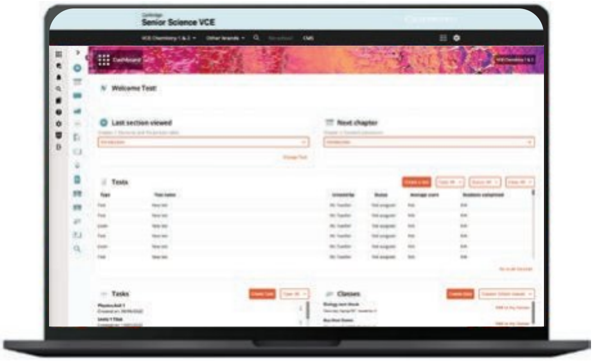
Aim

① To determine whether the presence of an enzyme increases the rate of a chemical reaction.

② To determine whether the presence of the enzyme invertase increases the rate of hydrolysis of sucrose by measuring the concentration of glucose produced using glucose test strips.

The aim includes explicit reference to the independent and dependent variable. This will be included in your introduction for the final scientific poster presentation.

Interactive Textbook features



The digital version of the textbook is hosted on the Edjin platform, offering easy navigation, excellent on-screen display and multimedia assets, as well as auto-marking of multiple-choice questions, and workspaces for other questions with self-assessment and confidence-rating tools. The different kinds of digital assets are listed below:

WORKSHEET 1A–1
COMPARING FUELS

VIDEO 3A–1
SKILLS: IMPORTANCE OF OXIDATION NUMBERS

- Printable **worksheets** with extra questions and activities (and content in some cases) are provided for most chapters, marked by an icon in the margin, as shown on the right.
- **Videos** are provided for all chapters and are of two kinds: **concept videos** demonstrate or illustrate important theory, while **skills and example videos** work through the textbook's skills and example boxes, providing extra explanation and guidance. Some videos are provided in the print pages as QR codes for immediate access and review.
- **Answers** (suggested responses) to questions are provided as printable documents in the teacher resources and, if enabled by the teacher, below the question there are workspaces for short-answer questions in the ITB.
- **Prior knowledge** can be tested with an auto-marked quiz with questions from the Year 9 and 10 titles in the *Cambridge Science for the Victorian Curriculum* series.

Online Teaching Suite features (teacher resources)

The OTS provides Edjin's learning management system, which allows teachers to set tasks, track progress and scores, prepare reports on individuals and the class, and give students feedback. The assets include:

- **Curriculum Grid** and **teaching programs**
- Editable and printable **Chapter tests** with answers
- **Checklists** with linkage to the success criteria for the chapter question sets and tests
- A **question bank** and test generator, with answers
- **Practice exams** and **assessment tasks**, with answers
- Editable versions of **Worksheets** in the Interactive Textbook, and answers to them
- Downloadable, editable and printable **practicals**
- Editable and printable chapter **summaries** (model answers for the chapter summary activity)
- **Teacher notes** on selected content with additional theory explanation and suggestions for further activities and resources
- **Curated links** to internet resources, such as videos and interactives.

Exam generator

The Online Teaching Suite includes a comprehensive bank of exam-style and actual VCAA exam questions to create custom trial exams to target topics that students are having difficulty with. Features include:

- Filtering by question-type, topic and degree of difficulty
- Answers provided to teachers
- VCAA marking scheme
- Multiple-choice questions that will be auto-marked if completed online
- Tests that can be downloaded and used in class or for revision.

Overview: Aboriginal and Torres Strait Islander knowledge, cultures and history

The VCE Chemistry Study Design includes aspects of Aboriginal and Torres Strait Islander knowledge, cultures and history. This overview is a guide to coverage in this resource.

Aboriginal and Torres Strait Islander peoples' world views are highly integrated: each aspect of culture, history and society connects with all other aspects. Each community has their own personalised system of thinking, doing and knowing based on sharing culture and adapting to the environment around them.

In order to gain an understanding of any system, Indigenous or not, time and effort is needed to appreciate it. That time is limited in this course; and it is wrong to try and generalise the Indigenous culture of Australia, or even of Victoria. Instead, the coverage in the resource should be taken as a collection of examples, and students should read up on or engage with their local Indigenous community to understand their cultural aspects.

This textbook includes examples of Aboriginal and Torres Strait Islander knowledge, cultures and history and in addition, for students, the Interactive Textbook includes an introductory guide prepared by First Nations consultants advising on approaches to studying this material, with links to further reading.

For teachers, the teacher resources include a guide to approaches to teaching Aboriginal and Torres Strait Islander knowledge, cultures and history in the VCE Chemistry course, with links to internet resources.

Guide to terms used in this resource

Language is very important in discussing Indigenous issues, especially given the past history of deliberately offensive usage in Australia, where language was used to oppress and control.

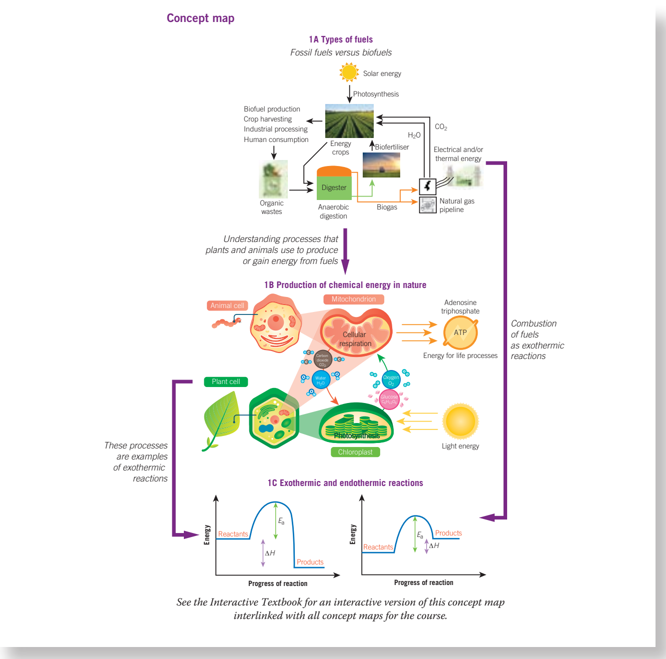
Indigenous First Australians and First Peoples of any country	Respectful usage requires a capital 'I'.
First Australians, First Nations or First Peoples Indigenous people of Australia	These terms have become more common in recent years, with 'Indigenous' as the adjective.
Aboriginal an Aboriginal person is someone who is of Aboriginal descent, identifies as being Aboriginal and is accepted as such by the Aboriginal community with which they originally identified	One of the reasons that 'First Nations' and allied forms have become more common is that the term 'Aboriginal' was sometimes used disrespectfully, and still is in some circles.
Aboriginal and Torres Strait Islander peoples the Australian Indigenous population includes Aboriginal People, Torres Strait Islander People, and people who have both Aboriginal and Torres Strait Islander heritage. The term 'Aboriginal and Torres Strait Islander' encompasses all three	While this is still used in official circles and is in the name or title of many organisations and documents, it is tending to be replaced by 'First Australians' and similar terms, especially in everyday use. This is partly because the abbreviation 'ATSI' is considered disrespectful by Indigenous people, who regard it as lazy not to use a full title. The abbreviation should not be used to refer to people.

Cambridge University Press & Assessment acknowledges the Australian Aboriginal and Torres Strait Islander peoples of this nation. We acknowledge the traditional custodians of the lands on which our company is located and where we conduct our business. We pay our respects to ancestors and Elders, past and present.

Concept maps for Units 3&4

Pages xiii–xvi display the concept maps for topics in Chapters 1–13. Access the digital version of this concept map in the ITB to zoom in on the details and click on hyperlinks to explore the interconnections of the topics.

Chapter 1
Carbon-based fuels


Concept map

1A Types of fuels
Fossil fuels versus biofuels

Understanding processes that plants and animals use to produce or gain energy from fuels

1B Production of chemical energy in nature

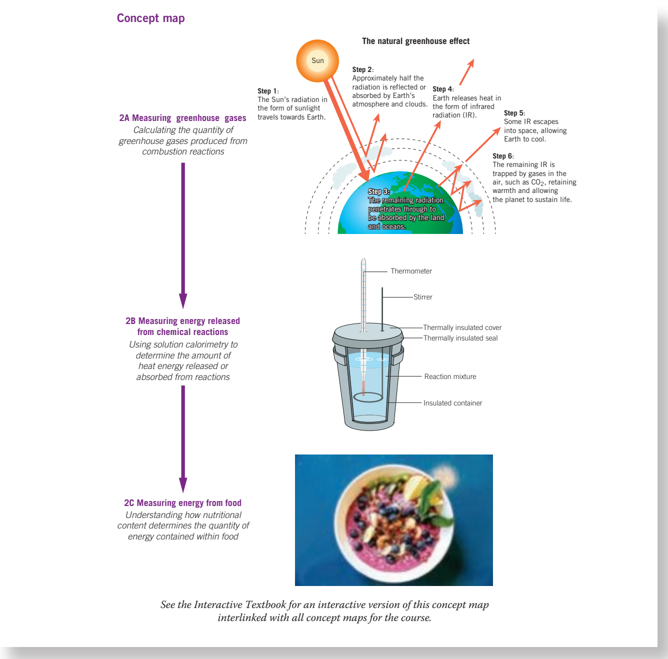
Combustion of fuels as exothermic reactions

These processes are examples of exothermic reactions

1C Exothermic and endothermic reactions

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 2 Measuring changes in chemical reactions


Concept map

2A Measuring greenhouse gases
Calculating the quantity of greenhouse gases produced from combustion reactions

2B Measuring energy released from chemical reactions
Using solution calorimetry to determine the amount of heat energy released or absorbed from reactions

2C Measuring energy from food
Understanding how nutritional content determines the quantity of energy contained within food

The natural greenhouse effect

Step 1: The Sun's radiation in the form of sunlight travels towards Earth.

Step 2: Approximately half the radiation is reflected or absorbed by Earth's atmosphere and clouds.

Step 3: The remaining radiation penetrates through to be absorbed by the land and oceans.

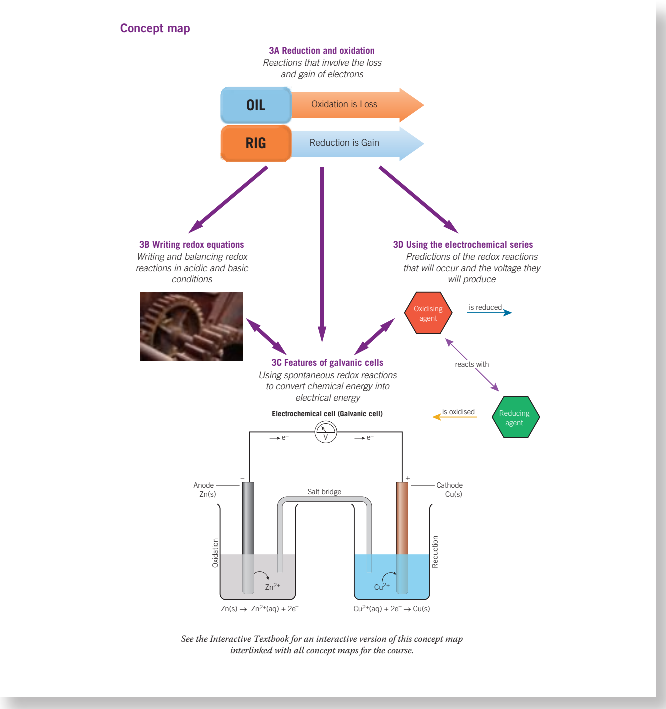
Step 4: Earth releases heat in the form of infrared radiation (IR).

Step 5: Some IR escapes into space, allowing Earth to cool.

Step 6: The remaining IR is trapped by gases in the air, such as CO$_2$, retaining warmth and allowing the planet to sustain life.

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 3 Galvanic cells


Concept map

3A Reduction and oxidation
Reactions that involve the loss and gain of electrons

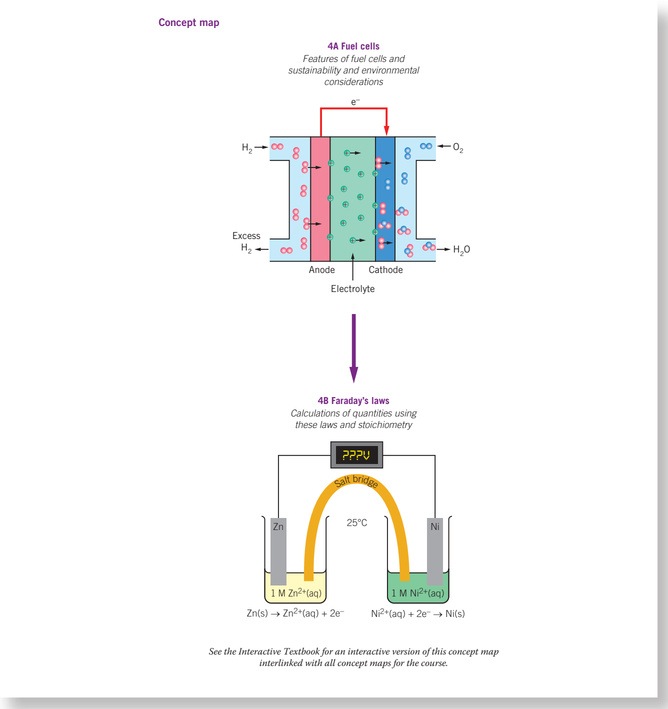
3B Writing redox equations
Writing and balancing redox reactions in acidic and basic conditions

3D Using the electrochemical series
Predictions of the redox reactions that will occur and the voltage they will produce

3C Features of galvanic cells
Using spontaneous redox reactions to convert chemical energy into electrical energy

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 4 Fuel cells

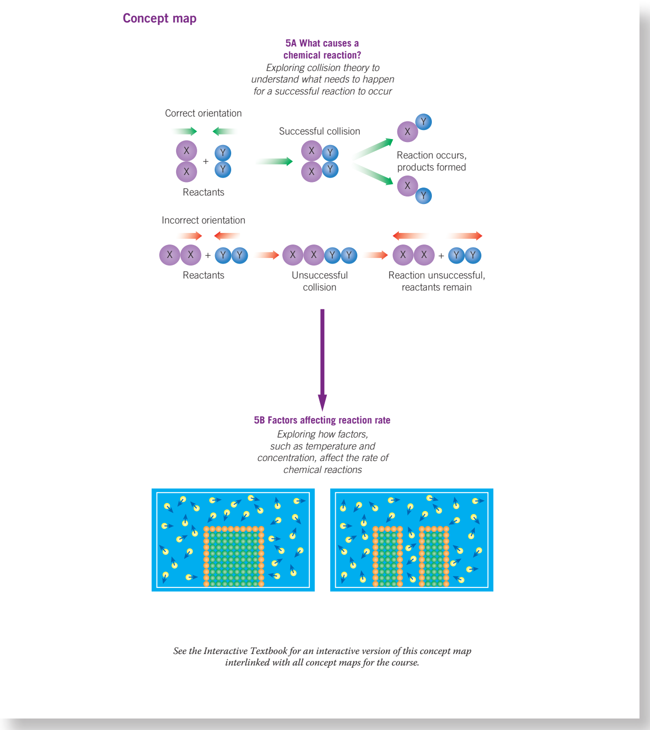

Concept map

4A Fuel cells
Features of fuel cells and sustainability and environmental considerations

4B Faraday's laws
Calculations of quantities using these laws and stoichiometry

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 5
Rates of reaction



Concept map

5A What causes a chemical reaction?

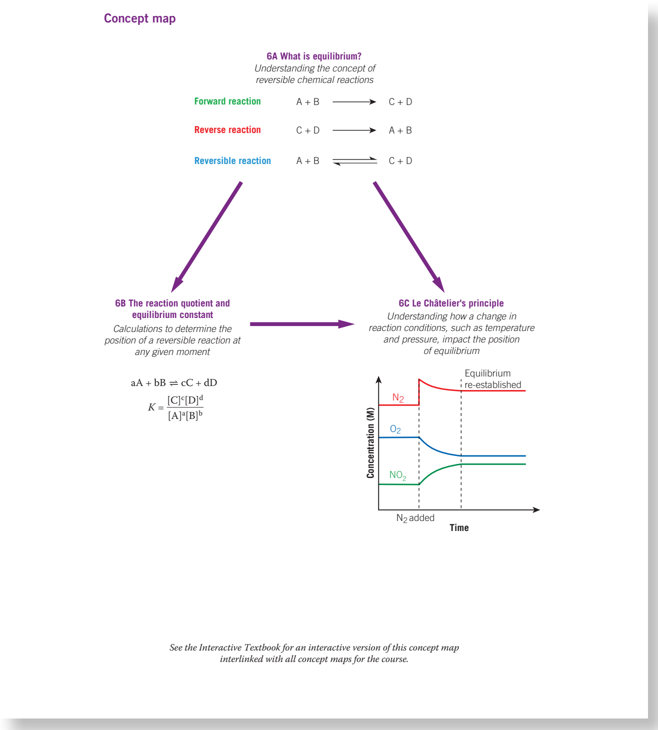
Exploring collision theory to understand what needs to happen for a successful reaction to occur

5B Factors affecting reaction rate

Exploring how factors, such as temperature and concentration, affect the rate of chemical reactions

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 6
Equilibrium



Concept map

6A What is equilibrium?

Understanding the concept of reversible chemical reactions

Forward reaction A + B $\rightarrow$ C + D

Reverse reaction C + D $\rightarrow$ A + B

Reversible reaction A + B $\rightleftharpoons$ C + D

6B The reaction quotient and equilibrium constant

Calculations to determine the position of a reversible reaction at any given moment

$aA + bB \rightleftharpoons cC + dD$

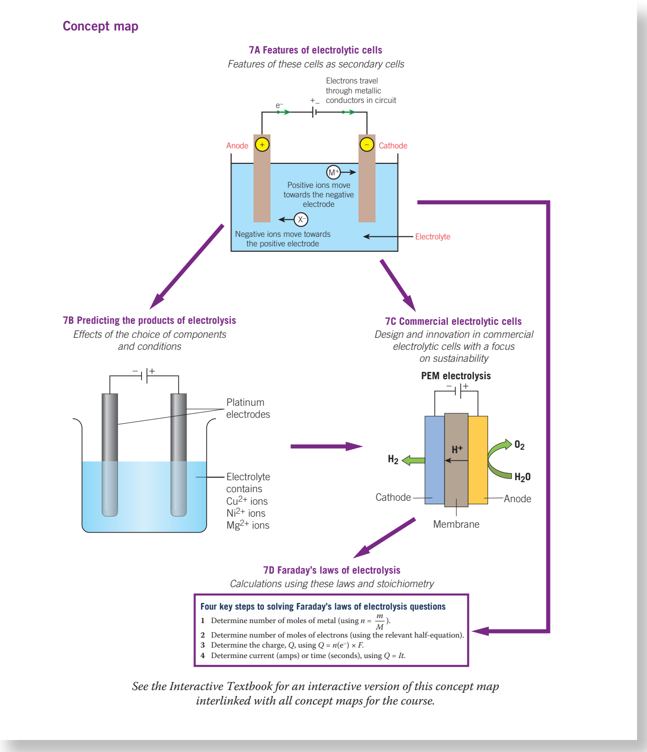
$$K = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

6C Le Châtelier's principle

Understanding how a change in reaction conditions, such as temperature and pressure, impact the position of equilibrium

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 7 Electrolytic cells



Concept map

7A Features of electrolytic cells

Features of these cells as secondary cells

7B Predicting the products of electrolysis

Effects of the choice of components and conditions

7C Commercial electrolytic cells

Design and innovation in commercial electrolytic cells with a focus on sustainability

7D Faraday's laws of electrolysis

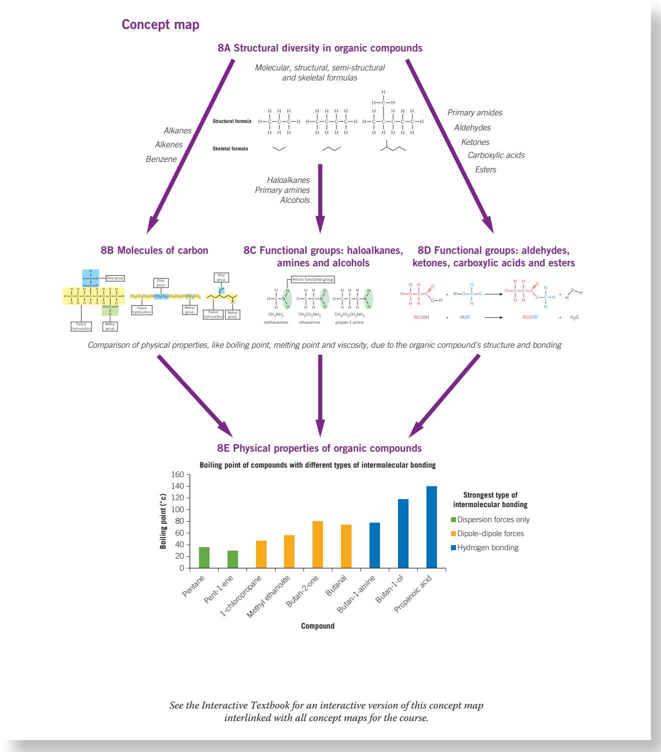
Calculations using these laws and stoichiometry

Four key steps to solving Faraday's laws of electrolysis questions

1 Determine number of moles of metal (using $n = \frac{m}{M}$).
2 Determine number of moles of electrons (using the relevant half-equation).
3 Determine the charge, Q, using $Q = n(e^-) \times F$.
4 Determine current (amps) or time (seconds), using $Q = It$.

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 8 Structure and properties of organic compounds



Concept map

8A Structural diversity in organic compounds

Molecular, structural, semi-structural and skeletal formulas

8B Molecules of carbon

8C Functional groups: haloalkanes, amines and alcohols

8D Functional groups: aldehydes, ketones, carboxylic acids and esters

Comparison of physical properties, like boiling point, melting point and viscosity, due to the organic compound's structure and bonding

8E Physical properties of organic compounds

Boiling point of compounds with different types of intermolecular bonding

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

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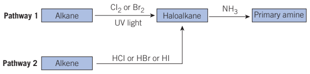
Chapter 9 Reactions of organic compounds

Concept map

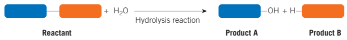
9A Organic reactions: substitution, addition and oxidation

Writing equations and drawing reaction pathways



9B Organic reactions: condensation and hydrolysis

Writing equations and drawing reaction pathways



Calculating % yield and atom economy with a view on Green Chemistry Principles

9C Designing sustainable organic reactions

1. Waste prevention
2. Atom economy
3. Less hazardous chemical syntheses
4. Design safer chemicals
5. Safer solvents and auxiliaries
6. Design for energy efficiency
7. Use renewable feedstocks
8. Reduce derivatives
9. Catalysis
10. Design for degradation
11. Real-time analysis for pollution prevention
12. Inherently safer chemistry for accident prevention

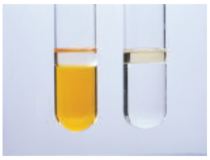
See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 10 Laboratory analysis of organic compounds

Concept map

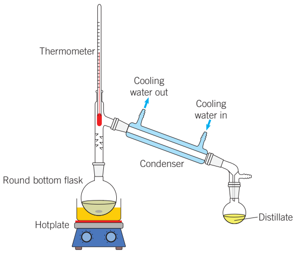
10A Analysis of functional groups

Qualitative tests to determine the presence of carbon-carbon double bonds and hydroxyl and carboxyl functional groups



10B Analysis of purity and concentration

Experimental techniques, including distillation, melting point determination and volumetric analysis, to determine purity and concentration



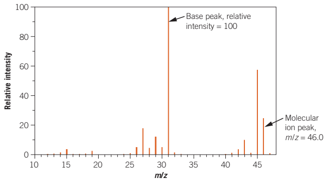
See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 11 Instrumental analysis of organic compounds

Concept map

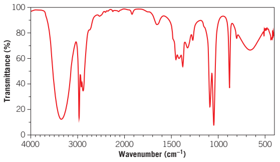
11A Mass spectrometry

Technique for determining the mass and identity of organic compounds



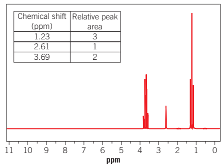
11B Infrared spectroscopy

Technique for identifying functional groups in organic compounds



11C Nuclear magnetic resonance spectroscopy

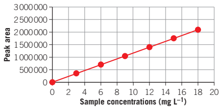
Technique for determining the identity and structure of organic compounds



Chemical shift (ppm)	Relative peak area
1.23	3
2.61	1
3.69	2

11D Chromatography

Technique for separating organic compounds in mixtures, analysing purity and determining concentration



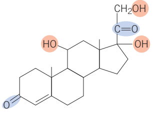
See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

Chapter 12 Medicinal chemistry

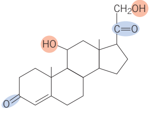
Concept map

12A Organic compounds as medicines

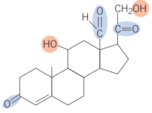
Developing medicine using compounds found in nature and identifying key functional groups that make medicine effective



Cortisol



Corticosterone

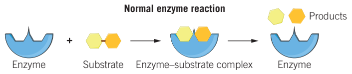


Aldosterone

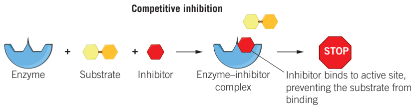
12B Enzymes

Biological catalysts that speed up chemical reactions and can be used as therapeutic targets

Normal enzyme reaction



Competitive inhibition



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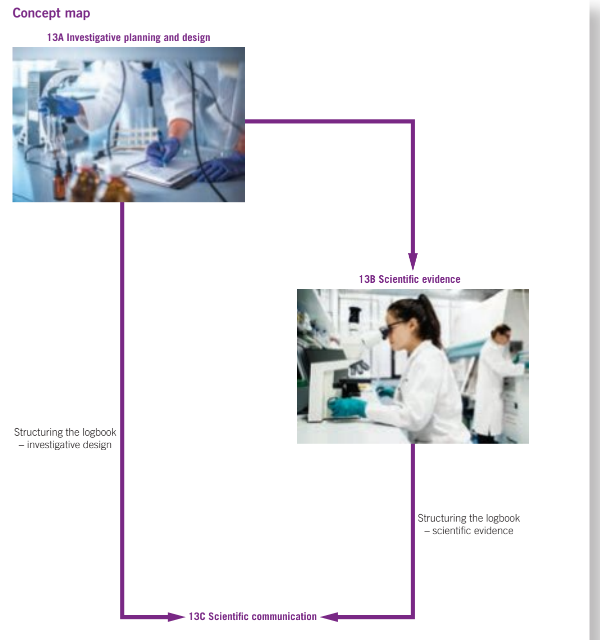
Chapter 13 Scientific investigations



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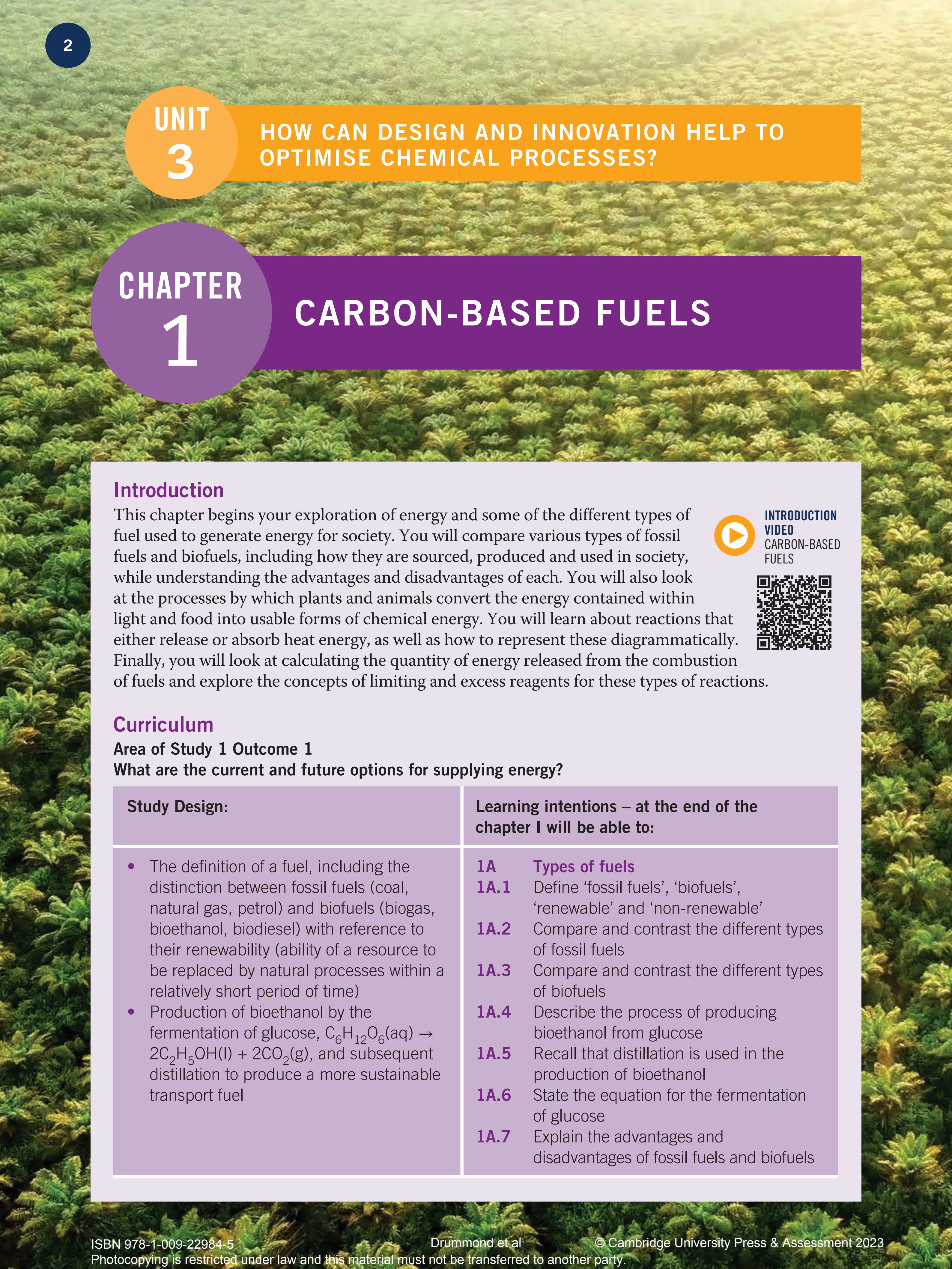

UNIT 3

HOW CAN DESIGN AND INNOVATION HELP TO OPTIMISE CHEMICAL PROCESSES?

CHAPTER 1

CARBON-BASED FUELS

Introduction

This chapter begins your exploration of energy and some of the different types of fuel used to generate energy for society. You will compare various types of fossil fuels and biofuels, including how they are sourced, produced and used in society, while understanding the advantages and disadvantages of each. You will also look at the processes by which plants and animals convert the energy contained within light and food into usable forms of chemical energy. You will learn about reactions that either release or absorb heat energy, as well as how to represent these diagrammatically. Finally, you will look at calculating the quantity of energy released from the combustion of fuels and explore the concepts of limiting and excess reagents for these types of reactions.

INTRODUCTION VIDEO
CARBON-BASED FUELS

Curriculum

Area of Study 1 Outcome 1
What are the current and future options for supplying energy?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• The definition of a fuel, including the distinction between fossil fuels (coal, natural gas, petrol) and biofuels (biogas, bioethanol, biodiesel) with reference to their renewability (ability of a resource to be replaced by natural processes within a relatively short period of time) • Production of bioethanol by the fermentation of glucose, $C_6H_{12}O_6(aq) \rightarrow 2C_2H_5OH(l) + 2CO_2(g)$, and subsequent distillation to produce a more sustainable transport fuel	**1A Types of fuels** **1A.1** Define 'fossil fuels', 'biofuels', 'renewable' and 'non-renewable' **1A.2** Compare and contrast the different types of fossil fuels **1A.3** Compare and contrast the different types of biofuels **1A.4** Describe the process of producing bioethanol from glucose **1A.5** Recall that distillation is used in the production of bioethanol **1A.6** State the equation for the fermentation of glucose **1A.7** Explain the advantages and disadvantages of fossil fuels and biofuels

Study Design:	**Learning intentions – at the end of the chapter I will be able to:**
- Photosynthesis as the process that converts light energy into chemical energy and as a source of glucose and oxygen for respiration in living things: $6CO_2(g) + 6H_2O(l) \rightarrow C_6H_{12}O_6(aq) + 6O_2(g)$ - Oxidation of glucose as the primary carbohydrate energy source, including the balanced equation for cellular respiration: $C_6H_{12}O_6(aq) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l)$	**1B Production of chemical energy in nature** **1B.1** Describe the process of photosynthesis **1B.2** State the equation for photosynthesis **1B.3** Describe the process of cellular respiration **1B.4** State the equation for cellular respiration
- Comparison of exothermic and endothermic reactions, with reference to bond making and bond breaking, including enthalpy changes (ΔH) measured in kJ, molar enthalpy changes measured in $kJ\,mol^{-1}$ and enthalpy changes for mixtures measured in $kJ\,g^{-1}$, and their representations in energy profile diagrams - Determination of limiting reactants or reagents in chemical reactions - Combustion (complete and incomplete) reactions of fuels as exothermic reactions; the writing of balanced thermochemical equations, including states, for the complete and incomplete combustion of organic molecules using experimental data and data tables	**1C Exothermic and endothermic reactions** **1C.1** Compare and contrast exothermic and endothermic reactions **1C.2** Define 'activation energy' **1C.3** Define 'enthalpy' and 'enthalpy change' **1C.4** Draw and fully label energy profiles for exothermic and endothermic reactions **1C.5** Identify the limiting reagent in a given chemical reaction **1C.6** Calculate the mass, concentration or volume of various reactants or products in a given chemical equation when a limiting reagent is present **1C.7** Compare complete and incomplete combustion reactions of fuels **1C.8** State that all combustion reactions are exothermic **1C.9** Determine the balanced thermochemical equation for complete and incomplete combustion of organic molecules

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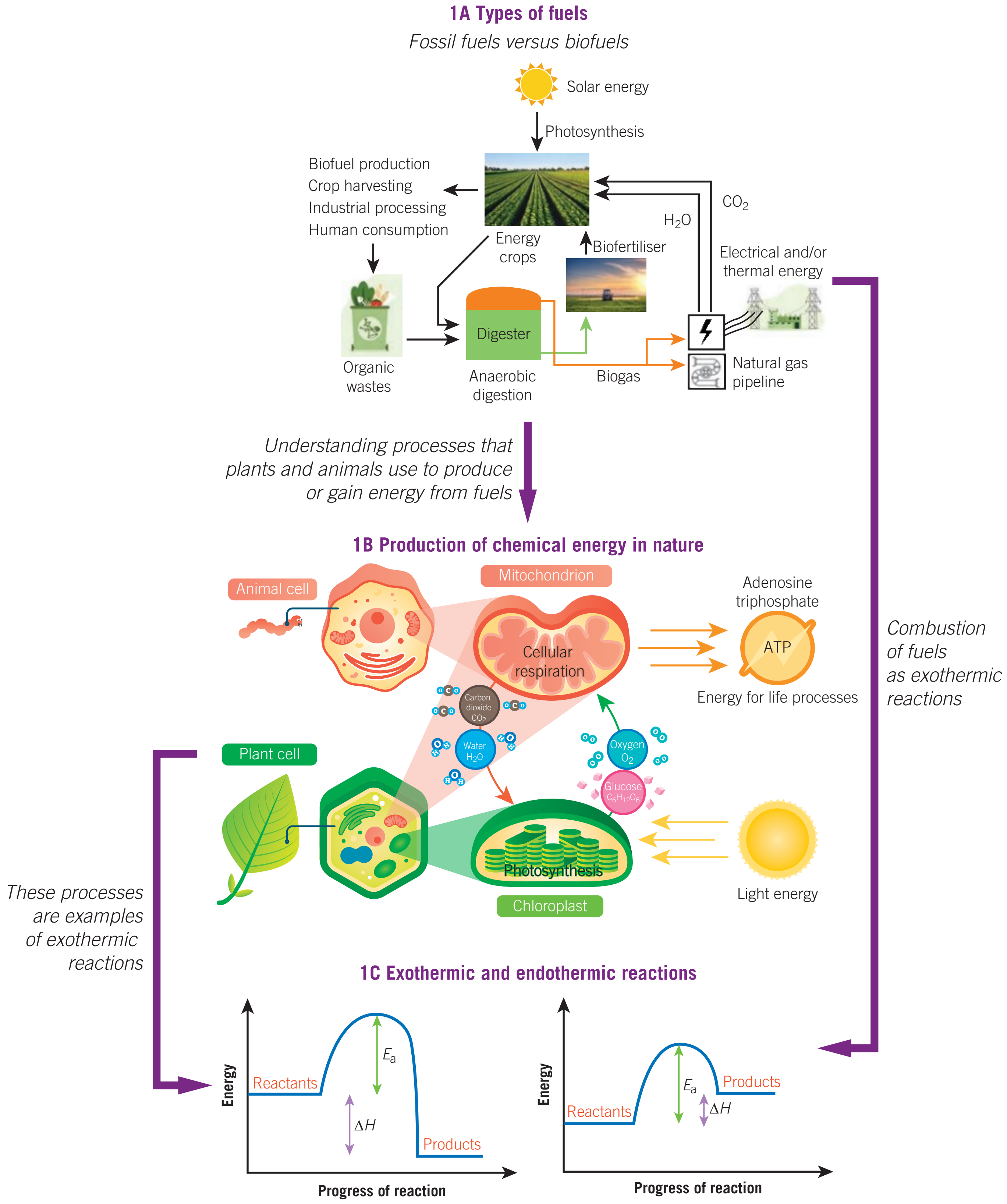
Glossary

Activation energy
Aerobic
Anabolic
Anaerobic
Biodiesel
Bioethanol
Biofuel
Biogas
Biomass
Catabolic
Cellular respiration
Coal
Complete combustion
Crude oil
Endothermic
Enthalpy
Enthalpy change
Enzyme
Exothermic
Fermentation
First-generation feedstock
Fossil fuel
Fracking
Fractional distillation
Fuel
Incomplete combustion
Inorganic
Natural gas
Non-renewable
Organic
Oxidation number
Oxidised
Photosynthesis
Renewable
Triglyceride

Concept map



See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

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1A

Types of fuels

Study Design:

- The definition of a fuel, including the distinction between fossil fuels (coal, natural gas, petrol) and biofuels (biogas, bioethanol, biodiesel) with reference to their renewability (ability of a resource to be replaced by natural processes within a relatively short period of time)
- Production of bioethanol by the fermentation of glucose, $C_6H_{12}O_6(aq) \rightarrow 2C_2H_5OH(l) + 2CO_2(g)$, and subsequent distillation to produce a more sustainable transport fuel

Glossary:

Anaerobic
Biodiesel
Bioethanol
Biofuel
Biogas
Biomass
Coal
Crude oil
Enzyme
Fermentation
First-generation feedstock
Fossil fuel
Fracking
Fractional distillation
Fuel
Inorganic
Natural gas
Non-renewable
Organic
Photosynthesis
Renewable
Triglyceride

ENGAGE

Australia's first petrol-driven car

When Harley Tarrant was young, his father owned the *Clunes Gazette*, the *St Kilda Chronicle* and the *Prahran Chronicle*. As such, Harley was surrounded by information from overseas publications, and from these articles he learned about, and became obsessed with, cars.

Figure 1A–1 The vehicle shown in this photo is the first two-seater, two-cylinder petrol engine automobile built and sold in Australia, by Harley Tarrant and Howard Lewis in 1901.

Later, when working on the Nullarbor Plain as a surveyor, he determined that steam and electric vehicles would not be suitable to tackle the harsh Australian outback. In 1897, he decided to build a kerosene engine with bicycle-maker, Howard Lewis. Due to the high temperature at which kerosene vaporises, it was not suitable as a fuel for a car engine, but it was ideal for pumping water. His engine sold extremely well across Australia, providing him funding to continue working on a suitable fuel and engine for an automobile.

Following this, Tarrant and Lewis set out to build their own petrol-driven car, which used an imported Benz engine. After successfully developing a two-cylinder petrol motor car in 1901, they refined it further with their own locally made engine. At the time, they decided to sacrifice speed for a car that would thrive in Australian conditions. Since then, and especially recently, the use of different fuels has continued to evolve from fossil fuels to biofuels, and now the push to fully electric vehicles. Fossil fuels and biofuels, with a focus on their renewability, are discussed further in this section.

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EXPLAIN

What are fuels and why do we need them?

Likely, when you hear the word ‘fuel’, you think about petrol, diesel or coal used to power planes, trains and automobiles. However, as you will see later in this chapter, food, such as sugar, is also used as a fuel for our bodies.

Fuel
any substance that stores chemical energy

1C EXOTHERMIC AND ENDOTHERMIC REACTIONS LINK

Fuels are both **organic** and **inorganic** substances capable of storing chemical energy. In this section, we will look at only organic fuels. As you will see in Section 1C, when a fuel is burned, the stored chemical energy is released as heat (thermal) energy, which can then be further used to power objects.

Organic
a chemical that contains both carbon and hydrogen (hydrocarbons) or substances obtained from plants and animals

Inorganic
a chemical that does not contain both carbon and hydrogen or contains substances obtained from minerals

You should be familiar with the units of energy from earlier years in science. The International System of Units (SI) unit for energy is the joule, J.

Fossil fuels

Fossil fuels are mostly hydrocarbons, with some other minor impurities, as you learned about in Unit 1 and will learn more about in Unit 4. They are called ‘fossil’ fuels, as they are formed through the fossilised remains and subsequent decay of plants, animals and microorganisms, which lived millions of years ago. The hydrocarbon remains are extracted through mining and the drilling of wells both on land and at sea. These remains still contain some of the chemical energy that the plants, and the plants consumed by animals at the time, originally stored from transforming light energy from the Sun when carrying out **photosynthesis**. Photosynthesis as a chemical process will be covered further in Section 1B.

UNIT 1 LINK

1B PRODUCTION OF CHEMICAL ENERGY IN NATURE LINK

Fossil fuels are **non-renewable**, meaning their availability is limited and they are being consumed at a rate faster than they are being produced. As these fossil fuels are formed over millions of years, once they are depleted, they will not be replaced any time soon.

Fossil fuels can be separated into three main categories: coal, natural gas and petroleum.

Fossil fuel
a source of fuel made from decomposing plants and animals over hundreds of millions of years. It consists mainly of carbon and hydrogen atoms

Photosynthesis
a chemical reaction in which light energy is used to convert the inorganic compounds carbon dioxide, CO_2, and water, H_2O, into the organic compound glucose; *photo* = light, *synthesis* = build or put together

Non-renewable
limited or not capable of being replenished at a rate equal to consumption

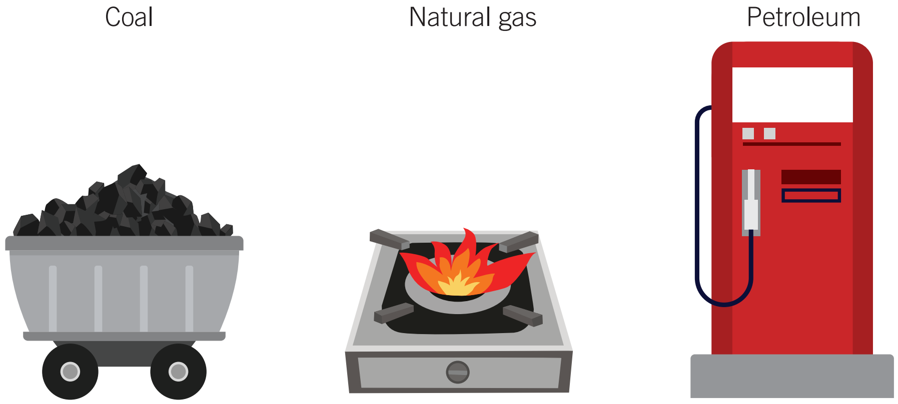

Figure 1A–2 The three main categories of fossil fuels, all of which contain carbon and hydrogen, with other minor impurities

Coal

Coal is a layer of sedimentary rock formed underground, containing mostly plant remains, that are then buried by further sediments. It is formed under low oxygen conditions at high temperatures and pressures over millions of years. Coal formations are called 'coal beds' and they exist globally. The deeper the coal bed, the higher its rank, where the ranking is based on how much it has changed over time. Deeper underground, the plant matter experiences higher temperatures and pressures, and so more of the plant remains are transformed into carbon, while water (H_2O), carbon dioxide (CO_2) and methane (CH_4) escape. The methane that is produced is trapped as coal seam gas. The higher the percentage of carbon, the better the coal fuel source.

Coal
sedimentary rock containing plant remains formed over millions of years

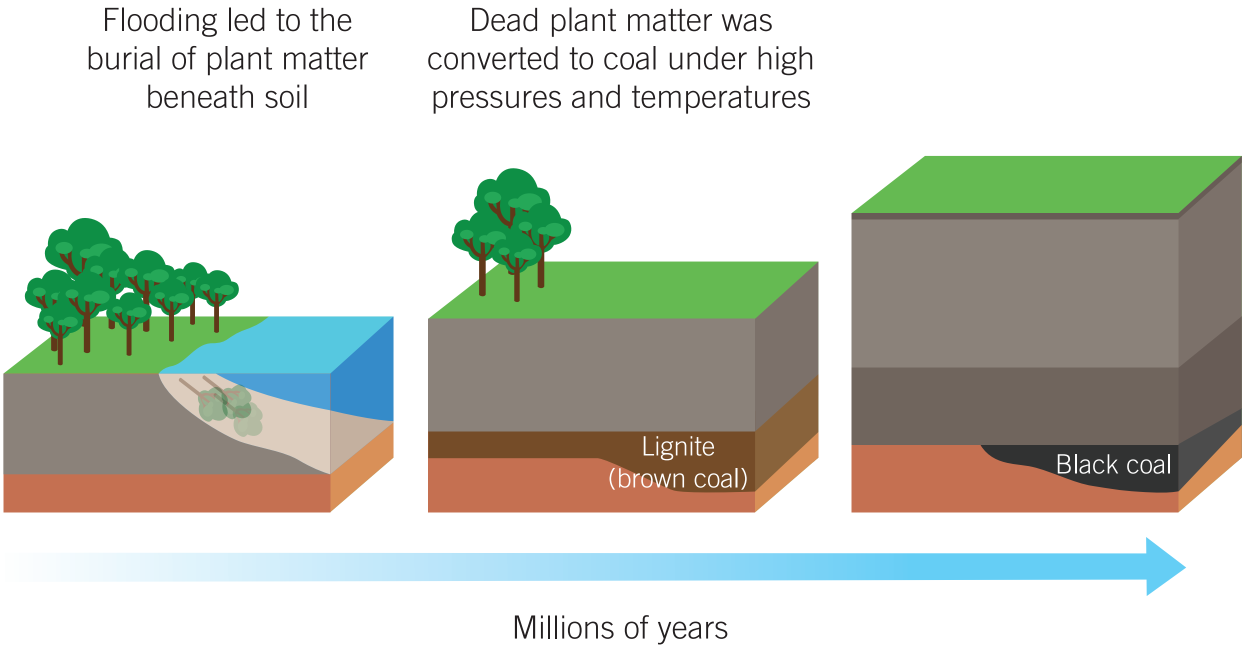

Figure 1A–3 The formation and existence of different coal layers

Coal is the most abundant of the fossil fuels and is the largest fuel source used for generating electricity in the world. Coal is Australia's largest energy resource. It is mined in every state in Australia, with the largest black coal resources located in New South Wales and Queensland. As Figure 1A–3 shows, black coal is buried deeper than other layers of coal, but because of the heat efficiency it provides, it is much more economical for mining. Approximately 70% of the coal mined in Australia is exported, mostly to eastern Asian regions. In 2019, pre-COVID, coal exploration expenditure was $229 million, which was an increase of 32% from 2018. In comparison, the combustion of brown coal produces approximately 85% of Australia's electricity.

UNIT 1 LINK

8B MOLECULES OF CARBON LINK

Natural gas

Natural gas is mostly methane (CH_4), with traces of other small hydrocarbons, such as ethane (C_2H_6), propane (C_3H_8) and butane (C_4H_{10}). Other substances including water, carbon dioxide, sulfur and nitrogen can also be present in the gas reservoirs.

You will recall that in the formation of coal, the increased pressure and temperature resulted in the physical and chemical change of the sedimentary rock, releasing methane, carbon dioxide and water.

8B MOLECULES OF CARBON LINK

Likewise, this pressure causes the natural gas found in rock formations to adsorb to the surface of the coal. When drilling wells fracture coal deposits, natural gas flows to the surface, as shown in Figure 1A–4. This process is called **fracking**. A fracking fluid is injected into the well to increase the permeability of the sediment, allowing an easier flow of gas to the surface. The fracking fluid contains sand, water and other chemicals. A chemical once used in fracking fluid was benzene, which you will learn about in Section 8B. However, this has been banned in Australia because it is carcinogenic, and there is a potential risk of it escaping and contaminating water supplies. Sand is convenient as a component of this fluid because it is often present at the site of drilling. However, water is not, and so this has to be transported to the drilling sites, which is environmentally unfriendly and economically costly.

One of the environmental concerns associated with fracking is that it releases methane, a greenhouse gas, into the atmosphere. It is predicted that approximately 4–8% leaks to the atmosphere from the well head, pipelines and storage facilities.

Natural gas
a fossil fuel formed when layers of decomposing plant and animal remains experience high temperatures and pressures

Fracking
a process in which fluid is injected at high pressure, fracturing sedimentary rocks, releasing gas or oil

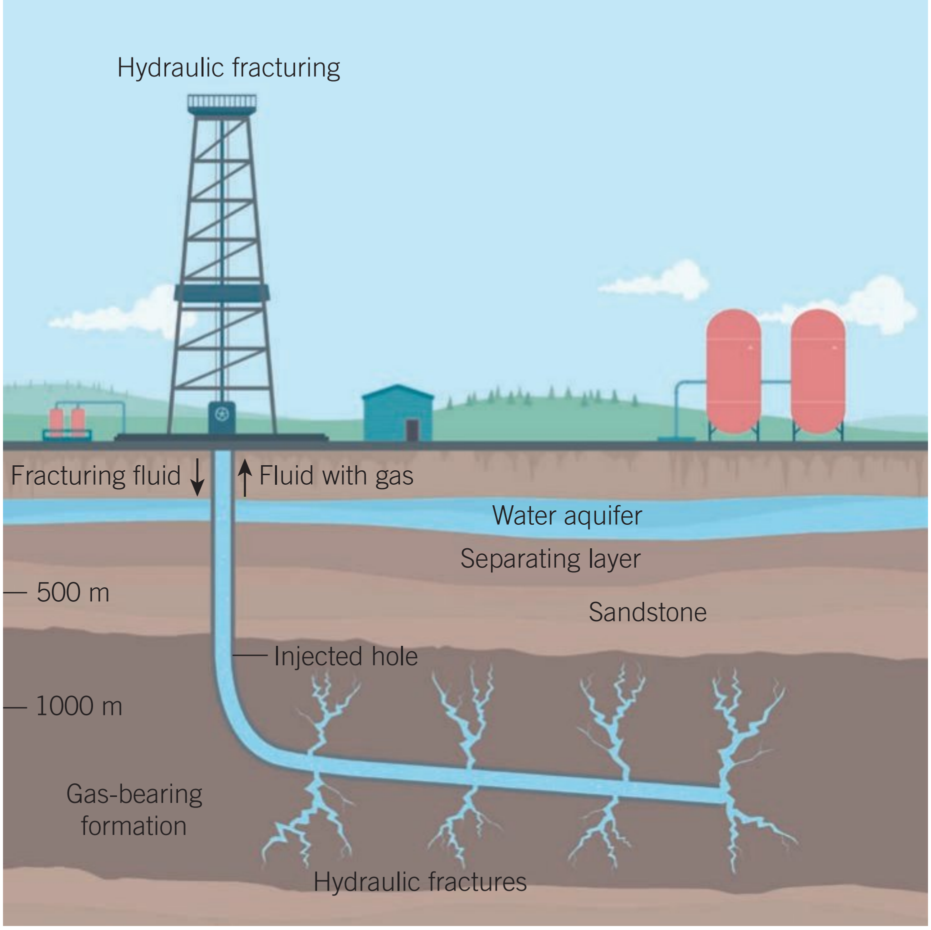

Figure 1A–4 The fracking process releases natural gas trapped above crude oil layers to the surface.

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Petroleum

In Unit 1, you learned about **crude oil** as being a mixture of predominantly alkanes, which are organic hydrocarbon molecules. Like coal and natural gas, crude oil is formed from plant and animal remains that decay over millions of years. However, crude oil is not as widespread or as easy to access as coal and natural gas.

Crude oil is essentially petrol (petroleum). However, because the crude oil mixture contains many hydrocarbons with varying sizes (based on their number of carbon atoms), it is not useful to mine and use directly once drilled and brought to the surface. The crude oil first needs to be separated into its various hydrocarbon fractions in a process called **fractional distillation**.

Fractional distillation works on the fundamental basis that different-sized hydrocarbons can be separated from each other because of their different boiling points, something you learned in Unit 1 and will again cover in Section 10B. Countries in the Middle East are the main sources and exporters of crude oil, including petrol, internationally. Australia, being one of their trade partners, imports 90% of all the crude oil it uses. Australia does have a few small crude oil reserves off the coast of northern Western Australia, South Australia and Bass Strait; however, these are likely to be depleted by 2100.

LINK **UNIT 1**

Crude oil a naturally occurring mixture of liquid hydrocarbons that can be used as a fuel source

Fractional distillation separation of a mixture of liquids into separate fractions based on their boiling points

LINK **UNIT 1**

LINK **10B** ANALYSIS OF PURITY AND CONCENTRATION

Check-in questions – Set 1

1 Recall the three different types of fossil fuels.
2 Which fossil fuels (from your answer to Question **1**) are associated with the following processes:
  a fractional distillation
  b fracking
3 Fossil fuels are described as being non-renewable. What does this mean?

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Biofuels

Biofuel
a renewable energy source produced from biological matter called biomass

Renewable
a resource that can be replenished at an equal or higher rate than it is consumed

Biomass
renewable organic matter that comes from plants, animals and other living organisms

While fossil fuels take millions of years to produce, and are being used up at a faster rate than which they are being replenished, **biofuels** are the opposite. Biofuels are classified as **renewable** because they can be produced at the same rate at which they are consumed. As the name suggests, they are produced from living (hence, *bio*) matter, called **biomass**. There are three types of biofuels covered in this chapter: biogas, bioethanol and biodiesel.

Figure 1A–5 shows the proportion of feedstocks in total biofuel production. As you will see in the following pages, different feedstocks can be used for different types of biofuel.

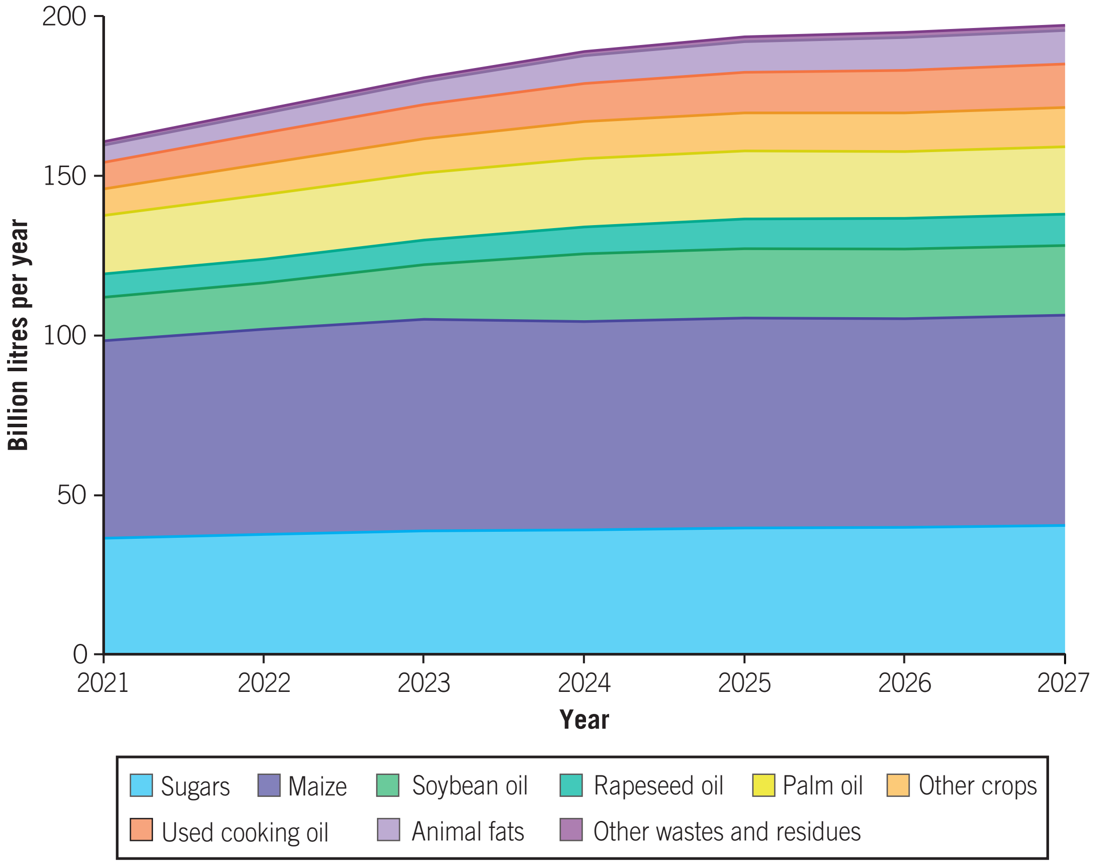

Figure 1A–5 Predicted total biofuel production by feedstock, 2021–2027. This is a work derived by Cambridge University Press & Assessment from International Energy Agency (IEA) material, and Cambridge University Press & Assessment is solely liable and responsible for this derived work. The derived work is not endorsed by the IEA in any manner.

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Biogas

Biogas is formed from the breakdown of organic biological waste, such as plant matter, by **anaerobic** bacteria. Anaerobic bacteria are those that thrive in the absence of oxygen. The bacteria break down complex carbohydrates, such as cellulose and starch, as well as proteins, into simpler molecules. The contents and percentage of these simpler molecules will depend on the starting organic material that is being decomposed. Approximate percentages are shown in Table 1A–1.

Biogas
a type of biofuel formed from the breakdown of organic waste by anaerobic bacteria

Anaerobic
an organism or process that does not require oxygen

Table 1A–1 Approximate percentages of contents within biogas

Molecule	Percentage (%)
Methane (CH_4)	50–75
Carbon dioxide (CO_2)	25–50
Nitrogen (N_2)	0–10
Hydrogen sulfide (H_2S)	0–3
Hydrogen (H_2)	0–1
Oxygen (O_2)	0–1

As you can see from the biogas cycle shown in Figure 1A–6, the original solar energy is captured by crops and transformed into chemical energy by photosynthesis, which will be explored in Section 1B. For large-scale production, the organic waste produced from harvesting crops, food waste and animal by-products is placed in a large tank called a digester. The digester is filled with anaerobic bacteria. Waste from this process can be used as a good biofertiliser and the biogas produced is useful for heating and electricity in homes and farms. This cycle further highlights the renewability and low impact of greenhouse gas emissions for this process.

LINK **1B** PRODUCTION OF CHEMICAL ENERGY IN NATURE

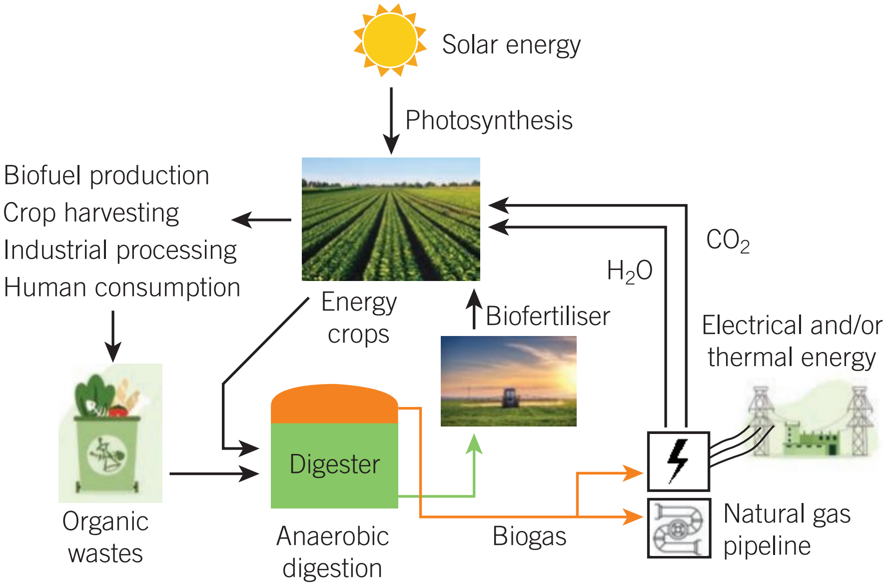


Figure 1A–6 The biogas cycle

The Australian biogas industry is still emerging. In 2017, there were 272 biogas plants, most of which use raw materials that would otherwise rot in landfill. In 2021, the first large-scale biogas plant was announced for Nowra, in NSW. According to the Australian Renewable Energy Agency (ARENA), the estimated biogas potential would place Australia on par with Germany, a leading country in the production of biogas.

You will learn more about biogas when discussing green chemistry in fuel cells in Section 4A.

LINK **4A** FUEL CELLS

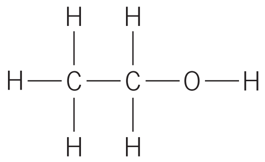
Bioethanol

Ethanol is a two-carbon hydrocarbon containing a hydroxyl (–OH) functional group. Its molecular formula, structural formula and semi-structural formula are shown in Table 1A–2.

Fermentation the process by which glucose is broken down in the absence of oxygen to produce energy (ATP); also called anaerobic cellular respiration

Bioethanol a type of biofuel produced by fermentation in plants and yeast

Table 1A–2 The molecular, structural and semi-structural formulas of ethanol

Name	Molecular formula	Structural formula	Semi-structural formula
Ethanol	C_2H_6O	 $\begin{array}{ccccccc} & & H & & H & & \\ & & \vert & & \vert & & \\ H & - & C & - & C & - & O-H \\ & & \vert & & \vert & & \\ & & H & & H & & \end{array}$	CH_3CH_2OH

Ethanol can be manufactured by the addition reaction of ethene with steam. You will encounter this reaction again in Section 9A.

9A ORGANIC REACTIONS: SUBSTITUTION, ADDITION AND OXIDATION LINK

More commonly and naturally, ethanol is produced in plants and yeast that undergo anaerobic **fermentation**. Typical crops grown globally for ethanol production include corn, maize and wheat, but Australia has a long history of fermenting native plants. The Palawa people of Tasmania have a history of using the sap of a cider gum to make the sweet fermented drink *wayalinah*, and the Noongar people in south-western Australia have fermented the fruit of the macrozamia plant (known as *by-yu* or *kwineen*) as a method of detoxification and to enhance its nutritional value.

Figure 1A–7 Cider gum tree leaves and flowers (left) and pollen cones of a *Macrozamia ridelei* plant (right). These Australian native plants are examples of those that have been fermented.

First-generation feedstock a biofuel produced from edible feedstocks (starch, glucose) from plants such as corn and wheat

Enzyme a protein molecule that acts as a catalyst in a specific biochemical reaction

The main feedstock used in Australia for producing **bioethanol** is wheat. Facilities are currently located in both New South Wales and Queensland, with plans for a large-scale facility to operate in regional Victoria in the future.

In wheat and other **first-generation feedstocks**, biological catalysts called **enzymes** speed up the breakdown of cellulose and starch to sucrose. Yeast is then added to this solution. The yeast contains another enzyme called invertase, which helps convert the sucrose into glucose. The glucose then binds with another enzyme in the yeast called zymase, which assists the final step of fermentation into ethanol (bioethanol) and carbon dioxide according to the following equation.

$$\text{glucose} \rightarrow \text{ethanol} + \text{carbon dioxide}$$

$$C_6H_{12}O_6(aq) \rightarrow 2CH_3CH_2OH(aq) + 2CO_2(g)$$

NOTE

As first-generation bioethanol feedstocks are also used for food, there is a tension between growing these crops for food versus fuel. This is called the 'food versus fuel debate'.

Notice that the ethanol produced from fermentation is in an aqueous (aq) state. This means that it is not pure and is hydrated by water molecules. These water molecules are removed by distillation, which will be covered in more detail in Section 10B.

10B ANALYSIS OF PURITY AND CONCENTRATION LINK

If you've got your learner permit or probationary licence and have driven to fill the car up at the petrol station, you will have noticed the fuel pump labelled 'E10'. It is called E10 as it contains a blend of 90% petrol and 10% ethanol. The addition of ethanol to petrol has several advantages, including:

- the use of petrol derived from crude oil is reduced
- the fuel is oxygenated so that it burns more completely
- the amount of greenhouse gas emissions is reduced
- the source of the bioethanol makes it a more sustainable transport fuel.

Biodiesel

Biodiesel is a mixture of organic compounds produced from vegetable oils, cooking oils and animal fats. Because it is produced from plant and/or animal products, it is renewable and often called 'green diesel'. A transesterification reaction between plant and/or animal **triglycerides** (fats, oils) and alcohol, typically methanol (CH_3OH), results in a mixture of methyl esters, or biodiesel. You will learn more about transesterification reactions in Section 9B; however, an example reaction is shown in Figure 1A–8 below. Note that this reaction also requires the presence of a strong base, such as sodium hydroxide (NaOH), acting as a catalyst. Biodiesel production in this way requires less energy and has less emissions than producing bioethanol.

Biodiesel
a type of biofuel composed of the esters of fatty acids

Triglyceride
an organic compound in which the three hydroxyl groups of glycerol form esters with three fatty acid molecules

LINK **9B** ORGANIC REACTIONS: CONDENSATION AND HYDROLYSIS

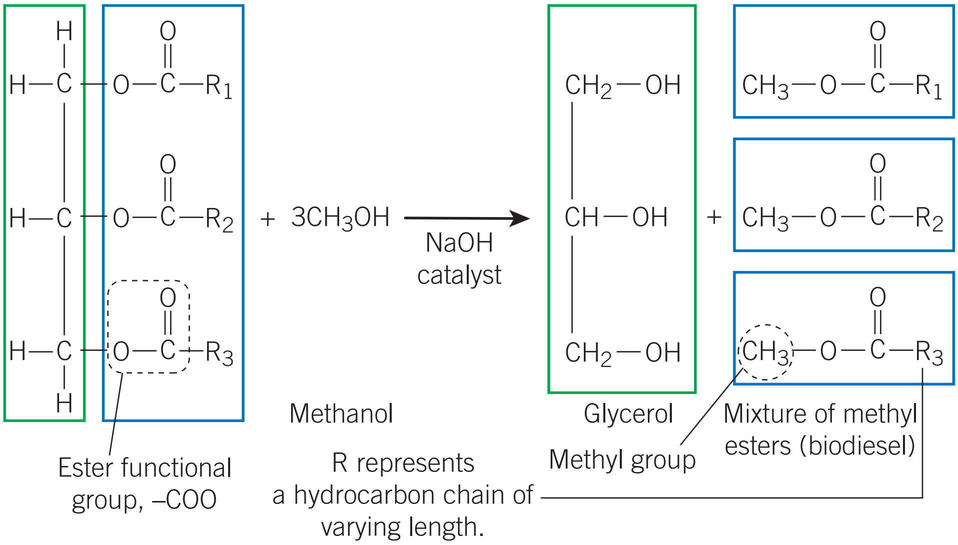


Figure 1A–8 Transesterification reaction between a triglyceride and methanol, producing a mixture of fatty acids, or biodiesel

> **NOTE**
>
> The other product in the transesterification reaction, glycerol, is commonly used in the manufacture of pharmaceuticals. You will learn more about medicinal chemistry in Chapter 12.

LINK **CHAPTER 12**

If you look back at Figure 1A–5 on page 10, you will see that a large number of the feedstocks used in biofuel production are vegetable oils, used for biodiesels.

There are currently three biodiesel plants operating in Australia. However, after peaking in the mid-2010s, they now operate at less than 40% capacity. With only around 0.2% blend rate with standard diesel, it is a fuel with very little focus in Australia. Globally, biodiesel can be used in most existing diesel engines without them needing further modifications. Like bioethanol, these blends are also labelled at the pump, typically as B5 or B20, indicating a 5% or 20% blend, respectively, of biodiesel with standard diesel.

WORKSHEET 1A–1
COMPARING FUELS

VIDEO 1A–1
RENEWABLE AND NON-RENEWABLE FUELS

Comparing fossil fuels and biofuels

In this chapter so far, you have learned about six different types of fuels. Three of these were fossil fuels and three were biofuels. Table 1A–3 highlights the key comparisons of these with a focus on their renewability and societal impacts.

Table 1A–3 Advantages and disadvantages of the different types of fossil fuels and biofuels

Fuel type		Advantages	Disadvantages
Fossil fuels (non-renewable)	Coal	• Mined easily • Large reserves remaining • Cheap • Can be converted to liquid and gas fuel, which is more portable if oil runs out	• Traces of sulfur and nitrogen react with atmospheric O_2 to form SO_2 and NO_2, which contribute to acid rain. • Finite supply so will eventually run out
	Natural gas	• Moderate cost for consumers • Easily converted to methanol • Produces least pollution	• Limited reserves remaining • Economically expensive to harness and transport • Environmental concerns over fracking
	Petrol	• Easily transported • Less pollution than coal • Many applications	• Limited reserves remaining globally, and availability will decline within decades • Expensive • Mining is destroying ecosystems (both on and offshore)
Biofuels (renewable)	Biogas	• Derived from plants, animals and humans • Utilisation of waste for heating, electricity and fertilisers, rather than letting it rot in landfills • Produces a circular economy • Good alternative for electricity and heating in rural areas or developing countries	• Very few technological advancements, so additional research and government funding required to make production efficient • Anaerobic digestion occurs optimally at 37°C, so in colder climates heat energy is required to generate biogas continually. • Odour is emitted from digesters used in this process, so a need to build these in locations away from residences
	Bioethanol	• Reduces greenhouse gas emissions, as crops used for fuel production absorb the CO_2 they emit when burned • Combining with oil extends the longevity of limited crude oil supplies	• Production requires large volumes of water. • The food vs fuel debate of growing crops
	Biodiesel	• New land not required for production • Reduces hydrocarbon emissions and the lifecycle of greenhouse gases • Reduces smog thereby reducing atmospheric pollution	• Farmland used for growing fuel instead of food • Large volumes of water (or availability) and fertilisers required

While biofuels might seem like a better alternative to fossil fuels, their increasing use in the immediate future raises a number of other important implications that need to be considered and managed, including:

- how much land degradation and forest destruction occurs to grow crops
- the percentage of crops grown for fuel versus that grown for food to meet the needs of increasing population sizes.

Research is underway to look at the potential for either algae or agave crops to be used as a feedstock for biodiesel production. The latter thrives in dry, arid desert environments with little water and produces a high oil yield. Therefore, land required for growing food would not be compromised.

1A SKILLS

VIDEO 1A–2
SKILLS: COMPARISON-BASED QUESTIONS

Comparison-based questions

In this section, you were presented with six different types of fuels. You learned about how and where each was sourced from, the chemical processes used in their production and their respective advantages and disadvantages. As such, it is predictable that assessment questions will require you to compare various aspects of different combinations of these fuels. In comparison or contrast questions, you are required to explain both the similarities and differences of each item in the question. Let's look at an example question, which has been adapted from the 2021 VCAA Exam and solution.

Question

Digesters use bacteria to convert organic waste into biogas. Both biogas and coal seam gas have the same hydrocarbon as their main component. Referring specifically to this hydrocarbon, compare biogas and coal seam gas.

VCAA 2021

Answer

Similarities:

Both are types of fuels that contain mainly methane, CH_4.

Differences:

- Coal seam gas is non-renewable as it originally comes from the increased temperature and pressure experienced by sedimentary rock deeper below Earth's surface and is not produced at a rate equal to or faster than it is consumed.
- On the other hand, biogas is renewable, as it is produced from the breakdown of plant matter, in particular cellulose and starch, by bacteria under anaerobic conditions.

Notice that in this answer, the comparison word 'whereas' was used to differentiate between the difference of the two fuels.

This was just one example for two fuels covered in this chapter, but other examples may require you to compare two different types of fossil fuels or two different types of biofuels, the advantages and/or disadvantages of different fuels or their renewability. Developing a clear set of notes with what makes each distinct from the other will be important for this section.

Section 1A questions

1 Bioethanol can be produced in organisms through a process known as fermentation.
   - a Write a balanced chemical equation for fermentation.
   - b Identify the reactants and products in the equation from your answer to part **a**.
   - c What conditions and other substances are required for the fermentation process to occur effectively?
   - d State the technique that is employed to purify bioethanol once it has been produced through fermentation.

2 Discuss the accuracy of the following statement:
‘Crude oil can be classified as a biofuel because it originally comes from plants.’

3 Fossil fuels are recognised as a significant contribution to the increase in greenhouse gas emissions. Alternative fuels to fossil fuels as an energy source exist but they are not yet at the stage where they can completely replace them. From different groups, there are concerns about the suitability of biofuels as a replacement for fossil fuels.
   - a Define ‘biofuel’.
   - b List three examples of biofuels.
   - c Compare bioethanol and biodiesel. In your answer, ensure you refer to how they are produced and the specific organic compounds they consist of.
   - d Explain the advantages for society of adding small quantities of these biofuels to current fossil fuels used for powering automobiles.
   - e Provide three reasons why it is currently unfeasible to incorporate a higher percentage of these biofuels into either petrol or diesel fuels.

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1B Production of chemical energy in nature

Study Design:

- Photosynthesis as the process that converts light energy into chemical energy and as a source of glucose and oxygen for respiration in living things: $6CO_2(g) + 6H_2O(l) \rightarrow C_6H_{12}O_6(aq) + 6O_2(g)$
- Oxidation of glucose as the primary carbohydrate energy source, including the balanced equation for cellular respiration: $C_6H_{12}O_6(aq) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l)$

Glossary:

Aerobic
Anabolic
Catabolic
Cellular respiration
Oxidation number
Oxidised

ENGAGE

The carbon economy

Have you heard of the carbon economy? Perhaps you're more familiar with the term 'carbon footprint'. Both of these relate to carbon dioxide emissions. As you learned in Unit 2, carbon dioxide emissions (a type of greenhouse gas) are primarily responsible for global warming and climate change. Carbon dioxide is released naturally through processes like cellular respiration, which you will learn more about in this chapter, and fermentation. However, other human activities, such as deforestation and the burning of fossil fuels, which you will learn more about in Section 1C, have been the main producers of the gas. For decades, efforts have been made to monitor and lower these emissions. Governments and industries are continually improving the efficiency of photosynthesis, which is the way carbon dioxide is naturally removed from the atmosphere. The benefits of this improvement will be twofold. The world's population is growing rapidly and greater quantities of food will be needed to support future generations. Not only will there be less carbon dioxide in the atmosphere, but it is thought that increasing the efficiency of photosynthesis will mean more nutrient-rich crops and increased crop yields. Governments and industries also want to increase the production of biomass, a sustainable and renewable energy resource, in the hope that this will reduce our reliance on fossil fuels and again reduce the volume of carbon dioxide in the atmosphere.

LINK UNIT 2

LINK 1C EXOTHERMIC AND ENDOTHERMIC REACTIONS

Figure 1B–1 The rise in carbon dioxide levels in the atmosphere is responsible for global warming and climate change.

EXPLAIN

Photosynthesis

Photosynthesis is an **anabolic** chemical reaction in which the Sun's light energy is used to convert the inorganic compounds carbon dioxide (CO_2) and water (H_2O) into the organic compound glucose ($C_6H_{12}O_6$). Glucose can then be used as a source of energy by the cells of living organisms, enabling growth and reproduction.

Anabolic
a biochemical process requiring energy, where simple molecules combine to generate complex molecules

Photosynthesis consists of a series of steps (a biochemical pathway), with each step controlled by a different enzyme. The overall process of photosynthesis can be written as both a word equation and a balanced chemical equation:

$$\text{carbon dioxide} + \text{water} \longrightarrow \text{oxygen} + \text{glucose}$$

$$6CO_2(g) + 6H_2O(l) \xrightarrow[\text{chlorophyll}]{\text{light energy}} 6O_2(g) + C_6H_{12}O_6(aq)$$

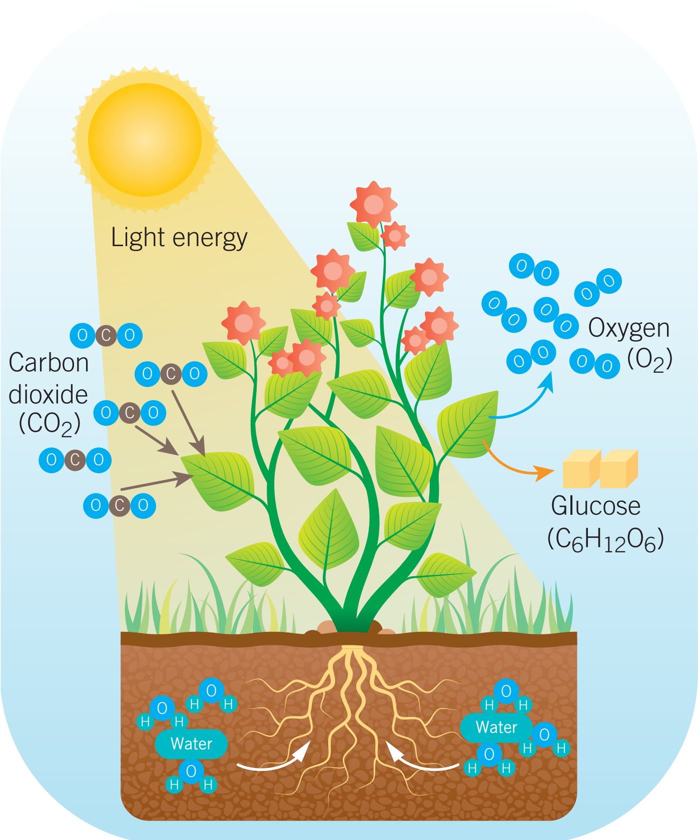

Figure 1B–2 The initial reactants and final products of photosynthesis

The oxygen released is considered a waste product from a photosynthesis perspective. However, this is a very important reactant for **cellular respiration** in both plants and animals. The glucose produced from photosynthesis in plants is the key reactant required for cellular respiration in living organisms, as you will see later in this chapter. As you learned in Section 1A, glucose is also the key input for fermentation in the production of bioethanol from plants and yeast.

Photosynthesis is an example of an endothermic reaction, which you will learn about in Section 1C.

Cellular respiration
the transformation of the chemical energy stored in glucose into usable energy (ATP) for cells

1A TYPES OF FUELS LINK

1C EXOTHERMIC AND ENDOTHERMIC REACTIONS LINK

NOTE

There are many factors that affect the rate of the photosynthesis reaction, such as temperature, light availability, water availability, carbon dioxide concentration and enzyme (catalyst) concentration. Factors affecting the frequency and success of collisions between reactants, and the subsequent rate of chemical reactions, are explored further in Section 5B.

5B FACTORS AFFECTING REACTION RATE LINK

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Check-in questions – Set 1

1 What is the purpose of photosynthesis?
2 a Write the word equation for photosynthesis.
  b Write the simplified balanced chemical equation for photosynthesis.

Cellular respiration

Like photosynthesis, cellular respiration occurs as a series of steps in a biochemical pathway, with each step controlled by a different enzyme. You do not need to be familiar with any of these steps in this chemistry course. The purpose of cellular respiration is the **catabolic** breakdown of glucose, which releases the chemical energy in a form more usable for cells, as a molecule called adenosine triphosphate (ATP).

Catabolic a biochemical process releasing energy, in which complex molecules are broken down into simple molecules

LINK **1A** TYPES OF FUELS

There are two types of cellular respiration. The first occurs in the absence of oxygen (anaerobic) and is commonly referred to as fermentation. You learned about this in Section 1A. This occurs in certain plants and yeast, resulting in the production of ethanol (bioethanol) and carbon dioxide, according to the following equation:

$$\text{glucose} \rightarrow \text{ethanol} + \text{carbon dioxide}$$

$$C_6H_{12}O_6(aq) \rightarrow 2CH_3CH_2OH(aq) + 2CO_2(g)$$

In animals, a slightly different form of anaerobic cellular respiration takes place. It is often called lactic acid fermentation and results in the production of lactic acid (lactate ions), which is associated with muscle cramping. This chemical reaction is represented according to the following equation:

$$\text{glucose} \rightarrow \text{lactic acid}$$

$$C_6H_{12}O_6(aq) \rightarrow 2CH_3CH(OH)COOH(aq)$$

The second form of cellular respiration occurs in the presence of oxygen (**aerobic**). This occurs in many plant and animal cells with some steps occurring inside the mitochondria, the energy powerhouse of the cell. Aerobic cellular respiration results in a much greater yield of energy per mole of glucose than that yielded by anaerobic cellular respiration.

Aerobic an organism or process that requires the presence of free oxygen

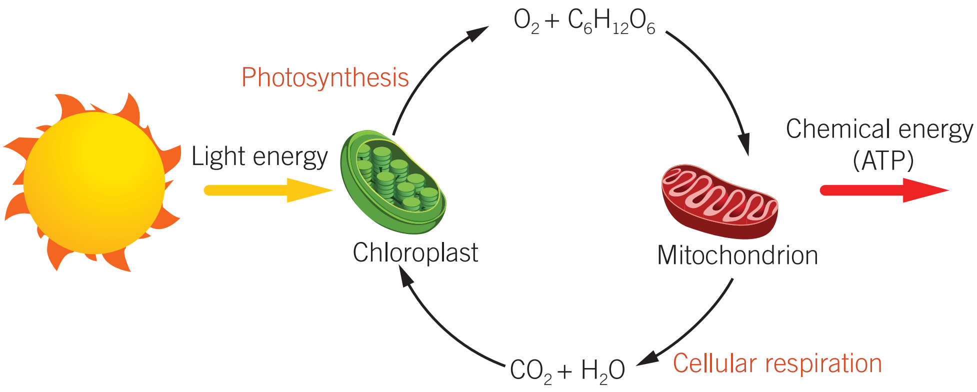

Figure 1B–3 An overview of the relationship between photosynthesis and aerobic cellular respiration

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Oxidised describes a chemical species that has undergone oxidation – that is, it has lost electrons in a reaction

In aerobic cellular respiration, glucose is **oxidised** to form carbon dioxide and water. The chemical reaction for aerobic cellular respiration is:

$$\begin{array}{llll} \text{glucose} & + \text{ oxygen} \rightarrow & \text{water} & + \text{ carbon dioxide} \\ 0\ {+1}\ {-2} & 0 & {+1}\ {-2} & {+4}\ {-2} \\ C_6H_{12}O_6(aq)\ + & 6O_2(g) \rightarrow & 6H_2O(l)\ + & 6CO_2(g) \end{array}$$

NOTE

You should notice from this equation that the products of this chemical reaction are the inputs for the photosynthesis reaction.

UNIT 2 LINK

3A REDUCTION AND OXIDATION LINK

1A TYPES OF FUELS LINK

1C EXOTHERMIC AND ENDOTHERMIC REACTIONS LINK

5B FACTORS AFFECTING REACTION RATE LINK

You will recall from Unit 2, and this will again be covered in Section 3A, that **oxidation** means a loss of electrons. If you look at the **oxidation numbers**, in red, shown above the balanced chemical equation, you will see that the carbon changes from a '0' to a '+4' oxidation number. This means it is losing electrons. Conversely, the oxygen gas reactant is being reduced, as it changes oxidation number from '0' to '+2'.

As glucose can be broken down to release the energy required for all metabolic reactions occurring in our bodies' cells, it is a type of fuel. Like the other fuels you learned about in Section 1A, it undergoes a combustion reaction that releases energy, which means it is an exothermic reaction. Exothermic combustion reactions will be discussed in more detail in Section 1C.

As in photosynthesis, there are many factors which affect the rate of cellular respiration reactions, such as temperature, glucose availability, oxygen concentration and enzyme (catalyst) concentration. Factors affecting the frequency and success of collisions between reactants, and the subsequent rate of chemical reactions, are explored further in Section 5B.

Oxidation number a measure of the degree of oxidation of an atom in a substance; defined as the charge an atom might have when electrons are counted to help identify redox reactions, oxidising agents and reducing agents

WORKSHEET 1B–1 ENERGY PRODUCTION IN PLANTS AND ANIMALS

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1B SKILLS

VIDEO 1B–1
SKILLS: UNDERSTANDING THE LINK BETWEEN PHOTOSYNTHESIS AND CELLULAR RESPIRATION

Understanding the link between photosynthesis and cellular respiration

An overview of the processes of photosynthesis and cellular respiration is given in the diagram below.

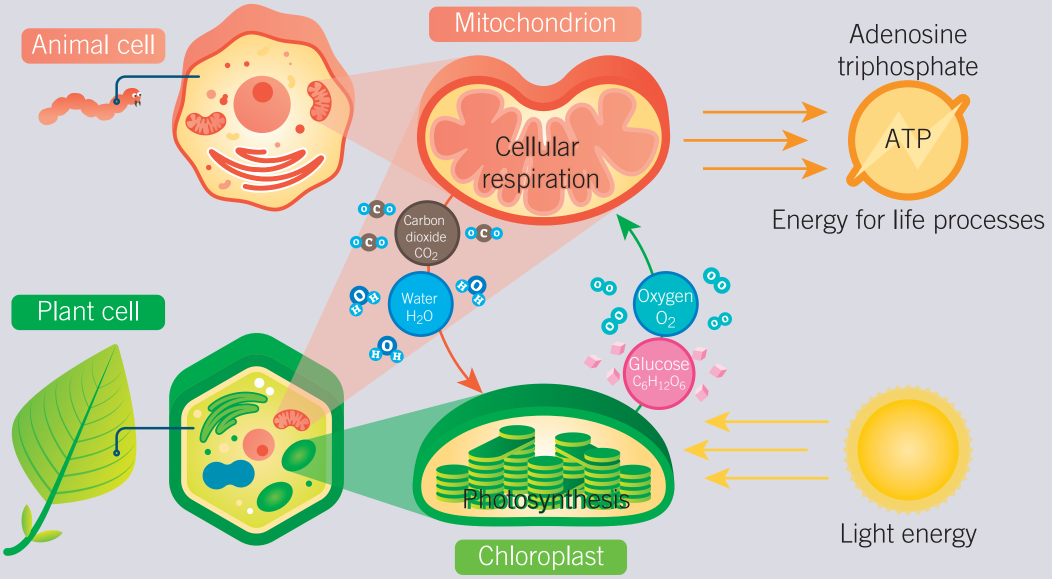


Figure 1B–4 The complementary nature of the photosynthesis and cellular respiration reactions means that carbon, hydrogen and oxygen cycle through organisms and their environments continually.

Referring to Figure 1B–4, note the following key points.

- Photosynthesis occurs in the chloroplast, an organelle found only in the cells of green plants and algae.
- The products of photosynthesis (oxygen and glucose) are used as reactants in the process of aerobic cellular respiration.
- Aerobic cellular respiration occurs mostly in mitochondria, organelles found in animal, plant and fungal cells, and protists.
- Aerobic cellular respiration uses the products of photosynthesis to produce ATP, an energy storage molecule, which can then release energy to meet the cell's requirements.
- In plants, the products of aerobic cellular respiration (water and carbon dioxide) can then be used as reactants in the process of photosynthesis.
- Although photosynthesis appears to be the reverse of cellular respiration, the processes are different and use different enzymes. (You will learn in general about enzymes in Section 12B.)

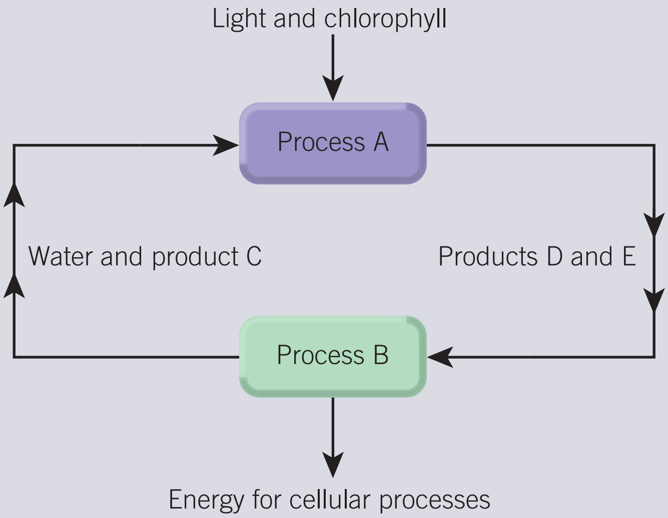
LINK **12B** ENZYMES

Using the Study Design to guide your preparation

The most important way of determining the detail you need to know is by looking at the Study Design and completing many practice questions. Keep focused on the terms used in the Study Design dot points and, when making notes, always use the dot points, or part of the dot points, as your headings. The Study Design was written specifically to cover what you need to know, and the success criteria have been written to guide you through the necessary material.

For example, the Study Design requires you to know that photosynthesis is a source of both glucose and oxygen, which are required for respiration in living things, and that it is in these living things where the glucose is oxidised as the primary energy source.

Additionally, both chemical equations are given for you. This suggests that, if you know these things, you will be able to work through and determine the answers to assessment questions. Consider the following diagram and predict what the questions could be, based on what you know of the Study Design.



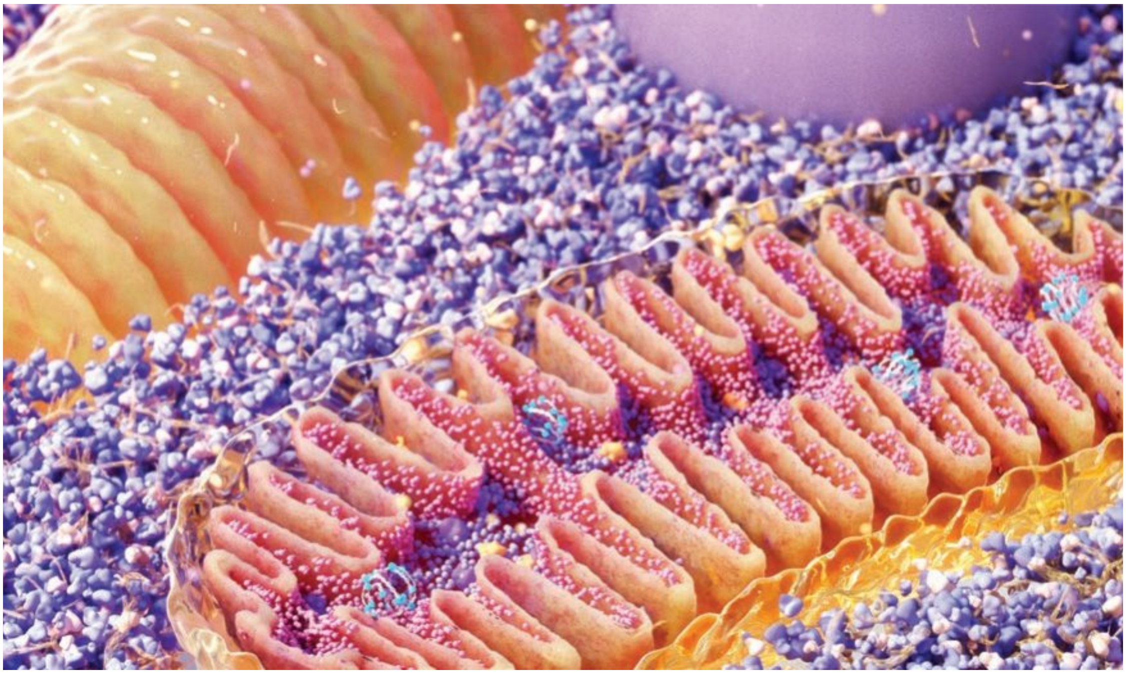
Possible questions could be:

- Determine what processes A and B are.
- Write word and balanced chemical equations for processes A and B.
- List where processes A and B occur.
- Identify products C, D and E.

12B ENZYMES LINK

5B FACTORS AFFECTING REACTION RATE LINK

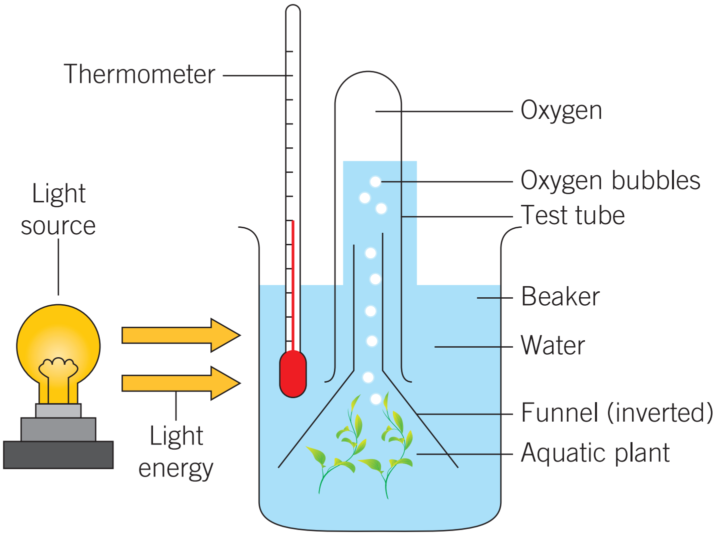
Also keep in mind the interrelationships between concepts. Section 12B will look in more detail at the structure and role of enzymes in helping catalyse (speed up) specific reactions. Chapter 5 will investigate the factors that affect rates of chemical reactions, which are relevant to these two processes.



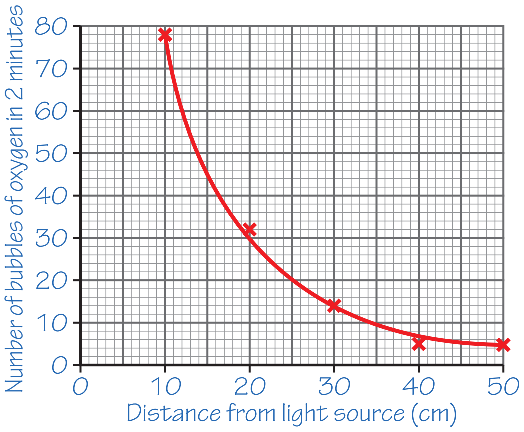
Section 1B questions

1 Light energy is converted into what form of energy during photosynthesis?

2 Students were investigating the relationship between the number of oxygen bubbles produced by an aquatic green plant and the light intensity it was exposed to. They set up two beakers with similarly sized sections of aquatic plant and placed one in the shade and one next to a light source. The students recorded the number of bubbles given off by each plant in two minutes. They then moved the plant near the light source, 10 cm away, and repeated their recordings. They continued moving the plant back in 10 cm intervals until the plant was 50 cm away from the light source.



Their results for the plant that was placed in the light were graphed and shown on the right.



- **a** What chemical reaction does the production of oxygen indicate is occurring in the aquatic green plant?
- **b** Write a balanced chemical equation to represent the reaction from your answer to part **a** above.
- **c** From your understanding of this process, which beaker is the students' control?
- **d** State the independent variable (what is being changed) and the dependent variable (what is being measured) in the students' investigation.
- **e** Explain the trend observed in the data shown on the graph. Make sure to refer to specific data in your answer.

3 Cells cannot directly use the chemical energy stored in glucose.

- **a** Compare and contrast the two processes that break down glucose in plants and animals. In your answer, include the chemical equation for each of these.
- **b** The Study Design refers to the 'oxidation of glucose as the primary carbohydrate energy source'. Explain what this sentence means to someone who has a limited understanding of chemistry.

4 Outline the relationship between the reactants and products of cellular respiration and photosynthesis.

1C Exothermic and endothermic reactions

Study Design:

- Comparison of exothermic and endothermic reactions, with reference to bond making and bond breaking, including enthalpy changes (ΔH) measured in kJ, molar enthalpy changes measured in kJ mol^{-1} and enthalpy changes for mixtures measured in kJ g^{-1}, and their representations in energy profile diagrams
- Determination of limiting reactants or reagents in chemical reactions
- Combustion (complete and incomplete) reactions of fuels as exothermic reactions; the writing of balanced thermochemical equations, including states, for the complete and incomplete combustion of organic molecules using experimental data and data tables

Glossary:

Activation energy
Complete combustion
Endothermic
Enthalpy
Enthalpy change
Exothermic
Incomplete combustion

ENGAGE

It's getting hot!

What do composting vegetable waste and burning a candle have in common? While it may seem like the answer should be 'not much at all', they are in fact linked as they both involve chemical reactions that release heat into the environment! In this section, you are going to gain an understanding of two different types of reactions and how they either release or absorb heat from the environment. You will also investigate a specific type of exothermic reaction, called combustion reactions, as a way of obtaining energy from fuels. Lastly, you will learn how to draw energy profile diagrams to represent the reactions occurring during these processes.

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EXPLAIN

Exothermic and endothermic reactions

For a chemical reaction to occur, the bonds within the reactants must first be broken. This requires energy and the exact quantity of energy is specific for each reaction. Every reaction has a minimum amount of energy that is needed for the reaction to occur – this is known as the **activation energy** and is represented by the symbol E_a. As a reaction proceeds, new bonds must be formed to generate the products. Unlike breaking bonds, this process releases energy. This can be summarised by the following statements:

Breaking bonds: requires energy from the environment

Forming bonds: releases energy to the environment

The chemical energy of a substance is called its **enthalpy** or heat content and has the symbol *H*. The overall change in energy from reactants to products is known as the **enthalpy change** (ΔH). The enthalpy change indicates whether more energy was required to break the reactant bonds than was released forming the product bonds or vice versa. It can be represented by the equation:

$$\Delta H_{\text{(reaction)}} = \Sigma H_{\text{(reactant bonds broken)}} - \Sigma H_{\text{(product bonds formed)}}$$

From this equation, we can see that there are two possible outcomes.

1 The energy required to break the bonds of the reactants is greater than the energy released from forming the bonds in the products. In this instance, the ΔH will be positive, and the reaction is referred to as an **endothermic** reaction.

2 The energy required to break the bonds of the reactants is less than the energy released from forming the bonds in the products. In this instance, the ΔH will be negative, and the reaction is referred to as an **exothermic** reaction.

Exothermic and endothermic reactions can be illustrated using energy profile diagrams (Figure 1C–1).

Activation energy
the minimum quantity of energy required so that a chemical reaction can proceed

Enthalpy
the internal energy of a chemical system (plus the product of pressure and volume)

Enthalpy change
the difference in enthalpy between reactants and products in a chemical reaction; symbol ΔH

Endothermic
a reaction that has a positive enthalpy change value and absorbs heat from the environment

Exothermic
a reaction that has a negative enthalpy change value and releases heat to the environment

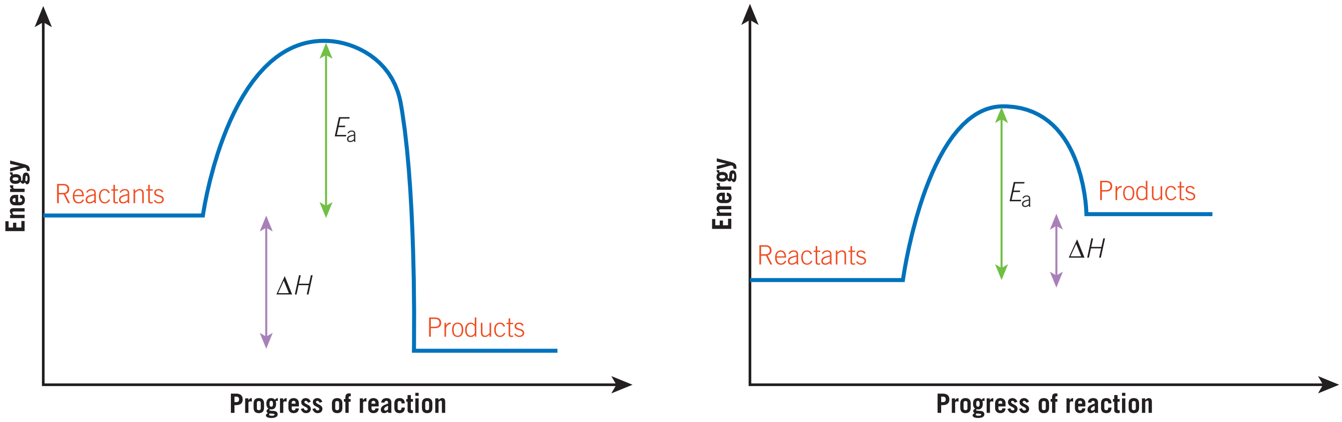

Figure 1C–1 Exothermic (left) and endothermic (right) reactions can be illustrated using energy profile diagrams. These diagrams show the activation energy (E_a) of the reaction, as well as the quantity of energy released or absorbed (ΔH).

Enthalpy change (ΔH) has the units of joules, J (or more commonly kJ), $kJ\,mol^{-1}$ or $kJ\,g^{-1}$.

Table 1C–1 Enthalpy change units and when they are commonly used

Unit	Circumstance when the unit is commonly used
J (or kJ)	When the overall energy released is the important consideration
$kJ\,mol^{-1}$	When the energy released per mole of compound is of interest. This should be used when a comparison of fuel sources is required and the fuels in question are composed of a single compound (e.g. pure substances only).
$kJ\,g^{-1}$	When the energy released per gram of a substance is of interest. This should be used when a comparison of fuel sources is required, but the fuels in question are composed of multiple compounds, making it impossible to accurately calculate $kJ\,mol^{-1}$. It can also be used as an alternative to $kJ\,mol^{-1}$ for fuels with only one compound.

2B MEASURING ENERGY RELEASED FROM CHEMICAL REACTIONS LINK

Calculating the value for the enthalpy change of a reaction can be important in understanding the energy content of fuels and foods. This will be covered in more depth in Section 2B.

It is important to note that in an exothermic reaction, where the ΔH is negative, the products are at a lower energy level than the reactants. This means that in an exothermic reaction the products are more stable than the reactants.

It is the opposite when considering an endothermic reaction, where the ΔH is positive. In these reactions, the reactants, which are at a lower energy level than the products, are more stable.

Key points and differences between exothermic and endothermic reactions are summarised in Table 1C–2.

Table 1C–2 Key features of exothermic and endothermic reactions

Exothermic	Endothermic
ΔH is negative	ΔH is positive
Reactions release energy/heat to the environment.	Reactions absorb energy/heat from the environment.
Products are more stable than the reactants.	Reactants are more stable than the products.
Must overcome the activation energy to proceed	Must overcome the activation energy to proceed

Check-in questions – Set 1

1 What is the difference between an exothermic reaction and an endothermic reaction?
2 Is the enthalpy change for an endothermic reaction positive or negative? Explain why.
3 What is the minimum quantity of energy required for a reaction to proceed?

Combustion of fuels

Earlier in this chapter, we discussed fuels as sources of energy. To obtain energy from these types of fuels, they must undergo combustion reactions. Combustion reactions involve reacting an organic fuel in the presence of oxygen gas, and produce carbon dioxide, water and heat energy. As heat energy is released as part of these reactions, all combustion reactions are exothermic.

LINK **1A** TYPES OF FUELS

Knowledge of combustion reactions means they can be employed in society's favour. This can allow for more efficient consumption of petrol in a car or to maximise the energy produced in thermal power plants. With the increasing severity of bushfires in Australia, there has been a growing resurgence of interest in examining the techniques of First Nations cultural (or cool) burning, the oldest known farming practice in the world. First Nations rangers and traditional owners in the Kimberley region in northern Western Australia perform targeted burnings during the early dry season (March to July) to minimise the most dangerous season for bushfires (August to November).

Combustion reactions can be represented by thermochemical equations, which not only show the reactants and products of the reaction, but also the energy released.

Let's start by writing the balanced equation for the **complete combustion** of methane:

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

Complete combustion a combustion reaction of organic fuel that takes place in the presence of excess oxygen gas to produce carbon dioxide and water

The first thing that you might notice in the above equation is that water is present in the gaseous state (that is, as water vapour), rather than as a liquid. This is because all combustion reactions occur at high temperatures that are above the boiling point of water.

This equation, however, is not a thermochemical equation. For this, we need to add in the enthalpy change data for the combustion of methane. For many common fuels, the heat of combustion has been determined experimentally, and the values are provided in the VCAA Data Book. Using this, we see that the heat of combustion for methane is given as 55.6 $kJ\,g^{-1}$ or 890 $kJ\,mol^{-1}$. This can then be added to our balanced equation to give us a complete thermochemical equation as follows:

$$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(l) \qquad \Delta H = -890\ kJ\,mol^{-1}$$

NOTE

You will notice that in the thermochemical equation, the state for the water produced is now liquid (l). This is because all reactants and products must be in their standard states at SLC (standard laboratory conditions; 25°C, 100 kPa).

With this information, it is possible to calculate the quantity of heat released from the combustion of methane in almost any given situation at 25°C and 100 kPa. This thermochemical equation tells us that the combustion of one mole of methane releases 890 kJ of energy. If two moles of methane underwent combustion, 1780 kJ of energy (that is, 2 × 890) would be released. You will learn more about how to perform these calculations in Section 2A. In these instances, we are assuming that the fuel continues to react until it is all gone. This is true if the reaction takes place with an abundance of oxygen gas; however, this isn't always the case. If the oxygen is depleted before the fuel, the reaction is known as **incomplete combustion**. Due to the lack of oxygen present, different carbon-containing products are formed from this reaction: solid carbon, carbon monoxide gas

LINK **2A** MEASURING GREENHOUSE GASES

Incomplete combustion a combustion reaction of organic fuel that takes place when oxygen is the limiting reagent to produce carbon monoxide and water and carbon dioxide gas. Shown below is one possible equation for the incomplete combustion of methane, where carbon monoxide, rather than carbon dioxide, is the only carbon-containing product generated:

$$2CH_4(g) + 3O_2(g) \rightarrow 2CO(g) + 4H_2O(l)$$

If incomplete combustion occurs, the energy released will be less than if complete combustion occurs. To determine whether complete or incomplete combustion will occur in certain circumstances, we need to understand the concept of limiting and excess reagents.

NOTE

In some cases of incomplete combustion, solid carbon, C(s), is also produced as a product. This can be observed as soot.

Limiting and excess reagents

UNIT 2 LINK

VIDEO 1C–1 LIMITING AND EXCESS REAGENTS

In Unit 2, you learned about a variety of different applications where you may be required to perform stoichiometric calculations. As part of this, you were introduced to the concept of mole ratios, which are represented by the coefficients in a chemical equation and provide information about the relative amounts of each compound needed for the reaction to occur. In a way, this is similar to how a recipe provides instructions on the different quantities of ingredients required to make a meal or bake a cake.

Let's look at part of a hypothetical recipe for a banana cake. As well as other ingredients, the recipe says that to make one cake we need:

- 3 bananas
- 2 eggs
- 1 cup of milk.

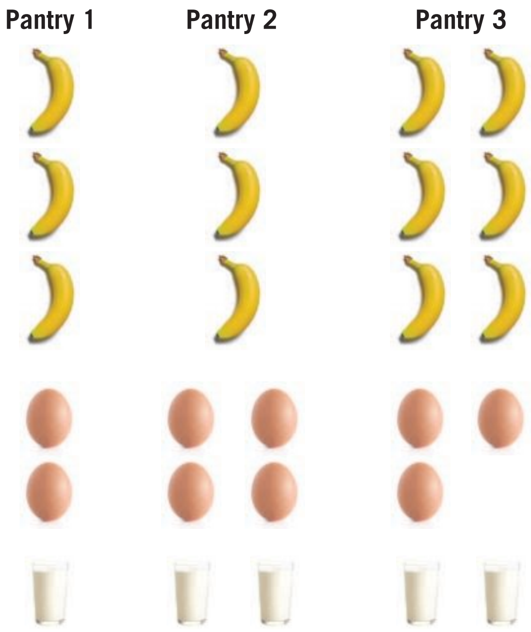

Figure 1C–2 Using cake ingredients to model mole ratios

We can essentially express this in the same way that we would a balanced chemical reaction:

$$3 \text{ bananas} + 2 \text{ eggs} + 1 \text{ cup of milk} \rightarrow 1 \text{ banana cake}$$

This shows us that the numbers (or coefficients) in front of each ingredient provide the ratio required to make our product, the banana cake. Now let's look at the ingredients contained within three potential pantries (Figure 1C–2).

Referring to our original recipe equation, we need: 3 bananas, 2 eggs and 1 cup of milk.

For each pantry, our equation looks like this:

Pantry 1: 3 bananas + 2 eggs + 1 cup of milk → ? banana cakes

Pantry 2: 3 bananas + 4 eggs + 2 cups of milk → ? banana cakes

Pantry 3: 6 bananas + 3 eggs + 2 cups of milk → ? banana cakes

In each instance, you can see that we need to work out the total number of banana cakes that we can make from the ingredients that we have.

In pantry 1, we have the exact number of each ingredient required by the original recipe to make a single banana cake.

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In pantry 2, we can see that we have double the number of eggs and double the number of cups of milk required to make a single banana cake. However, if we wanted to make two banana cakes, we would also need 6 bananas. We only have 3 bananas in this pantry, which is only enough to make 1 banana cake. In this instance, the bananas are our limiting ingredient (or reagent). In contrast, the eggs and milk will both be present in excess.

In pantry 3, we can see that we have double the number of bananas and double the number of cups of milk required to make a single banana cake. However, if we wanted to make 2 banana cakes, we would also need 4 eggs. While we have more eggs than we need to make a single cake (2 eggs), we still have less than we need to make 2 cakes (4 eggs). This means that in this pantry, the eggs are our limiting ingredient and the bananas and milk will both be present in excess.

From this example, it should be clear that we can only make as many cakes as our limiting ingredient allows. By applying our ingredient ratios to pantry 3 and only focusing on the limiting ingredient, we can calculate the following:

2 eggs: 1 cake

3 eggs: 1.5 cakes

While this example may have just made you crave banana cake, it also illustrates perfectly the concept of limiting and excess reagents and how they can be used to calculate the theoretical amount of product that can be generated from a chemical reaction.

Let's now look at a specific worked example using the combustion of methane.

Worked example 1C–1: Determining the limiting reagent

VIDEO
WORKED
EXAMPLE 1C–1

A 2.0 mol sample of methane (CH_4) reacts in the presence of 6.0 mol of oxygen (O_2) to produce carbon dioxide (CO_2) and water (H_2O). Determine the limiting reagent in this reaction.

Solution

	Logic	Process
Step 1	Write a balanced equation for the reaction.	$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$
Step 2	Write the relevant information provided in the question under the equation.	$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$ $n(CH_4) = 2.0$ mol; $n(O_2) = 6.0$ mol
Step 3	Calculate the number of moles of each reactant using coefficients in the equation.	$n(CH_4) : n(O_2) = 1 : 2$ So, 2 mol of CH_4 would react with 4 mol of O_2.
Step 4	Based on the moles present of one reactant, work out how much would be required of the other, based on the mole ratio in the equation.	4 mol of O_2 required 6 mol of O_2 present O_2 present > O_2 required
Step 5	Determine if the amount of the second reagent is more or less than what is required from Step 3.	There is more oxygen present than required.
Step 6	State the limiting reagent.	Methane is the limiting reagent.

As you can see in Worked example 1C–1, the oxygen is in excess and so this will lead to complete combustion. You can also see from this example that we need to know the moles of each reactant to determine the limiting and excess reagents. However, if you are given a mass, as in the following example, you need to complete an extra step.

VIDEO
WORKED
EXAMPLE 1C–2

Worked example 1C–2: Determining the limiting reagent in moles

Methane (CH_4) reacts in the presence of oxygen (O_2) to produce carbon monoxide (CO) and water (H_2O). Initially, 8.0 g of methane and 16.0 g of oxygen are present. Determine the limiting reagent in this reaction.

Solution

	Logic	Process
Step 1	Write a balanced equation for the reaction.	$2CH_4(g) + 3O_2(g) \rightarrow 2CO(g) + 4H_2O(g)$
Step 2	Write the relevant information provided in the question under the equation.	$2CH_4(g) \quad + \quad 3O_2(g) \rightarrow 2CO(g) + 4H_2O(g)$ $m = 8.0\text{ g} \quad m = 16.0\text{ g}$
Step 3	Calculate the amount, in mol, of each reactant.	$n(CH_4) = \frac{m}{M}$ $n(CH_4) = \frac{8.0\text{ g}}{16.0\text{ g mol}^{-1}}$ $n(CH_4) = 0.50\text{ mol}$ $n(O_2) = \frac{m}{M}$ $n(O_2) = \frac{16.0\text{ g}}{32.0\text{ g mol}^{-1}}$ $n(O_2) = 0.50\text{ mol}$
Step 4	Based on the moles present of one reactant, work out how much would be required of the other, based on the mole ratio in the equation.	$n(CH_4) : n(O_2) = 2 : 3$ 0.50 mol of O_2 would react with 0.33 mol of CH_4.
Step 5	Determine if the amount of the second reagent is more or less than what is required from Step 3.	0.33 mol of CH_4 required 0.50 mol of CH_4 present CH_4 present > CH_4 required
Step 6	State the limiting reagent.	As there is more CH_4 present than required, CH_4 is the excess reagent, making O_2 the limiting reagent.

Lastly, once we have determined the limiting reagent, we can also use this information to calculate the amount or mass of a product, or the quantity of heat in the case of combustion, that is generated from the reaction. This type of question is illustrated in Worked example 1C–3.

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Worked example 1C–3: Determining the mass of the product or the quantity of heat

VIDEO
WORKED EXAMPLE 1C–3

Using the reaction from Worked example 1C–2, determine the mass of carbon monoxide that would be produced. We will start from the beginning and add extra steps at the end to show how this question could be done in its entirety.

Solution

	Logic	Process
Step 1	Write a balanced equation for the reaction.	$2CH_4(g) + 3O_2(g) \rightarrow 2CO(g) + 4H_2O(g)$
Step 2	Write the relevant information provided in the question under the equation.	$2CH_4(g) \quad + \quad 3O_2(g) \rightarrow 2CO(g) + 4H_2O(g)$ $m = 8.0\text{ g} \quad m = 16.0\text{ g}$
Step 3	Calculate the amount, in mol, of each reactant.	$n(CH_4) = \frac{m}{M}$ $n(CH_4) = \frac{8.0\text{ g}}{16.0\text{ g mol}^{-1}}$ $n(CH_4) = 0.50\text{ mol}$ $n(O_2) = \frac{m}{M}$ $n(O_2) = \frac{16.0\text{ g}}{32.0\text{ g mol}^{-1}}$ $n(O_2) = 0.50\text{ mol}$
Step 4	Based on the moles present of one reactant, work out how much would be required of the other, based on the mole ratio in the equation.	$n(CH_4) : n(O_2) = 2 : 3$ 0.50 mol of O_2 would react with 0.33 mol of CH_4.
Step 5	Determine if the amount of the second reagent is more or less than what is required from Step 3.	0.33 mol of CH_4 required 0.50 mol of CH_4 present CH_4 present > CH_4 required
Step 6	State the limiting reagent.	As there is more CH_4 present than required, CH_4 is the excess reagent, making O_2 the limiting reagent.
Step 7	Use the number of moles of the limiting reagent and the mole ratio to calculate the number of moles of the desired product.	$n(O_2) : n(CO) = 3 : 2$ $n(O_2) = 0.50\text{ mol}$ $n(\text{CO produced}) = \frac{2}{3} \times 0.50 = 0.33\text{ mol}$
Step 8	Use $n = \frac{m}{M}$ to calculate the mass in grams produced.	$n(CO) = \frac{m}{M}$ $m(CO) = n \times M$ $m(CO) = 0.33\text{ mol} \times 28.0\text{ g mol}^{-1}$ $m(\text{CO produced}) = 9.3\text{ g}$

Linking this back to combustion reactions, we can now understand the main difference between complete and incomplete combustion and summarise it as follows:

- complete combustion: the fuel is the limiting reagent, oxygen is the excess reagent
- incomplete combustion: the fuel is the excess reagent, oxygen is the limiting reagent.

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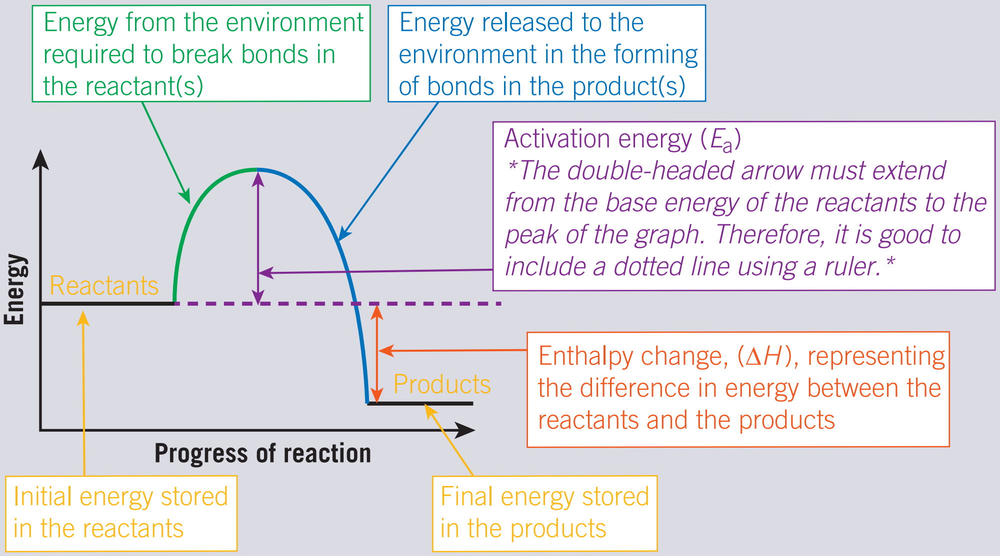
It is important to always be aware of limiting and excess reagents when performing calculations for chemical reactions. It will not always be clearly indicated that this is a required step, but it is important in order to obtain the correct answer.

VIDEO 1C–2
SKILLS: REPRESENTING AND ANALYSING ENERGY PROFILE DIAGRAMS

1C SKILLS

Representing and analysing energy profile diagrams

Being able to draw fully labelled energy profile diagrams is an important skill for assessments. However, you also need to be able to explain what each part of the energy profile diagram represents, as well as connect this to key chemistry terms for this topic. Consider the example shown below.



An energy profile diagram like the one above could be given to you in a question. The following are some example tasks that you may be asked to complete:

- Label the activation energy (answer shown in purple above).
- Label OR explain the enthalpy change (answer shown in orange above).
- Describe why the amount of energy increases initially in the energy profile diagram (answer shown in green above).
- Describe why the amount of energy decreases following the top of the peak in the energy profile diagram (answer shown in blue above).

Note, when labelling the activation energy or enthalpy change you need to be precise with placement of arrows otherwise you will lose marks. Using a ruler to draw a dotted horizontal line makes this labelling easier.

Another question may be: Does the energy profile diagram represent an exothermic or an endothermic reaction? Justify your reasoning.

For this question, you should note that as this is a 50:50 choice, you do not get a mark for making the correct selection. The term 'justify' means you need to provide evidence/reasons why the energy profile diagram is exothermic or why it is not endothermic. As such, if this was a 2-mark question, your answer should look as follows:

Exothermic (no mark)

The energy of the products is lower than the energy of the reactants (1 mark) OR the enthalpy change (ΔH) is negative. (1 mark)

Whereas, for endothermic reactions the energy of the products is higher than the energy of the reactants OR the enthalpy change (ΔH) is positive. (1 mark)

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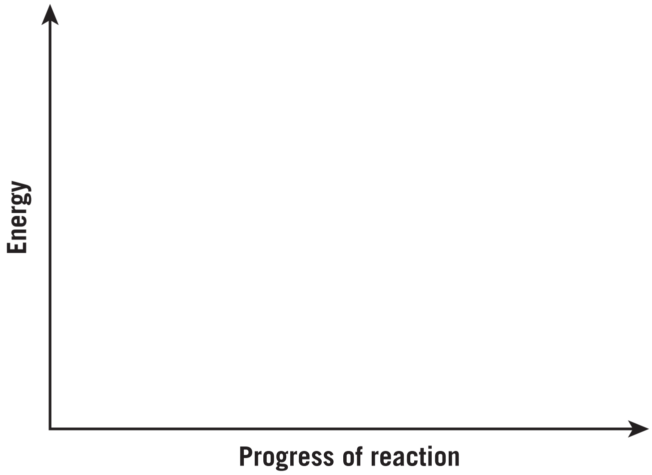
Section 1C questions

1 Compare and contrast exothermic and endothermic reactions.

2 Octane (C_8H_{18}) is a common hydrocarbon found in petrol.

  a Write a balanced thermochemical equation for the combustion of octane.

  b Copy the following axes into your workbook and draw the energy profile diagram for the combustion of octane. On your diagram, label the enthalpy change of the reaction, ΔH, and the activation energy, E_a.



3 Sodium metal undergoes a vigorous exothermic reaction with water to produce hydrogen gas and aqueous sodium hydroxide according to the equation:

$$2Na(s) + 2H_2O(l) \rightarrow 2NaOH(aq) + H_2(g) \qquad \Delta H = -368\ kJ\ mol^{-1}$$

A 0.500 g piece of sodium metal is placed in a beaker containing 100 mL of water.

  a Determine the limiting reagent in this reaction.

  b Determine the mass of hydrogen gas that would be produced.

  c Determine the concentration, in mol L^{-1}, of sodium hydroxide present after the reaction has gone to completion.

  d Determine the energy released, in kJ.

4 A mixture contains equal parts by mass of methanol and ethanol. (Heat of combustion of methanol = 22.7 kJ g^{-1}; Heat of combustion of ethanol = 29.6 kJ g^{-1})

A 100 g sample of this fuel mixture undergoes complete combustion in excess oxygen.

  a Calculate the mass of each product.

  b Calculate the energy released, in MJ.

  c Calculate the mass of carbon dioxide gas released.

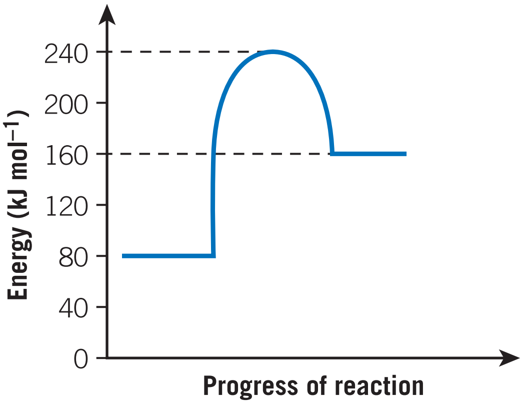
  d Calculate the mass of the fuel mixture required to undergo complete combustion to produce 100 kJ of energy.

5 Using the energy profile diagram on the right, answer the following questions.

  a Does the energy profile diagram depict an endothermic or an exothermic reaction? Justify your reasoning.

  b What is the enthalpy change, ΔH, of the reaction?

  c What is the activation energy, E_a, of the reaction?



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Chapter 1 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

	Success criteria – I am now able to:	Linked questions
1A.1	Define 'fossil fuels', 'biofuels', 'renewable' and 'non-renewable'	1☐, 11☐
1A.2	Compare and contrast the different types of fossil fuels	11☐
1A.3	Compare and contrast the different types of biofuels	4☐
1A.4	Describe the process of producing bioethanol from glucose	12☐
1A.5	Recall that distillation is used in the production of bioethanol	12☐
1A.6	State the equation for the fermentation of glucose	12☐
1A.7	Explain the advantages and disadvantages of fossil fuels and biofuels	11☐, 12☐
1B.1	Describe the process of photosynthesis	7☐
1B.2	State the equation for photosynthesis	9☐, 12☐
1B.3	Describe the process of cellular respiration	3☐
1B.4	State the equation for cellular respiration	12☐
1C.1	Compare and contrast exothermic and endothermic reactions	5☐, 11☐
1C.2	Define 'activation energy'	6☐
1C.3	Define 'enthalpy' and 'enthalpy change'	2☐, 6☐
1C.4	Draw and fully label energy profiles for exothermic and endothermic reactions	13☐
1C.5	Identify the limiting reagent in a given chemical reaction	10☐, 13☐
1C.6	Calculate the mass, concentration or volume of various reactants or products in a given chemical equation when a limiting reagent is present	13☐
1C.7	Compare complete and incomplete combustion reactions of fuels	13☐
1C.8	State that all combustion reactions are exothermic	8☐, 13☐
1C.9	Determine the balanced thermochemical equation for complete and incomplete combustion of organic molecules	13☐

Multiple-choice questions

1 Which of these statements best describes a fuel that is renewable?

A fossil fuels that are produced at the same rate at which they are consumed
B fossil fuels that are produced at a slower rate than they are consumed
C biofuels that are produced at the same rate at which they are consumed
D biofuels that are produced at a slower rate than they are consumed

2 What would be the most appropriate units to compare the enthalpy change of the combustion of two different fuels, both containing a mixture of components?

A kJ
B $\mathrm{kJ\,g^{-1}}$
C $\mathrm{kJ\,mol^{-1}}$
D $\mathrm{g\,mol^{-1}}$

3 What type of reaction does glucose undergo in cellular respiration?

A oxidation
B reduction
C displacement
D neutralisation

4 Which of the following biofuels is made from decomposing plant and animal materials?

A biogas
B biodiesel
C bioethanol
D biopetroleum

5 In an endothermic reaction, the

A enthalpy change is negative.
B products are more stable than the reactants.
C reaction releases energy in the form of heat.
D energy required to break bonds in the reactants is greater than the energy released to form the bonds in the products.

6 From the table below, identify the correct explanations for both enthalpy change and activation energy.

	Enthalpy change	Activation energy
A	The sum of the energy of the products minus the energy of the reactants	The minimum quantity of energy required so that a chemical reaction can proceed
B	The sum of the energy of the reactants and the products	The maximum quantity of energy required to break the bonds in the reactants so that new products can be formed
C	The difference in total energy between reactants and products in a chemical reaction	The minimum quantity of energy required so that a chemical reaction can proceed
D	The amount of energy released from the breaking of bonds	The quantity of energy required to form bonds in products

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7 In the process of photosynthesis, which of the following best outlines the main energy transformation taking place?

A light → heat

B light → chemical

C chemical → heat

D carbon dioxide → glucose

8 Both the complete and incomplete combustion of octane, C_8H_{18},

A occur in the presence of excess oxygen gas.

B produce carbon monoxide.

C are exothermic reactions.

D have positive enthalpies.

9 Which of the following shows the correctly balanced chemical equation for photosynthesis?

A $6CO_2(g) + 12H_2O(l) \rightarrow 6O_2(g) + C_6H_{12}O_6(aq)$

B $6CO_2(g) + 6H_2O(l) \rightarrow 6O_2(g) + C_6H_{12}O_6(aq)$

C $6CO_2(g) + 6H_2O(l) \rightarrow 6O_2(g) + C_6H_6O_{12}(aq)$

D $C_6H_{12}O_6(aq) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l)$

10 Ethane (C_2H_6) and oxygen react to form carbon dioxide and water. If 0.8 g of ethane reacts with 0.25 g of oxygen, which reactant is limiting?

A oxygen

B ethane

C carbon dioxide

D neither reactant is limiting

Short-answer questions

11 Concerns from society about the rising levels of greenhouse gas emissions are continuing to drive our focus on aspects of different types of fuels. Coal is one of Australia's largest exports; however, the mining and burning of coal is a major contributor to our greenhouse gas emissions.

a List the two forms of greenhouse gases that are released from the plant remains during the formation of coal. (1 mark)

b What conditions help to cause the release of these greenhouse gas emissions from the coal beds? (1 mark)

c Coal is an example of a fossil fuel. Explain why, by comparing this to biofuels. (2 marks)

In the Latrobe Valley, east of Melbourne, an electricity generation company is planning to replace a thermal power station fired by brown coal with a thermal plant fired by natural gas. Natural gas offers many potential benefits because it results in the release of less greenhouse gases.

d Using your knowledge of natural gas, explain why less greenhouse gases are emitted. (2 marks)

e Would you say that natural gas is renewable? Explain. (1 mark)

f Is the burning of natural gas an example of an exothermic or an endothermic reaction? Explain. (2 marks)

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- **g** One issue with the location of the natural gas plant further from Melbourne is that more energy is lost in the transmission of electricity through power lines than the amount of energy lost by the flow of gas in pipelines. What is one potential solution to this problem for the electricity company? (1 mark)
- **h** Outline why biogas is considered an example of a renewable energy resource. (2 marks)

12 Bioethanol is primarily produced by the fermentation of glucose and sucrose by yeast, such as *Saccharomyces cerevisiae*, or bacteria, such as *Escherichia coli.*

- **a** Define 'fermentation' and include both a word equation and a balanced chemical equation illustrating the type of fermentation *Saccharomyces cerevisiae* would carry out. (3 marks)
- **b** Bioethanol production can also use starch from corn. However, biomass of this sort must be pretreated prior to fermentation. Define 'biomass'. (1 mark)
- **c** Outline one advantage and one disadvantage with the use of bioethanol compared with petrol. (2 marks)

13 In the presence of oxygen, plants and animals can perform aerobic cellular respiration. Writing balanced chemical equations, explain how the processes of aerobic cellular respiration and photosynthesis are linked. (3 marks)

14 Propane is a common fuel used in portable burners, such as those found in camp stoves. In certain situations, there is not enough ventilation for the fuel to burn completely. This can be quite dangerous, as it leads to the production of carbon monoxide. Carbon monoxide is a colourless, odourless gas that can be poisonous if inhaled in large enough quantities. This is one reason why camp stoves have warnings not to be used inside a tent, as the carbon monoxide can build up quite quickly and lead to unconsciousness and death.

- **a** Write a balanced chemical equation for the incomplete combustion reaction of propane occurring at 25°C and 100 kPa, assuming that carbon monoxide is the only carbon-based product formed. (2 marks)
- **b** Describe how you know that oxygen will be the limiting reactant in this reaction. (1 mark)
- **c** A standard camping stove comes with 468 g of propane gas in a canister. If this is burned in the presence of 1050 g of oxygen gas, determine the mass (in g) of carbon monoxide that will be produced. (2 marks)
- **d** Determine the mass of fuel that remains following the reaction. (1 mark)
- **e** Calculate the energy released in MJ. (2 marks)
- **f** Draw a fully labelled energy profile diagram for this reaction. (4 marks)

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UNIT 3 HOW CAN DESIGN AND INNOVATION HELP TO OPTIMISE CHEMICAL PROCESSES?

CHAPTER 2 MEASURING CHANGES IN CHEMICAL REACTIONS

Introduction

Energy is involved in almost every aspect of our lives. The food we eat for breakfast, lunch and dinner provides our bodies with the energy that they need to function. The petrol that we use to fill up our cars and motorbikes provides the energy that they need to run. Electrical energy powers all our equipment and devices, lights up our homes and helps us communicate all over the world. In this chapter, we will focus on the energy that is generated from the chemical reactions involving fuel and food. You will apply stoichiometry to a real-world problem – the emission of greenhouse gases – and learn how to quantitate the energy produced from combustion reactions.

INTRODUCTION VIDEO
MEASURING CHANGES IN CHEMICAL REACTIONS

Curriculum

Area of Study 1 Outcome 1
What are the current and future options for supplying energy?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
- Calculations related to the application of stoichiometry to reactions involving the combustion of fuels, including mass–mass, mass–volume and volume–volume stoichiometry, to determine heat energy released, reactant and product amounts and net volume or mass of major greenhouse gases (CO_2, CH_4 and H_2O), limited to standard laboratory conditions (SLC) at 25°C and 100 kPa	**2A Measuring greenhouse gases** **2A.1** Recall principles of stoichiometry in balancing equations **2A.2** Determine the heat produced from combustion reactions using the equation $E = \Delta H \times n$ **2A.3** Use stoichiometry to calculate reactant and product amounts, and net volume or mass of major greenhouse gases **2A.4** Perform calculations involving excess and limiting reagents in combustion reactions

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Study Design:	Learning intentions – at the end of the chapter I will be able to:
• The use of the specific heat capacity of water to approximate the quantity of heat energy released during the combustion of a known mass of fuel and food • The principles of solution calorimetry, including determination of the calibration factor and consideration of the effects of heat loss; analysis of temperature–time graphs obtained from solution calorimetry • Energy from fuels and food: – calculation of energy transformation efficiency during combustion as a percentage of chemical energy converted to useful energy – comparison and calculations of energy values of foods containing carbohydrates, proteins and fats and oils	**2B** **Measuring energy released from chemical reactions** **2B.1** Define ‘specific heat capacity’ and its units **2B.2** Recall the properties of water that lead to its use in specific heat experiments **2B.3** Perform calculations using the equation $q = mc\Delta T$ **2B.4** State the principles of solution calorimetry **2B.5** Analyse graphical data to determine the calibration factor of a calorimeter **2B.6** Use experimental data to calculate the calibration factor of a calorimeter and energy produced from chemical reactions **2B.7** Calculate energy transformation efficiency from given experimental data
• Energy from fuels and food: – calculation of energy transformation efficiency during combustion as a percentage of chemical energy converted to useful energy – comparison and calculations of energy values of foods containing carbohydrates, proteins and fats and oils	**2C** **Measuring energy from food** **2C.1** Use reference tables for heats of combustion of different food groups **2C.2** Determine the energy content of a food based on food group composition **2C.3** Calculate the energy content of a food using calorimetry

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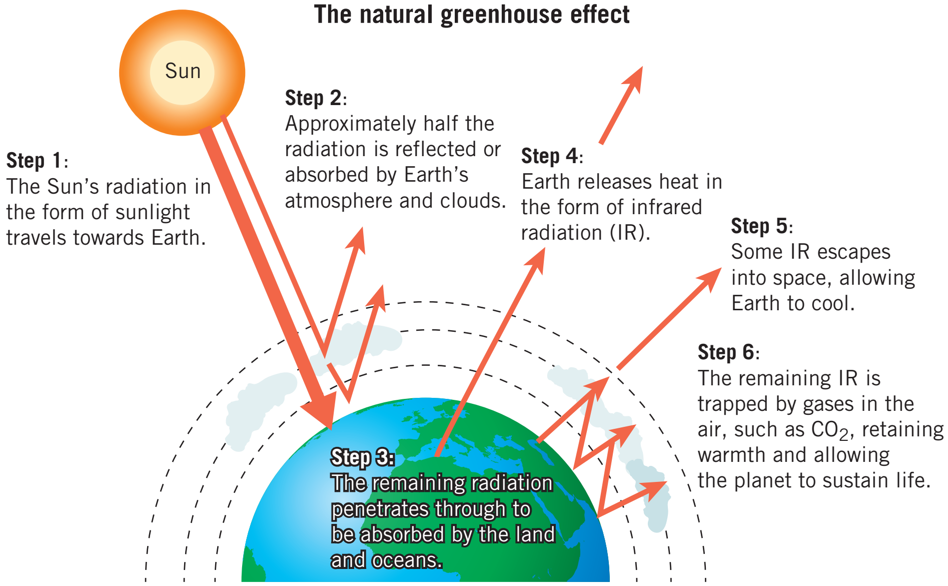
Glossary

Calorimetry
Enhanced greenhouse effect
Global warming
Greenhouse gas
Line of best fit
Molar volume
Solution calorimeter
Specific heat capacity
Standard laboratory conditions
Stoichiometry

Concept map

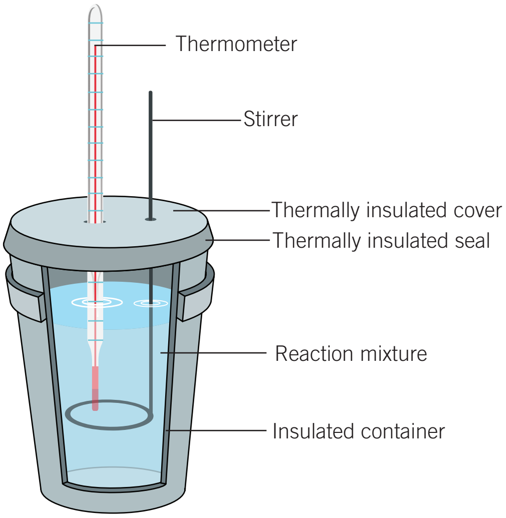
2A Measuring greenhouse gases

Calculating the quantity of greenhouse gases produced from combustion reactions



2B Measuring energy released from chemical reactions

Using solution calorimetry to determine the amount of heat energy released or absorbed from reactions



2C Measuring energy from food

Understanding how nutritional content determines the quantity of energy contained within food

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

2A Measuring greenhouse gases

Study Design:

- Calculations related to the application of stoichiometry to reactions involving the combustion of fuels, including mass–mass, mass–volume and volume–volume stoichiometry, to determine heat energy released, reactant and product amounts and net volume or mass of major greenhouse gases (CO_2, CH_4 and H_2O), limited to standard laboratory conditions (SLC) at 25°C and 100 kPa

Glossary:

Enhanced greenhouse effect
Global warming
Greenhouse gas
Molar volume
Standard laboratory conditions
Stoichiometry

ENGAGE

Lowering greenhouse gas emissions for global security

In 2015, the Conference of the Parties (COP) to the United Nations Framework Convention on Climate Change held a summit in Paris that set down a landmark treaty on greenhouse gas emissions targets that was supported by 196 member nations. In November 2016, that treaty was ratified and became legally binding. The goal is to limit global warming to 1.5°C compared to pre-industrial levels and reach peak greenhouse gas production as soon as possible.

In 2020, countries submitted their plans to reach their peak targets and the global warming limit. While COP27, held in Egypt in 2022, revealed the political difficulties in meeting the 1.5°C target, the 2015 Paris Agreement set the wheels in motion for many countries to set low-carbon solutions, carbon economies and carbon neutrality targets, all in the name of reaching this goal. This has led to new jobs, new industries and the hope that by 2030 zero-carbon solutions could be viable options in sectors that currently represent 70% of global greenhouse gas emissions.

Figure 2A–1 Heads of delegations at the United Nations Summit in Paris, 2015

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EXPLAIN

Greenhouse gases and chemical reactions

Before beginning to explore chemical reactions in more depth, let's first refresh our understanding of how greenhouse gases are produced.

Combustion reactions

1C EXOTHERMIC AND ENDOTHERMIC REACTIONS LINK

As you learned in Section 1C, combustion reactions occur when a hydrocarbon is burned in the presence of oxygen. This results in the production of carbon dioxide (CO_2) and water vapour (H_2O), which are **greenhouse gases**. Other well-known greenhouse gases include nitrous oxide (N_2O), ozone (O_3) and methane (CH_4). Methane is emitted during the extraction and transport of natural gas, as well as from livestock and other agricultural activities. These gases allow sunlight to pass through Earth's atmosphere, but they trap the heat that is reflected from the surface, preventing it from radiating out into space. This process is known as the greenhouse effect, and it is what makes Earth warm enough to support life as we know it.

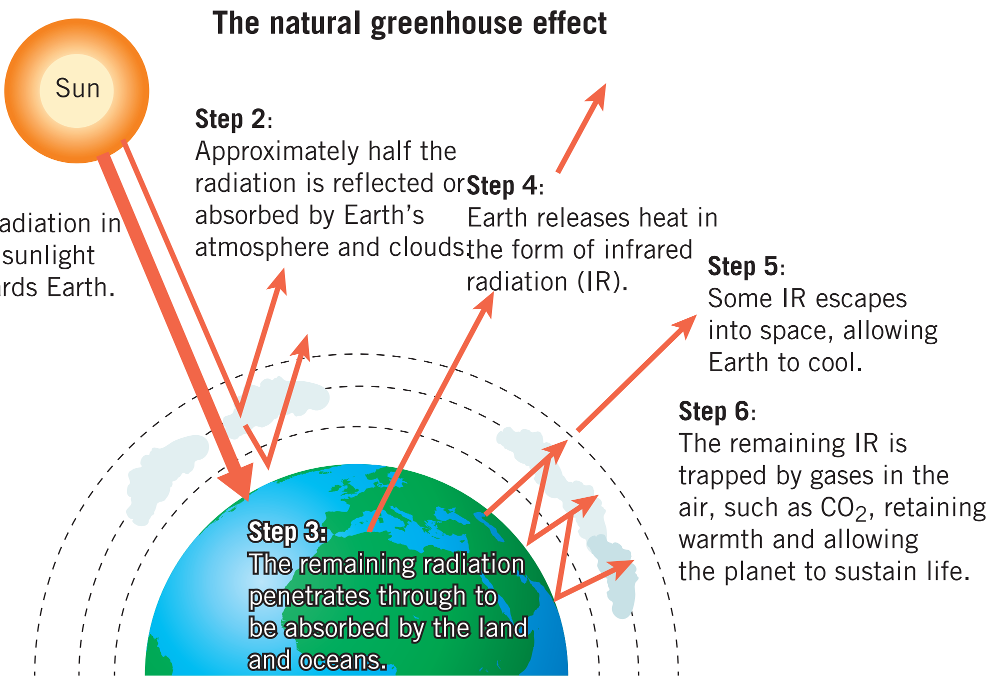

Figure 2A–2 A representation of the natural greenhouse effect

Greenhouse gas a gas that absorbs and emits infrared radiation in the atmosphere, causing warming of Earth's surface

Enhanced greenhouse effect the change of the normal climate equilibrium on Earth, primarily increased global temperatures; caused by increased emissions of greenhouse gases; also known as global warming

Global warming the long-term warming of Earth's surface temperature, observed since the pre-industrial period

However, an increase of these gases, particularly the ones caused by human activity, such as CO_2 and CH_4, causes an enhancement of the greenhouse effect, known as the **enhanced greenhouse effect**, which leads to **global warming** and climate change. Being able to calculate how much greenhouse gas will be produced from a reaction is therefore critical in determining the suitability of a reaction or process in line with the societal goals of decreasing global warming.

1C EXOTHERMIC AND ENDOTHERMIC REACTIONS LINK

When writing combustion reactions, it is also standard practice to state the enthalpy of the given reaction.

Common combustion reactions

LINK **1A** TYPES OF FUELS

LINK **1C** EXOTHERMIC AND ENDOTHERMIC REACTIONS

There are several common reactions that produce different greenhouse gases. Carbon dioxide (CO_2) is produced when fossil fuels, such as coal, petrol and natural gas, are burned for energy. For example, the combustion of octane in a car engine has the equation:

$$2C_8H_{18}(l) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O(l) \qquad \Delta H = -10\,920\ \text{kJ mol}^{-1}$$

Not all combustion reactions go to completion. For example, carbon monoxide (CO) is produced when fuels burn incompletely. For incomplete combustion reactions, the enthalpy value can vary depending on the conditions. This is because ‘imperfect’ conditions, such as a lack of oxygen or low temperatures, can lead to incomplete combustion.

Determining heat energy production from the combustion of fuels

Combustion is the chemical process that produces heat energy from the oxidation of fuels. We can experience the benefits directly around an open fire or indirectly in powering our homes and vehicles, where the energy from combusted fuels drives other processes. Combustion reactions are always exothermic – that is, they release heat energy.

To determine the energy released from the combustion of some fuels, we can use the reference tables found in the VCAA Data book for ‘Molar heat of combustion’, measured in kJ mol^{-1}, as shown below.

Table 2A–1 Molar heat of combustion values for some common fuels at 25°C and 100 kPa

Fuel	Molecular formula	Molar heat of combustion (kJ mol^{-1})
Methane	CH_4	890
Propane	C_3H_8	2220
Butane	C_4H_{10}	2880
Pentane	C_5H_{12}	3510
Octane	C_8H_{18}	5460
Methanol	CH_3OH	726
Ethanol	CH_3CH_2OH	1360
Hydrogen	H_2	282
Glucose	$C_6H_{12}O_6$	2840

While heat energy transformation into other forms isn’t 100% efficient, a large portion of this energy produced from combustion reactions can be put to use. Depending on the amount of fuel available, which is expressed in moles, a certain amount of energy can be released, as shown in Worked example 2A–1 on the following page.

VIDEO
WORKED
EXAMPLE 2A–1

Worked example 2A–1: Calculating heat energy produced from burning a fuel sample

A 100.0 kg quantity of ethanol, C_2H_5OH, is burned in an industrial stove with an open air-intake. How much energy, in MJ, will be produced if all the ethanol is burned?

Solution

	Logic	Process
Step 1	Write down the information that you have about the known substance.	$m(C_2H_5OH) = 100.0\text{ kg} = 100\,000\text{ g}$ $M(C_2H_5OH) = 46.0\text{ g mol}^{-1}$ $n(C_2H_5OH) = ?$
Step 2	Calculate the amount of substance being combusted in moles.	$n(C_2H_5OH) = \dfrac{m(C_2H_5OH)}{M(C_2H_5OH)}$ $= \dfrac{100\,000\text{ g}}{46.0\text{ g mol}^{-1}}$ $= 2173.9\text{ mol}$
Step 3	Determine the energy produced by multiplying $n(C_2H_5OH)$ by the molar heat of combustion of ethanol.	$E = 1360\text{ kJ mol}^{-1} \times 2173.9\text{ mol}$ $= 2\,956\,504\text{ kJ}$
Step 4	Convert result to MJ.	$E = \dfrac{2\,956\,504\text{ kJ}}{1000}$ $= 2960\text{ MJ}$

Special conditions of stoichiometry

The amount of energy emitted or required for a reaction can vary considerably, as can the amount of greenhouse gas produced. It is important to consider two things here:

- The energy value of the enthalpy is in kilojoules.
- The amounts are ‘per mole’ of reference material.

This last point should help us realise how important **stoichiometry** will be to success in calculations of greenhouse gas emissions. To do this, we must first be able to successfully balance an equation.

Stoichiometry the quantitative relationship between two or more substances during a reaction, based on the ratio in which they react

Converting stoichiometrically from different units

In addition to basic calculations, there are times when we don't need to convert to/from the amount in moles, *n*, and we can convert stoichiometrically from different units. This is represented diagrammatically in Figure 2A–3.

Worked example 2A–2: Calculating the moles of product in combustion

VIDEO
WORKED
EXAMPLE 2A–2

When 0.5 mole of pentane is burned in excess oxygen, how many moles of carbon dioxide are produced?

Solution

	Logic	Process
Step 1	Write a balanced equation for the reaction.	$C_5H_{12}(g) + 8O_2(g) \rightarrow 5CO_2(g) + 6H_2O(g)$
Step 2	Write down the information that you have about the known substance.	$n(C_5H_{12}) = 0.5$ mol
Step 3	Determine the stoichiometric ratio from the equation.	From the equation, the coefficient of pentane is 1 and CO_2 is 5. $n(C_5H_{12}) : n(CO_2) = 1:5$
Step 4	Use the stoichiometric ratio to determine the amount of unknown substance.	5 times the amount of CO_2 is produced per amount of pentane $\therefore n(CO_2) = 5 \times n(C_5H_{12}) = 5 \times 0.5 = 2.5$ mol

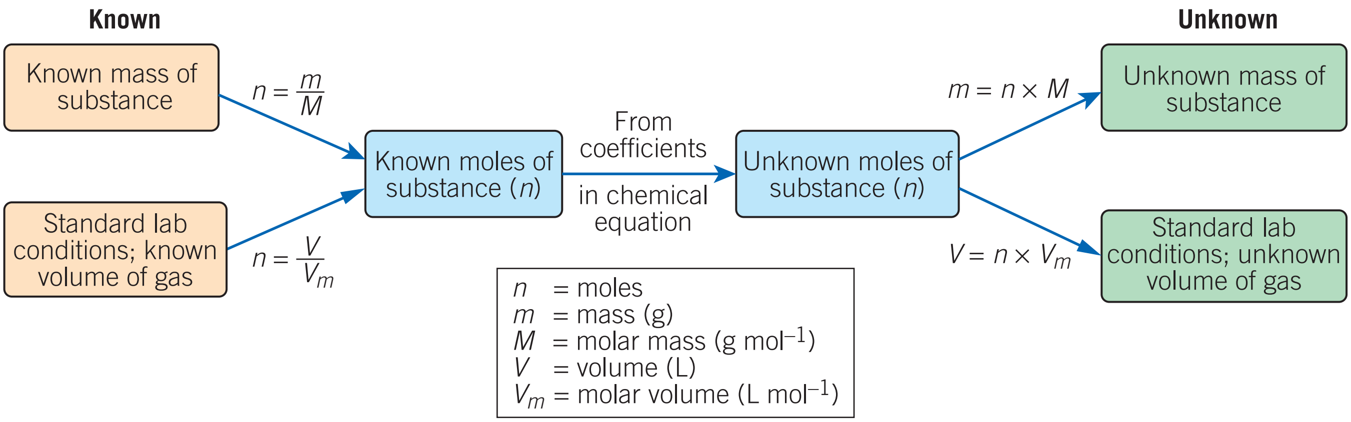

Figure 2A–3 Different inputs and how they can get to different outputs through stoichiometric ratios

For example, the result of Worked example 2A–2 can be represented as shown in Figure 2A–4.

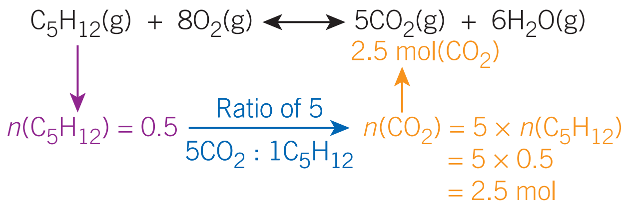

Figure 2A–4 Using stoichiometric ratios from Worked example 2A–2

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VIDEO
WORKED
EXAMPLE 2A–3

Worked example 2A–3: Calculating the moles of product in combustion

When 11 moles of octane are completely combusted in oxygen, how many moles of water are produced?

Solution

	Logic	Process
Step 1	Write a balanced equation for the reaction.	$2C_8H_{18}(g) + 25O_2(g) \rightarrow 16CO_2(g) + 18H_2O(l)$
Step 2	Write down the information that you have about the known substance.	$n(C_8H_{18}) = 11$ mol
Step 3	Determine the stoichiometric ratio from the equation.	From the equations, the number in front of octane is 2 and 18 for H_2O. $n(C_8H_{18}) : n(H_2O) = 2 : 18 = 1 : 9$
Step 4	Use the stoichiometric ratio to determine the amount of unknown substance.	$n(H_2O) = 9 \times n(C_8H_{18})$ $= 9 \times 11$ $= 99$ moles of water

Check-in questions – Set 1

1 Define the following terms: combustion, greenhouse gas, global warming.
2 Draw a diagram that shows the relationship between all the different formulas for amount of substance, mass, volume, pressure and temperature.
3 a A promising fuel is hydrogen, as water is the main by-product of its combustion reaction. What amount of water, in moles, is produced from the combustion of 3.33 moles of hydrogen fuel?
  b How much energy is released from the combustion of 3.33 moles of hydrogen fuel?

Mass–mass stoichiometry

For mass–mass stoichiometry, we're interested in the mass of product produced from a given mass of reactant or vice versa. To calculate this successfully, we need to determine the number of moles of the substance we have information for and then follow our 'down, across, up' process, as shown in Figure 2A–3.

1 Convert the given mass of a substance to moles using $n = \frac{m}{M}$.
2 Use the mole ratio in the thermochemical equation to determine the moles of the substance of interest.
3 Calculate the mass of the substance of interest from the moles determined in Step 2 using $m = n \times M$.

This is still making use of the techniques learned earlier but with a specific strategy for mass–mass questions. We see this in action in Worked example 2A–4.

VIDEO
WORKED EXAMPLE 2A–4

Worked example 2A–4: Calculating the mass of a product in combustion

If a 4.4 gram sample of propane is burned completely in oxygen, calculate the mass, in grams, of carbon dioxide produced.

Solution

	Logic	Process
Step 1	Write a balanced equation for the reaction.	$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$
Step 2	Write down the information you have and need about the substances.	$m(C_3H_8) = 4.4\ g$ $M(C_3H_8) = 44.0\ g\,mol^{-1}$ $M(CO_2) = 44.0\ g\,mol^{-1}$ $n(C_3H_8)$ = unknown
Step 3	Determine the number of moles of the known substance with known mass using $n = \frac{m}{M}$.	$n(C_3H_8) = \frac{m(C_3H_8)}{M(C_3H_8)}$ $= \frac{4.4\ g}{44.0\ g\ mol^{-1}}$ $= 0.10\ mol$
Step 4	Determine the stoichiometric ratio from the equation.	From the equations, the number before propane is 1 and CO_2 is 3. $n(C_3H_8) : n(CO_2) = 1:3$
Step 5	Use the ratio to determine the unknown number of moles.	$n(CO_2) = 3 \times n(C_3H_8)$ $= 3 \times 0.10\ mol$ $= 0.30\ mol$
Step 6	Calculate the unknown mass of the substance using $m = n \times M$.	$m(CO_2) = n(CO_2) \times M(CO_2)$ $= 0.30 \times 44.0\ g\ mol^{-1}$ $= 13\ g$

Mass–volume stoichiometry

Mass–volume stoichiometry is similar to mass–mass stoichiometry except we are interested in the volume of product produced from a given mass of reactant or vice versa. To calculate this correctly, we need to determine the number of moles of the substance we are given information for and then follow our 'down, across, up' process, as shown in Figure 2A–3 on page 45.

1 Convert the given mass to moles using $n = \frac{m}{M}$.
2 Use the mole ratio in the thermochemical equation to determine the moles the substance of interest.
3 Convert the moles to volume using the **molar volume** equation.

A special condition of Avogadro's law applies when a gas is being measured at **standard laboratory conditions** (SLC). For 1 mole of a gas at SLC, there is a known volume (as temperature and pressure are known at SLC). This means the molar volume at SLC is 24.8 L mol^{-1}. Based on this, Avogadro's law for measuring volume change becomes

$$n = \frac{V}{V_m}$$

where:

n = The moles of the gas
V = The volume of gas (in L)
V_m = The molar volume at SLC (in L mol^{-1}).

Molar volume a measure of how much product is formed in a reaction, which can be calculated quantitatively

Standard laboratory conditions refers to the standard laboratory conditions (SLC) of 25°C and 100 kPa, as specified by the International Union of Pure and Applied Chemistry (IUPAC)

This is still making use of the techniques learned earlier but with a specific strategy for mass–volume questions. We see this in action in Worked example 2A–5.

VIDEO WORKED EXAMPLE 2A–5

Worked example 2A–5: Calculating the mass of a product in combustion using the molar volume at SLC

What mass of water is produced when 20.0 mL of butane is completely combusted in oxygen under standard laboratory conditions?

Solution

	Logic	Process
Step 1	Write a balanced equation for the reaction.	$2C_4H_{10}(g) + 13O_2(g) \rightarrow 8CO_2(g) + 10H_2O(l)$
Step 2	Write down the information you have and need about the substances.	$V(C_4H_{10}) = 0.0200\ L$ Molar volume at SLC (V_M) = $24.8\ L\ mol^{-1}$ $n(C_4H_{10})$ = unknown
Step 3	Determine the number of moles of the substance with known volume using the molar volume at SLC.	$n(C_4H_{10}) = \frac{V(C_4H_{10})}{V_M}$ $= \frac{0.0200\ L}{24.8\ L\ mol^{-1}}$ $= 8.06 \times 10^{-4}\ mol$
Step 4	Determine the stoichiometric ratio from the equation.	From the equation, the number before butane is 2 and the number before water is 10. $n(C_4H_{10}) : n(H_2O) = 2 : 10 = 1 : 5$
Step 5	Use the ratio to determine the unknown number of moles of the substance.	$n(H_2O) = 5 \times n(C_4H_{10})$ $= 5 \times 8.06 \times 10^{-4}\ mol$ $= 4.03 \times 10^{-3}\ mol$
Step 6	Calculate the unknown mass using $m = n \times M$	$m(H_2O) = n(H_2O) \times M(H_2O)$ $= 4.03 \times 10^{-3}\ mol \times 18\ g\ mol^{-1}$ $= 0.0726\ g$

Volume–volume stoichiometry

Volume–volume stoichiometry is similar to mass–mass stoichiometry and mass–volume stoichiometry except we're interested in the volume of a gaseous product from a given volume of gaseous reactant or vice versa. If the following conditions are met, we can skip some steps in the overall process.

5A WHAT CAUSES A CHEMICAL REACTION? LINK

1 The system is a closed system. A closed system is one in which energy can be transferred between the reaction and the surroundings, but matter cannot. This is discussed further in Section 5A.
2 The pressure is kept constant.
3 The temperature is kept constant.

If these conditions are met, then the ratio of gas volumes is identical to the mole ratios and the coefficients in the reaction equation also apply for volume. For example, consider the following equation:

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

If 100 mL of methane is combusted in a reaction container, how much CO_2 will be produced?

As we have a system that meets the conditions of a volume–volume stoichiometry, we can say that 'one volume of methane produces one volume of CO_2, and therefore, 100 mL of methane will produce 100 mL of CO_2'.

Worked example 2A–6: Calculating the volume of a product in combustion using volume–volume stoichiometry

VIDEO WORKED EXAMPLE 2A–6

Methane is a common ingredient in biogas. If 4.0 L of methane is burned in excess oxygen in a closed reactor that is kept at constant temperature, how many litres of carbon dioxide are going to be produced?

Solution

	Logic	Process
Step 1	Write a balanced equation for the reaction.	$CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$
Step 2	Check whether we have the conditions for volume–volume stoichiometry.	Yes. Pressure is constant, temperature is constant, all species are gaseous and the container is sealed.
Step 3	Write the volume ratio.	$V(CH_4) : V(CO_2) = 1 : 1$
Step 4	Use the ratio to determine the unknown volume.	$V(CO_2) = 1 \times V(CH_4) = 1 \times 4.0\ \text{L}$ $= 4.0\ \text{L}$

Calculations involving limiting and excess reagents

LINK **1C** EXOTHERMIC AND ENDOTHERMIC REACTIONS

Determining whether a reactant is limiting, or in excess, was covered in Section 1C. Here we'll look at how this can apply to questions involving greenhouse gases.

Consider Worked example 2A–7 below. There are really two questions here:

- Which of the reagents is limiting, and therefore, which one is in excess? (This is shown in Steps 1–4.)
- What is the mass of methane gas formed? (You need to know which is limiting to calculate which is in excess. This is shown in Steps 5–7.)

Worked example 2A–7: Calculating the mass of a product when there is a limiting reactant

VIDEO WORKED EXAMPLE 2A–7

Determine the expected mass of methane produced in the below reaction when 25.0 g of hydrogen gas and 100.0 g of carbon dioxide gas are mixed and reacted.

$$CO_2(g) + 4H_2(g) \rightarrow CH_4(g) + 2H_2O(l) \qquad \Delta H = -165.0\ \text{kJ mol}^{-1}$$

Solution

	Logic	Process
Step 1	Write a balanced equation for the reaction.	$CO_2(g) + 4H_2(g) \rightarrow CH_4(g) + 2H_2O(l)$
Step 2	Calculate the moles of both reactants using $n = \frac{m}{M}$.	$n(CO_2) = \frac{m(CO_2)}{M(CO_2)} = \frac{100.0\ \text{g}}{44.0\ \text{g mol}^{-1}} = 2.27\ \text{mol}$ $n(H_2) = \frac{m(H_2)}{M(H_2)} = \frac{25.0\ \text{g}}{2.0\ \text{g mol}^{-1}} = 12.5\ \text{mol}$

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Step 3	Write the stoichiometric ratio and the experimental ratio of both reactants.	Stoichiometric = 1 : 4 Experimental = 2.27 : 12.5 = 1 : 5.5
Step 4	Write which species is in excess and which is limiting.	Carbon dioxide is limiting; hydrogen is in excess.
Step 5	Write the stoichiometric ratio for the limiting reactant and the product in question.	$n(CO_2) : n(CH_4) = 1:1$
Step 6	Use the stoichiometric ratio to determine the unknown number of moles.	$n(CH_4) = 1 \times n(CO_2) = 2.27$ mol
Step 7	Calculate the unknown mass using $m = n \times M$.	$m(CH_4) = n(CH_4) \times M(CH_4)$ $= 2.27 \text{ mol} \times 16.0 \text{ g mol}^{-1}$ $= 36.3$ g

WORKSHEET 2A–1
CALCULATING GREENHOUSE GAS EMISSIONS

Check-in questions – Set 2

1 Explain the process for calculating energy produced from combustion of *n* moles of fuel, given that the heat of combustion of this fuel is *h* kJ mol^{-1}.

2 A car petrol tank can hold 45 L of octane at SLC. How much energy can be produced from a full tank of fuel, assuming the fuel is 100% octane?

3 Which of the reactants in the following equations is in excess and which is limiting?
   a $C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(g)$ with 0.5 g of propane and 2.5 g of oxygen
   b $H_2(g) + 4O_2(g) \rightarrow CH_4(g) + 2H_2O(g)$ with 0.2 g of oxygen and 0.4 g of hydrogen
   c $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$ with 2.22 g of methane and 1.11 g of oxygen

4 An experiment on human cells looks at the metabolism of glucose in different environments. If an experiment provides 3.2 g of glucose in a oxygen-limited environment with 2 g of available oxygen, how much CO_2 is produced? Which reactants are limiting and which are in excess?

$$C_6H_{12}O_6(s) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(g)$$

VIDEO 2A–1
SKILLS: IDENTIFYING LIMITING REAGENTS

2A SKILLS

Identifying limiting reagents

In this section, you have learned more about calculations that require you to identify the limiting reagent in combustion reactions. As described in the text, this involves calculating the number of moles of each reactant and applying stoichiometric ratios to determine which is in excess and which is limiting.

When the stoichiometric ratio is 1 : 1, this is a relatively simple process whereby the reagent with the lowest number of moles is limiting. However, it can become trickier when other stoichiometric ratios are involved. To help with that, there are many tips and strategies that people employ to make sure they solve the problem correctly. It is important that you find a method that makes sense and works well for you, but we will describe one below that you may find useful. It can be summarised as follows.

Strategy: Once you have calculated the number of moles of each reactant, divide that value by the stoichiometric coefficient from the equation. Whichever number is lower after you do this will correspond to the limiting reagent.

To understand this better, let's look at an example. In this instance, we won't go through the process of calculating the number of moles, we will just provide them in the question.

Question: The combustion of ethane can be represented by the following balanced equation:

$$2C_2H_6(g) + 7O_2(g) \rightarrow 4CO_2(g) + 6H_2O(g)$$

If 0.5 moles of ethane reacts with 2.1 moles of oxygen, which is the limiting reagent?

Solution: Using the strategy that we have above, we can set out our calculation as follows.

	C_2H_6	O_2
Number of moles (*n*)	0.5	2.1
Stoichiometric coefficient	2	7
	$\frac{0.5}{2} = 0.25$	$\frac{2.1}{7} = 0.3$

Therefore, C_2H_6 is the limiting reagent as it has the lowest value after dividing the number of moles by the stoichiometric coefficient.

Go back over some practice questions that you have done involving a limiting reagent and use this method to see if it helps.

Section 2A questions

1 Calculate the heat energy produced from each of the following combustion reactions.
  a 32 g of methanol
  b 126 mL of hydrogen gas
  c a petrol composed of 91% octane and 9% butane

2 Explain the difference between mass–mass, mass–volume and volume–volume calculations for determining the amount of products produced from reactants.

3 Water is a common by-product of combustion reactions. For a 5.8 g sample of butane, how much water vapour will be produced at SLC?

4 When butane is burned in air, water vapour and carbon dioxide are produced. Balance the equation and state the stoichiometric ratio for butane and water vapour.

5 Draw a diagram that shows the method for obtaining the unknown mass of a substance from the known mass of a second substance.

6 Daryl loves barbecuing and wants to get the most value for money.
  a Daryl is worried about the water by-product from his butane four-burner barbecue. If he plans to completely burn 25 kg of butane, how much water vapour will he produce?
  b Daryl has a new barbecue that uses propane, which advertises 'less food spoilage due to water vapour compared to butane'. If he plans to completely burn 25 kg of propane at SLC, how much water vapour will he produce, in mL? Is this better than butane?
  c Daryl has figured it out now and will only be using gas fuels from now on, so he purchases a new barbecue that uses methane in the annual sale at his camping store. If he plans to empty a 25 kg tank of methane that completely combusts (which is advertised as 18 L of methane at SLC), how much water vapour will he produce, in mL?
  d Is this the best barbecue of the three used?

7 A 62.0 g sample of propane is ignited in 100 L of oxygen. The gas volume is measured at SLC. Calculate the volume of carbon dioxide produced, in L, if the equation for the reaction is:

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l)$$

Also note which species is in excess and which is limiting.

2B Measuring energy released from chemical reactions

Study Design:
- the use of the specific heat capacity of water to approximate the quantity of heat energy released during the combustion of a known mass of fuel and food
- the principles of solution calorimetry, including determination of the calibration factor and consideration of the effects of heat loss; analysis of temperature–time graphs obtained from solution calorimetry
- energy from fuels and food:
  - calculation of energy transformation efficiency during combustion as a percentage of chemical energy converted to useful energy
  - comparison and calculations of energy values of foods containing carbohydrates, proteins and fats and oils

Glossary:
Calorimetry
Line of best fit
Solution calorimeter
Specific heat capacity

ENGAGE

Guinea pigs: nature's calorimeter?

In 1789, Antione Lavoisier conducted a series of experiments on guinea pigs. These are not the experiments for which he was famed and which led to the discovery of the principle of conservation of mass but, equally, they're not far off. Lavoisier was able to measure the heat of respiration by guinea pigs and, in doing so, also invented the world's first calorimeter, a device for detecting the energy change in a chemical reaction. He did this by placing the guinea pigs in a small ice calorimeter (a container inside another container that's filled with ice) and measured how much ice was melted. He then used this to determine the amount of energy produced by the guinea pigs and their rate of respiration. Therefore, the guinea pigs themselves were not the calorimeter, but they were useful test subjects in determining the energy produced when animals undergo respiration.

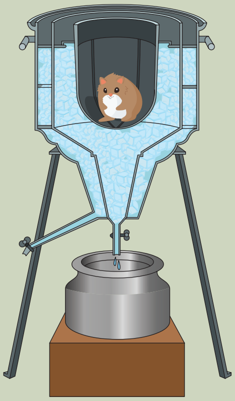

Figure 2B–1 A schematic diagram of the calorimeter, with a guinea pig inside, used by Lavoisier for his experiments on respiration

Specific heat capacity the amount of energy required to raise the temperature of one gram of a substance by one degree Celsius; symbol *c*

EXPLAIN

Measuring energy from fuels

1C EXOTHERMIC AND ENDOTHERMIC REACTIONS
2A MEASURING GREENHOUSE GASES
LINK

UNIT 2 LINK

In Section 1C and Section 2A, we discussed the release of energy from the combustion reaction of fuels using thermochemical equations. However, what hasn't yet been discussed is how these energy values are calculated. To do this experimentally, it is useful to be able to utilise a material known for its energy storage properties – water. Water is excellent for measuring energy changes as it has a uniquely high **specific heat capacity**. We remember from Unit 2 that the specific heat capacity of a material is the energy required to raise the temperature of one gram of a given substance by one degree Celsius.

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Table 2B–1 Specific heat capacities of some common materials

Material	Specific heat ($J\,g^{-1}\,°C^{-1}$)
Liquid water	4.18
Solid water (ice)	2.11
Gaseous water (steam)	2.00
Air (dry)	1.01
Basalt	0.84
Granite	0.79
Iron	0.45
Copper	0.38
Lead	0.13

As Table 2B–1 shows, liquid water stands out in its ability to store energy with little change in temperature.

From this, we can understand that a relatively large quantity of energy is required to raise the temperature of water, but how does that help us determine the actual quantity of energy released from the combustion of fuels? The answer lies in the use of the following formula, which links together energy (q) with the specific heat capacity (c):

$$q = mc\Delta T$$

where:

q = The energy produced or used in joules
c = The specific heat capacity in $J\,g^{-1}°C^{-1}$
m = The mass of the substance in grams
ΔT = The change in temperature in degrees Celsius.

Worked example 2B–1: Calculating heat energy using $q = mc\Delta T$

VIDEO WORKED EXAMPLE 2B–1

Determine how much heat energy is required to raise the temperature of 100 grams of water by 10 degrees Celsius.

Solution

	Logic	Process
Step 1	Write down everything you have and need, ensuring to convert units where appropriate.	$m(H_2O) = 100\text{ g}$ $\Delta T = 10°C$ $c(H_2O) = 4.18\ J\,g^{-1}°C^{-1}$ $q = ?$
Step 2	Write down the relevant equation.	$q = mc\Delta T$
Step 3	Substitute and solve.	$q = mc\Delta T$ $= 100\text{ g} \times 4.18\ J\,g^{-1}°C^{-1} \times 10°C$ $= 4180\text{ J}$

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Calorimetry

Calorimetry an experimental method by which the heat energy of food or a fuel is measured

To measure the quantity of energy released or absorbed in a chemical reaction, we use a technique called calorimetry. The analytical equipment used to perform **calorimetry** is the calorimeter. All calorimeters have the same goals in their design:

- isolate the reaction taking place
- have well insulated walls
- have a reference material to reduce the effects of imperfect isolation
- use stirrers to ensure that temperatures measured are even
- use thermometers to measure the temperature in the calorimeter
- have negligible heat capacity (or a known accurate heat capacity), so the loss of heat in heating the calorimeter can be taken into account.

One such technique, which can be used to measure the energy contained within food or fuel, is known as simple calorimetry. The experimental set-up for simple calorimetry is shown in Figure 2B–2.

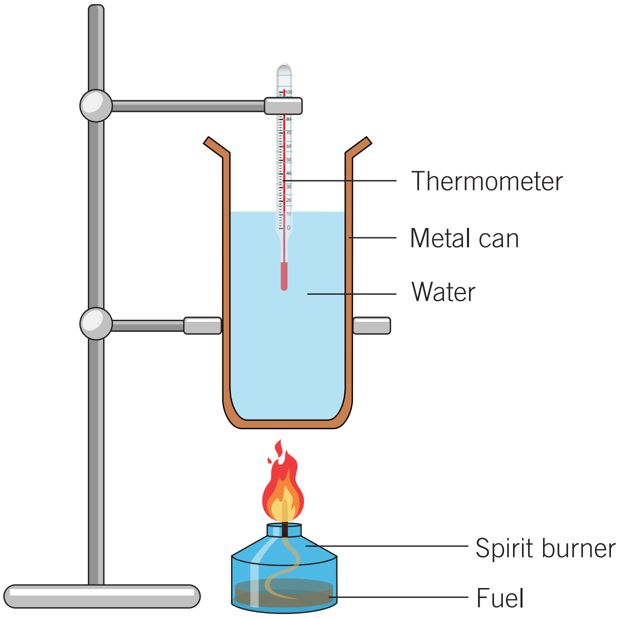

Figure 2B–2 A simple calorimetry set-up like this can be used for measuring the quantity of energy released or absorbed in a chemical reaction.

In these experiments, the fuel or food is burned (or combusted) above a spirit burner that is positioned beneath a container filled with water. As the fuel or food is burned, energy is released. The energy that is released will gradually heat the water in the container. Using the equation, $q = mc\Delta T$, above, the change in temperature can be used to calculate the quantity of energy that is released from the fuel source.

The basic experimental procedure for this follows these steps:

1. Accurately measure and record the mass of water added to the metal can.
2. Record the initial temperature of the water.
3. Weigh your fuel source and place into the spirit burner.
4. Light the spirit burner.
5. Using the thermometer, record the change in temperature of the water over time.
6. Stop heating the water before all the fuel has been used and well before the water boils.

To help understand how this can be used to measure energy, let's consider Worked example 2B–2.

Worked example 2B–2: Measuring energy from the combustion of a fuel

VIDEO
WORKED EXAMPLE 2B–2

A 13.5 g sample of octane is burned below 50.0 g of water contained in a copper container. The water temperature changed from 20.2°C to 22.8°C. How much energy, in joules, was released from the octane?

Solution

	Logic	Process
Step 1	Write down everything you have and need, ensuring to convert units where appropriate.	Have: $m(H_2O) = 50.0\text{ g}$ $c(H_2O) = 4.18\text{ J g}^{-1}\text{°C}^{-1}$ $\Delta T = 22.8\text{°C} - 20.2\text{°C} = 2.60\text{°C}$
Step 2	Write down the specific heat equation and rearrange if required.	$q = mc\Delta T$
Step 3	Substitute and solve.	$q = mc\Delta T$ $= 50.0\text{ g} \times 4.18\text{ J g}^{-1}\text{°C}^{-1} \times 2.60\text{°C}$ $= 543\text{ J}$

Solution calorimetry

Solution calorimeters measure the enthalpies associated with reactions that occur in solution, including heat of precipitation, heat of solution and heat of neutralisation. These reactions can be endothermic or exothermic. The container is thermally insulated, preventing heat loss to the surroundings. Gas samples can be measured through solution calorimetry using an ampoule. Ampoules are small (typically glass) sealed containers that are used to preserve samples but can be broken open to release their sample safely.

Solution calorimeter an instrument used to measure the heat absorbed or released during a chemical reaction, dissolution or neutralisation occurring in a liquid solution

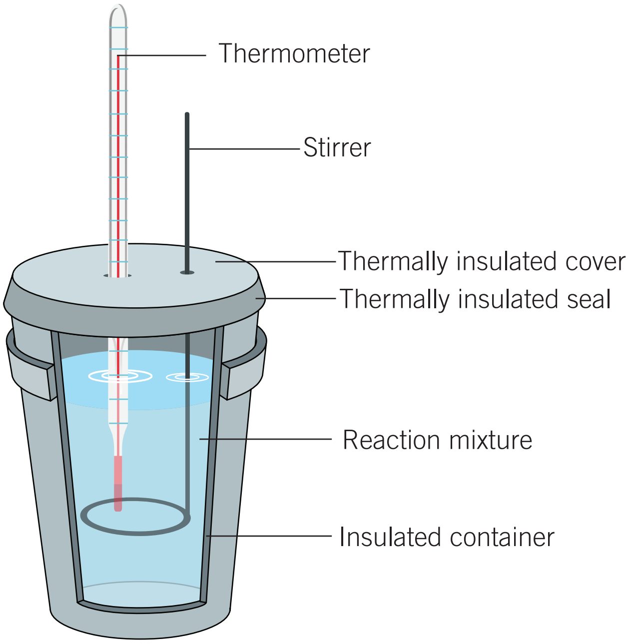

Figure 2B–3 A solution calorimeter, sometimes referred to as a 'coffee cup' calorimeter, showing the internal structures that allow for the measurement of heat of reactions in solution

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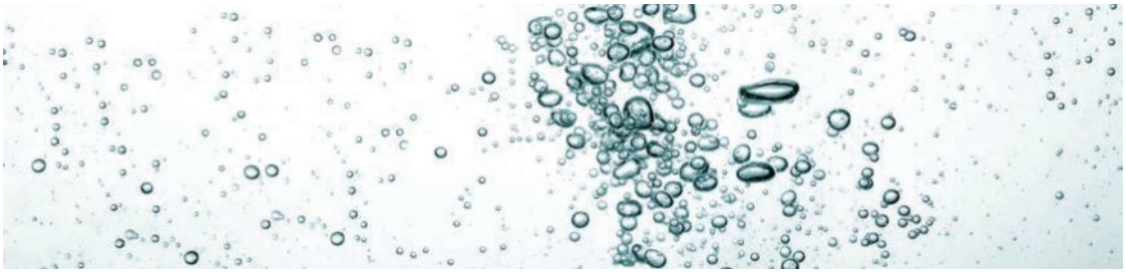
VIDEO
WORKED EXAMPLE 2B–3

Worked example 2B–3: Calculating the molar heat of solution using a solution calorimeter

A student wants to determine the heat of mixing methane gas through an experiment. They place an ampoule containing 3.00×10^{-3} moles of methane gas in a solution calorimeter of 100 g of distilled water at 20.00°C. After breaking the ampoule and releasing the methane, the solution reached a maximum temperature of 22.00°C. Calculate the molar heat of solution for the dissolution $CH_4(g) \rightarrow CH_4(aq)$.

Solution

	Logic	Process
Step 1	Write down everything you have and need, ensuring to convert units where appropriate.	Have: $n(CH_4) = 3.00 \times 10^{-3}$ mol $M(CH_4) = 16\ g\ mol^{-1}$ $\Delta T = 22 - 20 = 2.00°C$ $m(\text{water}) = 100\ g$ $c(\text{water}) = 4.18\ J\ g^{-1}°C^{-1}$ Need to find q in kilojoules to solve for $\Delta H(CH_4)$.
Step 2	Write down the specific heat equation and rearrange if required.	$q = mc\Delta T$
Step 3	Substitute and solve.	$q = mc\Delta T$ $= 100 \times 4.18 \times 2$ $= 836$ J $= 0.84$ kJ $\Delta H = \frac{q}{n}$ $= \frac{0.84}{0.003}$ $= 278.67\ kJ\ mol^{-1}$



WORKSHEET
2B–1
CALCULATIONS USING $q = mc\Delta T$

Energy transformation efficiency

As the experimental set-up on page 54 suggests, the fuel in the spirit burner is undergoing combustion and the heat energy produced is being used to heat the water. However, this process is not 100% efficient. There are several reasons that can contribute to a reduced efficiency, such as heat being lost to the surrounding environment or incomplete combustion. By calculating the thermal energy absorbed by the water, as described in the examples above and on page 55, and then comparing this to the known theoretical enthalpy of combustion of the fuel being used, it is possible to calculate the energy transformation efficiency. This is highlighted through Worked example 2B–4.

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Worked example 2B–4: Calculating the percentage energy transformation efficiency

VIDEO
WORKED EXAMPLE 2B–4

A 1.50 g sample of ethanol is combusted in a spirit burner, which is placed underneath a can containing 100.0 g of water. The water changed temperature from 20.2°C to 57.4°C. What is the percentage efficiency of this process?

Solution

	Logic	Process
Step 1	Write down all relevant information from the question.	$m(H_2O) = 100.0\ \text{g}$ $c(H_2O) = 4.18\ \text{J g}^{-1}\text{°C}^{-1}$ $\Delta T = 57.4\text{°C} - 20.2\text{°C} = 37.2\text{°C}$ $m(C_2H_5OH) = 1.5\ \text{g}$
Step 2	Calculate the energy used to heat the water, using $q = mc\Delta T$.	$q = mc\Delta T$ $q = 100.0\ \text{g} \times 4.18\ \text{J g}^{-1}\text{°C}^{-1} \times 37.2\text{°C}$ $q = 15549.6\ \text{J} = 15.5\ \text{kJ}$
Step 3	Calculate the theoretical maximum energy released by the ethanol using the VCAA Data Book.	$m(C_2H_5OH) = 1.5\ \text{g}$ $\Delta H°c\ (C_2H_5OH) = 29.6\ \text{kJ g}^{-1}$ $\Delta H(C_2H_5OH) = 1.5\ \text{g} \times 29.6\ \text{kJ g}^{-1}$ $= 44.4\ \text{kJ}$
Step 4	Calculate the percentage efficiency using % efficiency = $\frac{\text{experimental value}}{\text{theoretical value}} \times 100$	$\%\ \text{efficiency} = \frac{15.5\ \text{kJ}}{44.4\ \text{kJ}} \times 100$ $= 34.9\%$

Calibrating a calorimeter

To help reduce systematic errors, calibration of the apparatus is performed before each experiment.

This can be done by either using a known chemical reference material such as a metal or a well-studied compound like potassium chloride, or by using an electric heating element as a known provider of energy based on the power supply.

Chemical calibration

Chemicals with well-characterised enthalpies of dissolution are often used as reference materials for solution calorimetry. Potassium chloride is a common reference material, as it is solid at room temperature and has a well-characterised enthalpy of dissolution of 17.2 kJ mol^{-1}.

For calibration to occur, a known amount of potassium chloride is placed in the calorimeter and dissolved. The temperature change is recorded. We then use two equations to determine the calibration factor:

$$E = n \times \Delta H_c$$

$$\text{Calibration factor} = \frac{E}{\Delta T}$$

where:

E = The energy released in kilojoules
n = The number of moles of reference material
ΔH_C = The heat of combustion for the reference material
ΔT = The change in temperature recorded.

Calibration factor may also be written as CF.

Figure 2B–4 Potassium chloride is a common staple of laboratories that conduct a lot of solution calorimetry experiments as it is a widely available, cheap and well-studied compound.

VIDEO
WORKED
EXAMPLE 2B–5

Worked example 2B–5: Calculating the calibration factor of a solution calorimeter by chemical calibration

A 1.00 g sample of potassium nitrate ($M(KNO_3) = 101.1\ g\,mol^{-1}$) was dissolved in a solution calorimeter containing water with an initial temperature of 20.06°C. Once the potassium nitrate was completely dissolved, a final temperature of 18.05°C was recorded. Potassium nitrate dissolves in water according to the following equation:

$$KNO_3(s) \rightarrow K^+(aq) + NO_3^-(aq) \quad \Delta H = +34.9\ kJ\,mol^{-1}$$

Determine the calibration factor of the calorimeter in $J\,°C^{-1}$.

Solution

	Logic	Process
Step 1	Write down everything you have and need, ensuring to convert units where appropriate.	Have: $m(KNO_3) = 1.00\ g$ $M(KNO_3) = 101.1\ g\,mol^{-1}$ $\Delta H(NO_3) = +34.9\ kJ\,mol^{-1}$ $= +34\,900\ J\,mol^{-1}$ $T_{initial} = 20.06°C$ $T_{final} = 18.05°C$ Need n to find calibration factor.
Step 2	Write down the calibration equations and rearrange, if required.	$E = n \times \Delta H$ $CF = \frac{E}{\Delta T} = \frac{n \times \Delta H}{\Delta T}$
Step 3	Substitute and solve.	$n = \frac{m}{M} = \frac{2.00}{101.1} = 0.0099\ mol$ $CF = \frac{n \times \Delta H}{\Delta T}$ $= \frac{0.0099 \times 34900}{2.01}$ $= 172\ J\,°C^{-1}$

Electrical calibration

Calorimeters can also be calibrated electrically, as the heating element that heats the solution has a constant power supply from the socket. This means that you can link the energy produced by the element to a change in temperature of the water within the calorimeter. The energy produced from electricity passing through the heating element is calculated from the following equation:

$$E = V \times I \times t$$

where:

E = The energy produced in joules
V = The voltage in volts
I = The current in amperes
t = The time in seconds.

This allows us to combine equations as we did in the chemical calibration method:

$$\text{Calibration factor} = \frac{E}{\Delta T} = \frac{VIt}{\Delta T}$$

Worked example 2B–6: Calculating the calibration factor of a solution calorimeter by electrical calibration

VIDEO
WORKED EXAMPLE 2B–6

A solution calorimeter was calibrated by passing a current of 2.25 A through an electric heating element for 45.75 s. The potential difference was 5.25 V, and the temperature of the water in the calorimeter increased from 20.25°C to 21.89°C. Using this information, calculate the calibration factor of the calorimeter.

Solution

	Logic	Process
Step 1	Write down everything you have and need, ensuring to convert units where appropriate.	Have: $I = 2.25$ A $t = 45.75$ s $V = 5.25$ V $T_{\text{initial}} = 20.25°\text{C}$ $T_{\text{final}} = 21.89°\text{C}$ Need to find calibration factor.
Step 2	Write down the calibration equations and rearrange if required.	$E = V \times I \times t$ $\text{CF} = \frac{E}{\Delta T} = \frac{V \times I \times T}{\Delta T}$
Step 3	Substitute and solve.	$\text{CF} = \frac{E}{\Delta T} = \frac{V \times I \times T}{\Delta T}$ $= \frac{5.25 \times 2.25 \times 45.75}{1.64}$ $= 330\ \text{J°C}^{-1}$

Check-in questions – Set 1

1. A solution calorimeter was calibrated by passing 1.50 A through the electric heater for 90 s at a potential difference of 6.50 V. The temperature of the water in the calorimeter was initially 18.00°C and rose to 20.50°C during the calibration. Determine the calibration factor of the calorimeter.

This method is commonly used for solution calorimeters and data can be acquired graphically to determine ΔT for the experiment either by direct reading or via extrapolation back to the point where a current was applied using a **line of best fit**. Both methods are shown in Figure 2B–5 on the following page.

Line of best fit a line on a graph that shows the general trend of the data points; the distance to the points above the line should equal the distance to the points below the line

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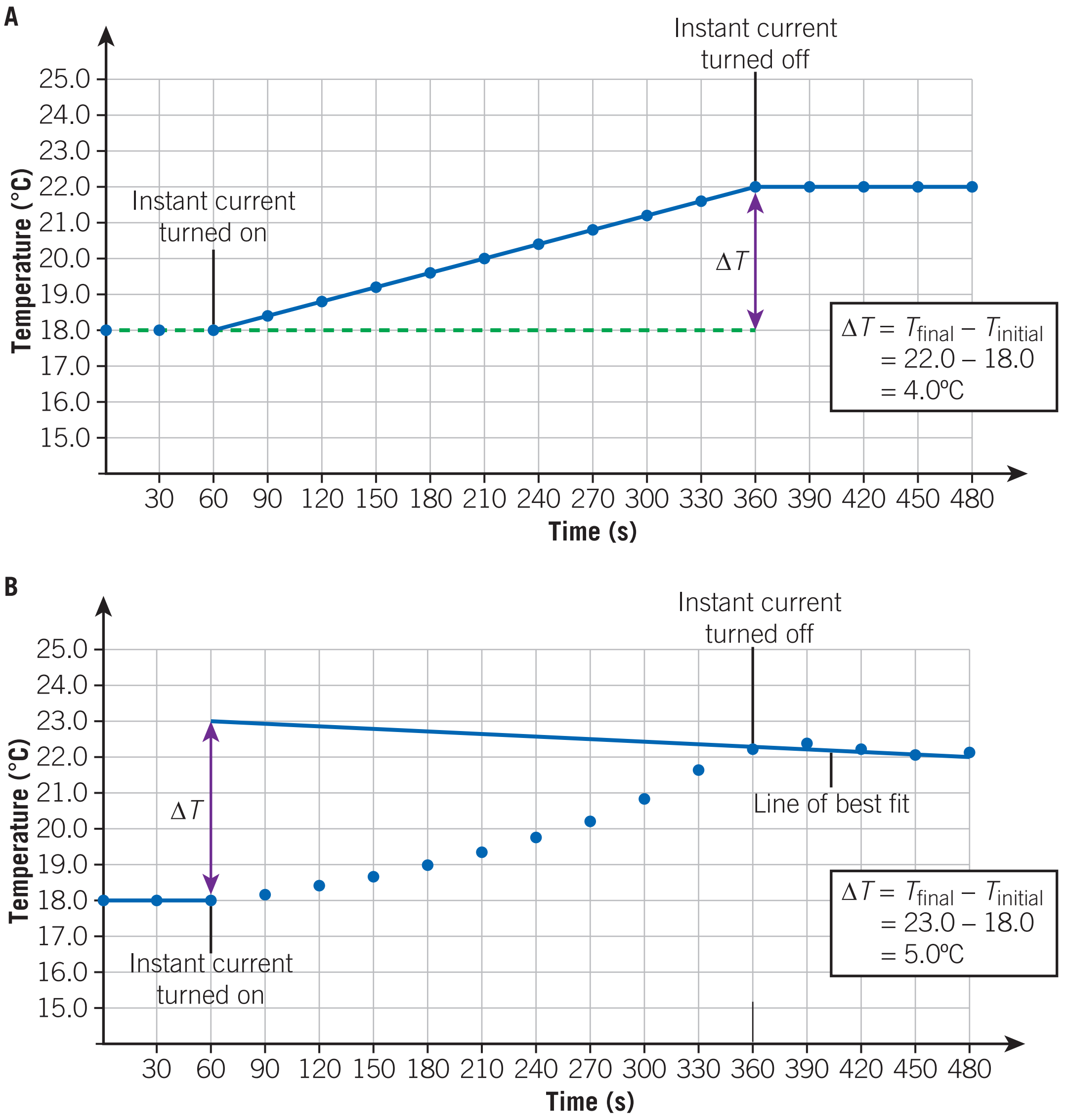


Figure 2B–5 These graphs show the results of two experiments to determine the calibration factor by electrical methods. The current is turned on at 60 seconds and turned off at 360 seconds. In graph A, the change in temperature can be read accurately; however, in graph B an extrapolation back to the point where the current was turned on is required via a line of best fit.

If you know the calibration factor for a calorimeter, the results for energy changes you produce will be more accurate. This allows us to put together a complete procedure for using a calorimeter and getting the best possible results with minimal experimental error.

Overall experimental process

Earlier in the chapter, we looked at calculating the energy produced from combustion reactions using simple calorimeters and from other types of reactions using solution calorimetry. However, as we've just seen, we also need to ensure the calorimeter is calibrated before making the measurement. This means our overall process for performing a calorimetric measurement to determine the enthalpy change of a reaction should be as follows:

1. Calibrate your calorimeter using the most appropriate method.
2. Perform your experiment.
3. Interpret your data.
4. Perform your calculations to determine the calibration factor, CF.
5. Use the calibration factor to determine ΔH.

Worked example 2B–7: Calculating the energy released by a reaction using the calibration factor

VIDEO
WORKED
EXAMPLE 2B–7

A solution calorimeter containing 150.0 mL of distilled water at 25.00°C is calibrated electrically by applying a potential difference of 4.00 V of electricity and a current of 2.00 A passed through the electric heater for 60.0 seconds, causing the temperature to increase to 26.50°C. The distilled water was then removed and replaced with 75.0 mL of 0.150 M hydrochloric acid and 75.0 mL of 0.100 M sodium hydroxide, which were both at an initial temperature of 22.0°C. The temperature of the solution increased to 23.23°C. Calculate the energy released, in kJ, by the neutralisation reaction between hydrochloric acid and sodium hydroxide.

Solution

	Logic	Process
Step 1	Write down everything you have and need, ensuring to convert units where appropriate.	Calibration data: $I = 2.00$ A $V = 4.00$ V $t = 60.0$ s $T_{\text{initial}} = 25.00$°C $T_{\text{final}} = 26.50$°C Neutralisation reaction data: $n(\text{NaOH}) = 0.0075$ mol (limiting reagent) $T_{\text{initial}} = 22.00$°C $T_{\text{final}} = 23.23$°C Need calibration factor to determine ΔH.
Step 2	Write down the calibration equations and rearrange if required.	$E = V \times I \times t$ $\text{CF} = \dfrac{E}{\Delta T}$ $= \dfrac{V \times I \times T}{\Delta T}$ $E = n \times \Delta H$ $\text{CF} = \dfrac{E}{\Delta T}$ $= \dfrac{n \times \Delta T}{\Delta T}$
Step 3	Calculate the calibration factor.	$\text{CF} = \dfrac{E}{\Delta T}$ $= \dfrac{V \times I \times T}{\Delta T}$ $= \dfrac{4.00\text{ V} \times 2.00\text{ A} \times 60.0\text{ s}}{1.5°\text{C}}$ $= 320\text{ J°C}^{-1}$
Step 4	Calculate the energy released by the neutralisation reaction using the calibration factor.	$E = \text{CF} \times \Delta T$ $= 320\text{ J°C}^{-1} \times 1.23°\text{C}$ $= 393.6$ J
Step 5	Calculate the molar heat of solution.	$\Delta H = \dfrac{E}{n}$ $= \dfrac{393.6\text{ J}}{0.0075\text{ mol}}$ $= 52.5\text{ kJ mol}^{-1}$

WORKSHEET 2B–2 CALIBRATING CALORIMETERS

VIDEO 2B–1 SKILLS: RANDOM VERSUS SYSTEMATIC ERRORS

2B SKILLS

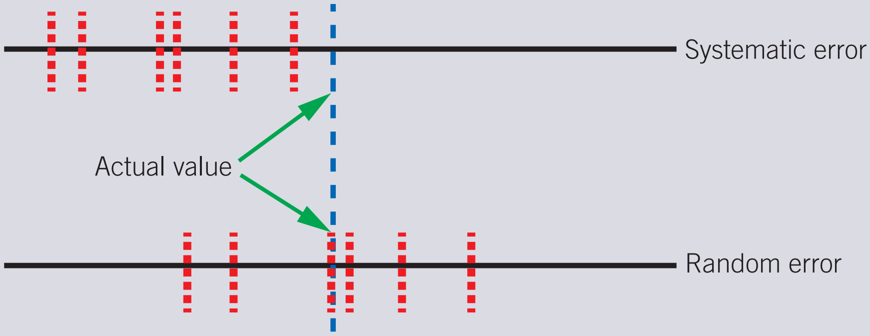
Random versus systematic errors

In the context of chemistry, particularly in an experiment such as calorimetry, two types of errors commonly occur: random and systematic.

Random errors occur unpredictably and differ in each measurement. They're caused by unpredictable fluctuations in the experimental process, such as variations in temperature, slight inconsistencies in material, or even human error during observation. In a calorimetry experiment, a random error could be the minor fluctuation in the temperature readings of the calorimeter. While these errors can't be completely eliminated, they can be minimised by conducting multiple trials and calculating an average result.

On the other hand, systematic errors are predictable and consistent in each measurement. They're caused by faulty equipment, incorrect calibration or bias in the method of measurement. For instance, if the calorimeter isn't perfectly insulated, heat may escape or enter, leading to a consistent underestimation or overestimation of energy changes in the system, respectively. This is a systematic error. Systematic errors can be identified because they skew results in a particular direction and their effect remains consistent irrespective of the number of trials. To eliminate systematic errors, equipment should be properly calibrated, and methods should be evaluated and adjusted if necessary.

The difference between these two types of errors can be demonstrated visually, as shown below.



Therefore, while both random and systematic errors affect the accuracy of experimental results, they have different sources and strategies for minimisation or elimination. The identification and understanding of these errors are key to improving the reliability and validity of experimental outcomes.

We can also look at these through a question, in which you might be asked to identify the type of error that has occurred.

Question: During a calorimetry experiment to determine the energy released from the combustion of a fuel, the recorded temperature change is consistently lower than the expected value. Is this error likely to be random or systematic? Provide some potential sources of the error.

Answer: The consistently lower temperature change observed in the calorimetry experiment suggests that the error is likely to be systematic rather than random. Systematic errors are characterised by consistent deviations in the same direction and magnitude. In this case, the lower recorded temperature change indicates a systematic bias that may be attributed to a flaw in the experimental set-up or procedure. It is important to carefully examine factors such as insulation, calorimeter calibration, heat loss and combustion efficiency to identify and rectify the source of this systematic error. By addressing the underlying issue causing the consistent deviation, scientists can improve the accuracy and reliability of the results obtained from the calorimetry experiment.

Section 2B questions

1 In a calorimetry experiment, the combustion of a small piece of chocolate-chip cookie released 1260 J of energy, which was used to heat a quantity of water in a can. If the temperature of this water increased by 3.25°C, determine the mass of water in the can.

2 Explain the following observations in terms of specific heat capacity.

- a Running water over a burn quickly helps reduce the burning feeling.
- b Copper heats up much quicker than wood on a hot day.
- c A quantity of 10 J of heat energy causes a larger temperature shift in 1 g of water vapour and 1 g of solid water compared with 1 g of liquid water.

3 Solve the following problems using the values for specific heat capacity from Table 2B–1 on page 53 where required.

- a the heat energy required to increase the temperature of 2.66 g of solid water from −6.2°C to −1.1°C
- b the temperature change in a 3.32 g piece of copper wire that absorbs 423 J of energy
- c the mass of basalt rock required to absorb 330 kJ of energy while only allowing a temperature shift from 15.16°C to 18.77°C
- d the specific heat capacity of liquid benzene, if 3 g of benzene increases from 13.13°C to 17.22°C with 1.63 kilojoules of energy

4 Calorimetry is the analytical technique that allows us to measure the heat released in a chemical reaction.

- a What are the two common types of calorimetry and how do they differ structurally?
- b What are the key requirements for a calorimeter to work effectively?
- c Give two experimental errors that could indicate a calorimeter is not set up properly and the cause.

5 Give a possible cause for each of the following experimental observations in an experiment using a calorimeter.

- a The temperature does not change during a reaction between butane and oxygen.
- b The temperature is not constant from the start to the end of the experiment.
- c The temperature increases sharply then starts to gradually decline.

6 An electric heating coil was placed in a solution calorimeter containing 150 mL of water. A current of 2.50 amps with a potential difference of 13 volts was applied to the heating coil for a period of 90 seconds. A temperature increase of 3.4°C was recorded.

After calibration, 10.3 g of sodium chloride was added to the calorimeter and the temperature was observed to decrease by 0.80°C.

- a Calculate the calibration factor of the calorimeter.
- b Calculate the heat of solution of sodium chloride.

7 Consider the following reaction involving ammonium chloride:

$$NH_4Cl(s) \rightarrow NH_4Cl(aq)$$

When completed, a final temperature of 24.91°C is reached.
Calculate the molar heat of solution, ΔH, in $kJ\,mol^{-1}$ if 100 mL of distilled water at 25.00°C is used in a solution calorimeter and 133.75 g of ammonium chloride is dissolved.

8 A student performed an experiment to determine the enthalpy change of the following reaction:

$$CaO(s) + H_2O(l) \rightarrow Ca(OH)_2(s)$$

The student placed 100 mL of water at an initial temperature of 25°C in a solution calorimeter. The calorimeter was calibrated using a known amount of heat and determined to have a calibration factor of 85 $J°C^{-1}$. The student added 0.90 grams of CaO powder to the calorimeter, causing the temperature to rise to 36.6°C. Calculate the enthalpy change of the reaction.

9 A 0.10 g piece of magnesium ribbon is placed in a solution calorimeter. A quantity of 100 mL of a 0.5 M HCl solution is added with an initial temperature of 18.32°C. The following reaction occurs:

$$Mg(s) + 2HCl(aq) \rightarrow H_2(g) + MgCl_2(aq)$$

Once completed, the final temperature of water is 22.87°C. Calculate the enthalpy change for the reaction. Assume that the specific heat capacity and density of the dilute solution are the same as pure water.

10 A 1.57 g sample of ammonium nitrate ($M(NH_4NO_3) = 80.04\ g\ mol^{-1}$) is dissolved in 100 mL of water in a calorimeter. The temperature of the calorimeter is observed to increase by 15.7°C. The enthalpy of solution of ammonium nitrate is 25.7 $kJ\ mol^{-1}$.

- a Determine the calibration factor of the calorimeter in $J°C^{-1}$.
- b Another student uses the calorimeter but calibrates it using potassium nitrate. They get a calibration factor of 27.2 $J°C^{-1}$. Explain a possible source of error that has led to two different calibration factor values.

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2C Measuring energy from food

Study Design:

- energy from fuels and food:
- calculation of energy transformation efficiency during combustion as a percentage of chemical energy converted to useful energy
- comparison and calculations of energy values of foods containing carbohydrates, proteins and fats and oils

ENGAGE

Energy: It's all in a label

When we think of food packaging, we usually think of brands, logos and advertisements. However, did you know that food packaging has a major legal responsibility to provide consumers with the information available to them around the energy provided in a food? Not only do labels provide us with a list of ingredients, they also provide us with the energy content information of the product. This allows us to make informed choices about the nutritional value of food, as well as the way the energy in food is being provided. This is because different food types provide energy differently, depending on the make-up of proteins, fats and carbohydrates within the food.

Figure 2C–1 A medium cheeseburger meal (left) provides 3515 kJ of energy, whereas a regular Acai bowl (right) provides 1760 kJ.

EXPLAIN

Food: a biochemical energy source

While we often think of food in terms of taste, our body views food as energy. When digested, the main food groups are broken down into smaller molecules that can be used directly as a source of energy or stored for later use. While we do also use food for structural components associated with growth, repair and daily function, food still comes down to the balance between energy taken in and energy used in the activities of daily life.

The main nutrients are carbohydrates, fats and proteins. As all of these groups are comprised of a mixture of different substances (for example, proteins refers to a number of different proteins, not a 'pure' protein), we measure energy value in food in kJ g^{-1}, not kJ mol^{-1} as we did with energy from reactions in the previous section. Equally, just because a nutrient has a certain energy content doesn't mean that the energy can be fully extracted from that food. This is shown in Table 2C–1.

LINK **2B** MEASURING ENERGY RELEASED FROM CHEMICAL REACTIONS

Table 2C–1 The heat of combustion of different food groups

Nutrient	Heat of combustion (kJ g^{-1})
Fats and oils	37
Proteins	17
Carbohydrates	16

The heat of combustion assumes we are completely burning the nutrient in an environment containing excess oxygen. The energy value, however, can be less than expected and can be due to factors such as the following:

- Cellulose can be combusted to release energy, but the human body can't metabolise or digest it.
- Nutrients move through the digestive system too fast for all of the carbohydrates, fats and proteins to be absorbed.

These factors help us understand why sugars are excellent for quick energy, whereas proteins are used for energy only when other sources are not readily available.

Table 2C–2 The composition of common foods

Food	% Protein	% Fats/Oils	% Carbohydrates
Peanuts	26	49	16
Bread	9.0	4.0	49
Bananas	1.1	0.3	23
Lettuce	1.4	0.2	2.9
Ice cream	1.7	6.5	29

We also need to remember that foods themselves are mixtures of these different nutrients and as such offer us different energy amounts in different ways. This is illustrated with different examples in Table 2C–2. One thing that you may notice about this table is that the values don't add up to 100%. This is because there are other substances in the food that don't contribute to the energy content (such as water and cellulose), which have been omitted.

We can then combine the information contained within Table 2C–1 and Table 2C–2 to provide an estimation for the overall energy content of food. The process for doing this is explained in Worked example 2C–1.

VIDEO
WORKED
EXAMPLE 2C–1

Worked example 2C–1: Calculating the overall energy content of food

The nutritional information on a bag of unsalted almonds states that they consist of 21.0% water, 21.0% carbohydrates, 6.0% protein and 52.0% fat. Given that water provides no energy, determine the energy value of a 100 g bag of unsalted almonds, in kJ g^{-1}.

Solution

	Logic	Process
Step 1	Refer to tables to determine the available energy for the nutrients in the nuts.	Fats = 37 kJ g^{-1} Proteins = 17 kJ g^{-1} Carbohydrates = 16 kJ g^{-1}
Step 2	Convert the percentages to a mass assuming 100 g is equivalent to 100% and multiply by energy availability.	Fats = 37 kJ g^{-1} × 52.0 g = 1924 kJ Proteins = 17 kJ g^{-1} × 6.0 g = 102 kJ Carbohydrates = 16 kJ g^{-1} × 21.0 g = 336 kJ
Step 3	Add all available energy.	Total energy = 1924 kJ + 102 kJ + 336 kJ = 2362 kJ
Step 4	Divide by the mass of the sample to get units of energy value, kJ g^{-1}.	Energy value = $\frac{2383\ \text{kJ}}{100\ \text{g}}$ = 23.62 kJ g^{-1}

Check-in questions – Set 1

1 The nutritional information on a bag of plain salted chips states that they consist of 10.0% water, 11.0% carbohydrates, 2.0% protein and 77.0% fat. Given that water provides no energy, determine the energy value of a 100 g bag of chips, in kJ g^{-1}.

Food and calorimetry

Just like fuels, the energy contained within food can be determined by calorimetry. From these measurements we can arrive at an overall estimate for the energy content of food.

VIDEO
WORKED EXAMPLE 2C–2

Worked example 2C–2: Calculating the energy content of a specific food

A potato chip weighing 0.150 g was partially burned under a metal can containing 150 g of water. By the end of the experiment, the temperature of the water had increased by 22.5°C, and the remaining mass of the potato chip was 0.030 g. Calculate the energy value of the potato chip in kJ g^{-1}.

Solution

	Logic	Process
Step 1	Calculate the heat transferred to the water from the burning potato chip using $q = mc\Delta T$.	$q = mc\Delta T$ $q = 150 \text{ g} \times 4.18 \text{ J g}^{-1}\text{°C}^{-1} \times 22.5\text{°C}$ $= 14\,107.5 \text{ J}$
Step 2	Convert the energy into kilojoules.	$14\,107.5 \text{ J} = 14.11 \text{ kJ}$
Step 3	Calculate the mass of food burned.	Total mass burned $= m_{\text{initial}} - m_{\text{final}}$ $= 0.15 \text{ g} - 0.03 \text{ g}$ $= 0.12 \text{ g}$
Step 4	Calculate the energy value by dividing the energy calculated in step 2 by the mass from step 3.	Energy value $= \dfrac{14.11}{0.12}$ $= 120 \text{ kJ g}^{-1}$

VIDEO 2C–1
MEASURING ENERGY FROM FOOD

WORKSHEET 2C–1
CALCULATING ENERGY FROM FOOD

Check-in questions – Set 2

1 A 1.340 g chocolate-chip biscuit was burned under a simple calorimeter. By the end of the experiment, the temperature of the water had increased by 3.85°C, and the remaining mass of the burned biscuit was considered negligible. Calculate the energy value of the biscuit in kJ g^{-1}.

VIDEO 2C–2
SKILLS: SIGNIFICANT FIGURES

2C SKILLS

Significant figures

At the end of any calculation question in chemistry, you should check two things: units and significant figures. It is frustrating to have done your working out correctly and obtained the right value, only to lose marks because you haven't included (or have used the wrong) units or written your answer to the correct number of significant figures.

Depending on the assessment, you may lose marks every time you do this ... so these mistakes can really add up!

In terms of significant figures, there are a few rules that you should know:

1. Any digit that isn't a zero is significant (for example, 19.782 has five significant figures).
2. Any zero that is found between two significant numbers is significant (for example, 19.702 has five significant figures).
3. After the decimal point, a zero that doesn't come between two significant numbers is only significant if it comes at the end (for example, 0.78200 has five significant figures, whereas 0.00782 has three significant figures).

If you are multiplying or dividing, you consider all significant figures provided in the question. For your answer, you will use the same number of significant figures as the value in the question that contains the LEAST number of significant figures (not just after the decimal point).

Let's do an example.

Question: Multiply the following values: 54.7 and 0.02.

Answer: 1.094. However, our answer should use the smallest number of significant figures in the question. Therefore, our actual answer is 1 (because 0.02 is only one significant figure).

If you are adding or subtracting, the number of digits to the right of the decimal point in the answer will be the same as the number of digits to the right of the decimal point in the number with the fewest digits to the right of the decimal point.

Let's look at the question above, but instead of multiplying the values, we will add them.

Question: Add the following values: 54.7 and 0.02.

Answer: 54.72. However, our answer should only include one digit to the right of the decimal point, as this is the fewest provided in the question. Therefore, our actual answer is 54.7.

Section 2C questions

1 Use the heat of combustion values from Table 2C–1, where applicable, to calculate:
   a the total energy in 14 g of protein bar.
   b the available energy in a 150 g piece of celery if it is 62% water, 18% glucose and 20% fibre.
   c the energy stored in a 3 kg calf muscle, assuming muscles are 87% protein and 13% fat.
   d the difference in total energy between a dried apple and a fresh apple of the same variety, assuming apples are predominantly carbohydrates and fibre.

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2 The nutritional information from a packet of food is shown below. Use this information and Table 2C–1 to answer the following questions.

Nutrition Facts

8 servings per container

Serving size **2/3 cup (55g)**

Amount per serving

Kilojoules **962**

	% Daily Value*
Total Fat 8g	**10%**
Saturated Fat 1g	**5%**
Trans Fat 0g	
Cholesterol 0mg	**0%**
Sodium 160mg	**7%**
Total Carbohydrate 37g	**13%**
Dietary Fibre 4g	**14%**
Total Sugars 12g	
Includes 10g Added Sugars	**20%**
Protein 3g	
Vitamin D 2mcg	10%
Calcium 260mg	20%
Iron 8mg	45%
Potassium 235mg	6%

* The % Daily Value (DV) tells you how much a nutrient in a serving of food contributes to a daily diet. 2,000 calories a day is used for general nutrition advice.

a How much energy is provided by protein in one serve of this food?

b For one serve of this food, how much energy from carbohydrates is available energy?

c For one serve of this food, how much energy is available from fats?

d How much total energy can be released from the food under combustion for the entire packet of food?

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Chapter 2 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
2A.1	Recall principles of stoichiometry in balancing equations	1☐
2A.2	Determine the heat produced from combustion reactions using the equation $E = \Delta H \times n$	2☐, 13☐
2A.3	Use stoichiometry to calculate reactant and product amounts, and net volume or mass of major greenhouse gases	3☐, 13☐
2A.4	Perform calculations involving excess and limiting reagents in combustion reactions	13☐
2B.1	Define 'specific heat capacity' and its units	5☐
2B.2	Recall the properties of water that lead to its use in specific heat experiments	4☐
2B.3	Perform calculations using the equation $q = mc\Delta T$	7☐, 13☐
2B.4	State the principles of solution calorimetry	6☐, 10☐, 11☐
2B.5	Analyse graphical data to determine the calibration factor of a calorimeter	14☐
2B.6	Use experimental data to calculate the calibration factor of a calorimeter and energy produced from chemical reactions	12☐, 13☐
2B.7	Calculate energy transformation efficiency from given experimental data	13☐
2C.1	Use reference tables for heats of combustion of different food groups	8☐
2C.2	Determine the energy content of a food based on food group composition	9☐
2C.3	Calculate the energy content of a food using calorimetry	13☐

Multiple-choice questions

1 Which of the following equations is correctly balanced?

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

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

C $3C_4H_{10}(g) + 19.5O_2(g) \rightarrow 12CO_2(g) + 15H_2O(g)$

D $4C_4H_{10}(g) + 26O_2(g) \rightarrow 16CO_2(g) + 20H_2O(g)$

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2 For the combustion of 44 g of propane, which of the following gives the correct amount of heat energy produced?

$$C_3H_8(g) + 5O_2(g) \rightarrow 3CO_2(g) + 4H_2O(l) \qquad \Delta H = 2220 \text{ kJ mol}^{-1}$$

A −2220 kJ

B +2220 kJ

C −50.45 kJ

D +50.45 kJ

3 Which of the following is **not** required to solve for the amount of a greenhouse gas produced in a combustion reaction?

A stoichiometric ratio

B the amount of reactant

C the presence or absence of a catalyst

D the amount of product

4 Which material would have the highest specific heat capacity at SLC?

A methane

B ethanol

C aluminium

D water

5 Which of the following gives the correct units for the specific heat capacity of a material?

A kJ mol^{-1}

B J °C mol^{-1}

C $\text{J g}^{-1}\text{ mol}^{-1}$

D $\text{J g}^{-1}\text{°C}^{-1}$

6 Which of the following is common to a solution calorimeter?

A stirrer and pH meter

B bomb chamber and stirrer

C thermometer and stirrer

D thermometer and pH meter

7 A burning candle was used to heat water in a can. The equation $q = mc\Delta T$ was used to determine the amount of heat released by the combustion of the candle. Which of the following is incorrect?

A The value of c in the specific heat equation depends on the material being heated.

B The value of m in the specific heat equation is based on the mass of the material reacting.

C The change in temperature refers to the temperature change in the water.

D The units for q are joules.

8 Which of the following nutrients produces the most energy when completely combusted?

A 12 g of protein

B 9 g of carbohydrates

C 11 g of fat

D 6 g of fat and 8 g of protein

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9 The label on a 100 g can of baked beans says it consists of 28% carbohydrates, 41% protein and 8% fat, with the remaining mass being water. What is the energy value of the baked beans?

A 19 kJ g^{-1}

B 8.3 kJ g^{-1}

C 14 kJ g^{-1}

D 21 kJ g^{-1}

10 Which of the following is **not** a type of calibration method for calorimeters?

A electrical

B reference material

C benzoic acid

D pure oxygen

Short-answer questions

11 Draw and label a solution calorimeter. (5 marks)

12 List the steps in calibrating a calorimeter using a single approach. (5 marks)

13 A student performed a calorimetry experiment to determine the heat of combustion of propan-2-ol, according to the following procedure.

1. Add 500 mL of cold water to a beaker. Record the initial temperature.
2. Fill a spirit burner with propan-2-ol. Record the mass of the spirit burner.
3. Ignite the spirit burner and place directly below the beaker. Stir the water gently while monitoring the temperature.
4. When the temperature has risen by approximately 10°C, extinguish the flame.
5. Record the final mass of the spirit burner.

The student recorded the following data.

Initial temperature of water (°C)	15.1
Final temperature of water (°C)	25.3
Initial mass of spirit burner (g)	124.5
Final mass of spirit burner (g)	125.8

a Calculate the heat of combustion of propan-2-ol. (2 marks)

b Given the theoretical molar heat of combustion for propan-2-ol is 2017.7 kJ mol^{-1}, calculate the percentage energy efficiency. (3 marks)

c Suggest a possible explanation for why the heat of combustion determined by the student is significantly lower than the reported value. (1 mark)

d Suggest one improvement to the experimental set-up that could be made to improve accuracy. (1 mark)

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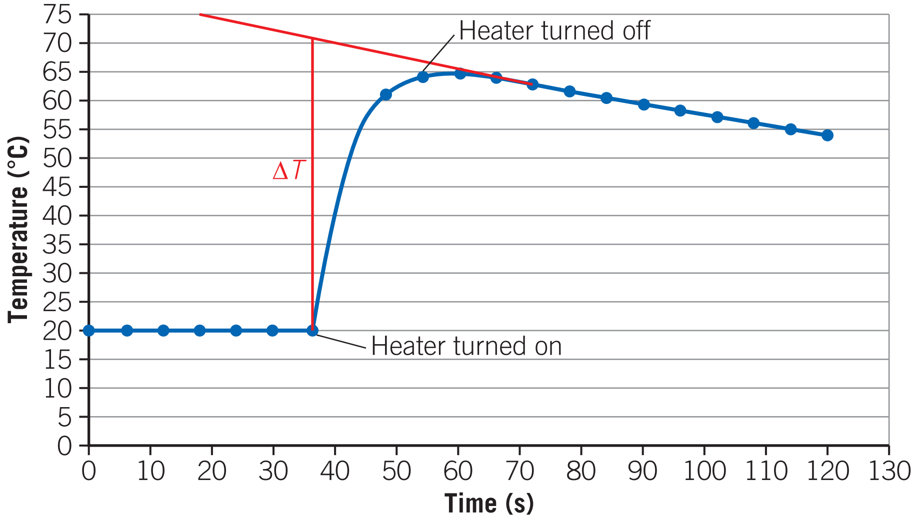
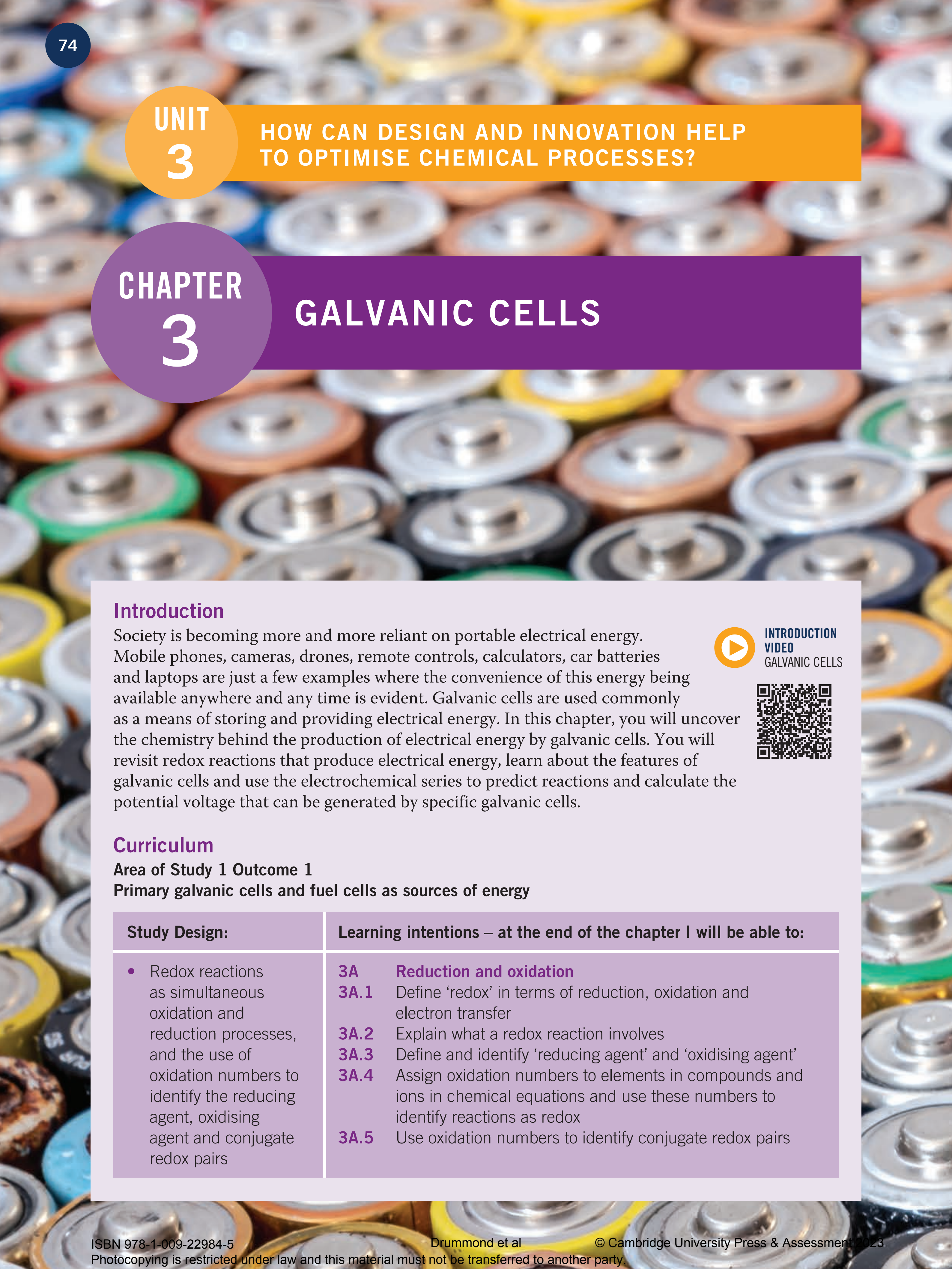
14 The table and graph below show data from the manual calibration of a calorimeter.

Volume of water in calorimeter	150 g
Current (*I*)	3.00 A
Time (s)	20 s
Voltage (*V*)	2.5 V
Initial temperature	22.2°C
Final temperature	65.1°C



a Calculate the calibration factor for this calorimeter. (3 marks)

b Comment on how the shape of the temperature–time graph would change if the lid was leaking, the heating element was faulty or the surrounding water had contaminants. (3 marks)



UNIT 3 HOW CAN DESIGN AND INNOVATION HELP TO OPTIMISE CHEMICAL PROCESSES?

CHAPTER 3 GALVANIC CELLS

Introduction

Society is becoming more and more reliant on portable electrical energy. Mobile phones, cameras, drones, remote controls, calculators, car batteries and laptops are just a few examples where the convenience of this energy being available anywhere and any time is evident. Galvanic cells are used commonly as a means of storing and providing electrical energy. In this chapter, you will uncover the chemistry behind the production of electrical energy by galvanic cells. You will revisit redox reactions that produce electrical energy, learn about the features of galvanic cells and use the electrochemical series to predict reactions and calculate the potential voltage that can be generated by specific galvanic cells.

INTRODUCTION VIDEO
GALVANIC CELLS

Curriculum

Area of Study 1 Outcome 1
Primary galvanic cells and fuel cells as sources of energy

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Redox reactions as simultaneous oxidation and reduction processes, and the use of oxidation numbers to identify the reducing agent, oxidising agent and conjugate redox pairs	**3A Reduction and oxidation** **3A.1** Define ‘redox’ in terms of reduction, oxidation and electron transfer **3A.2** Explain what a redox reaction involves **3A.3** Define and identify ‘reducing agent’ and ‘oxidising agent’ **3A.4** Assign oxidation numbers to elements in compounds and ions in chemical equations and use these numbers to identify reactions as redox **3A.5** Use oxidation numbers to identify conjugate redox pairs

Study Design:	Learning intentions – at the end of the chapter I will be able to:
- The writing of balanced half-equations (including states) for oxidation and reduction reactions, and the overall redox cell reaction in both acidic and basic conditions	**3B** **Writing redox equations** **3B.1** Write and balance simple and complex half-equations for oxidation and reduction reactions **3B.2** Write and balance overall redox equations, including states, in acidic conditions **3B.3** Write and balance overall redox equations, including states, in basic conditions **3B.4** Write and balance half-equations by identifying redox couples in overall equations
- The common design features and general operating principles of non-rechargeable (primary) galvanic cells converting chemical energy into electrical energy, including electrode polarities and the role of the electrodes (inert and reactive) and electrolyte solutions (details of specific cells not required)	**3C** **Features of galvanic cells** **3C.1** Recall and explain the importance of the key design features of galvanic cells **3C.2** Identify, name, draw and label features of galvanic cells **3C.3** Identify the chemical processes involved in primary galvanic cells, including the type of redox reaction occurring at each electrode **3C.4** Identify the direction of electron flow and ion flow in galvanic cells **3C.5** Write the half-equation for the reaction occurring at each electrode in a galvanic cell **3C.6** Write the overall equation for a galvanic cell **3C.7** Describe the importance of separating two half-cells to facilitate the transformation of chemical energy to electrical energy in a galvanic cell **3C.8** Explain the role of inert and reactive electrodes and electrolyte solutions in the reactions taking place in a galvanic cell
- The use and limitations of the electrochemical series in designing galvanic cells and as a tool for predicting the products of redox reactions, for deducing overall equations from redox half-equations and for determining maximum cell voltage under standard conditions	**3D** **Using the electrochemical series** **3D.1** Apply information presented in the elcetrochemical series to questions **3D.2** Predict whether certain combinations of reactants will produce electrical energy in a galvanic cell **3D.3** Compare the relative strengths of reducing agents and oxidising agents **3D.4** Predict the products, and therefore the overall equation, of a redox reaction in a galvanic cell **3D.5** Use the electrochemical series to calculate the maximum cell voltage generated under standard laboratory conditions

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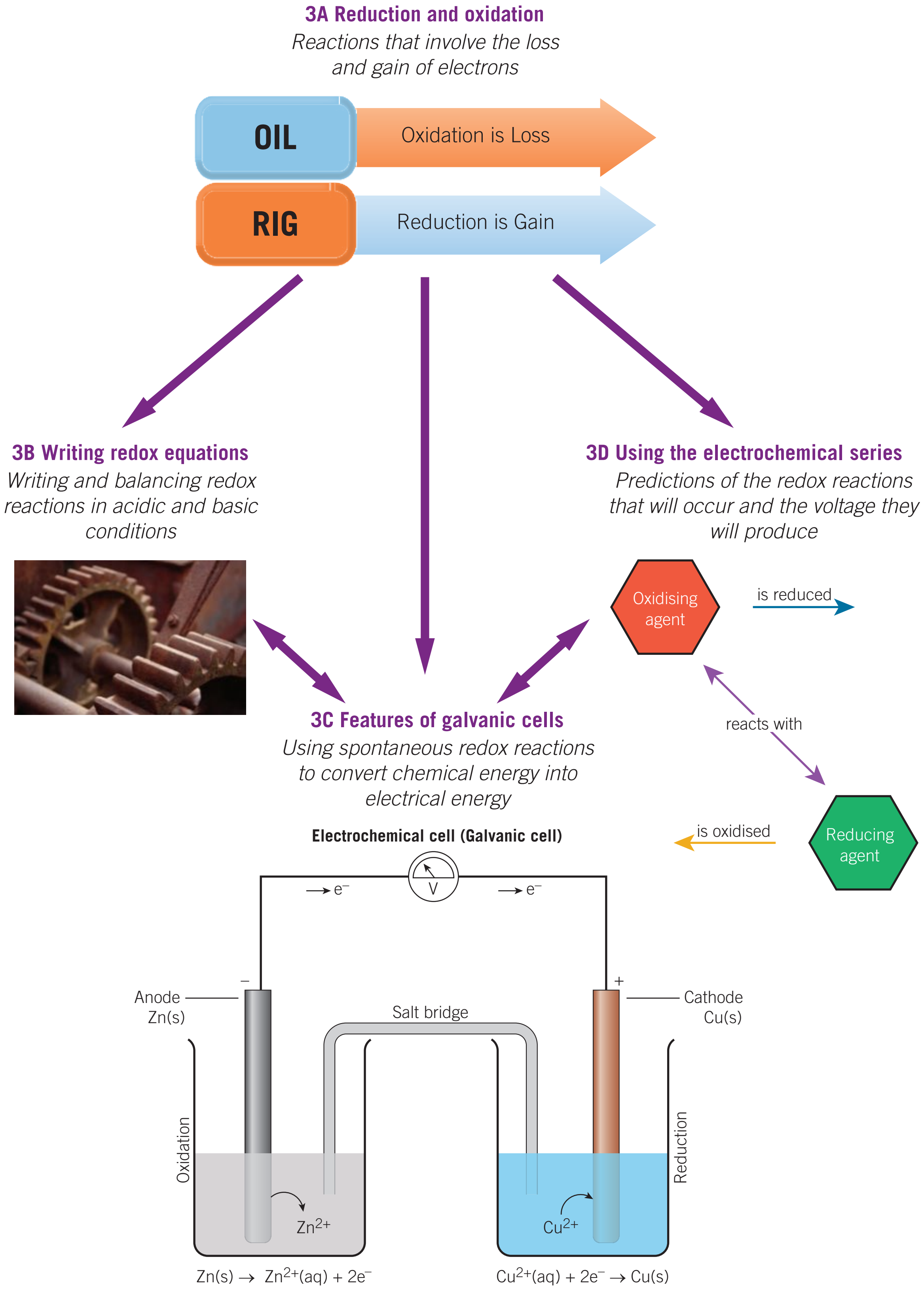
Glossary

- Anode
- Cathode
- Chemical energy
- Complex half-equation
- Conjugate redox pair
- Electrical energy
- Electrochemical cell
- Electrochemical series
- Electrode
- Electrode polarity
- Electrolyte
- Electron transfer
- Galvanic cell
- Half-cell
- Half-equation
- Inert
- Ion
- Oxidation
- Oxidation number
- Oxidising agent
- Potential difference
- Primary cell
- Redox couple
- Redox reaction
- Reducing agent
- Reduction
- Salt bridge
- Simple half-equation
- Species
- Spontaneous reaction
- Standard cell potential
- Standard electrode potential
- Standard hydrogen electrode
- Voltage
- Voltmeter

Concept map



3A Reduction and oxidation

Reactions that involve the loss and gain of electrons

OIL Oxidation is Loss

RIG Reduction is Gain

3B Writing redox equations

Writing and balancing redox reactions in acidic and basic conditions

3D Using the electrochemical series

Predictions of the redox reactions that will occur and the voltage they will produce

3C Features of galvanic cells

Using spontaneous redox reactions to convert chemical energy into electrical energy

Electrochemical cell (Galvanic cell)

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

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

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

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3A Reduction and oxidation

Study Design:

- Redox reactions as simultaneous oxidation and reduction processes, and the use of oxidation numbers to identify the reducing agent, oxidising agent and conjugate redox pairs

Glossary:

Electron transfer
Half-equation
Oxidation
Oxidation number
Oxidising agent
Redox couple
Redox reaction
Reducing agent
Reduction
Species

ENGAGE

What is oxidation?

You have likely heard of reduction and oxidation from your study of chemistry. However, where did these terms come from, and when and how were redox reactions first discovered?

The terms ‘reduction’ and ‘oxidation’ stem from the historical exploration of combustion, which was the first type of oxidation studied. In 1775, English scientist, Joseph Priestley, who had discovered oxygen about a year earlier, met with French chemist, Antoine Lavoisier, who went on to revolutionise the field of chemistry by investigating the role of oxygen in combustion reactions. Lavoisier’s work helped to later establish that combustion reactions involved materials combining with oxygen, and these reactions were classified as oxidation reactions. Alternatively, those reactions where oxygen was produced were classified as reduction reactions.

Often, when oxygen is involved in a reaction, it will be acting as an oxidising agent. However, this is not always the case; but when redox reactions were first discovered by Priestley and Lavoisier, they believed that oxygen was always involved, which is another reason why the term ‘oxidation’ was adopted.

Figure 3A–1 French chemist Antoine Lavoisier revolutionised the field of chemistry with his discovery of the role oxygen plays in combustion reactions.

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EXPLAIN

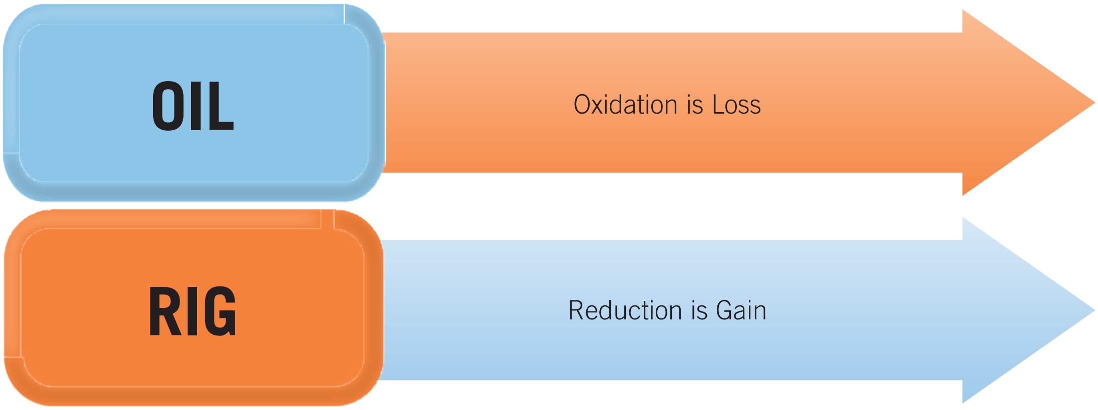
Most of the material in the following two sections is also covered in Units 1 and 2. However, it is also assessable in Units 3 and 4, hence its inclusion. Where possible, questions and examples have been altered. However, please note that in Section 3B, new material has been added in order to cover redox reactions under basic conditions. This was not required learning for the Units 1 and 2 course and is potentially examinable content.

LINK **UNITS 1 & 2**
3B WRITING REDOX EQUATIONS

What is redox?

The word **redox** is a combined abbreviation for ***red***uction and ***ox***idation, which are two different processes that occur simultaneously during a redox reaction. A **redox reaction** involves an **electron transfer** from one chemical **species** to another.

Therefore, **reduction** can be defined as the *gain* of electrons and **oxidation** as the *loss* of electrons. A nice way to remember this is using the mnemonic OILRIG – Oxidation Is Loss (of electrons), Reduction Is Gain (of electrons).



NOTE

There is also a 'rule of thumb', most often used by organic chemists, which identifies a species in a reaction as being oxidised due to a gain of oxygen or loss of hydrogen, or being reduced due to a loss of oxygen or gain of hydrogen. Note, however, that redox reactions do not always involve hydrogen or oxygen.

The reaction between solid magnesium ribbon and oxygen gas, if performed at high temperatures, produces solid magnesium oxide. The redox equation for this reaction can be written as

$$2Mg(s) + O_2(g) \rightarrow 2Mg^{2+}(s) + 2O^{2-}(s)$$

Reducing agents and oxidising agents

You should recall that ionic compounds are formed when there is a large difference in the electronegativities of the bonding atoms. This commonly occurs between a non-metal and a group 1 metal, a group 2 metal or a transition metal with a low **oxidation number**. In a similar way, the redox reaction between magnesium and oxygen involves a transfer of electrons from the magnesium atoms to the oxygen atoms. Given that oxidation is the loss of electrons, in this reaction magnesium has undergone oxidation; it has been oxidised. Similarly, the oxygen has undergone reduction; it has been reduced, since it is the molecule that gained the electrons.

Redox reaction
a reaction involving a transfer of electrons. Both reduction and oxidation occur simultaneously

Electron transfer
the exchange of electrons that occurs during a redox reaction. Electrons are transferred from the reducing agent to the oxidising agent

Species
any reactant or product in a chemical reaction

Reduction
a gain of electrons

Oxidation
a loss of electrons

Oxidation number
a measure of the degree of oxidation of an atom in a substance; defined as the charge an atom might have when electrons are counted to help identify redox reactions, oxidising agents and reducing agents

Oxidising agent the reactant in a redox reaction that causes oxidation. It is itself reduced and therefore will gain electrons – its oxidation number will decrease

Reducing agent the reactant in a redox reaction that causes reduction. It is itself oxidised and therefore will lose electrons – its oxidation number will increase

It is also useful to identify the reducing agent and the oxidising agent in a reaction. The species that causes oxidation of the other reactant (species) is termed the **oxidising agent**. The species that causes reduction to occur to the other species is termed the **reducing agent**.

In the example on the previous page, magnesium causes the reduction of oxygen gas and at the same time undergoes oxidation itself, losing electrons. Thus, magnesium can be identified as the reducing agent in this reaction. Similarly, oxygen causes the oxidation of magnesium and at the same time undergoes reduction itself, gaining electrons. Thus, oxygen can be identified as the oxidising agent in this reaction.

electron transfer

$$2Mg(s) + O_2(g) \rightarrow 2Mg^{2+}(s) + 2O^{2-}(s)$$

Reducing agent (undergoes oxidation)

Oxidising agent (undergoes reduction)

> **NOTE**
>
> It is helpful to remember that the species that undergoes reduction will be the oxidising agent, and the species that undergoes oxidation will be the reducing agent.

Check-in questions – Set 1

1 Define the following terms.
   - a reduction
   - b oxidation
   - c redox reaction

2 Describe what happens to the oxidising agent during a redox reaction.

VIDEO 3A–1 USING OXIDATION NUMBERS

Oxidation numbers

It is not always easy to identify whether electrons are being transferred or not in a chemical reaction, nor is it obvious which species is gaining or losing them. To help identify whether a species is gaining or losing electrons and consequently whether it is undergoing reduction or oxidation, we can use oxidation numbers.

Writing oxidation numbers

While not official IUPAC convention, oxidation numbers are easily represented when written directly above the element as –1, 0, +1, +2 and so on. It is important to distinguish between this format and that of an ion. For example, the magnesium ion, Mg^{2+}, has an ionic charge of 2+, but its oxidation number is written as +2, usually like this:

$$\overset{+2}{Mg}{}^{2+}$$

Oxidation number

Assigning oxidation numbers

You can work out the oxidation number of an unknown element by applying several rules to identify the oxidation numbers in other elements present in a species. Although many elements will often have the same oxidation number, some elements can have multiple oxidation numbers. One example of this is nitrogen, which can have oxidation numbers ranging from –3 to +5!

The rules to follow when assigning oxidation numbers, as well as exceptions to some rules that are particularly important to remember, are summarised in Table 3A–1.

Table 3A–1 Oxidation numbers rules and examples

Category	Rule	Example(s)
Free elements Oxidation number = 0 (zero)	A free element is any element that exists on its own and that is not a charged ion. It may be monoatomic or polyatomic but must contain only one type of element.	Solid iron metal, Fe(s) Hydrogen gas, $H_2(g)$ Oxygen gas, $O_2(g)$ Sulfur, $S_8(s)$ Carbon, C(s)
Hydrogen Typical oxidation number = +1 Alternative oxidation number = –1	The alternative oxidation number only occurs when hydrogen is part of a metal hydride. This is because metal hydrides are ionic compounds, and as such, the metal ion will have an oxidation number equal to its charge. To achieve an overall neutral charge for metal hydrides, hydrogen must have an oxidation number of –1.	Methane, CH_4 In this neutral molecule, hydrogen will have its typical oxidation number of +1. Exception: Sodium hydride, NaH. In this case, the sodium ion will have an oxidation number of +1, and the hydrogen will have an oxidation number of –1.
Oxygen Typical oxidation number = –2 Alternative oxidation number = –1	Oxygen will typically have an oxidation number of –2 when it is not a free element. The alternative oxidation number occurs only when oxygen is part of a peroxide, such as hydrogen peroxide, H_2O_2.	Carbon dioxide, CO_2 In this neutral molecule, oxygen will have an oxidation number of –2. Exception: Hydrogen peroxide, H_2O_2. In this molecule, hydrogen will have an oxidation number of +1, and oxygen will have an oxidation number of –1.
Pure ions Oxidation number = ionic charge	Pure ions have an oxidation number equal to their ionic charge.	Aluminium ions, Al^{3+} These ions will have an ionic charge of 3+ and an oxidation number of +3.
Neutral compounds The sum of the oxidation numbers will be 0 (zero).	Neutral compounds, as well as having an overall neutral charge, will also be neutral in their overall oxidation number total.	Water, H_2O In the neutral molecule of water, hydrogen has an oxidation number of +1 and oxygen has an oxidation number of –2. There are two hydrogen atoms, so overall: $(2 \times +1) + (-2) = 0$.
Polyatomic ions The sum of the oxidation numbers = charge on the ion	Polyatomic ions have an overall oxidation number equal to the charge on the polyatomic ion.	Sulfate ions, SO_4^{2-} These polyatomic ions have an overall ionic charge of 2–. Oxygen has an oxidation number of –2, and there are four atoms of oxygen, so $4 \times -2 = -8$. Sulfur must have an oxidation number of +6, to match the overall charge on the ion. $-8 + (+6) = -2$.

NOTE

The most electronegative element in a compound must be assigned a negative oxidation number. Therefore, fluorine, being the most electronegative element, will always have an oxidation number of –1. There are no exceptions to this scenario. More generally, group 17 halogens *usually* have an oxidation number of –1, but not always. Chlorine, in some cases, can have a positive oxidation number. An example of this is chlorine dioxide, ClO_2, where chlorine has an oxidation number of +4 because oxygen is more electronegative than chlorine and hence is assigned the oxidation number of –2.

VIDEO WORKED EXAMPLE 3A–1

Worked example 3A–1: Assigning oxidation numbers

Determine the oxidation number for each of the elements in the permanganate ion, MnO_4^-.

Solution

	Logic	Process
Step 1	Oxygen has an oxidation number of –2 (unless in a peroxide, which the permanganate ion is not). Then determine the total number of oxygen atoms.	O = –2 Four oxygen atoms $4 \times -2 = -8$
Step 2	Need to recognise that this is a polyatomic ion, so the sum of the oxidation numbers must add up to the corresponding charge on the ion.	Charge on permanganate ion = 1–, so sum of oxidation numbers must equal –1.
Step 3	Determine the oxidation number of the unknown atom, taking into consideration the number of these.	There is one Mn atom. Use algebra and assign Mn as 'x'. $x + (-8) = -1$ $x = -1 - (-8)$ $x = +7$
Step 4	Write down the oxidation numbers of all elements.	Mn = +7 O = –2 $\overset{+7}{Mn}\overset{-2}{O_4^-}$

Check-in questions – Set 2

1 Assign oxidation numbers to each element in the species below.

- a Na
- b NaCl
- c SO_2
- d CO_3^{2-}
- e $NaBrO_3$

2 Determine the oxidation number for sulfur, **S**, in each of the following compounds.

- a $\mathbf{S}_8$
- b $\mathbf{S}O_4^{2-}$
- c $\mathbf{S}O_2$
- d $H_2\mathbf{S}$
- e $\mathbf{S}^{2-}$
- f $\mathbf{S}O_3$

Using oxidation numbers

Identifying reducing agents and oxidising agents

A change in oxidation number of an element can be used to identify reducing agents and oxidising agents. If the oxidation number *increases* for an element during a reaction, it indicates that it has undergone oxidation, losing electrons (hence becoming 'more positive') and is therefore called the **reducing agent**. Similarly, if the oxidation number *decreases* for an element during a reaction, it indicates that it has undergone reduction, gaining electrons (hence becoming 'less positive') and is therefore identified as the **oxidising agent**.

$$\overset{+2}{Fe^{2+}}(aq) + 2e^- \rightarrow \overset{0}{Fe}(s)$$

In the equation shown above, Fe^{2+}(aq) ions are reduced because the oxidation number of iron decreases from +2 to 0. Fe(s) has gained electrons.

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In **half-equations** such as this, an alternative way to determine whether reduction or oxidation is taking place is to identify on which side of the equation the electrons are present. If electrons are on the left-hand side, as shown in Figure 3A–2, then it is a reduction half-equation. If electrons are on the right-hand side, then it is an oxidation half-equation.

Half-equation either the reduction or oxidation part of a redox reaction

$$Cu^{2+}(aq) + \underset{\text{electrons gained}}{\boxed{2e^-}} \rightarrow Cu(s) \quad \text{Reduction} \qquad Zn(s) \rightarrow Zn^{2+}(aq) + \underset{\text{electrons lost}}{\boxed{2e^-}} \quad \text{Oxidation}$$

Figure 3A–2 Reduction and oxidation half-equations showing location of electrons

This is useful when dealing with half-equations where electrons are shown. However, for more complex redox reactions, oxidation numbers are necessary, as shown in Worked example 3A–2.

WORKSHEET
3A–1 OXIDATION NUMBERS

VIDEO
WORKED EXAMPLE 3A–2

Worked example 3A–2: Identifying reducing and oxidising agents

Determine the reducing agent and oxidising agent in the reaction between lead ions, Pb^{2+}, and zinc metal, Zn, that produces lead metal, Pb, and zinc ions, Zn^{2+}.

Solution

	Logic	Process
Step 1	Write out the full balanced equation, including states.	$Pb^{2+}(aq) + Zn(s) \rightarrow Pb(s) + Zn^{2+}(aq)$
Step 2	Assign oxidation numbers to each species present in the equation.	$\overset{+2}{Pb^{2+}}(aq) + \overset{0}{Zn}(s) \rightarrow \overset{0}{Pb}(s) + \overset{+2}{Zn^{2+}}(aq)$
Step 3	Answer the question by using the change in oxidation numbers of the atoms/ions.	$Pb^{2+}(aq)$ ions have been reduced since the oxidation number decreases from +2 to 0. Zn(s) has been oxidised to $Zn^{2+}(aq)$ ions because its oxidation number has increased from 0 to +2. Zn(s) can be identified as the reducing agent, and $Pb^{2+}(aq)$ ions are therefore the oxidising agent.

Important considerations when using oxidation numbers

In many redox reactions, the same elements are often involved as reactants and as products. It is particularly important to note the difference in states and charges when you are describing changes in a redox reaction or when you are asked to identify reducing agents or oxidising agents. For example, copper ions, $Cu^{2+}(aq)$, are a different chemical species compared to copper solid, Cu(s).

In addition, where the element whose oxidation number changes during a redox reaction belongs to a polyatomic species, you should include the *entire reactant compound* that contains the element when naming the reducing agent or oxidising agent. Consider Worked example 3A–3 on the following page, where oxidation numbers are shown.

NOTE

Recall from Units 1 & 2 that roman numerals are used for oxidation numbers.

VIDEO
WORKED
EXAMPLE 3A–3

Worked example 3A–3: Identifying reducing and oxidising agents

Determine the reducing agent and oxidising agent in the reaction between iron(III) oxide and carbon monoxide.

Solution

	Logic	Process
Step 1	Write out the full balanced equation, including states.	$Fe_2O_3(s) + 3CO(g) \rightarrow 2Fe(s) + 3CO_2(g)$
Step 2	Assign oxidation numbers to each species present in the equation.	reduction oxidation $\overset{+3}{Fe_2}\overset{-2}{O_3}(s) + 3\overset{+2}{C}\overset{-2}{O}(g) \rightarrow 2\overset{0}{Fe}(s) + 3\overset{+4}{C}\overset{-2}{O_2}(g)$
Step 3	Answer the question by using the change in oxidation numbers of the atoms/ions.	Iron, Fe, shows an oxidation number change from +3 to 0, meaning that it has been reduced (gained electrons). However, if you were stating the oxidising agent, you would state iron oxide, $Fe_2O_3(s)$, as this is the chemical species causing the oxidation of the carbon monoxide. Similarly, the reducing agent for this reaction would be identified as carbon monoxide, CO(g), even though only the carbon undergoes an oxidation number increase (due to oxidation, loss of electrons).

Identifying redox couples

Redox couple a reducing agent, which donates electrons, and its corresponding oxidising agent, which accepts electrons

During a redox reaction, the species acting as a reducing agent on the reactant side donates (loses) electrons and in doing so forms a product that is an oxidising agent. At the same time, the reactant acting as the oxidising agent is converted into a product that is a reducing agent. The association of each reactant and the product it forms during a redox reaction is referred to as a **redox couple**.

For example, when copper metal undergoes oxidation, losing electrons, the copper ions produced could act as an oxidising agent, gaining electrons.

$$\overbrace{\underset{\text{Reducing agent}}{Cu(s)} \rightleftharpoons \underset{\text{Oxidising agent}}{Cu^{2+}(aq)}}^{\text{Redox couple}} + 2e^-$$

In a similar way, when zinc ions undergo reduction to zinc solid, the zinc solid could then act as a reducing agent.

$$\overbrace{\underset{\text{Oxidising agent}}{Zn^{2+}(aq)} + 2e^- \rightleftharpoons \underset{\text{Reducing agent}}{Zn(s)}}^{\text{Redox couple}}$$

NOTE

The complete electrochemical series can be found in the Units 3 & 4 VCE Chemistry Exam Data Book, as well as in the appendix on page 542 of this textbook, and shows an extensive list of these redox couples, arranged in order of increasing strength of the reducing agent.

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Your ability to identify redox couples will be equally important in the next section of this chapter when you explore how to write half-equations from full redox equations. In most cases, you will be required to identify redox couples in full redox reactions rather than in half-equations. Each redox reaction will therefore have *two* redox couples.

To identify a redox couple, the following are required:

1 There must be one species on the reactant side and one species on the product side of the equation containing the same element.
2 There must be a change in oxidation number.

Figure 3A–3 shows that copper has an oxidation number of +2 in copper oxide, CuO, on the reactant side, which decreases to 0 in copper (solid) on the product side. This is the first redox couple. In a similar way, the hydrogen gas and water can be identified as the second redox couple, where hydrogen shows an increase in oxidation number from 0 to +1.

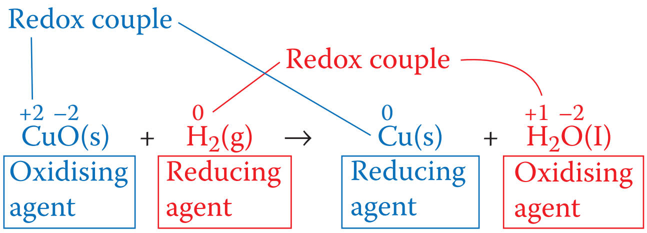


Figure 3A–3 Each redox reaction has two redox couples.

NOTE

You may have noticed that Figure 3A–3 also includes an element that does not change oxidation number. In this case, it is oxygen. If an element does not have a change in oxidation number during a redox reaction, it means that element is not undergoing reduction or oxidation.

Check-in questions – Set 3

1 State whether the following reactions are redox or not and explain why.
  - a $Mn(s) + Cu^{2+}(aq) \rightarrow Mn^{2+}(aq) + Cu(s)$
  - b $Na_2CO_3(aq) + 2HCl(aq) \rightarrow CO_2(g) + H_2O(l) + 2NaCl(aq)$

2 Identify whether the following are reduction or oxidation reactions.
  - a $K(s) \rightarrow K^+(aq) + e^-$
  - b $2Br^-(aq) \rightarrow Br_2(l) + 2e^-$

3 Assign oxidation numbers to each element in the following reactions.
  - a $Na_2CO_3 \rightarrow Na_2O + CO_2$
  - b $C_6H_{12}O_6 + 6O_2 \rightarrow 6CO_2 + 6H_2O$

4 For each reaction in Question **3**, state whether carbon has been reduced or oxidised.

5 For each reaction in Question **3**, identify which species is the reducing agent and which species is the oxidising agent.

VIDEO 3A–2
SKILLS: IMPORTANCE OF OXIDATION NUMBERS

3A SKILLS

Importance of oxidation numbers

In this section, you have seen the value of being able to assign and use oxidation numbers. The following important steps help you to do this.

1 Identify reactions as redox reactions (or not).
2 Identify reduction.
3 Identify oxidation.
4 Identify reducing agents.
5 Identify oxidising agents.
6 Identify redox couples.
7 Identify the movement of electrons.

Concept-mapping from key glossary terms

This section has explored much of the underlying chemistry and key definitions for redox reactions, including how to identify reduction, oxidation, reducing agents, oxidising agents, redox couples and ways of assigning and using oxidation numbers. Table 3A–2 and Figure 3A–4 summarise the key concepts covered but also highlight how the language you need to know and understand has a lot of similarities. This can sometimes cause confusion initially, so it is important to use the glossary terms throughout this chapter to help you solidify your understanding of the language used. A useful activity to consolidate your ability to correctly use these terms is to create your own concept map showing connections between the terms. You could also annotate the concept map at the beginning of the chapter to further consolidate the connections between the related terminology used.

Table 3A–2 Comparing oxidation and reduction

Oxidation	Reduction
Loss of electrons	Gain of electrons
Electrons on right-hand side of half-equations	Electrons on left-hand side of half-equations
Oxidation number increases	Oxidation number decreases
Caused by oxidising agent	Caused by reducing agent
Reducing agent undergoes oxidation	Oxidising agent undergoes reduction

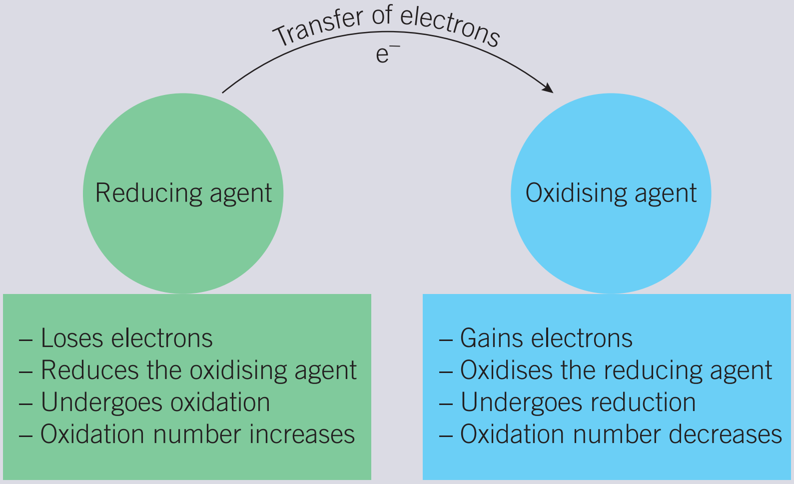


Figure 3A–4 Summary of key terms and concepts for reducing agents and oxidising agents

Section 3A questions

1 Use these terms to correctly complete the sentences below.

decreases
electrons
gain
increases
loss
oxidation
oxidised
reduced

Redox reactions involve a transfer of __________. During a redox reaction, both reduction and ___________ occur simultaneously. Oxidation is the ______ of electrons and reduction is the _____ of electrons. Oxidation numbers can be used to identify the reducing agent and oxidising agent. During a redox reaction, the oxidising agent is __________, and its oxidation number ___________. At the same time, the reducing agent is ______________, and its oxidation number ___________.

2 Write a definition for oxidation in terms of oxidation numbers.

3 Use oxidation numbers to identify which of the following reactions is **not** a redox reaction.

- a $Ag(s) + H_2S(g) \rightarrow Ag_2S(s) + H_2(g)$
- b $HCl(aq) + KOH(aq) \rightarrow H_2O(l) + KCl(aq)$
- c $Zn(s) + O_2(g) \rightarrow Zn_2O_3(s)$
- d $2Ag^+(aq) + Sn(s) \rightarrow Sn^{2+}(aq) + Ag(s)$

4 Classify each half-equation as reduction or oxidation.

- a $Sn^{4+}(aq) + 2e^- \rightarrow Sn^{2+}(aq)$
- b $2Cl^-(aq) \rightarrow Cl_2(g) + 2e^-$
- c $Fe^{2+}(aq) + e^- \rightarrow Fe^+(aq)$

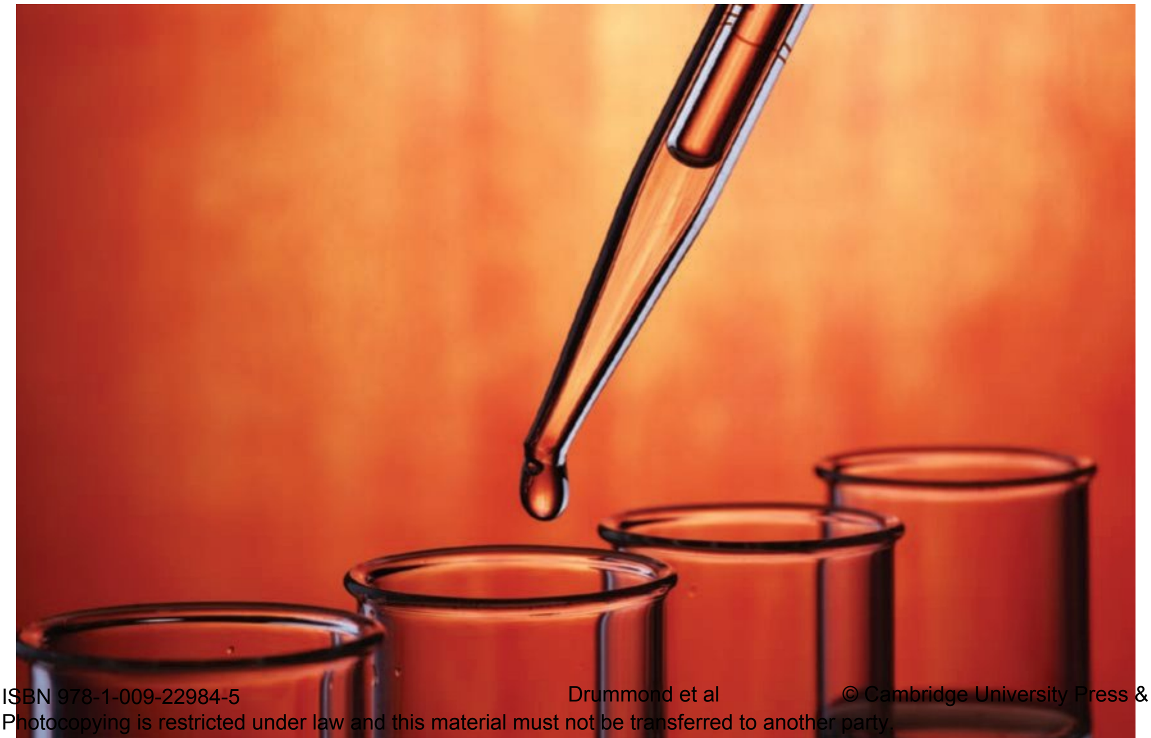
5 For each of the reactions below, explain how you would determine oxidation numbers to help you identify the reducing agent and the oxidising agent.

- a $Ni^{2+}(aq) + Zn(s) \rightarrow Zn^{2+}(aq) + Ni(s)$
- b $Zn(s) + Cl_2(g) \rightarrow ZnCl_2(s)$

6 Consider the reaction:

$$ZnO(s) + H_2(g) \rightarrow Zn(s) + H_2O(l)$$

- a Identify the two redox couples.
- b State which species is being reduced and which is being oxidised.



3B Writing redox equations

Study Design:

- The writing of balanced half-equations (including states) for oxidation and reduction reactions, and the overall redox cell reaction in both acidic and basic conditions

Glossary:

Complex half-equation
Simple half-equation

ENGAGE

What conditions are needed for redox reactions?

What conditions are needed for a redox reaction to take place? Do they even matter? Redox reactions can take place in a range of conditions, including neutral, basic or acidic conditions. These conditions do have some influence over what species are involved during a redox reaction and are important to consider when writing balanced equations for a given scenario.

In basic conditions, the OH^- ions play a role in the redox reactions that can take place. You might already be familiar with alkaline batteries; these are examples of redox reactions taking place in basic conditions. Car batteries, on the other hand, are an example of redox reactions taking place in acidic conditions. You will learn more about batteries and cells and their conditions in Section 3C.

3C FEATURES OF GALVANIC CELLS LINK

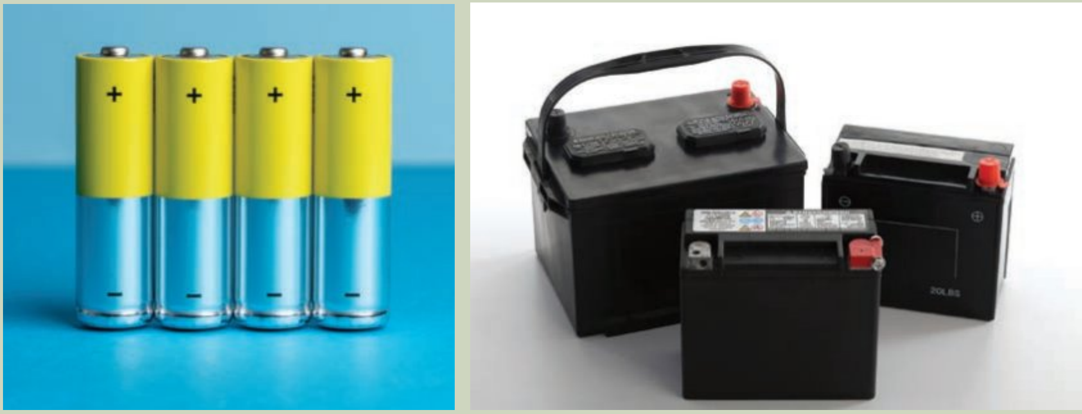


Figure 3B–1 AA batteries (left) are an example of redox reactions occurring under basic conditions. Car batteries (right) are an example of redox reactions occurring under acidic conditions.

VIDEO 3B–1 HALF-EQUATIONS

EXPLAIN

While most of this material is repeated from Units 1 and 2, please note that new material has been added to cover redox reactions under basic conditions. This was not required learning for the Units 1 and 2 course and is potentially examinable content.

UNIT 2 LINK

Writing redox half-equations

Simple half-equations

You should recall that redox reactions involve *both* reduction and oxidation. As you have already seen in Section 3A, reduction and oxidation reactions can be written as separate half-equations, which show the electrons either as reactants in reduction half-equations or as products in oxidation half-equations. These are referred to as **simple half-equations**.

Simple half-equation either the reduction or oxidation part of a redox reaction involving only one element

3A REDUCTION AND OXIDATION LINK

When writing simple half-equations, which contain only one type of element, there are a few steps that you need to follow. Applying the acronym **ECS** will help you to remember these three critical steps.

1. Write the species on the correct side of the equation and then balance the **E**lement involved.
2. Balance the **C**harges in the equation. This is done by adding the appropriate number of electrons to the *more positive* side of the half-equation. Note that you can apply your understanding of oxidation numbers to each element in an equation to determine this.
3. Finally, ensure that you have included correct **S**tates for each element listed.

NOTE

When assigning states for redox equations in this course, note the following points.

1. Ions are always aqueous, (aq).
2. Electrons have **no** state.
3. Water, H_2O, is always liquid, (l).

Worked example 3B–1: Writing oxidation half-equations

VIDEO
WORKED EXAMPLE 3B–1

Write the half-equation to represent the oxidation of solid zinc, Zn(s), to zinc ions, $Zn^{2+}(aq)$.

Solution

	Logic	Process
Step 1 **E**	From the description provided, write the species on the appropriate side of the equation. In this example, the moles of Zn is the same on each side, so the **E**lements are balanced.	$Zn \rightarrow Zn^{2+}$
Step 2 **C**	Identify which side is more positive and by how many units. This can be done by applying oxidation numbers. Add the appropriate number of electrons to that side. In this example, the right-hand side is more positive by 2, meaning that two electrons need to be added to this side, which balances the **C**harges.	$\overset{0}{Zn} \rightarrow \overset{+2}{Zn^{2+}} + 2e^-$
Step 3 **S**	Add **S**tates to each element as required.	$Zn(s) \rightarrow Zn^{2+}(aq) + 2e^-$

Figure 3B–2 In the above reaction, solid zinc (Zn) is converted to Zn^{2+} ions. These ions then go on to react with oxygen, forming zinc oxide.

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NOTE

The charges on each side of an equation *do not* necessarily have to equal zero. You must only balance the charges so that they are the *same* on each side of the half-equation.

VIDEO WORKED EXAMPLE 3B–2

Worked example 3B–2: Writing reduction half-equations

Write the redox half-equation to represent the reduction of bromine gas, $Br_2(g)$, to bromide ions, $Br^-(aq)$.

Solution

	Logic	Process
Step 1 **E**	From the description provided, write the species on the appropriate side of the equation. In this example, there are two bromine atoms on the left-hand side, but only one on the right-hand side. To balance the elements, we need to add an extra bromide ion, written as a coefficient in front of the species.	$Br_2 \rightarrow Br^-$ $Br_2 \rightarrow 2Br^-$
Step 2 **C**	Identify which side is more positive and by how many units. Add the appropriate number of electrons to that side. In this example, the left-hand side is more positive by 2, meaning that two electrons need to be added to this side.	$Br_2 + 2e^- \rightarrow 2Br^-$
Step 3 **S**	Add states to each element as required.	$Br_2(g) + 2e^- \rightarrow 2Br^-(aq)$

Check-in questions – Set 1

1 Balance the following half-equations and identify each as either reduction or oxidation.

- **a** $Cl_2(g) \rightarrow Cl^-(aq)$
- **b** $Mn^{2+}(aq) \rightarrow Mn(s)$
- **c** $K(s) \rightarrow K^+(aq)$

Complex half-equations

Complex half-equations contain more than one element and therefore require a different approach to balance them correctly.

Complex half-equation either the reduction or oxidation component of a redox reaction involving more than one element

Balancing in acidic conditions

Applying the acronym **KOHES** shown below will help ensure you follow the appropriate order to write and balance the half-equation if the reaction is taking place in acidic conditions.

	Step	Explanation
K	Balance the **K**ey element	This will be the element that is not oxygen or hydrogen. This is done by placing the correct coefficient in front of the required species.
O	Balance the **O**xygen	This is done by adding water, H_2O, to the opposite side of the equation to the oxygen.
H	Balance the **H**ydrogen	This is done by adding hydrogen ions, H^+, to the appropriate side of the equation.
E	Balance the **E**lectrons	Add the appropriate number of electrons to the more positive side of the equation.
S	It is imperative that you include **S**tates on all species	Water should be given a liquid state, (l), and the hydrogen ions will be written as aqueous, (aq).

Worked example 3B–3: Writing half-equations in acidic conditions

VIDEO
WORKED
EXAMPLE 3B–3

Dichromate ions, $Cr_2O_7^{2-}$, are a strong oxidising agent and as such can be reduced to chromium ions, Cr^{3+}. Write the half-equation to represent this, assuming the reaction takes place in acidic conditions.

Solution

	Logic	Process
Step 1 **K**	Start by writing each species on the appropriate side of the equation. Balance the **K**ey element, in this case the chromium, Cr. There are two chromium atoms on the left-hand side, but only one on the right-hand side. Balance by placing a 2 in front of the Cr^{3+}.	$Cr_2O_7^{2-} \rightarrow Cr^{3+}$ $Cr_2O_7^{2-} \rightarrow \mathbf{2}Cr^{3+}$
Step 2 **O**	Balance the **O**xygen. Do this by adding seven water (H_2O) molecules to the right-hand side.	$Cr_2O_7^{2-} \rightarrow 2Cr^{3+} + \mathbf{7H_2O}$
Step 3 **H**	Balance the **H**ydrogen. Do this by adding 14 H^+ ions to the left-hand side.	$Cr_2O_7^{2-} + \mathbf{14H^+} \rightarrow 2Cr^{3+} + 7H_2O$
Step 4 **E**	Balance the charges by adding **E**lectrons to the more positive side. In this example, the total of the charges is +12 on the left-hand side and +6 on the right-hand side. As such, six electrons are needed on the left-hand side.	$Cr_2O_7^{2-} + 14H^+ + \mathbf{6e^-} \rightarrow 2Cr^{3+} + 7H_2O$
Step 5 **S**	Add **S**tates to the half-equation.	$Cr_2O_7^{2-}\mathbf{(aq)} + 14H^+\mathbf{(aq)} + 6e^- \rightarrow$ $2Cr^{3+}\mathbf{(aq)} + 7H_2O\mathbf{(l)}$

Balancing in basic conditions

Balancing redox reactions in basic, or alkaline, conditions is slightly more complicated than the steps involved for acidic conditions. The main reason is that each redox half-equation will have *both* hydrogen ions, H^+, **and** hydroxide ions, OH^-, added to it. These ions then combine to make water, so there is some additional cancelling that takes place. We can still use the KOHES method, but remember to include the two additional steps, which are shown below.

	Step	Explanation
K	Balance the **K**ey element	This will be the element that is not oxygen or hydrogen. This is done by placing the correct coefficient in front of the required species.
O	Balance the **O**xygen	This is done by adding water, H_2O, to the opposite side of the equation to the oxygen.
H	Balance the **H**ydrogen	This is done by adding hydrogen ions, H^+, to the appropriate side of the equation.
Additional step **OH^-**	Neutralise any H^+ ions	This is done by adding hydroxide ions, OH^-, to both sides of the equation.
Additional step **H_2O**	Combine the H^+ and OH^- ions	Combine any H^+ and OH^- ions that appear on the same side of the equation, to make water. These water molecules can then potentially cancel with any other water molecules on the opposite side of the equation.
E	Balance the **E**lectrons	Add the appropriate number of electrons to the more positive side.
S	It is imperative that you include **S**tates on all species	Water should be given a liquid state, (l), and the hydrogen ions will be written as aqueous, (aq).

VIDEO
WORKED
EXAMPLE 3B–4

Worked example 3B–4: Writing half-equations in basic conditions

The dichromate ion, $Cr_2O_7^{2-}$, is a strong oxidising agent and as such can be reduced to a chromium ion, Cr^{3+}. Write the half-equation to represent this assuming the reaction takes place in alkaline conditions.

Solution

	Logic	Process
Step 1 **K**	Start by writing each species on the appropriate side of the equation. Balance the **K**ey element, in this case the chromium, Cr. There are two chromium atoms on the left-hand side, but only one on the right-hand side. Balance by placing a 2 in front of the Cr^{3+}.	$Cr_2O_7^{2-} \rightarrow Cr^{3+}$ $Cr_2O_7^{2-} \rightarrow \mathbf{2}Cr^{3+}$
Step 2 **O**	Balance the **O**xygen. Do this by adding seven water molecules to the right-hand side.	$Cr_2O_7^{2-} \rightarrow 2Cr^{3+} + \mathbf{7H_2O}$
Step 3 **H**	Balance the **H**ydrogen. Do this by adding 14 H^+ ions to the left-hand side.	$Cr_2O_7^{2-} + \mathbf{14H^+} \rightarrow 2Cr^{3+} + 7H_2O$
Step 4 **OH–**	Neutralise the H^+ ions by adding OH^-. Do this by adding 14 OH^- ions to both sides of the equation.	$Cr_2O_7^{2-} + 14H^+ + \mathbf{14OH^-} \rightarrow 2Cr^{3+} + 7H_2O + \mathbf{14OH^-}$
Step 5 **H_2O**	Combine the H^+ and OH^- ions to make water, then cancel the water molecules on each side of the equation where possible. In this example, there are seven H_2O that cancel on each side.	$Cr_2O_7^{2-} + \mathbf{14H_2O} \rightarrow 2Cr^{3+} + 7H_2O + \mathbf{14OH^-}$ $Cr_2O_7^{2-} + \mathbf{\cancel{14}H_2O} \rightarrow 2Cr^{3+} + \cancel{7H_2O} + \mathbf{14OH^-}$ $Cr_2O_7^{2-} + \mathbf{7H_2O} \rightarrow 2Cr^{3+} + \mathbf{14OH^-}$
Step 6 **E**	Balance the charges by adding **E**lectrons to the more positive side. In this example, the total of the charges is –2 on the left-hand side and –8 on the right-hand side. As such, six electrons are needed on the right-hand side.	$\mathbf{6e^-} + Cr_2O_7^{2-} + 7H_2O \rightarrow 2Cr^{3+} + \mathbf{14OH^-}$
Step 7 **S**	Add **S**tates to the half-equation.	$6e^- + Cr_2O_7^{2-}(aq) + 7H_2O(l) \rightarrow 2Cr^{3+}(aq) + 14OH^-(aq)$

Check-in questions – Set 2

1 Balance the following half-equations, assuming acidic conditions, and identify each half-equation as reduction or oxidation.

a $MnO_4^-(aq) \rightarrow Mn^{2+}(aq)$ **b** $H_2SO_3(aq) \rightarrow SO_4^{2-}(aq)$

2 Balance the following half-equations, assuming basic conditions, and identify each half-equation as reduction or oxidation.

a $MnO_4^-(aq) \rightarrow Mn^{2+}(aq)$ **b** $H_2SO_3(aq) \rightarrow SO_4^{2-}(aq)$

Combining half-equations

You should recall that redox reactions involve a transfer of electrons, where reduction and oxidation both occur simultaneously. That is, you can't have one without the other, and the number of electrons that the oxidising agent gains, *must be equal to* the number of electrons that the reducing agent loses. When considering half-equations, this means that the number of electrons on the left-hand side of a reduction half-equation *must be equal to* the number of electrons on the right-hand side of the corresponding oxidation half-equation.

In situations where the number of electrons differ in each half-equation, you must find the lowest common multiple for the number of electrons. Do this by multiplying one or both half-equations to ensure that the numbers of electrons are equal to this lowest common multiple value. The half-equations can then be added or combined to give the full, overall redox equation. Worked example 3B–5 shows you how to do this.

VIDEO
WORKED
EXAMPLE 3B–5

Worked example 3B–5: Combining redox half-equations

Write the combined redox equation for the reaction between silver ions and nickel metal.

Solution

	Logic	Process
Step 1	Write each of the balanced half-equations that take place.	$Ag^+(aq) + e^- \rightarrow Ag(s)$ $Ni(s) \rightarrow Ni^{2+}(aq) + 2e^-$
Step 2	Balance the electrons in each equation by finding the lowest common multiple. The silver half-equation only has one electron, whereas the nickel half-equation contains two electrons. To balance the electrons, we need to multiply the silver half-equation by 2.	$2 \times (Ag^+(aq) + e^- \rightarrow Ag(s))$ $2Ag^+(aq) + 2e^- \rightarrow 2Ag(s)$
Step 3	Combine the half-equations by adding them together. A simple way of doing this is to write each species that is on the left of the arrow of the half-equations together on the left and write each species that is on the right of the arrow of the half-equations together on the right. Note that it is important to place the arrows directly below each other.	$2Ag^+(aq) + 2e^- \rightarrow 2Ag(s)$ $Ni(s) \rightarrow Ni^{2+}(aq) + 2e^-$ $2Ag^+(aq) + 2e^- + Ni(s) \rightarrow 2Ag(s) + Ni^{2+}(aq) + 2e^-$
Step 4	The electrons on the left-hand side of the arrow cancel out those on the right-hand side, leaving the full balanced redox equation.	$2Ag^+(aq) + \cancel{2e^-} + Ni(s) \rightarrow 2Ag(s) + Ni^{2+}(aq) + \cancel{2e^-}$ $2Ag^+(aq) + Ni(s) \rightarrow 2Ag(s) + Ni^{2+}(aq)$

The final equation in the solution to Worked example 3B–5 is an example of a redox equation that can also be classified as an ionic equation. It shows the species reacting and their charges and states but does not show the electrons that are being transferred.

Writing balanced half-equations from full redox reactions

3A REDUCTION AND OXIDATION LINK

Sometimes you may be given an ionic equation, or full redox equation, from which you need to identify what the half-equations are. This involves applying most of the skills that you have been looking at in this chapter. You will need to identify the *redox couples* and follow the steps to balance each half-equation that were covered in Worked examples 3B–1, 3B–2 and 3B–3.

VIDEO WORKED EXAMPLE 3B–6

Worked example 3B–6: Writing half-equations from full equations

Use the following redox reaction to write the two half-reactions. Also identify which half-reaction is reduction and which is oxidation.

$$F_2(g) + 2Fe^{2+}(aq) \rightarrow 2F^-(aq) + 2Fe^{3+}(aq)$$

Solution

	Logic	Process
Step 1	Identify the redox couples and write each pair on appropriate sides of the half-equation.	$F_2(g) + 2Fe^{2+}(aq) \rightarrow 2F^-(aq) + 2Fe^{3+}(aq)$ $F_2 \rightarrow F^-$ $Fe^{2+} \rightarrow Fe^{3+}$
Step 2 **E**	Balance the **E**lements by adding coefficients where necessary. Only the F^- ion requires the coefficient 2 in this example.	$F_2 \rightarrow 2F^-$ $Fe^{2+} \rightarrow Fe^{3+}$
Step 3 **C**	Balance the **C**harges by adding electrons to the more positive side of each half-equation.	$F_2 + 2e^- \rightarrow 2F^-$ $Fe^{2+} \rightarrow Fe^{3+} + e^-$
Step 4 **S**	Include **S**tates.	$F_2(g) + 2e^- \rightarrow 2F^-(aq)$ $Fe^{2+}(aq) \rightarrow Fe^{3+}(aq) + e^-$
Step 5	Identify which is reduction and which is oxidation. The simplest way to do this is to identify on which side of the half-equation the electrons are shown. Another method is to use oxidation numbers.	Reduction (electrons on the left-hand side): $F_2(g) + 2e^- \rightarrow 2F^-(aq)$ Oxidation (electrons on right-hand side): $Fe^{2+}(aq) \rightarrow Fe^{3+}(aq) + e^-$

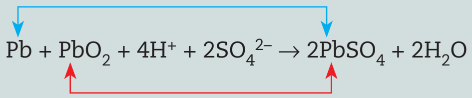
WORKSHEET 3B–1 WRITING SIMPLE AND COMPLEX HALF-EQUATIONS

NOTE

There is sometimes a rare case where the reduction and oxidation reactions both result in the *same* product being formed. An example of this is shown below.

$$Pb(s) + PbO_2(s) + 4H^+(aq) + 2SO_4^{2-}(aq) \rightarrow 2PbSO_4(s) + 2H_2O(l)$$

The redox couples for such a reaction would each have the same product as indicated below.



$$Pb + PbO_2 + 4H^+ + 2SO_4^{2-} \rightarrow 2PbSO_4 + 2H_2O$$

Sometimes it is possible for the opposite to happen, where the same species in a redox reaction acts as both the reducing agent and the oxidising agent. In one half-reaction it would undergo reduction, and in the other half-reaction it would undergo oxidation. These are uncommon circumstances but are important to be aware of.

Check-in questions – Set 3

1 Write the full ionic equation by combining the following half-equations.
   - a $Al^{3+}(aq) + 3e^- \rightarrow Al(s)$ and $Ca(s) \rightarrow Ca^{2+}(aq) + 2e^-$
   - b $O_2(g) + 4H^+(aq) + 4e^- \rightarrow 2H_2O(l)$ and $K(s) \rightarrow K^+(aq) + e^-$

2 Write the reduction and oxidation half-equations for the full redox equations shown, assuming they take place in acidic conditions. Label each half-equation as either reduction or oxidation.
   - a $2H^+(aq) + 2Li(s) \rightarrow 2Li^+(aq) + H_2(g)$
   - b $2MnO_4^-(aq) + 6H^+(aq) + 5H_2O_2(aq) \rightarrow 2Mn^{2+}(aq) + 8H_2O(l) + 5O_2(g)$

3 Identify the conjugate redox pairs and use these to determine the overall equation for the following reaction occurring in basic conditions.

$$MnO_4^-(aq) + Zn(s) \rightarrow MnO_2(s) + Zn(OH)_4^{2-}(aq)$$

3B SKILLS

VIDEO 3B–2
SKILLS: WRITING BALANCED EQUATIONS

Key things to check when writing balanced equations

It is important that you are able to write balanced equations, particularly in this section of the course. Below are a few points to remember that you may find helpful.

1 Never change the subscripted numbers in a formula. This is only done when balancing the formula of ionic compounds based on the individual charges of the cation and the anion.

2 Only ever change coefficients to balance elements.

3 A balanced equation must have the same number of each element on both the reactant and product sides.

4 Charges on both the reactant and product sides must always be the same. One common mistake is adding electrons to each side of a redox equation to make the charges equal zero on both sides. Sometimes the charges will be zero, other times positive or negative. They simply need to be the same on each side.

5 Finally, always make sure that you add states to any equations you write.

Let's look at an example to apply these rules.

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In the 1840s, a telegraph system used an early version of an electric primary cell that consisted of two half-cells, each with an electrode and an aqueous electrolyte, which were:

- a zinc electrode (Zn) in dilute sulfuric acid solution (H_2SO_4).
- a platinum electrode (Pt) in concentrated nitric acid (HNO_3).

In the nitric acid half-cell, aqueous nitrate ions, NO_3^-, were converted into nitrogen dioxide, NO_2.

Write the half-equation for this reaction by following these steps.

1 Write the initial reactant and products without changing the subscripts present

$$NO_3^- \rightleftharpoons NO_2$$

2 Balance the elements by following the steps in KOHES, which will change the coefficients.

$$NO_3^- + 2H^+ \rightleftharpoons NO_2 + H_2O$$

3 Check that the same number of elements is present on both the reactant and product sides of the equation – which they are.

4 The reactant side of the equation has an overall charge of +1 (−1 + 2), whereas the product side of the equation has an overall charge of 0. Therefore, balance the charges by adding electrons to the more positive side, in this case the reactant side (one electron needed).

$$NO_3^- + 2H^+ + e^- \rightleftharpoons NO_2 + H_2O$$

5 Make sure that you write a state for each species.

$$NO_3^-(aq) + 2H^+(aq) + e^- \rightleftharpoons NO_2(g) + H_2O(l)$$

Section 3B questions

1 Explain the difference between a redox half-equation and a full redox equation.

2 Balance the following half-equations.

- a $H_2(g) \rightarrow H^+(aq)$
- b $Cr^{3+}(aq) \rightarrow Cr(s)$
- c $Ag(s) \rightarrow Ag^+(aq)$

3 Balance the following half-equation using KOHES.

$$HNO_2(aq) \rightarrow NO_3^-(aq)$$

4 Write the full ionic equation by combining the following half-equations.

- a $Pb^{2+}(aq) + 2e^- \rightarrow Pb(s)$ and $Co(s) \rightarrow Co^{2+}(aq) + 2e^-$
- b $F_2(g) + 2e^- \rightarrow 2F^-(aq)$ and $K(s) \rightarrow K^+(aq) + e^-$
- c Explain the importance of multiplying the potassium, K, half-equation in part **b** when determining the overall equation.

5 Write the reduction and oxidation half-equations for the full redox equations shown below. Label each half-equation as either reduction or oxidation.

- a $Zn^{2+}(aq) + 2Li(s) \rightarrow 2Li^+(aq) + Zn(s)$
- b $3CH_3CH_2OH(aq) + 2Cr_2O_7^{2-}(aq) + 16H^+(aq) \rightarrow 4Cr^{3+}(aq) + 11H_2O(l) + 3CH_3COOH(aq)$

6 For each of the following reactions, write the balanced half-equations, identifying which is oxidation and which is reduction, as well as writing the overall redox equation.
   a $I_2(s) + H_2S(g) \rightarrow I^-(aq) + S(s)$
   b $NO_3^-(aq) + H_2S(g) \rightarrow NO(g) + S(s)$
   c $SO_3^{2-}(aq) + MnO_4^-(aq) \rightarrow SO_4^{2-}(aq) + Mn^{2+}(aq)$
   d $Cr_2O_7^{2-}(aq) + CH_3CH_2OH(g) \rightarrow CH_3COOH(g) + Cr^{3+}(aq)$

7 When a piece of copper metal is placed into a silver nitrate solution, silver metal is formed and the solution gradually turns blue, indicating the presence of copper(II) ions in solution. The oxidation and reduction reactions can be represented by two half-equations.
Write these half-equations and identify which substances are oxidised and which are reduced.

8 Form an overall equation by combining the following pair of half-equations:

$$VO^{2+}(aq) + H_2O(l) \rightarrow VO_2^+(aq) + 2H^+(aq) + e^-$$
$$VO^{2+}(aq) + 2H^+(aq) + 2e^- \rightarrow V^{2+}(aq) + H_2O(l)$$

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3C

Features of galvanic cells

Study Design:

- The common design features and general operating principles of non-rechargeable (primary) galvanic cells converting chemical energy into electrical energy, including electrode polarities and the role of the electrodes (inert and reactive) and electrolyte solutions (details of specific cells not required)

Glossary:

Anode
Cathode
Chemical energy
Conjugate redox pair
Electrical energy
Electrochemical cell
Electrode
Electrode polarity
Electrolyte
Galvanic cell
Half-cell
Inert
Ion
Primary cell
Salt bridge
Spontaneous reaction
Voltmeter

ENGAGE

Batteries are everywhere!

Figure 3C–1 Italian scientist Alessandro Volta and his voltaic pile 'battery' consisting of alternating silver and zinc discs

In a world where technology is advancing and the number of portable and mobile gadgets is increasing, have you ever wondered when batteries were first invented, or what is it about a battery that makes it possible to provide the electrical energy to power these devices?

There are many different types of batteries in use today. Some larger batteries store huge amounts of power generated by solar farms, others may be used to power electric cars, while many are much smaller and can be found in watches and hearing aids. Despite their size differences, essentially all of them have a similar design enabling a redox chemical reaction to take place that converts stored chemical energy into usable electrical energy.

American scientist and inventor, Benjamin Franklin, first used the term 'battery' in the mid-1700s but it is believed that the first true battery was made by Italian scientist Alessandro Volta in 1800. He created a stack of alternating discs of silver and zinc, separated by cloth soaked in salt water, to generate a current. Since there were no instruments available to detect weak currents at the time, he tested his batteries by using his tongue! Volta discovered that changing the types of metals used, as well as changing the number of discs, had an effect on the amount of current that the battery could produce.

Another battery that you might already be familiar with is the lead–acid battery, which was invented in the mid-1800s. It was the first-ever rechargeable battery and is still commonly used today to provide the electrical energy needed to start cars and other vehicles. Batteries are examples of galvanic cells, which are central to this section of the Study Design.

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EXPLAIN

Electrochemical cells

Electrochemical cells are systems that can convert stored **chemical energy** into **electrical energy** *or* that can use electrical energy supplied to facilitate chemical reactions. Some can even do both! In this chapter, we will focus on the former, also referred to as 'galvanic cells'. **Galvanic cells** are one type of electrochemical cell and involve **spontaneous** redox **reactions**.

NOTE

It is helpful to recognise that there are a number of interchangeable terms used when discussing galvanic cells: 'voltaic cell', '**primary cell**' and even the term 'battery' may all be used to reference a galvanic cell. Essentially, they are equivalent in that they refer to an electrochemical cell that spontaneously produces electrical energy from chemical energy.

Energy transformation

Figure 3C–2 shows the spontaneous redox reaction that occurs when solid zinc metal, Zn(s), is placed directly into a solution of copper(II) sulfate containing copper ions, $Cu^{2+}(aq)$. The overall redox reaction for this process is:

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

Since the reactants are in direct contact with each other, when the reaction takes place, electrons are exchanged directly in an exothermic reaction, and chemical energy is converted into thermal energy, which is released into the surroundings as heat.

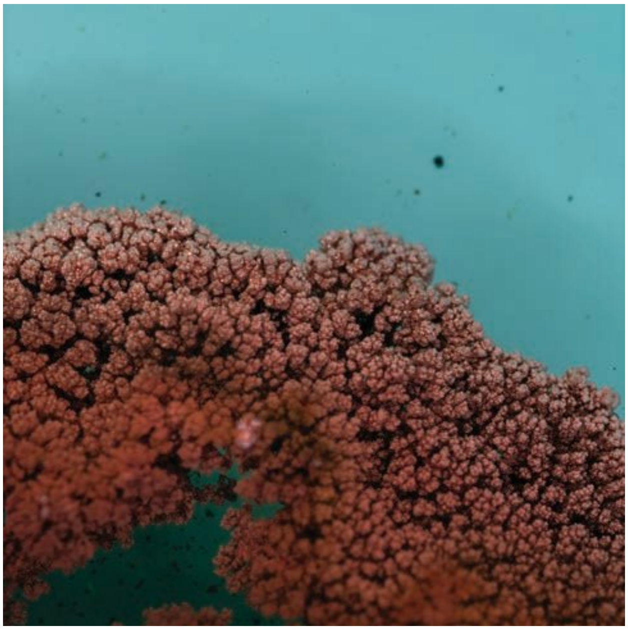

Figure 3C–2 A piece of solid zinc placed into copper sulfate solution undergoes a spontaneous exothermic reaction.

To be effective in producing electrical energy, galvanic cells are systems that separate the two reactants instead of allowing them to be in direct contact with one another. This allows for the transformation of chemical energy into electrical energy that can be harnessed and used to provide power. Without this separation, a spontaneous exothermic reaction would still occur, involving a direct exchange of electrons between the reactants. This would produce heat energy instead of the electrical energy that can be generated by a galvanic cell.

Check-in questions – Set 1

1 What type of energy transformation takes place when the reactants for a spontaneous redox reaction are in direct contact with one another?

2 What type of energy transformation takes place when the reactants for a spontaneous redox reaction are separated from one another in a galvanic cell?

Electrochemical cell
a system where electrical energy can be converted to chemical energy or vice versa

Chemical energy
energy stored within the bonds between atoms

Electrical energy
energy that involves the flow of electrons and/or charged particles

Galvanic cell
a system in which a spontaneous redox reaction takes place, converting chemical energy to electrical energy

Spontaneous reaction
a reaction that takes place without the input of external energy

Primary cell
a type of electrochemical cell that spontaneously produces electrical energy from chemical energy; also referred to as a voltaic cell or battery

Features of galvanic cells

Galvanic cells are designed with a number of important features to ensure that electrical energy can be produced. Figure 3C–3 shows a representation of a specific galvanic cell called the Daniell cell, which was one of the first galvanic cells, invented by English chemist John Daniell in 1836. It includes many of the essential features common to all galvanic cells and is simple enough that you can reproduce it in the laboratory.

3A REDUCTION AND OXIDATION LINK

Half-cell one half of a galvanic cell that contains an electrode submerged in a solution of ions

Electrode solid conducting material that can carry electric current; a connecting terminal that allows current to flow

Ion a positively or negatively charged atom that has either lost or gained electron(s)

Cathode the electrode at which reduction occurs. In a galvanic cell, the cathode is positive

Anode the electrode at which oxidation occurs. In a galvanic cell, the anode is negative

Electrode polarity the positive or negative charge associated with electrodes in an electrochemical cell because of reduction or oxidation occurring on their surface. In a galvanic cell, the cathode is positive and the anode is negative

Conjugate redox pair a reducing agent and its corresponding conjugate oxidising agent

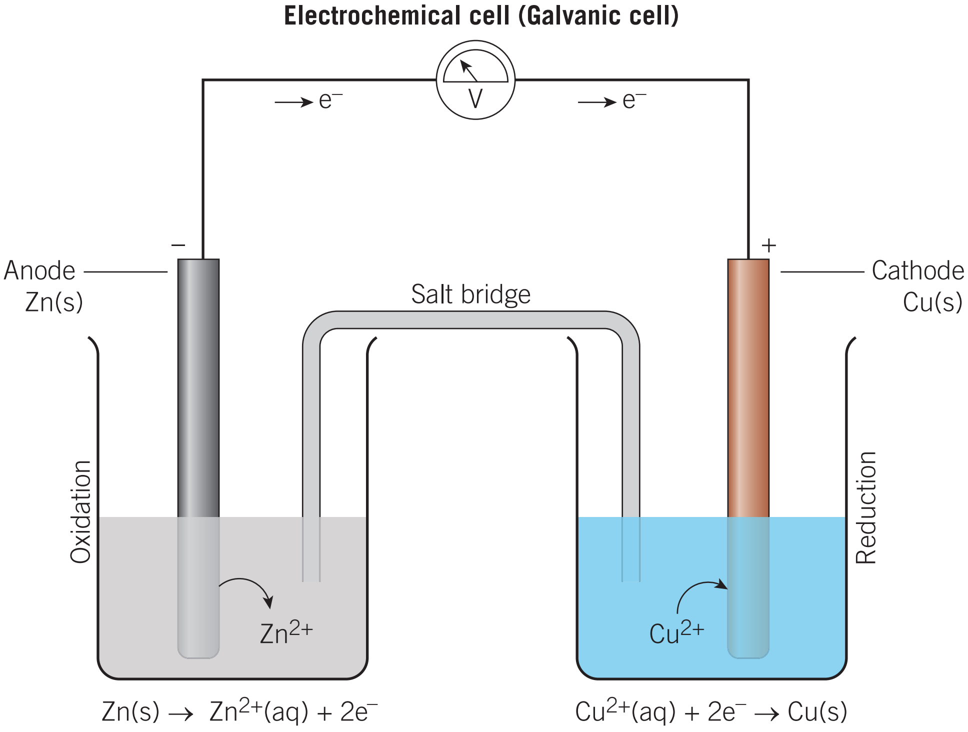

Figure 3C–3 A simple representation of the Daniell cell invented in 1836 by English chemist, John Daniell

Half-cells

Galvanic cells are comprised of two **half-cells**, which *must* be separated in order to produce electrical energy. In Figure 3C–3 above, the Daniell cell has two beakers separating the reactants. Each half-cell contains a solid conducting **electrode** partially submerged in a solution of **ions**. It is on the *surface* of these electrodes where the reduction and oxidation reactions take place. From Section 3A, we know that reduction involves a 'gain' of electrons, while oxidation involves the production or 'loss' of electrons. In a galvanic cell, the electrode where reduction occurs is called the **cathode**, which is also the *positive* terminal of the cell. The electrode where oxidation occurs is called the **anode**, which in a galvanic cell is also the *negative* terminal of the cell. The positive or negative 'charge' on these electrodes is more accurately referred to as the **electrode polarity**.

Electrodes

In Figure 3C–4, solid zinc, Zn(s), is acting as the anode in the oxidation half-cell, which also contains a solution of zinc ions, $Zn^{2+}(aq)$. Solid copper, Cu(s), is the cathode in the reduction half-cell, which also contains a solution of copper(II) ions, $Cu^{2+}(aq)$. You might recognise the species in each half-cell as **conjugate redox pairs**. Each half-cell contains a reducing agent and a conjugate oxidising agent. In most galvanic cells, a metal is part of the conjugate redox pair and is therefore often used as an electrode. When this is the case, the electrodes are *reactive* and take part in the redox reactions occurring. During such reactions, it is possible to observe an *increase* in mass at the cathode, where ions are converted to solid metal atoms (reduction occurs). Conversely, at the anode, where metal atoms are converted into ions, it is possible to observe a *decrease* in the mass of the metal electrode being used (oxidation occurs).

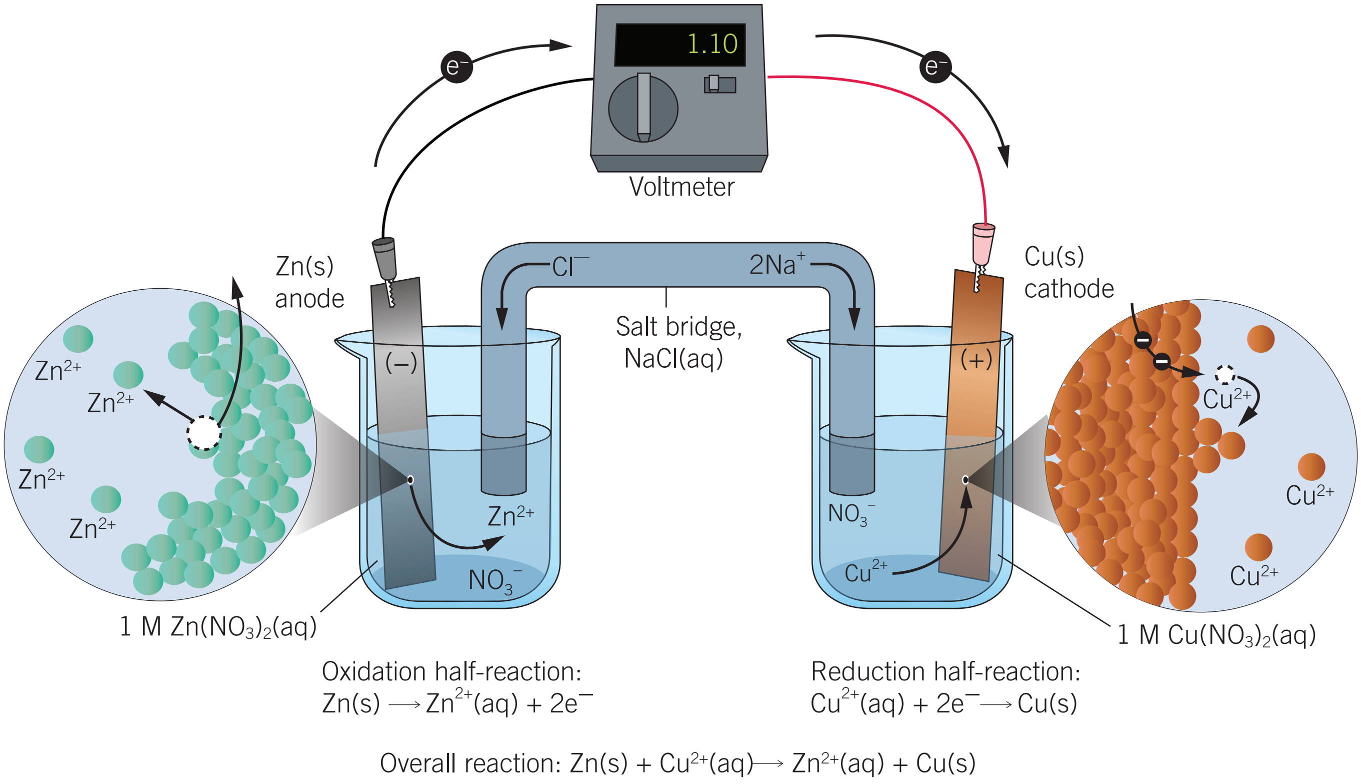

Figure 3C–4 Solid zinc, $Zn(s)$, is acting as the anode and solid copper, $Cu(s)$, is acting as the cathode.

Sometimes the conjugate redox pair in a half-cell does *not* include a metal, in which case an **inert** electrode, such as graphite or platinum, may be used instead. These materials still conduct electricity, but importantly, are *not* involved in the actual half-reactions that take place on their surfaces. A final point worth noting about electrodes is that some half-cells involving gases, such as hydrogen, oxygen or chlorine, may even have a special 'gas electrode'. Where the gas is a product of the reaction, there needs to be a way for the gas to escape. If the gas is a reactant, however, it is usually necessary for the gas to be bubbled into the solution surrounding the electrode. Figure 3C–5 shows an electrochemical cell that uses these gas electrodes.

Inert
largely non-reactive; does not take part in a reaction

Figure 3C–5 An electrochemical cell showing a set-up with two gas electrodes

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NOTE

Half-cells usually contain the species that react, but it is important to note that it is also possible for other species that are not involved in the reaction to be present. Sometimes there may be multiple ions present in a solution, often used to supply the reactive ions to the solution. For example, in the Daniell cell, the copper ions are supplied by copper(II) sulfate. Sulfate ions, SO_4^{2-} are also present but would be considered spectator ions as they do not take part in the actual reaction.

The salt bridge

Salt bridge connects the circuit in a galvanic cell and contains ions that balance the charges formed from each half-cell

Electrolyte a non-reactive solution or paste that enables the flow of charged particles and helps to facilitate the redox reactions

The **salt bridge** plays three important roles in a galvanic cell:

1. It connects the circuit, allowing for the flow of charged particles through the circuit
2. It allows for the physical separation of half-cells, preventing reactants from coming into direct contact with each other
3. It is usually soaked in a non-reactive **electrolyte** solution consisting of cations and anions that can migrate into the solutions to balance the charges of the reaction occurring in each half-cell (as shown in Figure 3C–4 with Na^+ and Cl^- ions).

Without a salt bridge, charge would accumulate in each of the cells and the redox reaction would soon cease.

Two common electrolytes used in galvanic cells are concentrated potassium nitrate, KNO_3, and concentrated potassium chloride, KCl; however, other substances may also be used, including sodium sulfate, Na_2SO_4, and sodium chloride, NaCl. Often the salt bridge is simply a piece of filter paper soaked in the electrolyte and draped across the two solutions in each beaker.

Migration of ions from the salt bridge

Consider the redox reactions taking place in the Daniell cell shown in Figure 3C–4.

Reduction at the cathode: $Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)$

Oxidation at the anode: $Zn(s) \rightarrow Zn^{2+}(aq) + 2e^-$

If we focus on the reduction reaction, we can see that it is using positive cations from the solution and converting them to neutral solid metal atoms. As a result, those cations are essentially removed from the solution as they take part in the reaction, so there would start to be an imbalance between the cations and anions in the solution. To balance the charges, positively charged cations from the salt bridge migrate into the solution of the reduction half-cell. For example, if NaCl is the electrolyte solution being used in the cell, it would be sodium ions, Na^+, that migrate towards the cathode. It is important to note that this 'balancing' of charge is happening in real-time and that if it did not, the galvanic cell would cease to function.

Looking at the anode reaction, the opposite is occurring, as solid zinc metal atoms are oxidised to zinc ions, Zn^{2+}. In this half-cell, the balance of charge in the solution would start to shift to have more cations than anions, so to balance this change, negatively charged anions migrate from the salt bridge towards the anode. If NaCl is the electrolyte solution being used in the cell, it would mean chloride ions, Cl^-, perform this function.

NOTE

An easy way to remember this movement of ions in the electrolyte (salt) bridge is:
- anions to the anode
- cations to the cathode.

As well as observing a change in mass at the cathode and anode, sometimes other important observations can be made that provide some indication that a reaction is taking place within a galvanic cell. In some half-cells, gases may be produced in a half-reaction that result in bubbles forming on the surface of the electrode. Another observation might be a change in appearance of the solvent used in a half-cell. For example, in the Daniell cell, the copper(II) sulfate solution has a blue colour. However, as the reaction proceeds and copper ions in that solution undergo reduction, the concentration of copper ions, Cu^{2+}, will decrease and the intensity of that blue coloured solution will also decrease over time.

The external circuit

The separation of reactants in a galvanic cell is crucial and allows the electrons produced by oxidation at the anode to flow to the cathode where they then take part in the reduction reaction. It is important to recognise that the electrons *do not* move into the solutions. Instead, the electrons flow from one electrode to the other via the external circuit, which is made up of wires connecting the electrodes. In some cell diagrams you may see light globes used in place of the **voltmeter** shown in Figure 3C–3 or 3C–4, which would glow when current flows through the external circuit.

Voltmeter an instrument used for measuring electrical potential

NOTE

An important skill is to determine the direction of flow of electrons. Although it should be possible to work out the direction by looking at the half-equations to see where the electrons are being used and where they are being produced, another convenient way to remember the direction is that they travel from the anode to the cathode (A to the C), which is in alphabetical order.

Check-in questions – Set 2

1 Explain the function of each galvanic cell design feature listed below.
  a salt bridge
  b electrolyte solution
  c electrode
  d external circuit
  e separated half-cells

2 State the direction of flow for the following particles during a spontaneous reaction occurring in a galvanic cell.
  a anion in the salt bridge solution
  b cation in the salt bridge solution
  c electron

3 In the Daniell cell shown in Figure 3C–3, predict which electrode would show an increase in mass and which would show a decrease in mass.

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Drawing and labelling galvanic cell diagrams

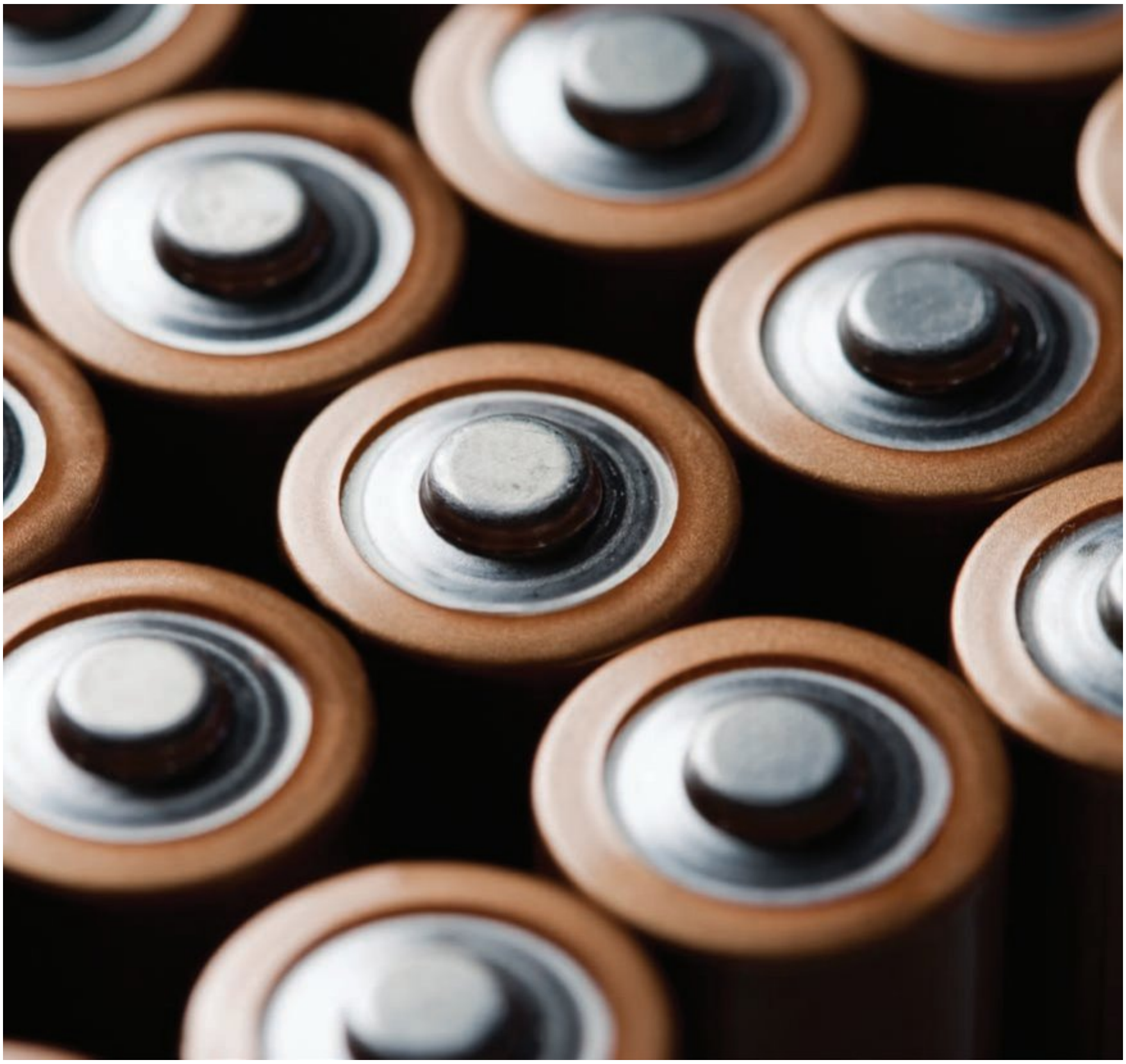
A key skill is being able to use the information about a reaction taking place in a galvanic cell to draw and/or label key aspects of the cell. This might include:

- writing the half-reactions or overall reaction occurring in the cell
- labelling the anode and cathode
- labelling the polarity of the electrodes
- labelling the direction of electron flow
- labelling the direction of flow of ions from the salt bridge.

Being able to determine many of these characteristics relies on identifying the cathode and the anode. To assist with this, make use of the galvanic cell mnemonic (memory aid): the **Happy Red Cat**.

- *Happy* corresponds to the *positive* terminal.
- *Red* corresponds to *red*uction.
- *Cat* corresponds to *cat*hode.

In galvanic cells, these three aspects *always* combine in the reduction half-cell, so you only need to identify one of the three aspects to quickly work out the other two. The opposite holds true for the oxidation half-cell: negative, oxidation and anode.

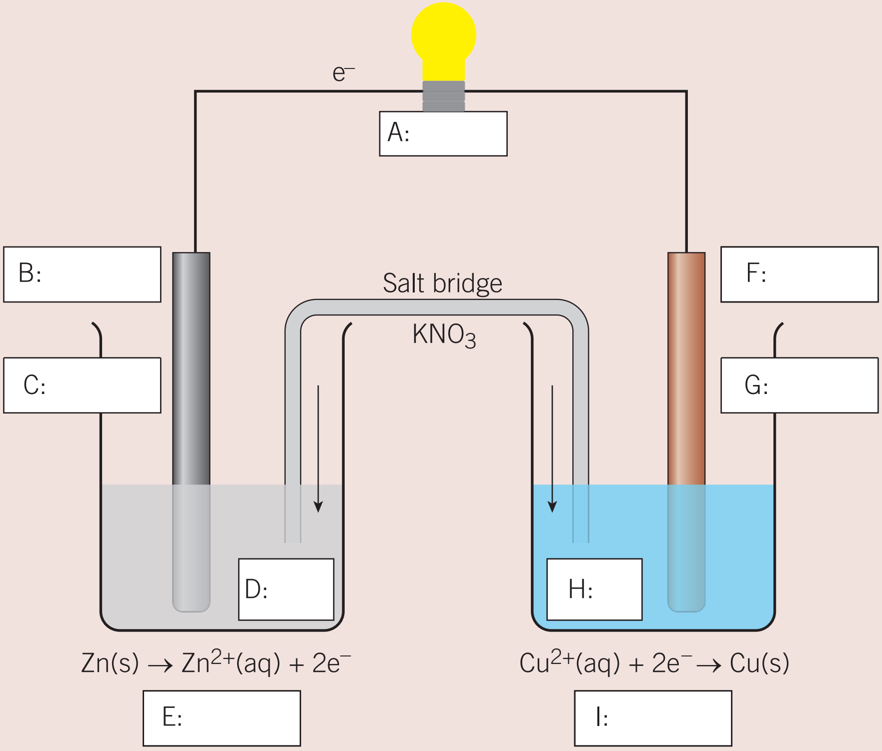


Worked example 3C–1: Identifying the features of a galvanic cell

VIDEO WORKED EXAMPLE 3C–1

Draw a copy of the galvanic cell shown below and label the following features.

A: direction of electron flow
B: name of zinc electrode (anode or cathode)
C: polarity of zinc electrode
D: ion migrating from salt bridge
E: name of reaction (reduction or oxidation)
F: name of copper electrode (anode or cathode)
G: polarity of copper electrode
H: ion migrating from salt bridge
I: name of reaction (reduction or oxidation)



Solution

	Logic	Process
Step 1	There is no specific order in which to approach a question like this, but the key is to identify what information you are given and to then try to apply the ‘happy red cat’ mnemonic. By identifying the reactions shown for each half-cell, and applying what we already understand about redox reactions, we can see the equation on the left for zinc is producing two electrons. Therefore, ‘E’ is oxidation. We can also see that in the half-reaction on the right the copper ions are combining with two electrons, which means that ‘I’ is reduction.	Loss of electrons: $Zn(s) \rightarrow Zn^{2+}(aq) + 2e^-$ Therefore, ‘E’ is oxidation. Gain of electrons: $Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)$ Therefore, ‘I’ is reduction.

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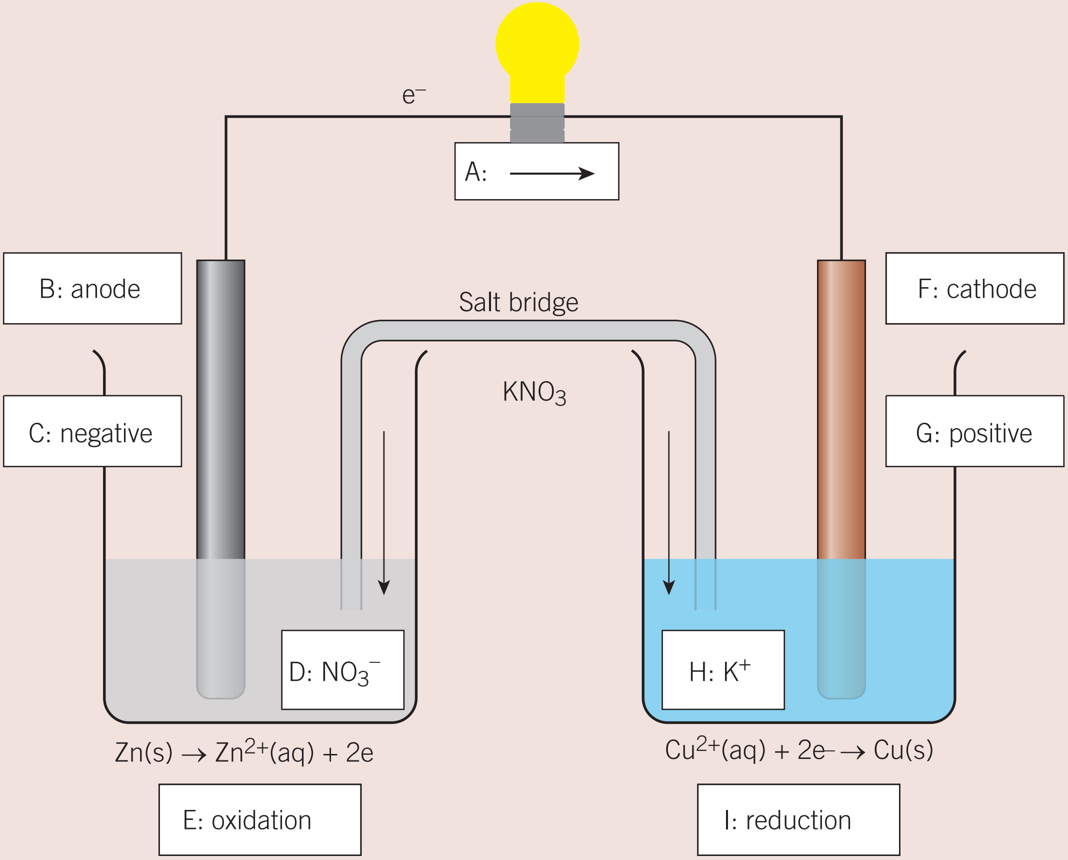
Step 2	We can then apply the 'happy red cat' to labels F and G.	Happy red cat: *Happy:* positive *Red:* reduction, which occurs on the right-hand side. *Cat:* cathode must also be on the right-hand side. Therefore, 'F' is cathode and 'G' is positive.
Step 3	By elimination, this tells us which terms correspond to labels B and C.	If 'F' is the cathode, 'B' is the anode and 'C' is negative.
Step 4	The direction of electron flow can now be determined, as we know electrons flow from anode to the cathode (A to the C).	Electrons flow from left to right in this cell, so an arrow pointing right is appropriate for 'A' on the diagram.
Step 5	For ion flow, we know that anions flow to the anode and cations flow to the cathode.	Because KNO_3 is shown as the electrolyte solution, the anions would be nitrate ions, NO_3^-, and the cations would be potassium ions, K^+. We can now add these species to labels D and H respectively.
Step 6	Complete the diagram.	See below.



Summarising the design features of galvanic cells

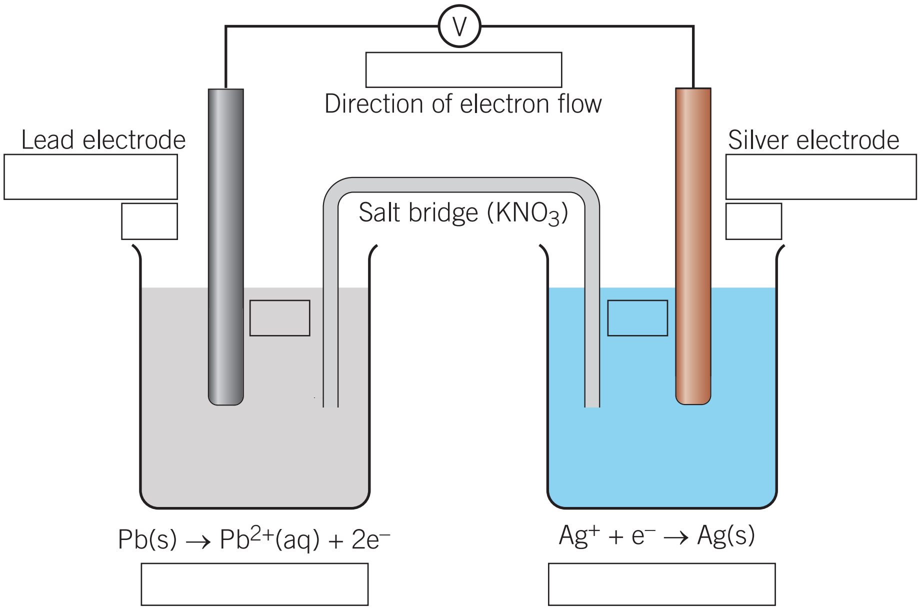
The design features of a galvanic cell play an important role in allowing for the conversion of chemical energy into usable electrical energy. Table 3C–1 provides a summary of the key design features of galvanic cells and their importance.

Table 3C–1 Essential features of a galvanic cell

Design feature	Function
Two separated half-cells	Allows for reduction and oxidation reactions to take place without direct contact between reactants so that electrons are forced to flow through the external circuit to provide electrical energy
External circuit	Consists of the wires connecting electrodes, as well as any device that is connected for electrons to flow though. Electrons flow from the anode to the cathode (A to the C).
Salt bridge	Allows half-cells to be physically separated. Connects the circuit allowing for charged particles (ions) to flow; supplies cations and anions to balance the charges in each half-cell
Electrodes	Provide a surface for the reduction and oxidation reactions to take place on. In most half-cells, they are made from the metal that forms part of the redox conjugate pair in that half-cell.
Electrolyte solution	Non-reactive solution that allows for flow of charge. Anions migrate towards the anode and cations migrate towards the cathode.
Anode	Negative electrode where oxidation half-reaction takes place
Cathode	Positive electrode where reduction half-reaction takes place

Check-in questions – Set 3

1 Draw a copy of the galvanic cell below and label the missing features.
   - a direction of electron flow
   - b name of each electrode (anode or cathode)
   - c polarity of each electrode
   - d ions migrating from salt bridge to each electrode (assume KNO_3 is the electrolyte)
   - e name of each half-reaction (reduction or oxidation)



VIDEO 3C–1
SKILLS: LABELLING GALVANIC CELL DIAGRAMS

3C SKILLS

Labelling galvanic cell diagrams

An important skill as part of this section is that you are able to draw and fully label a galvanic cell when given the electrode and electrolyte for two half-cells. You should as part of this be able to include the following information in your labelled diagram:

- relevant half-equations
- the polarity of the electrodes
- direction of electron flow through the wires (Remember: electrons flow away from the anode: A to C)
- direction and movement of ions from salt bridge (assume KNO_3 is being used) – remember positive ions migrate from the salt bridge to the cathode (+ with +)
- the anode and cathode
- the reducing agent and oxidising agent
- the overall equation
- the cell potential difference (theoretical voltage produced). This is discussed in more detail in the next section.

Let's look at an example question to apply all these things you should include.

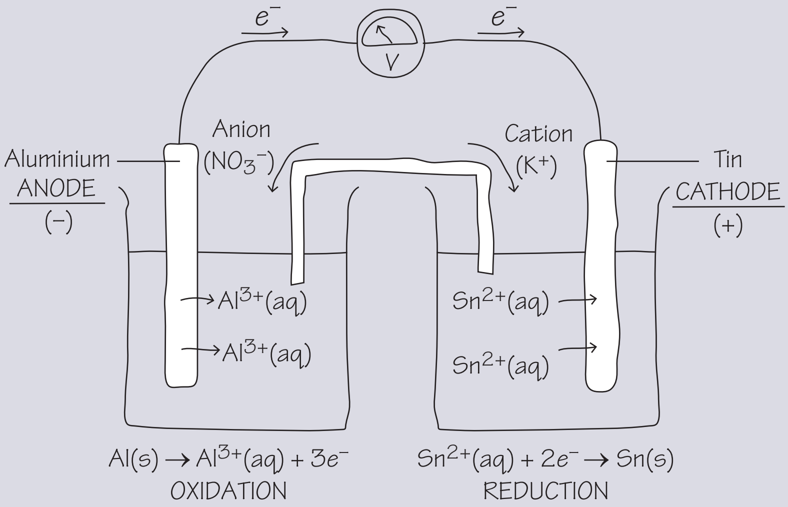
Question:

A galvanic cell is made up of two half-cells containing the following:

$Al^{3+}(aq)$ / Al(s) and $Sn^{2+}(aq)$ / Sn

Draw a fully labelled diagram for this galvanic cell, including all the points identified above.

Answer:



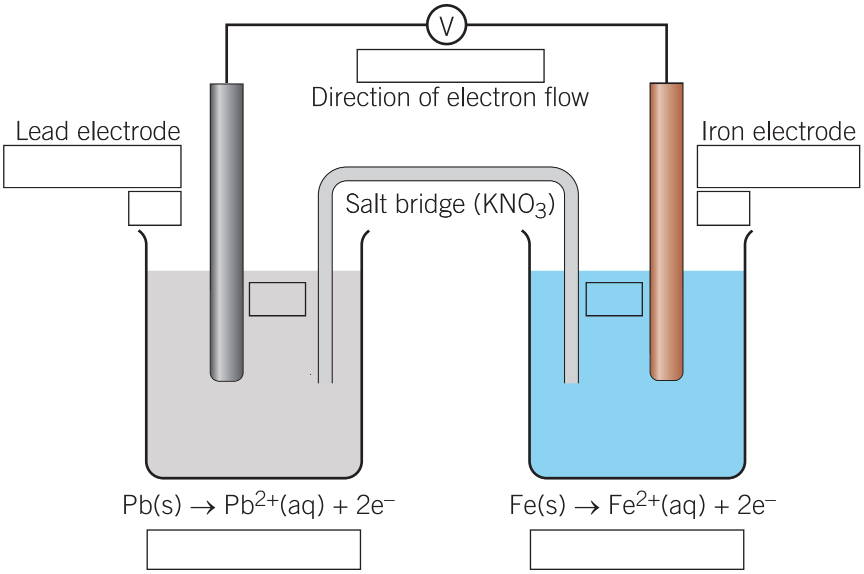
Section 3C questions

1 State whether the following statements are true or false for galvanic cells. Justify your response for each.

  a Electrons flow through the salt bridge from the anode to the cathode.
  b Cations flow from the salt bridge to the cathode.
  c Reduction occurs at the cathode.
  d Electrical energy is converted to chemical energy.
  e The polarity of the anode is negative.
  f The cathode can show an increase in mass during a reaction.

2 Copy the diagram of the galvanic cell below and label the missing features.

- **a** direction of electron flow
- **b** name of each electrode (anode or cathode)
- **c** polarity of each electrode
- **d** ions migrating from salt bridge to each electrode (assume KNO_3 is the electrolyte)
- **e** name of each half-reaction (reduction or oxidation)



3 A galvanic cell consists of one half-cell with a lead electrode placed in an aqueous lead ion electrolyte, and the other half-cell, which is a standard hydrogen half-cell with aqueous hydrogen ions.

Draw a fully labelled galvanic cell for this set-up, showing and labelling the following:

- anode and cathode
- electrode and electrolyte for each of the half-cells
- direction of electron flow
- salt bridge with the direction of ion flow into each half-cell
- oxidation and corresponding half-equation
- reduction and corresponding half-equation
- overall redox equation.

3D Using the electrochemical series

Study Design:

- The use and limitations of the electrochemical series in designing galvanic cells and as a tool for predicting the products of redox reactions, for deducing overall equations from redox half-equations and for determining maximum cell voltage under standard conditions

Glossary:

Electrochemical series
Potential difference
Standard cell potential
Standard electrode potential
Standard hydrogen electrode
Voltage

ENGAGE

The southern hemisphere's largest battery is right here in Victoria!

Did you know that, as of 2023, the largest lithium-ion battery in the southern hemisphere is located near Geelong? The Victorian Big Battery (VBB) stores enough energy to power more than 1 million homes for 30 minutes. In this section, you will look at how changing the reactants used in galvanic cells can have an effect on the reactions taking place as well as the amount of electrical energy they can produce.

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EXPLAIN

Potential difference

Under the same conditions, the type of reactants being used will influence the amount of **voltage** that can be produced by a galvanic cell. The voltage produced is caused by the **potential difference** in the amount of energy that the valence electrons have in atoms of different elements. Electrons flow through the external circuit because of this difference in potential energy between the two electrodes. More simply, the reactant in one half-cell has a stronger tendency to move electrons through the circuit compared to the other half-cell. The greater the difference between the two reactants, the greater the potential voltage the cell will be.

Voltage the amount of electrical potential that exists between two points

Potential difference a difference in the amount of energy that the valence electrons have in atoms of different reactants used in galvanic cells. The greater the potential difference, the greater the voltage produced

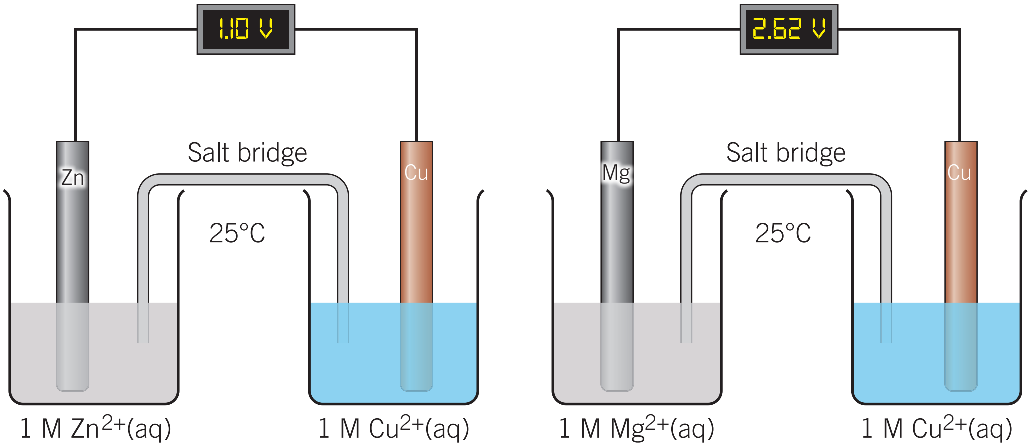

Figure 3D–1 Two similar galvanic cells. The voltage produced in the Daniell cell on the left is 1.10 volts compared to the cell on the right, which can produce 2.62 volts under the same conditions. In the cell on the right, the zinc half-cell has been replaced with a magnesium half-cell.

On the Daniell cell represented in Figure 3D–1, on the left-hand side, the voltmeter measuring the flow of electric current moving between the two half-cells shows that 1.10 volts is being produced. In the cell shown on the right-hand side, the zinc half-cell has been substituted with a magnesium half-cell. Under the same conditions, the second cell is able to produce 2.62 volts. This difference is due to magnesium being more reactive and having a greater tendency to move electrons through the external circuit compared to the zinc half-cell.

Standard electrode potential

Each half-cell has a unique **standard electrode potential**, which is the amount of voltage it can produce at standard conditions. For these experiments, standard conditions refers to a temperature of 25°C (298 K), solvent concentrations of 1 M and a pressure of 100 kPa. As redox reactions involve both reduction and oxidation occurring simultaneously, it is not possible to measure the electrode potential of one half-cell without connecting it to another. Reduction occurs in one half-cell, while oxidation occurs simultaneously in the other. For this reason, a **standard hydrogen electrode** has been used to determine the comparative electrode potentials of other half-reactions – this is then referred to as their standard electrode potentials.

Standard electrode potential the amount of voltage that can be produced by a half-cell, with reference to the standard hydrogen electrode

Standard hydrogen electrode the hydrogen half-cell consisting of hydrogen gas, $H_2(g)$, and hydrogen ions, $H^+(aq)$. It is used as a reference against which the standard electrode potentials for all other half-cells are determined

The standard hydrogen electrode

The value of the standard electrode potential for different half-cells has been experimentally determined using the standard hydrogen electrode as a reference. To develop the scale, this half-cell was arbitrarily assigned an electrode potential of 0.00 volts under standard conditions. Other half-cells were then measured against the standard hydrogen electrode to

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determine their comparative values. In the standard hydrogen electrode, hydrogen gas, $H_2(g)$, is bubbled around an inert platinum electrode at a pressure of 100 kPa. As shown in Figure 3D–2, the electrode sits in an aqueous solution of 1 M $H^+(aq)$ ions. The reaction for the half-cell can be written as:

$$2H^+(aq) + 2e^- \rightleftharpoons H_2(g)$$

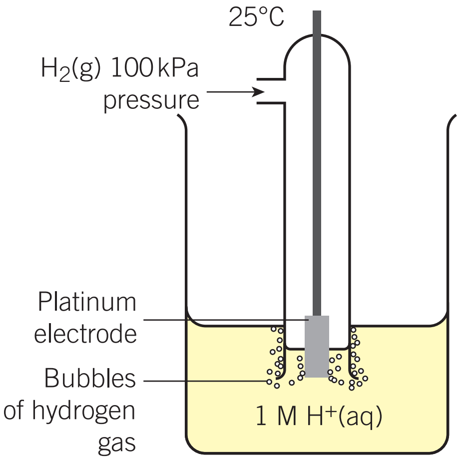

Figure 3D–2 The standard hydrogen electrode

The electrochemical series

Electrochemical series series of reduction half-cell reactions and their corresponding standard electrode potentials in order of strongest oxidising agent to weakest oxidising agent listed on the left-hand side

Standard cell potential the theoretical amount of voltage that a galvanic cell can produce under standard conditions; also referred to as electromotive force (emf)

The **electrochemical series** shown in Table 3D–1 on the opposite page is a list of *reduction* half-reactions in order of strongest oxidising agent to weakest oxidising agent, listed as the species on the *left-hand side* of the half-equation. It also includes the standard electrode potential for each reduction half-reaction. The most positive value is associated with the strongest oxidising agent, at the top of the table. The electrochemical series allows us to not only predict which reduction and oxidation reactions will occur in a galvanic cell, but also the magnitude of the voltage, or **standard cell potential**, that a particular galvanic cell can produce. This voltage may also be referred to as electromotive force, or emf, and is measured in volts.

Calculating cell potential

Consider the zinc–nickel galvanic cell shown on the right in Figure 3D–3. Oxidation is occurring in the zinc half-cell, while reduction is occurring in the nickel half-cell.

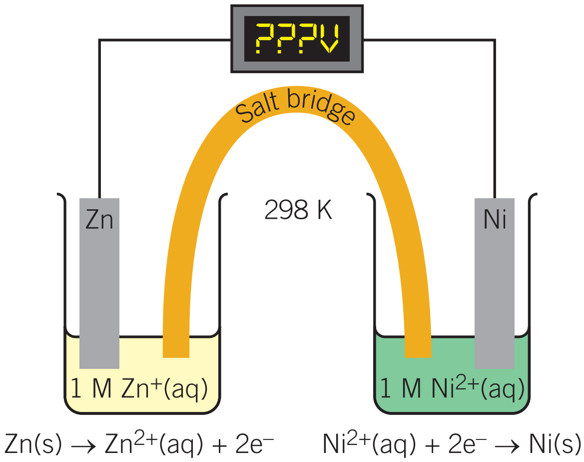

Figure 3D–3 A zinc–nickel cell

The two half-reactions occurring in the galvanic cell have been highlighted below in a small section of the electrochemical series. It is vital to remember that these are both represented as reduction reactions, and the electrode potential shown is the value for the forward *reduction* half-reaction. This will be the half-reaction listed *highest* on the electrochemical series. However, at the anode, oxidation is taking place, not reduction, so this half-reaction must be reversed. Whenever a reaction is reversed, the sign for the value of the standard electrode potential must also be reversed. The oxidation reaction will be the one listed *lowest* on the electrochemical series, as shown:

Reaction	Standard electrode potential (E^0) in volts at 25 °C
$Ni^{2+}(aq) + 2e^- \rightleftharpoons Ni(s)$	–0.25
$Zn^{2+}(aq) + 2e^- \rightleftharpoons Zn(s)$	–0.76

With the zinc half-cell reaction reversed, the reactions occurring in the zinc–nickel galvanic cell can be represented as follows:

Reduction at the cathode: $Ni^{2+}(aq) + 2e^- \rightarrow Ni(s)$ $E^0 = -0.25$ volts

Oxidation at the anode: $Zn(s) \rightarrow Zn^{2+}(aq) + 2e^-$ $E^0 = +0.76$ volts

Table 3D–1 The electrochemical series

Reaction	Standard electrode potential (E^0) in volts at 25°C
$F_2(g) + 2e^- \rightleftharpoons 2F^-(aq)$	+2.87
$H_2O_2(aq) + 2H^+(aq) + 2e^- \rightleftharpoons 2H_2O(l)$	+1.77
$Au^+(aq) + e^- \rightleftharpoons Au(s)$	+1.68
$Cl_2(g) + 2e^- \rightleftharpoons 2Cl^-(aq)$	+1.36
$O_2(g) + 4H^+(aq) + 4e^- \rightleftharpoons 2H_2O(1)$	+1.23
$Br_2(l) + 2e^- \rightleftharpoons 2Br^-(aq)$	+1.09
$Ag^+(aq) + e^- \rightleftharpoons Ag(s)$	+0.80
$Fe^{3+}(aq) + e^- \rightleftharpoons Fe^{2+}(aq)$	+0.77
$O_2(g) + 2H^+(aq) + 2e^- \rightleftharpoons H_2O_2(aq)$	+0.68
$I_2(s) + 2e^- \rightleftharpoons 2I^-(aq)$	+0.54
$O_2(g) + 2H_2O(l) + 4e^- \rightleftharpoons 4OH^-(aq)$	+0.40
$Cu^{2+}(aq) + 2e^- \rightleftharpoons Cu(s)$	+0.34
$Sn^{4+}(aq) + 2e^- \rightleftharpoons Sn^{2+}(aq)$	+0.15
$S(s) + 2H^+(aq) + 2e^- \rightleftharpoons H_2S(g)$	+0.14
$2H^+(aq) + 2e^- \rightleftharpoons H_2(g)$	0.00
$Pb^{2+}(aq) + 2e^- \rightleftharpoons Pb(s)$	–0.13
$Sn^{2+}(aq) + 2e^- \rightleftharpoons Sn(s)$	–0.14
$Ni^{2+}(aq) + 2e^- \rightleftharpoons Ni(s)$	–0.25
$Co^{2+}(aq) + 2e^- \rightleftharpoons Co(s)$	–0.28
$Cd^{2+}(aq) + 2e^- \rightleftharpoons Cd(s)$	–0.40
$Fe^{2+}(aq) + 2e^- \rightleftharpoons Fe(s)$	–0.44
$Zn^{2+}(aq) + 2e^- \rightleftharpoons Zn(s)$	–0.76
$2H_2O(l) + 2e^- \rightleftharpoons H_2(g) + 2OH^-(aq)$	–0.83
$Mn^{2+}(aq) + 2e^- \rightleftharpoons Mn(s)$	–1.18
$Al^{3+}(aq) + 3e^- \rightleftharpoons Al(s)$	–1.66
$Mg^{2+}(aq) + 2e^- \rightleftharpoons Mg(s)$	–2.37
$Na^+(aq) + e^- \rightleftharpoons Na(s)$	–2.71
$Ca^{2+}(aq) + 2e^- \rightleftharpoons Ca(s)$	–2.87
$K^+(aq) + e^- \rightleftharpoons K(s)$	–2.93
$Li^+(aq) + e^- \rightleftharpoons Li(s)$	–3.04

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NOTE

Strong reducing agents:
- are located towards the bottom and on the right-hand side of the electrochemical series.
- donate electrons more readily.
- have weak conjugate oxidising agents.
- usually undergo oxidation.

Strong oxidising agents:
- are located towards the top and on the left-hand side of the electrochemical series.
- accept electrons more readily.
- have weak conjugate reducing agents.
- usually undergo reduction.

To determine the overall cell potential, or voltage, that can be produced by the zinc–nickel cell from page 112 under standard conditions, simply *add* the two standard electrode potentials together:

$-0.25 + (+0.76) = +0.51$ volts

7A FEATURES OF ELECTROLYTIC CELLS LINK

A *positive* value obtained for the cell potential indicates that the reaction is *spontaneous*, which is expected in a galvanic cell. This is useful to remember when performing calculations of cell potentials. A negative value would mean that the electrochemical cell is an electrolytic cell, not a galvanic cell. Electrolytic cells are covered further in Section 7A.

NOTE

The values should *only* be added together if the half-equation and standard electrode potentials are reversed for the anode half-reaction.

A useful way to calculate the cell potential directly from the electrochemical series, without reversing equations and values, is to use the following rule:

$$E^0_{\text{cell}} = E^0_{\text{Reduction reaction}} - E^0_{\text{Oxidation reaction}}$$

In Figure 3D–3, notice that the reduction half-equation for nickel appears higher up in the electrochemical series, compared to the oxidation reaction for zinc. This will be true for *ALL* galvanic cells. This is another alternative way to remember which electrode potential should be subtracted from the other when calculating cell potentials in galvanic cells, as in the following rule:

$$E^0_{\text{cell}} = E^0_{\text{Higher half-reaction}} - E^0_{\text{Lower half-reaction}}$$

NOTE

As well as stressing the importance of always including units, it is essential to note that the value for cell potential is directional, and the positive or negative sign must always be written in front of the value to indicate this.

VIDEO WORKED EXAMPLE 3D–1

Worked example 3D–1: Calculating the standard cell potential for a galvanic cell

Calculate the standard cell potential for the galvanic cell consisting of a $Sn(s)/Sn^{2+}(aq)$ half-cell and a $Fe(s)/Fe^{2+}(aq)$ half-cell.

Solution

	Logic	Process
Step 1	Identify the two relevant half-reactions in the electrochemical series.	Referring to Table 3D–1: $Sn(s)/Sn^{2+}(aq)$: –0.14 $Fe(s)/Fe^{2+}(aq)$: –0.44
Step 2	Recall that the top reaction will proceed in the forwards direction, as reduction. The bottom reaction will occur in reverse, as oxidation. Substitute the values into the equation.	$E^0_{\text{cell}} = E^0_{\text{Reduction reaction}} - E^0_{\text{Oxidation reaction}}$ $E^0_{\text{cell}} = -0.14 - (-0.44) = +0.30$
Step 3	Write the cell potential value, making sure to include units (volts).	+0.30 volts

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Check-in questions – Set 1

1 Explain the difference between standard cell potential and standard electrode potential.

2 Using the electrochemical series shown below, identify which of the labelled species (in red text and with the asterisk next to them) is:

- a the strongest oxidising agent
- b the weakest oxidising agent
- c the strongest reducing agent
- d the weakest reducing agent.

	Reaction	Standard electrode potential (E^0) in volts at 25°C
	$F_2(g) + 2e^- \rightleftharpoons 2F^-(aq)$	+2.87
	$H_2O_2(aq) + 2H^+(aq) + 2e^- \rightleftharpoons 2H_2O(l)$	+1.77
*	$Au^+(aq) + e^- \rightleftharpoons Au(s)$	+1.68
	$Cl_2(g) + 2e^- \rightleftharpoons 2Cl^-(aq)$	+1.36
	$O_2(g) + 4H^+(aq) + 4e^- \rightleftharpoons 2H_2O(1)$	+1.23
	$Br_2(l) + 2e^- \rightleftharpoons 2Br^-(aq)$	+1.09
*	$Ag^+(aq) + e^- \rightleftharpoons Ag(s)$	+0.80
	$Fe^{3+}(aq) + e^- \rightleftharpoons Fe^{2+}(aq)$	+0.77
	$O_2(g) + 2H^+(aq) + 2e^- \rightleftharpoons H_2O_2(aq)$	+0.68
	$I_2(s) + 2e^- \rightleftharpoons 2I^-(aq)$	+0.54
	$O_2(g) + 2H_2O(l) + 4e^- \rightleftharpoons 4OH^-(aq)$	+0.40
*	$Cu^{2+}(aq) + 2e^- \rightleftharpoons Cu(s)$	+0.34
	$Sn^{4+}(aq) + 2e^- \rightleftharpoons Sn^{2+}(aq)$	+0.15
	$S(s) + 2H^+(aq) + 2e^- \rightleftharpoons H_2S(g)$	+0.14
	$2H^+(aq) + 2e^- \rightleftharpoons H_2(g)$	0.00
	$Pb^{2+}(aq) + 2e^- \rightleftharpoons Pb(s)$	–0.13

3 Calculate the standard cell potential using the electrochemical series for a galvanic cell consisting of $Au^+(aq)/Au(s)$ and $Ag^+(aq)/Ag(s)$ half-cells.

Predicting redox reactions in galvanic cells

The electrochemical series can be used to help identify whether a reaction will occur spontaneously. For a reaction to occur, the oxidising agent **must** be located *higher* on the left-hand side of the series, compared to the reducing agent, which **must** be located lower and on the right-hand side of the series. If the species are not positioned in this way, *no reaction* will occur.

Worked example 3D–2: Predicting whether a redox reaction will occur

VIDEO
WORKED
EXAMPLE 3D–2

Consider the following three equations that appear in the same order in the electrochemical series:

$$Pb^{2+}(aq) + 2e^- \rightleftharpoons Pb(s) \quad E^0 = -0.13V$$

$$Ni^{2+}(aq) + 2e^- \rightleftharpoons Ni(s) \quad E^0 = -0.25V$$

$$Cd^{2+}(aq) + 2e^- \rightleftharpoons Cd(s) \quad E^0 = -0.40V$$

Predict whether a reaction will occur between the following species.

- **a** $Pb^{2+}(aq)$ and $Cd(s)$
- **b** $Pb^{2+}(aq)$ and $Cd^{2+}(aq)$
- **c** $Ni^{2+}(aq)$ and $Pb(s)$

Solution

a $Pb^{2+}(aq)$ is the oxidising agent, as it is the species highest on the left-hand side and Cd(s) is the reducing agent, as it is located lower on the right-hand side. As such they will undergo a spontaneous reaction.

b No reaction will occur, since both species are oxidising agents and are both located on the left-hand side of the electrochemical series.

c No reaction will occur, since $Ni^{2+}(aq)$, as the oxidising agent on the left-hand side is lower than $Pb^{2+}(aq)$, which is the reducing agent, located higher on the right-hand side.

Identifying reactions using the electrochemical series

The half-equations occurring in a galvanic cell are not always provided. However, if all the species present are known, the electrochemical series can be used to identify the half-reactions occurring, to then determine the overall redox reaction and to calculate the cell potential for a given combination of reactants. On the electrochemical series, the species that is *highest on the left-hand side* of the electrochemical series will undergo reduction. The species that is *lowest on the right-hand side* will undergo oxidation, meaning the reaction on the electrochemical series for this half-reaction must be written in reverse.

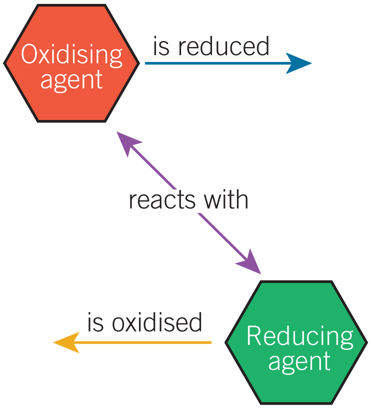

Figure 3D–4 On the electrochemical series, a spontaneous redox reaction takes place between the oxidising agent located higher on the left-hand side and the reducing agent located lower on the right-hand side.

VIDEO WORKED EXAMPLE 3D–3

Worked example 3D–3: Identifying reactions using the electrochemical series

Consider a galvanic cell consisting of a $Ag(s)/Ag^{+}(aq)$ half-cell and a $Pb(s)/Pb^{2+}(aq)$ half-cell.

a Identify the strongest reducing agent and oxidising agent.

b Write the half-reactions occurring at the anode and cathode.

c Calculate the standard cell potential.

d Write the overall equation for the cell.

Solution

	Logic	Process
Step 1	Use the electrochemical series to highlight the four species present.	$Ag^{+}(aq) + e^{-} \rightleftharpoons Ag(s) \quad E^{0} = +0.80$ $Pb^{2+}(aq) + 2e^{-} \rightleftharpoons Pb(s) \quad E^{0} = -0.13$
Step 2	The species highest on the left-hand side will be the strongest oxidising agent, and as such will undergo reduction. In this example, silver ions, Ag^{+} are the strongest oxidising agent. The species lowest on the right-hand side will be strongest reducing agent, and as such will undergo oxidation. In this example, solid lead, Pb(s) is the strongest reducing agent.	**a** Strongest oxidising agent: $Ag^{+}(aq)$ Strongest reducing agent: Pb(s)

Step 3	Write the equations for reduction and oxidation, remembering to reverse the oxidation reaction, which is the lower of the two. It is important to note the use of correct arrows when writing these half-equations. The electrochemical series represents each reduction half-equation with equilibrium arrows because it can be reversed, depending on what else it is reacting with. However, when writing half-equations for a particular cell, a critical part of what we are predicting is the direction in which these reactions will occur, and hence the use of a solid forward arrow is appropriate.	**b** $Ag^+(aq) + e^- \rightarrow Ag(s)$ $E^0 = +0.80$ $Pb(s) \rightarrow Pb^{2+}(aq) + 2e^-$ $E^0 = +0.13$
Step 4	To determine the cell potential, the values in Step 3 can be added, since the oxidation reaction and its standard electrode potential have been reversed. Alternatively, the values can be substituted straight into the following equation from the electrochemical series.	**c** $+0.80 + (+0.13) = +0.93$ volts $E^0_{cell} = E^0_{Reduction\ reaction} - E^0_{Oxidation\ reaction}$ $E^0_{cell} = +0.80 - (-0.13) = +0.93$ volts
Step 5	Write the overall equation by balancing electrons and combining the half-equations. In this example, there are two electrons in the oxidation half-equation but only one electron in the reduction half-equation, which consequently needs to be doubled. Now that the number of electrons is the same on each side, the electrons can be cancelled to leave the full redox equation.	$2 \times (Ag^+(aq) + e^- \rightarrow Ag(s))$ $2Ag^+(aq) + \cancel{2e^-} \rightarrow 2Ag(s)$ $Pb(s) \rightarrow Pb^{2+}(aq) + \cancel{2e^-}$ $2Ag^+(aq) + Pb(s) \rightarrow 2Ag(s) + Pb^{2+}(aq)$
Step 6	Add the cell potential value to the overall equation, making sure to include units (volts).	**d** $2Ag^+(aq) + Pb(s) \rightarrow 2Ag(s) + Pb^{2+}(aq)$ $E^0 = +0.93$ volts

NOTE

The standard electrode potential indicates the potential for a reaction to occur – it is never multiplied when calculating cell potentials.

Check-in questions – Set 2

1 Consider the four reactions highlighted in the electrochemical series:

Reaction	Standard electrode potential (E^0) in volts at 25°C
$Ni^{2+}(aq) + 2e^- \rightleftharpoons Ni(s)$	–0.25
$Fe^{2+}(aq) + 2e^- \rightleftharpoons Fe(s)$	–0.44
$Mn^{2+}(aq) + 2e^- \rightleftharpoons Mn(s)$	–1.18
$Mg^{2+}(aq) + 2e^- \rightleftharpoons Mg(s)$	–2.37

Predict whether a spontaneous reaction would occur between the following species.

- **a** $Mn^{2+}(aq)$ and $Mg(s)$
- **b** $Mg^{2+}(aq)$ and $Fe(s)$
- **c** $Ni^{2+}(aq)$ and $Mn(s)$
- **d** $Fe^{2+}(aq)$ and $Ni(s)$
- **e** $Fe(s)$ and $Mn(s)$

2 Consider a galvanic cell consisting of a $Co(s)/Co^{2+}(aq)$ half-cell and a $Al(s)/Al^{3+}(aq)$ half-cell.

- **a** Identify the strongest reducing agent and oxidising agent.
- **b** Write the half-reactions occurring at the anode and cathode.
- **c** Calculate the standard cell potential.
- **d** Write the overall equation for the cell.

Limitations of the electrochemical series

Recall that the electrochemical series was derived using standard laboratory conditions. This means that unpredictable things may occur when a galvanic cell is placed under conditions that vary significantly from SLC. Sometimes a different reaction may take place, or there may in fact be no reaction at all, even if a reaction is predicted to occur spontaneously. Changing the temperature from 25°C or using solutions that have a concentration different to 1 M, may result in different reactions taking place. The increased concentration of one particular ion may mean that it reacts instead of the ions predicted on the electrochemical series. This can be seen when the electrode potential values, E^0, are close together.

One final consideration is that the electrochemical series does not provide any indication of the *reaction rate*. Sometimes reactions may be predicted to occur, but they may do so very slowly. Sometimes reactions may be taking place at such a slow rate that they appear not to react, even though the electrochemical series predicts that a reaction is taking place. For example, observing a galvanic cell for 20 minutes may not be sufficient time to observe products of reactions being formed or other changes expected in the half-cells. You will study rates of reaction more in Section 5B.

5B FACTORS AFFECTING REACTION RATE LINK

Sometimes, as well as the same species appearing in multiple positions on the electrochemical series, some half-reactions may also include *multiple* species. Two examples of this are shown below where there are hydrogen ions, $H^+(aq)$ shown as part of the half-reaction. This indicates that for the reaction to proceed, there must also be a suitable supply of hydrogen ions, which would usually mean using an acidic solution. It is important to consider all species when predicting whether reactions will occur, but also when predicting what the products of a particular galvanic cell may be. Measuring pH changes or using acid–base indicators may be one additional way to detect whether a reaction is taking place.

UNIT 2 LINK

Table 3D–2 Examples of half-reactions with multiple species

Reaction	Standard electrode potential (E^0) in volts at 25°C
$H_2O_2(aq) + 2H^+(aq) + 2e^- \rightleftharpoons 2H_2O(l)$	+1.77
$O_2(g) + 4H^+(aq) + 4e^- \rightleftharpoons 2H_2O(l)$	+1.23

3D SKILLS

Predicting reactions with more than one type of ion present

VIDEO 3D–1
SKILLS: PREDICTING REACTIONS WITH MORE THAN ONE TYPE OF ION PRESENT

In some galvanic cells, electrodes can be inert, in which case they are not considered when trying to predict the reactions occurring. Similarly, solutions in each half-cell may contain more than one type of reactive ion. In such cases, it is important to remember redox reactions will only occur between the *strongest* oxidising agent in the reduction half-cell and the *strongest* reducing agent in the oxidation half-cell. If there are many ion species present, only two will react, and the rest will be considered to be spectator ions.

Some species appear more than once on the electrochemical series on both the left-hand side and right-hand side of the series. When predicting reactions, all occurrences of each species must be considered to accurately identify the strongest reducing agent and strongest oxidising agent.

Further consideration should also be given regarding what would happen in a galvanic cell where one of these ions is completely used up by the reaction. If one completely reacts, the next strongest species will start to react, provided there is another species available. There would be a decrease in the amount of voltage produced, but it is important to recognise that whenever other species are present, the reaction may not simply 'stop'.

The example below highlights a type of question where more than one type of ion is present, as well as the worked solution for this example.

Question

A galvanic cell consists of one half-cell with an inert platinum, Pt(s), electrode in a 1 M solution of $Cu^{2+}(aq)$, $Zn^{2+}(aq)$ and $Ni^{2+}(aq)$ ions. The other half-cell has a solid iron electrode, Fe(s), in a 1 M solution containing iron(II) ions, $Fe^{2+}(aq)$.

a Identify the strongest reducing agent and oxidising agent.
b State which electrode is the anode, and which is the cathode.
c Write the half-reactions occurring **initially** at the anode and cathode.
d Calculate the standard cell potential.
e Explain what you would expect to observe at the cathode over time.

Solution

<table>
<tr><th></th><th>Logic</th><th>Process</th></tr>
<tr><td>Step 1</td><td>Use the electrochemical series to highlight all the reactive species present. It is often useful to highlight the species present in one half-cell differently from those in the other. This can make it easier to identify the reduction and oxidation reactions that will take place.
The species highest on the left-hand side of a reaction arrow will be the strongest oxidising agent.
The species lowest on the right-hand side of a reaction arrow will be the strongest reducing agent.</td><td>
<table>
<tr><td>$Ag^+(aq) + e^- \rightleftharpoons Ag(s)$</td><td>+0.80</td><td>$Pb^{2+}(aq) + 2e^- \rightleftharpoons Pb(s)$</td><td>–0.13</td></tr>
<tr><td>$Fe^{3+}(aq) + e^- \rightleftharpoons Fe^{2+}(aq)$</td><td>+0.77</td><td>$Sn^{2+}(aq) + 2e^- \rightleftharpoons Sn(s)$</td><td>–0.14</td></tr>
<tr><td>$O_2(g) + 2H^+(aq) + 2e^- \rightleftharpoons H_2O_2(aq)$</td><td>+0.68</td><td>$Ni^{2+}(aq) + 2e^- \rightleftharpoons Ni(s)$</td><td>–0.25</td></tr>
<tr><td>$I_2(s) + 2e^- \rightleftharpoons 2I^-(aq)$</td><td>+0.54</td><td>$Co^{2+}(aq) + 2e^- \rightleftharpoons Co(s)$</td><td>–0.28</td></tr>
<tr><td>$O_2(g) + 2H_2O(l) + 4e^- \rightleftharpoons 4OH^-(aq)$</td><td>+0.40</td><td>$Cd^{2+}(aq) + 2e^- \rightleftharpoons Cd(s)$</td><td>–0.40</td></tr>
<tr><td>$Cu^{2+}(aq) + 2e^- \rightleftharpoons Cu(s)$</td><td>+0.34</td><td>$Fe^{2+}(aq) + 2e^- \rightleftharpoons Fe(s)$</td><td>–0.44</td></tr>
<tr><td>$Sn^{4+}(aq) + 2e^- \rightleftharpoons Sn^{2+}(aq)$</td><td>+0.15</td><td>$Zn^{2+}(aq) + 2e^- \rightleftharpoons Zn(s)$</td><td>–0.76</td></tr>
<tr><td>$S(s) + 2H^+(aq) + 2e^- \rightleftharpoons H_2S(g)$</td><td>+0.14</td><td>$2H_2O(l) + 2e^- \rightleftharpoons H_2(g) + 2OH^-(aq)$</td><td>–0.83</td></tr>
<tr><td>$2H^+(aq) + 2e^- \rightleftharpoons H_2(g)$</td><td>0.00</td><td></td><td></td></tr>
</table>
a strongest oxidising agent: $Cu^{2+}(aq)$
strongest reducing agent: Fe(s)</td></tr>
</table>

Step 2	To identify the cathode, apply the 'happy red cat'. Given that the iron electrode is the strongest reducing agent, undergoing oxidation, it must be the anode. Therefore, the strongest oxidising agent, copper ions undergo reduction in the other half-cell, where platinum is the electrode, the cathode must be platinum.	**b** Anode: Fe(s) Cathode: Pt(s)
Step 3	Having identified the strongest oxidising agent, $Cu^{2+}(aq)$ and strongest reducing agent, Fe(s), use the electrochemical series to write the equations for each species, remembering to reverse the oxidation reaction, being the lower of the two.	**c** Reduction: $Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)$ Oxidation: $Fe(s) \rightarrow Fe^{2+}(aq) + 2e^-$
Step 4	Substitute the values straight into the following equation from the electrochemical series.	**d** $E^0_{cell} = E^0_{\text{Reduction reaction}} - E^0_{\text{Oxidation reaction}}$ $E^0_{cell} = +0.34 - (-0.44) = +0.78$ volts
Step 5	Write your explanation of what you would expect, given the cell potential.	**e** At the cathode: Initially copper ions, $Cu^{2+}(aq)$ would be reduced to solid copper, Cu(s). This would appear as a thin coating on the surface of the platinum electrode. The mass of the electrode would be increasing. Over time, all the copper ions may react. At this point, the next strongest oxidising agent present in the half-cell solution would be nickel ions, $Ni^{2+}(aq)$, which would be reduced to solid nickel, Ni(s). This would create another thin layer on the platinum electrode, over the top of the copper layer and would result in a further increase in mass of the electrode. During this time, the cell potential would be reduced to +0.19 volts. $E^0_{cell} = -0.25 - (-0.44) = +0.19$ volts

Once all of the nickel ions have reacted, the reaction would cease to produce any electrical energy since the remaining ions at the cathode are zinc ions, $Zn^{2+}(aq)$, and these occur lower on the electrochemical series than the strongest reducing agent, which is still Fe(s).

Section 3D questions

1 A galvanic cell consists of $Cu^{2+}(aq)/Cu(s)$ and $Sn^{2+}(aq)/Sn(s)$ half-cells.
  - a Write the reduction and oxidation half-equations.
  - b Write the overall cell equation.
  - c Calculate the standard cell potential.
  - d Identify which half-cell is the cathode, and which is the anode.

2 Draw a labelled diagram of a galvanic cell made from a hydrogen half-cell, $H^+(aq)/H_2(g)$ and a zinc half-cell, $Zn^{2+}(aq)/Zn(s)$ with a salt bridge soaked in KNO_3. Include:
   - a half-reactions for each half-cell
   - b anode and cathode
   - c polarity of each electrode
   - d direction of electron flow
   - e direction of cation and anion flow
   - f overall reaction
   - g cell potential.

3 State whether the following reactions would take place. For those where there is a reaction, write the balanced equation.
   - a silver ions, $Ag^+(aq)$, being mixed into a 1 M solution of hydrogen peroxide, H_2O_2
   - b copper ions, $Cu^{2+}(aq)$, being mixed into a 1 M solution of hydrogen peroxide, H_2O_2
   - c chlorine gas, $Cl_2(g)$, being bubbled through a 1 M solution of hydrogen peroxide, H_2O_2
   - d solid copper placed into a 1 M solution of hydrogen peroxide, H_2O_2.

4 A galvanic cell consists of one half-cell with an inert carbon C(s) electrode with a 1 M solution of $Pb^{2+}(aq)$, $Sn^{2+}(aq)$ and $Co^{2+}(aq)$ ions. The other half-cell has a solid zinc electrode, Zn(s), in a 1 M solution containing zinc ions, $Zn^{2+}(aq)$.
   - a Identify the strongest reducing agent and oxidising agent.
   - b State which electrode is the anode, and which is the cathode.
   - c Write the half-reactions occurring initially at the anode and cathode.
   - d Calculate the standard cell potential.
   - e Explain what you would expect to observe at the cathode over time.

5 A student uses the electrochemical series to create a galvanic cell in their school laboratory that is predicted to undergo a spontaneous reaction. Suggest two reasons why they may not observe any changes, even after several minutes.

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Chapter 3 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
3A.1	Define ‘redox’ in terms of reduction, oxidation and electron transfer	18☐
3A.2	Explain what a redox reaction involves	18☐
3A.3	Define and identify ‘reducing agent’ and ‘oxidising agent’	18☐
3A.4	Assign oxidation numbers to elements in compounds and ions in chemical equations and use these numbers to identify reactions as redox	18☐
3A.5	Use oxidation numbers to identify conjugate redox pairs	18☐
3B.1	Write and balance simple and complex half-equations for oxidation and reduction reactions	18☐
3B.2	Write and balance overall redox equations, including states, in acidic conditions	19☐
3B.3	Write and balance overall redox equations, including states, in basic conditions	19☐
3B.4	Write and balance half-equations by identifying redox couples in overall equations	18☐
3C.1	Recall and explain the importance of the key design features of galvanic cells	11☐
3C.2	Identify, name, draw and label features of galvanic cells	6☐, 13☐
3C.3	Identify the chemical processes involved in primary galvanic cells, including the type of redox reaction occurring at each electrode	1☐
3C.4	Identify the direction of electron flow and ion flow in galvanic cells	2☐, 7☐
3C.5	Write the half-equation for the reaction occurring at each electrode in a galvanic cell	16☐
3C.6	Write the overall equation for a galvanic cell	17☐
3C.7	Describe the importance of separating two half-cells to facilitate the transformation of chemical energy to electrical energy in a galvanic cell	12☐
3C.8	Explain the role of inert and reactive electrodes and electrolyte solutions in the reactions taking place in a galvanic cell	14☐
3D.1	Apply information presented in the electrochemical series to questions	8☐, 14☐

3D.2	Predict whether certain combinations of reactants will produce electrical energy in a galvanic cell	3☐, 4☐
3D.3	Compare the relative strengths of reducing agents and oxidising agents	10☐
3D.4	Predict the products, and therefore the overall equation, of a redox reaction in a galvanic cell	8☐
3D.5	Use the electrochemical series to calculate the maximum cell voltage generated under standard laboratory conditions	5☐, 9☐, 15☐

Multiple-choice questions

1 Identify the correct statement. In a galvanic cell

- **A** cations flow from the salt bridge to the anode.
- **B** electrons are produced at the cathode.
- **C** oxidation occurs at the cathode.
- **D** chemical energy is converted to electrical energy.

2 Identify the incorrect statement. In a galvanic cell

- **A** reduction occurs at the cathode.
- **B** cations flow from the salt bridge to the cathode.
- **C** electrons flow from the cathode to the anode.
- **D** the polarity of the anode is negative.

3 Which of the following combinations would **not** react?

- **A** cadmium ions, $Cd^{2+}(aq)$, and solid iron, $Fe(s)$
- **B** calcium ions, $Ca^{2+}(aq)$, and solid iron, $Fe(s)$
- **C** cobalt ions, $Co^{2+}(aq)$, and solid iron, $Fe(s)$
- **D** copper ions, $Cu^{2+}(aq)$, and solid iron, $Fe(s)$

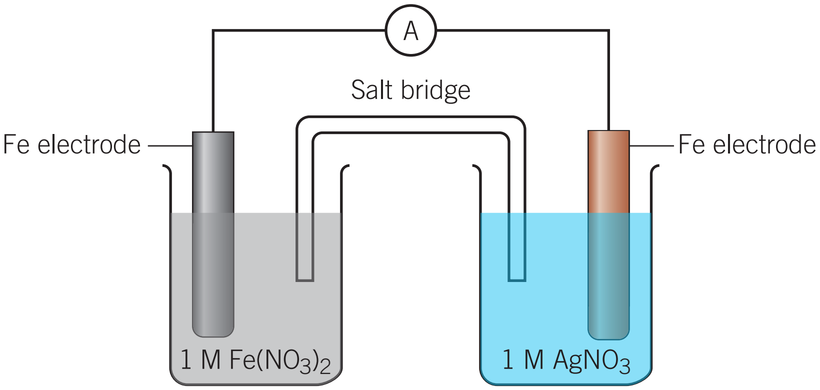
4 Identify which one of the following would react with solid iron, $Fe(s)$, but **not** react with solid lead, $Pb(s)$.

- **A** nickel ions, $Ni^{2+}(aq)$
- **B** aluminium ions, $Al^{3+}(aq)$
- **C** copper ions, $Cu^{2+}(aq)$
- **D** chlorine gas, $Cl_2(g)$

5 What is the standard cell potential when an iron half-cell ($Fe^{3+}(aq)/Fe^{2+}(aq)$) is connected to a chlorine half-cell ($Cl_2(g)/Cl^-(aq)$)?

- **A** –0.59 volts
- **B** +2.13 volts
- **C** +0.59 volts
- **D** +0.18 volts

6 Select the correct statement for the galvanic cell shown below.



A Electrons flow from the Ag electrode to the Fe electrode.

B The mass of the Ag electrode increases.

C The Ag electrode will be the anode.

D The polarity of the Fe electrode is positive.

7 In a galvanic cell, the flow of electrons is from the

A reducing agent to the oxidising agent through the salt bridge.

B oxidising agent to the reducing agent through the salt bridge.

C anode to the cathode through the external circuit.

D cathode to the anode through the external circuit.

8 Some galvanic cells are made using four half-cells (W/W^{2+}, X/X^{2+}, Y/Y^{2+} and Z/Z^{2+}) set up under standard conditions. Using the information about the combinations shown, what is the order of cell potential, E^0, in order from highest to lowest?

$X(s) + W^{2+}(aq) \rightarrow X^{2+}(aq) + W(s)$

$Z(s) + X^{2+}(aq) \rightarrow$ No Reaction

$Y(s) + Z^{2+}(aq) \rightarrow$ No Reaction

$W(s) + Z^{2+}(aq) \rightarrow W^{2+}(aq) + Z(s)$

A $Y > Z > W > X$

B $X > Z > W > Y$

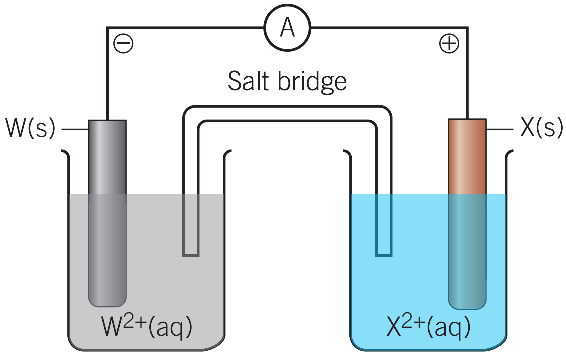
C $Y > W > Z > X$

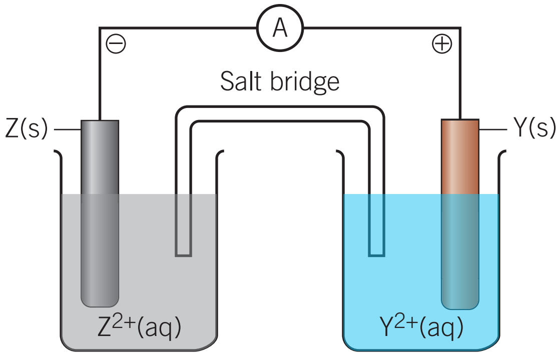
D $X > W > Z > Y$

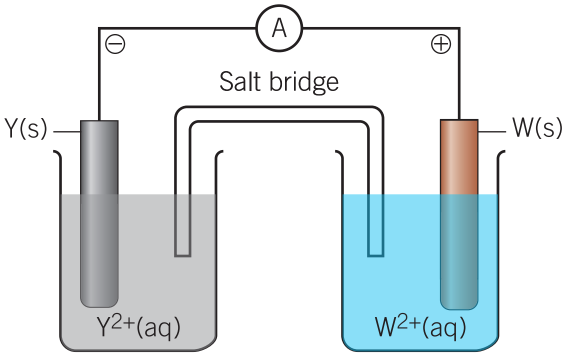
9 A galvanic cell potential consists of two connected half-cells. Identify which combination below would be expected to result in a cell potential of 1.08 V.

A	Ni electrode with $Ni(NO_3)_2$	Al electrode with $Al(NO_3)_3$
B	Al electrode with $Al(NO_3)_3$	Ag electrode with $AgNO_3$
C	Co electrode with $Co(NO_3)_2$	Ag electrode with $AgNO_3$
D	Ni electrode with $Ni(NO_3)_2$	Co electrode with $Co(NO_3)_2$

10 The diagrams below show combinations of galvanic cells made from four half-cells (W/W^{2+}, X/X^{2+}, Y/Y^{2+} and Z/Z^{2+}) set up under standard conditions. Use the polarity of each electrode shown to identify the order of half-cells, from highest E^0 value to the lowest.







A W^{2+}/W, X^{2+}/X, Y^{2+}/Y, Z^{2+}/Z

B X^{2+}/X, W^{2+}/W, Y^{2+}/Y, Z^{2+}/Z

C Z^{2+}/Z, Y^{2+}/Y, X^{2+}/X, W^{2+}/W

D X^{2+}/X, Y^{2+}/Y, Z^{2+}/Z, W^{2+}/W

Short-answer questions

11 Explain the difference between the internal and external circuit of a galvanic cell. (2 marks)

12 In a galvanic cell, one of the key design features is the separation of half-cells.

a Explain the importance of this separation in terms of energy conversions. (2 marks)

b Explain the role of the salt bridge in allowing for the separation of half-cells. (2 marks)

13 Draw a diagram of the galvanic cell containing a chlorine half-cell ($Cl_2(g)/Cl^-(aq)$) and a copper half-cell ($Cu^{2+}(aq)/Cu(s)$). Chlorine gas is supplied to the electrode.

a On your diagram, label the following: (6 marks)

- anode and cathode
- polarity of each electrode
- direction of electron flow
- direction of ion flow from the salt bridge (assuming KCl is the electrolyte).

b Write the half-reaction occurring at the anode and cathode. (2 marks)

c Write the overall equation. (1 mark)

d Calculate the cell potential. (1 mark)

14 Zinc strips are placed into 1 M solutions of $Cu(NO_3)_2$, $Al(NO_3)_3$, $Pb(NO_3)_2$ and $Mg(NO_3)_2$. Using the electrochemical series, predict which solutions would result in a different metal coating being deposited on the surface of the zinc strip. (2 marks)

$Cu^{2+}(aq) + 2e^- \rightleftharpoons Cu(s)$	+0.34
$Sn^{4+}(aq) + 2e^- \rightleftharpoons Sn^{2+}(aq)$	+0.15
$S(s) + 2H^+(aq) + 2e^- \rightleftharpoons H_2S(g)$	+0.14
$2H^+(aq) + 2e^- \rightleftharpoons H_2(g)$	0.00
$Pb^{2+}(aq) + 2e^- \rightleftharpoons Pb(s)$	–0.13
$Sn^{2+}(aq) + 2e^- \rightleftharpoons Sn(s)$	–0.14
$Ni^{2+}(aq) + 2e^- \rightleftharpoons Ni(s)$	–0.25
$Co^{2+}(aq) + 2e^- \rightleftharpoons Co(s)$	–0.28

$Cd^{2+}(aq) + 2e^- \rightleftharpoons Cd(s)$	–0.40
$Fe^{2+}(aq) + 2e^- \rightleftharpoons Fe(s)$	–0.44
$Zn^{2+}(aq) + 2e^- \rightleftharpoons Zn(s)$	–0.76
$2H_2O(l) + 2e^- \rightleftharpoons H_2(g) + 2OH^-(aq)$	–0.83
$Mn^{2+}(aq) + 2e^- \rightleftharpoons Mn(s)$	–1.18
$Al^{3+}(aq) + 3e^- \rightleftharpoons Al(s)$	–1.66
$Mg^{2+}(aq) + 2e^- \rightleftharpoons Mg(s)$	–2.37

15 Consider the different combinations of four unknown species, W, X, Y and Z, and their respective ions shown in the three equations below.

$X^{2+}(aq) + Y(s) \rightarrow Y^{2+}(aq) + X(s)$

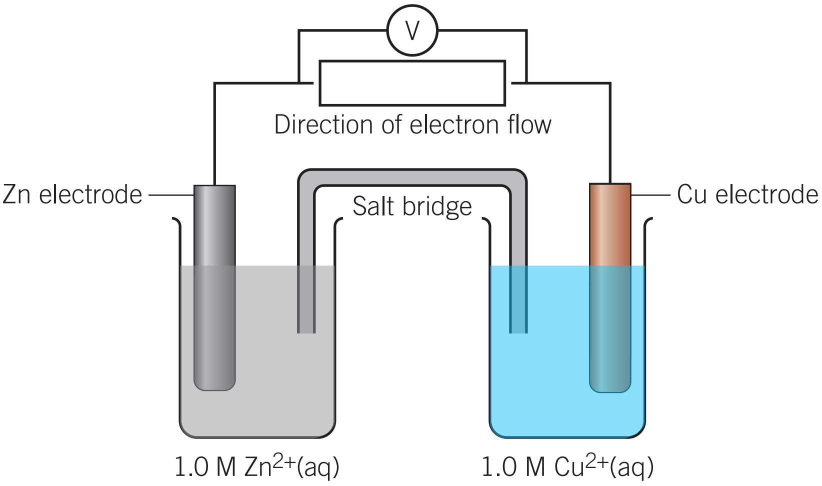
$W^{2+}(aq) + X(s) \rightarrow W(s) + X^{2+}(aq)$

$Z^{2+}(aq) + W(s) \rightarrow Z(s) + W^{2+}(aq)$

a Identify the relative position of each species on the electrochemical series ordering them from highest E^0 value to lowest. (3 marks)

b State which of the species listed is the strongest reducing agent and which is the strongest oxidising agent. (2 marks)

16 A representation of the Daniell cell is shown below.



a State two features of this cell that allow chemical energy to be converted to usable electrical energy. (2 marks)

b State the polarity of each electrode. (1 mark)

c State which electrode is the cathode. (1 mark)

d Write the half-equation for the reaction occurring at the cathode. (1 mark)

e State the direction of electron flow. (1 mark)

f The electrolyte used in the salt bridge is KNO_3. State which ion would migrate to the anode. (1 mark)

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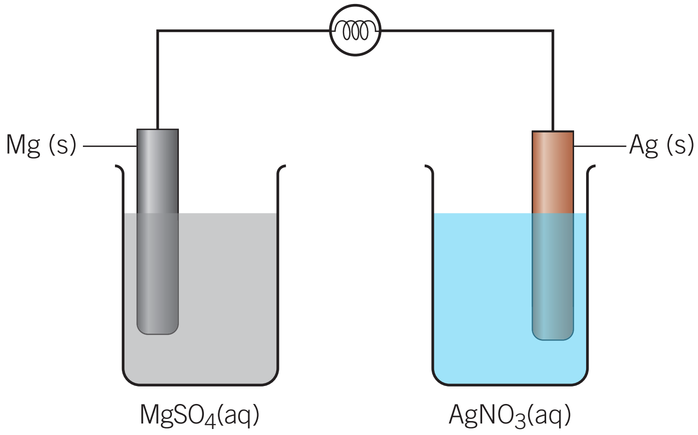
g Calculate the cell potential using the electrochemical series. (1 mark)

h List two visible changes that you expect to observe after the cell has been operating for some time. (2 marks)

17 The diagram below shows an incomplete galvanic cell.



a Identify the missing component in this cell diagram. (1 mark)

b Determine whether electrons travel towards the magnesium or silver electrode. (1 mark)

c Write the half-equations occurring in each half-cell. (2 marks)

d Write the overall reaction occurring in the cell. (2 marks)

e Calculate the standard cell potential. (1 mark)

18 Look at the following reaction between iron(III) oxide and carbon monoxide:

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

a Rewrite the reaction above in your workbook, then assign oxidation numbers to each of the elements present in the reaction. (1 mark)

b Using the terms 'redox', 'reduction', 'oxidation' and 'electron transfer', explain why this reaction is an example of a redox reaction. (4 marks)

c Identify both the reducing agent and oxidising agent in this reaction. (2 marks)

d Write balanced half-equations for the reduction and oxidation reactions occurring. (2 marks)

19 The following chemical equation shows the redox reaction between solutions of sulfite ions and permanganate ions.

$$SO_3^{2-}(aq) + MnO_4^{-}(aq) \rightarrow SO_4^{2-}(aq) + Mn^{2+}(aq)$$

a Write the half-equations and the balanced overall equation for this redox reaction under **acidic** conditions. (3 marks)

b Write the reduction half-equation for the conversion of permanganate ions into manganese ions under **alkaline (basic)** conditions. (1 mark)

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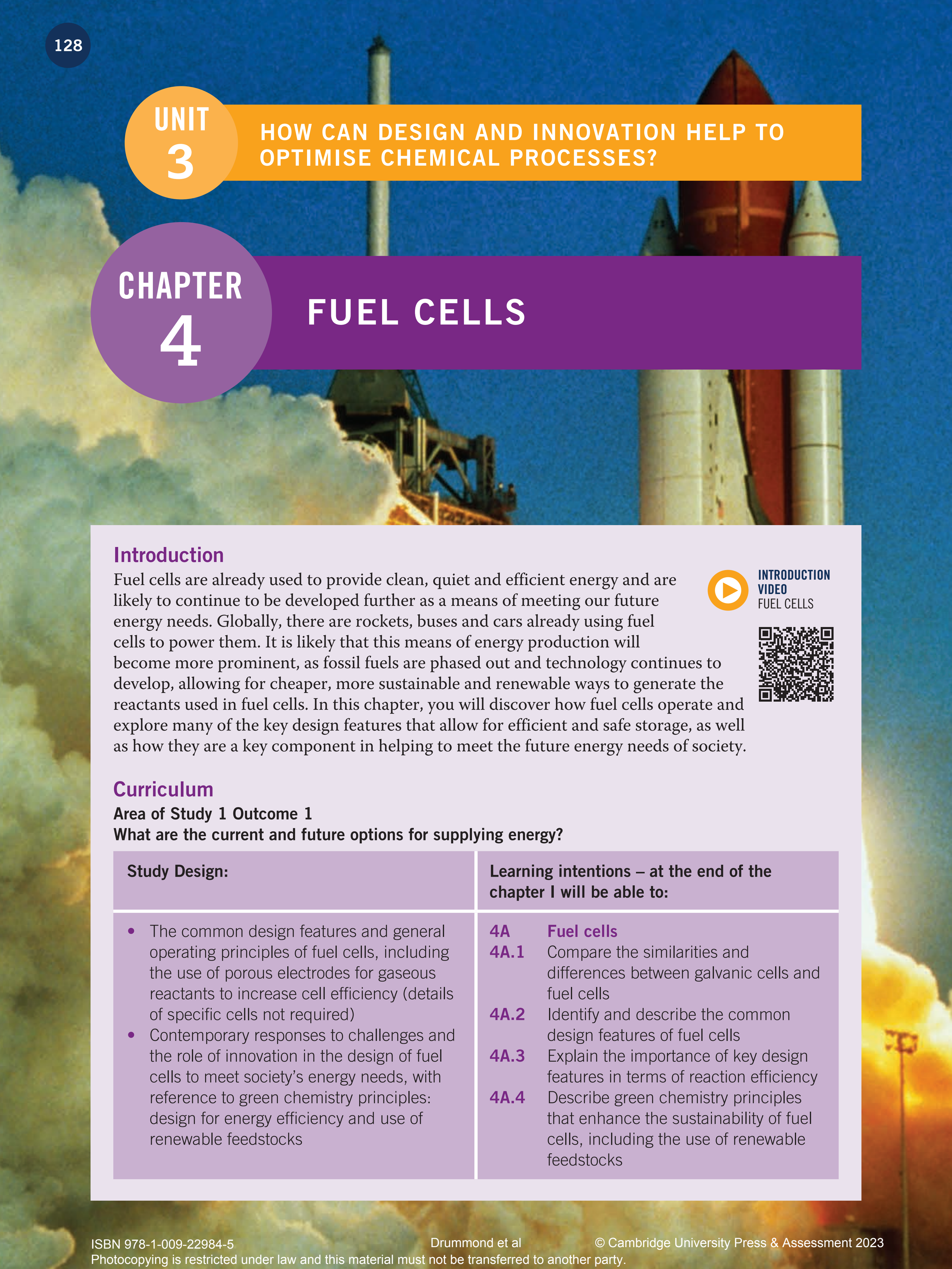

UNIT 3
HOW CAN DESIGN AND INNOVATION HELP TO OPTIMISE CHEMICAL PROCESSES?

CHAPTER 4
FUEL CELLS

Introduction

Fuel cells are already used to provide clean, quiet and efficient energy and are likely to continue to be developed further as a means of meeting our future energy needs. Globally, there are rockets, buses and cars already using fuel cells to power them. It is likely that this means of energy production will become more prominent, as fossil fuels are phased out and technology continues to develop, allowing for cheaper, more sustainable and renewable ways to generate the reactants used in fuel cells. In this chapter, you will discover how fuel cells operate and explore many of the key design features that allow for efficient and safe storage, as well as how they are a key component in helping to meet the future energy needs of society.

INTRODUCTION VIDEO
FUEL CELLS

Curriculum

Area of Study 1 Outcome 1
What are the current and future options for supplying energy?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• The common design features and general operating principles of fuel cells, including the use of porous electrodes for gaseous reactants to increase cell efficiency (details of specific cells not required) • Contemporary responses to challenges and the role of innovation in the design of fuel cells to meet society's energy needs, with reference to green chemistry principles: design for energy efficiency and use of renewable feedstocks	**4A Fuel cells** **4A.1** Compare the similarities and differences between galvanic cells and fuel cells **4A.2** Identify and describe the common design features of fuel cells **4A.3** Explain the importance of key design features in terms of reaction efficiency **4A.4** Describe green chemistry principles that enhance the sustainability of fuel cells, including the use of renewable feedstocks

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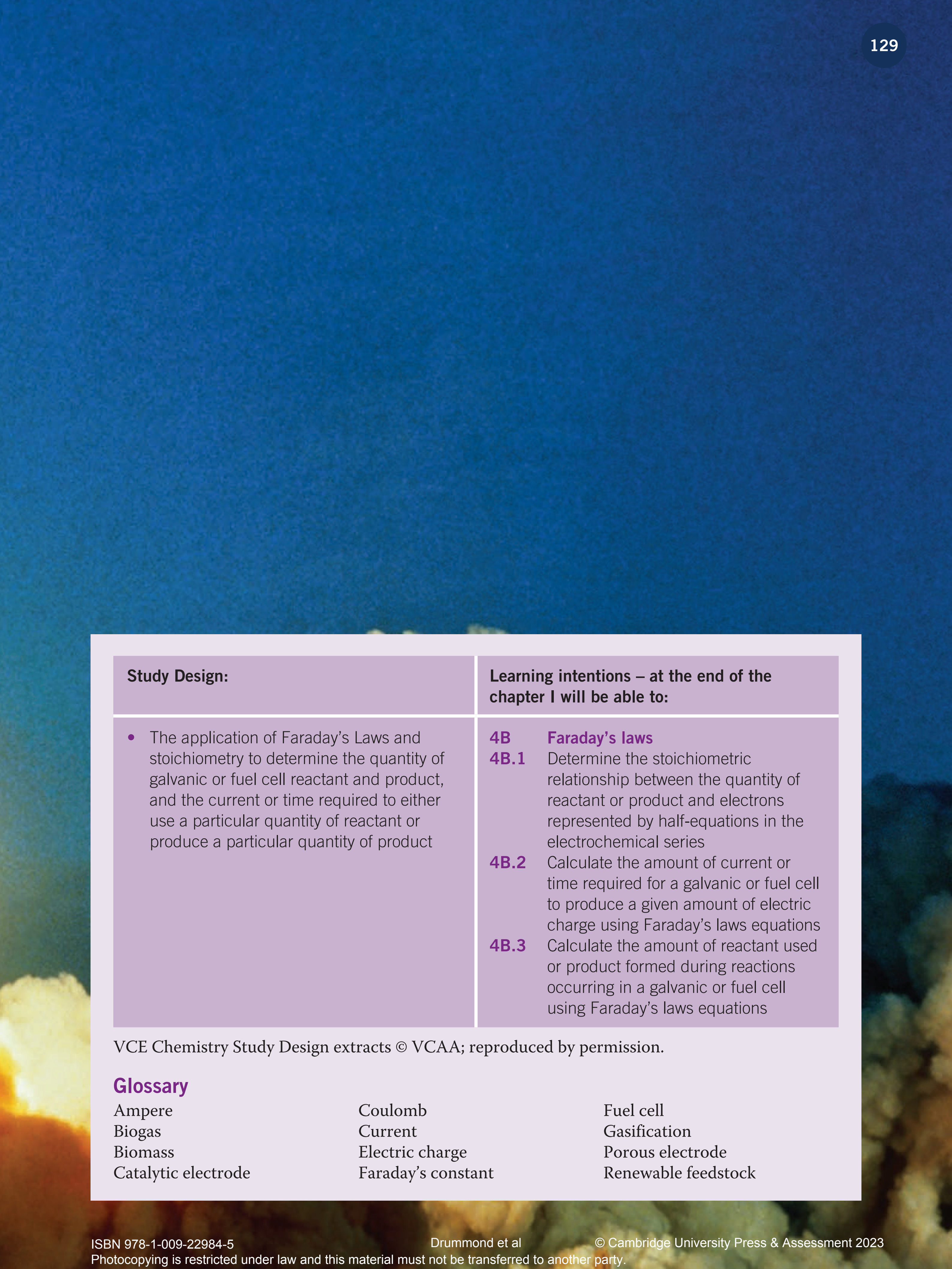

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• The application of Faraday's Laws and stoichiometry to determine the quantity of galvanic or fuel cell reactant and product, and the current or time required to either use a particular quantity of reactant or produce a particular quantity of product	**4B Faraday's laws** **4B.1** Determine the stoichiometric relationship between the quantity of reactant or product and electrons represented by half-equations in the electrochemical series **4B.2** Calculate the amount of current or time required for a galvanic or fuel cell to produce a given amount of electric charge using Faraday's laws equations **4B.3** Calculate the amount of reactant used or product formed during reactions occurring in a galvanic or fuel cell using Faraday's laws equations

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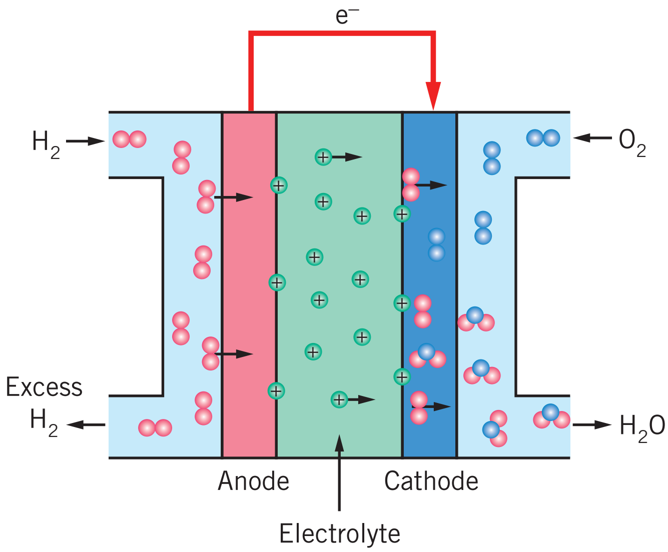
Glossary

Ampere
Biogas
Biomass
Catalytic electrode
Coulomb
Current
Electric charge
Faraday's constant
Fuel cell
Gasification
Porous electrode
Renewable feedstock

Concept map

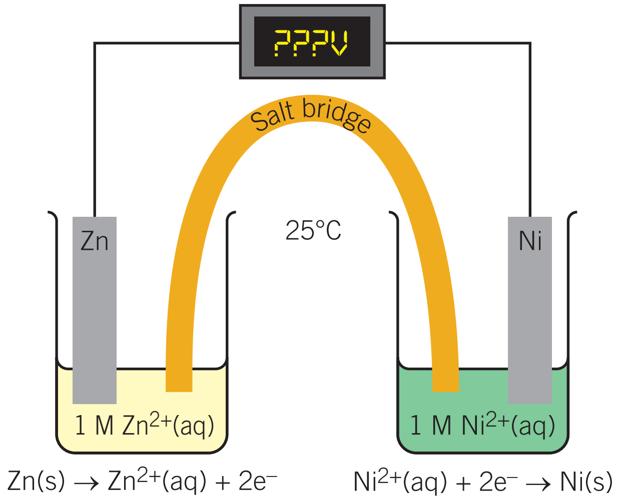
4A Fuel cells

Features of fuel cells and sustainability and environmental considerations



4B Faraday's laws

Calculations of quantities using these laws and stoichiometry



See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

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4A Fuel cells

Study Design:

- The common design features and general operating principles of fuel cells, including the use of porous electrodes for gaseous reactants to increase cell efficiency (details of specific cells not required)
- Contemporary responses to challenges and the role of innovation in the design of fuel cells to meet society's energy needs, with reference to green chemistry principles: design for energy efficiency and use of renewable feedstocks

Glossary:

Biogas
Biomass
Catalytic electrode
Fuel cell
Gasification
Porous electrode
Renewable feedstock

ENGAGE

Fuel cell electric vehicles

Electric cars are becoming more and more common, such as those made by Tesla. Tesla make battery-powered vehicles, in which the battery stores up energy (via charging) that is then used to power the electric motor. Another type of electric car is also available: the fuel cell electric vehicle (FCEV). In FCEVs, such as the Toyota Mirai and Hyundai Nexo, hydrogen and oxygen combine in the fuel cell to generate electricity. Compared to batteries, which take considerable time to charge, FCEVs can be refuelled in less than four minutes. They can also travel further on average than battery-powered vehicles, which is often one of the main reasons people are reluctant to switch to electric cars.

So why are FCEVs so much less popular? One of the biggest problems is that of infrastructure. While hydrogen fuel cells have had plenty of success in powering non-consumer engines, such as those of space shuttles and aircraft, their use in daily life is limited by the need for vehicle refuelling stations to be common and easily accessible. Currently, it is simply too costly and difficult to implement such infrastructure compared to battery-charging stations. If hydrogen could be more readily available, and sourced renewably, FCEVs could become much more common.

Figure 4A–1 A hydrogen fuel cell sign on a car (left); a hydrogen refuelling station (right)

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EXPLAIN

Fuel cells

3C
FEATURES OF GALVANIC CELLS
LINK

Fuel cell
a type of electrochemical cell that produces electrical energy from chemical energy, requiring a continuous supply of reactants

7C
COMMERCIAL ELECTROLYTIC CELLS
LINK

Fuel cells work in a similar way to other types of galvanic cells (which were discussed in Section 3C), using spontaneous reactions to convert chemical energy into electrical energy. Unlike primary galvanic cells, which eventually reach a state of equilibrium and no longer produce electrical energy, fuel cells are a type of galvanic cell that *do not* store the reactants in the cell. Instead, the reactants must be supplied from an external source. The huge advantage of this is that the fuel cells are able to produce a *continuous* supply of electricity, provided the supply of reactants into the cell is maintained. As well as this, they do not require recharging like secondary cells do.

There are many different types of fuel cell, including the hydrogen-fuelled polymer electrolyte membrane (also known as a proton exchange membrane or PEM) fuel cell, methanol fuel cells, alkaline fuel cells (such as potassium hydroxide cells), phosphoric acid fuel cells and solid oxide fuel cells. Regardless of the type of fuel cell, they share many advantages, such as:

- They have higher efficiency than coal-fired power stations or combustion car engines. This is because they directly convert chemical energy into electrical energy, rather than relying on a number of energy transformation steps, which ultimately result in a decrease in efficiency.
- They are relatively quiet when operating and the products of the reactions are generally more environmentally friendly.
- Unlike other galvanic cells, the fuels used are not stored in the cell itself and so must be generated and supplied from an external source. However, provided that there is a constant supply of reactants, fuel cells are able to sustain long-term continuous energy production (without needing to be recharged or replaced regularly).
- Catalysts and modifications to electrode design can be used to increase the rate of reaction.
- Fuel cells are portable. Although they can’t necessarily be packaged into small battery-sized compartments, their ability to produce electricity directly where it is needed makes them suitable for use in vehicles, including space shuttles.
- There are a range of reactants that are suitable for use in fuel cells.
- They also generate heat, which can be used to minimise energy needs to fulfill heating requirements.

VIDEO 4A–1
HOW DO FUEL CELLS WORK?

Design features of fuel cells

Each fuel cell has similar design features, including:

- an anode and cathode, separated by an electrolyte
- inlets that allow for the continuous supply of fuel
- inlets that supply the other reactants for the reactions
- outlets for the products to leave the cell
- an external circuit where electrons flow as electrical energy is produced.

These features can be seen in Figure 4A–2 on the following page.

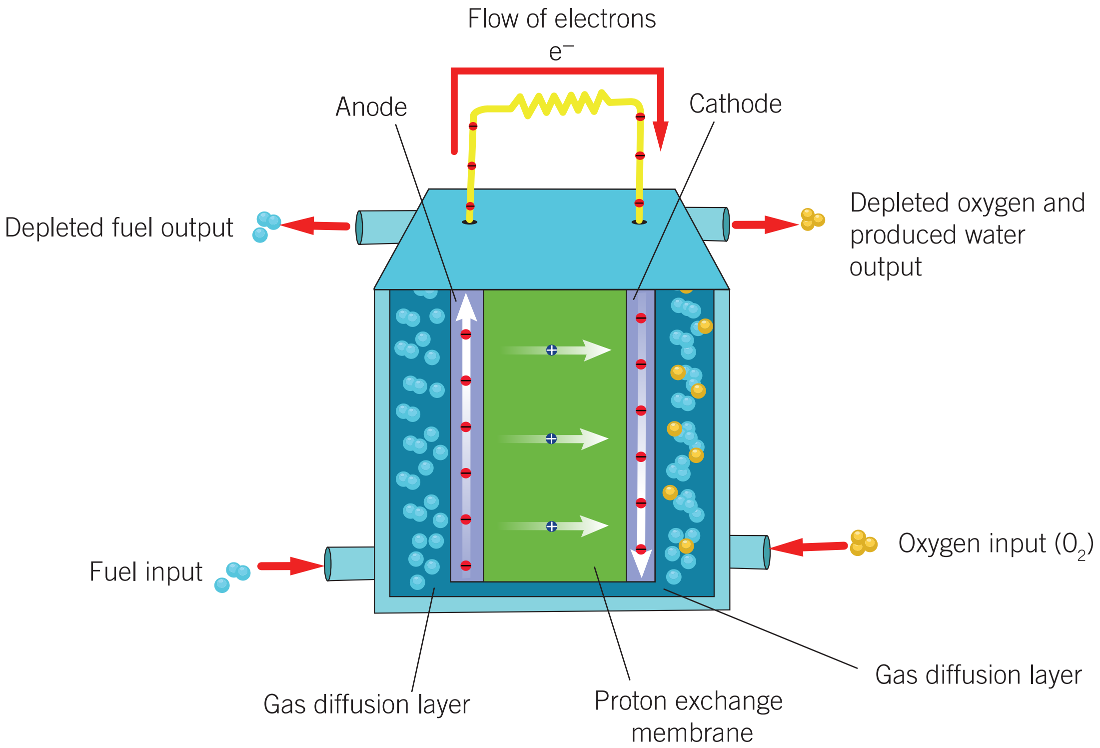

Figure 4A–2 A proton-exchange membrane fuel cell, highlighting features common to all fuel cells

WORKSHEET 4A–1 FEATURES OF FUEL CELLS

Fuel cells often have design features that enhance the efficiency of the cells. Some of these include:

- the use of **catalytic electrodes** to speed up the reactions taking place. One such example is the use of powdered platinum anodes that help break fuel molecules into electrons and ions. Another example is the use of a nickel cathode, which catalyses the conversion of excess ions into water molecules.
- oxidation-resistant gas diffusion layers made from carbon-based materials. These maintain an optimal flow rate of reactant gases and also ensure minimal water retention within the cell, which can reduce the power being generated by the cell.
- **porous electrodes** to increase the effective surface area of the electrode, enhancing the ability for gaseous reactants to diffuse through them easily and react with the ions present in the electrolyte solution of the cell. This also distributes the current more evenly within the electrode, improving the efficiency of the cell.

Catalytic electrode an electrode made from or coated with a substance that acts to speed up the rate of a reaction in an electrolytic cell

Porous electrode an electrode with tiny spaces or holes through which substances, in particular gases, can diffuse easily

Sustainability and environmental considerations

With the current challenges of meeting society's energy needs, there is more emphasis than ever on researching and exploring innovative ways to design fuel cells in a way that increases energy efficiency and minimises fuel consumption. Currently, fuel cells are used mainly for space exploration, vehicle transportation and stationary power generation, the latter of which can be configured to provide both heat and power. Using fuel cells in this way improves energy efficiency as, in addition to the electrical energy that the cells produce, the heat from the fuel cells can be used to generate hot water and low-pressure steam. An absorption chiller can also be employed to use otherwise wasted energy to produce chilled water.

One of the most discussed fuel cells to improve the environmental impact of energy production is the hydrogen fuel cell. While there are many potential applications where hydrogen fuel cells may prove to be useful, there is particular interest in how they could be implemented in cars.

Figure 4A–3 Cars powered by hydrogen fuel cells may produce less than 50% of the greenhouse gas emissions of vehicles currently running on petrol.

Hydrogen fuel cells have the same basic structure as other fuel cells but specifically have hydrogen as the input. Importantly, the 'waste' products that are generated from these fuel cells are heat and water (Figure 4A–4). As mentioned earlier, not only are these more environmentally friendly than the outputs of traditional engines, but they can be useful to help drive other processes.

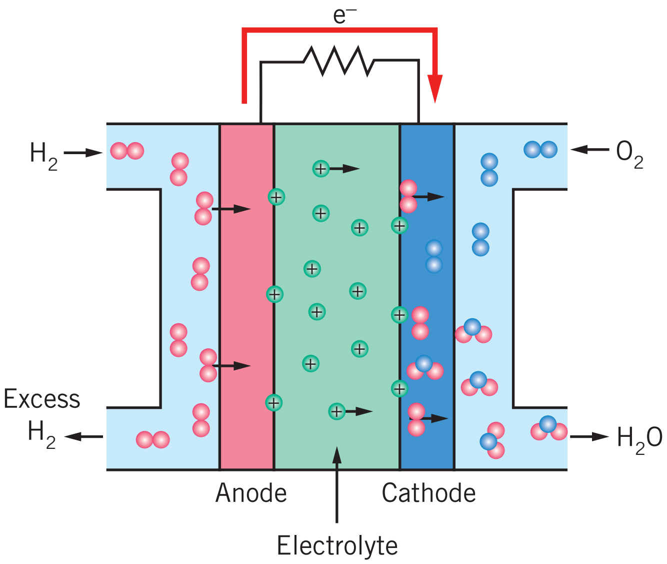

Figure 4A–4 A hydrogen fuel cell is an environmentally friendly approach to energy production that uses hydrogen gas to produce electricity, while reducing carbon emissions.

According to a report by the United States Government Department of Energy, these fuel cell-powered vehicles have the following benefits:

- They can generate energy with an efficiency of around 60%, whereas conventional petrol engines are less than 20% efficient.
- Using natural gas as a source of hydrogen, these vehicles would have total greenhouse gas emissions that are less than 50% of those produced by current vehicles.

As mentioned, as well as the improved efficiency, fuel cells use natural gas, or better still, **biogas** or **biomass**, which can be re-formed into hydrogen. It is the hydrogen that then reacts in the fuel cell to provide the electrical energy. Biogas can be generated from **renewable feedstocks**, such as corn starch, switchgrass and soybean oil, as well as food scraps and animal waste. However, classification of what is considered renewable can be debated. There are huge advantages to the use of this material to produce energy. It is estimated that every year in the United States alone, there could be up to one trillion kilograms of biomass available for energy use. Biomass is converted to hydrogen gas, and other products, through a process known as **gasification**.

LINK **1A** TYPES OF FUELS

Biogas
a type of biofuel formed from the breakdown of organic waste by anaerobic bacteria

Biomass
renewable organic matter that comes from plants, animals and other living organisms

Renewable feedstock
raw material that is used to supply an industrial process and can be readily replenished

Gasification
the process through which carbon-based material is converted into gas products that can be used for fuel

Figure 4A–5 Biomass, such as corn, can be used to generate biogas that can power hydrogen fuel cells.

The utilisation of organic and renewable feedstocks is one of the most important and significant challenges that chemists face in the world today as society moves to eliminate the use of non-renewable carbon resources such as coal, oil and natural gas. However, our conceptions of what feedstocks should be considered renewable is still developing. In December 2022, Australia became the first major economy to exclude native forest biomass from being considered a renewable energy source. This is different from other regions, such as the European Union (EU), which significantly relies on 'woody biomass' (the term for trees and woody plants) to meet its renewable energy targets. Only time will tell if this leads to any further global shift in the understanding of renewability, but regardless, there will continue to be innovation and developments in the drive to produce fuel cells that are designed to run more efficiently on affordable, scalable and sustainable fuels that have low emissions to make them more environmentally friendly.

LINK **9C** SUSTAINABLE PRODUCTION OF ORGANIC COMPOUNDS

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4A SKILLS

1A TYPES OF FUELS LINK

Using tables for comparison

In Section 1A, the Skills section described important things to remember when writing answers that require you to perform a comparison. To expand on these comments, another useful technique when writing answers that involve a comparison is the use of a table. Using a table is a really helpful method for ensuring that you illustrate your answer clearly and cover all of the required points.

As an example, based on the material covered in this section, you could reasonably expect to receive a question that asked the following:

Question: Compare the features and function of primary galvanic cells and fuel cells.

Answer: Instead of answering this as a paragraph of text, you may find it suits you better to use a table. There are a couple of different ways that you could structure your tables.

Firstly, as shown below, you could have one column for galvanic cells and one column for fuel cells. Each line in the table could then be used to describe a specific aspect, such as the overall purpose, which has been filled in already. Any differences between the two regarding that aspect would be highlighted by the text in each column.

Primary galvanic cells	Fuel cells
Convert or make the header row singular chemical energy into electrical energy	Convert chemical energy into electrical energy

Secondly, as shown below, you could set up your table in a way that has a column for similarities and a column for differences. This allows you to specifically highlight the aspects in common and those that differ, but it doesn't necessarily align them by an overall theme.

Similarities	Differences

Either method is effective, and it is important to work out what suits you personally. For revision, you may wish to fill in the tables above with the information you have learned so far.

Section 4A questions

1 State two similarities and two differences between primary galvanic cells and fuel cells.

2 State three advantages of using fuel cells.

3 Explain the importance of the following design features used in fuel cells:

  a porous electrodes

  b catalytic electrodes

4 Explain the importance of using renewable feedstocks to generate the reactants, including hydrogen, used in fuel cells.

4B Faraday's laws

Study Design:

- The application of Faraday's laws and stoichiometry to determine the quantity of galvanic or fuel cell reactant and product, and the current or time required to either use a particular quantity of reactant or produce a particular quantity of product

Glossary:

Ampere
Coulomb
Current
Electric charge
Faraday's constant

ENGAGE

Who was Faraday?

Michael Faraday, born in 1791, was a scientist who made incredible discoveries in the fields of chemistry and physics. He discovered several organic compounds, including bicarburet of hydrogen (which we now call benzene), and many of his scientific contributions laid the foundations for electromagnetic field theory. In this section, we will look at two laws described by Faraday in 1833. These laws directly relate the amount of reactant or product formed over time in an electrochemical cell with the electric charge that runs through it. In commercial chemistry, where large amounts of compounds need to be generated with a level of exactness, being able to apply these laws is particularly significant. In this section, you will learn how to perform calculations related to galvanic and fuel cells using Faraday's laws.

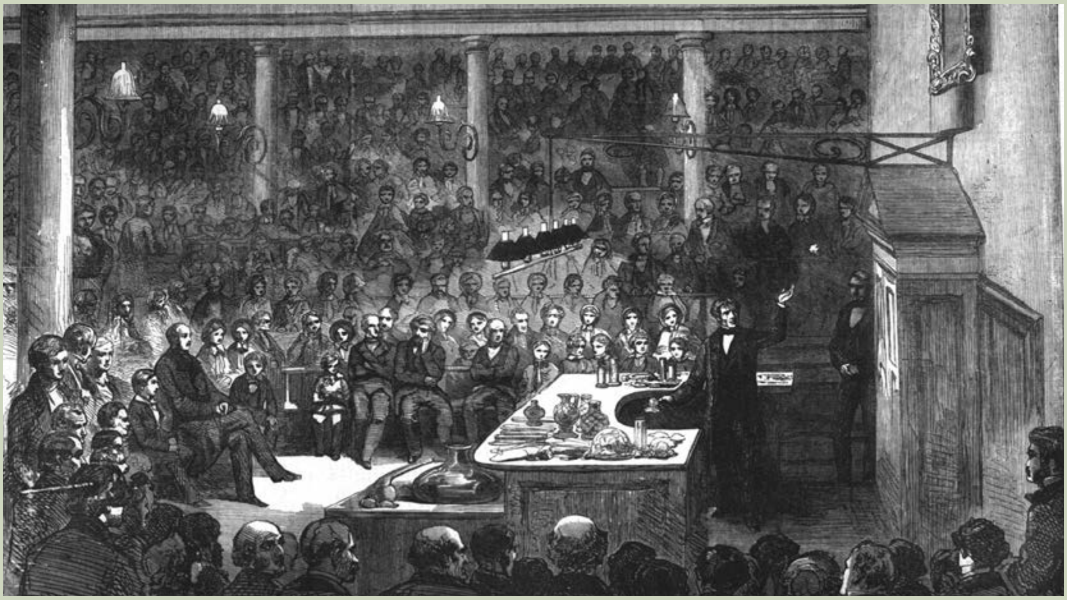

Figure 4B–1 Illustration of Michael Faraday delivering a lecture in 1856

EXPLAIN

Faraday's laws

It is important to be able to control or predict the outcomes in electrochemical cells. For example, how much metal will be deposited at the cathode? How much reactant is needed to produce a certain amount of electrical energy? How long will the cell operate for?

To help understand how the number of electrons flowing through a circuit can be related to the mass of the reactants consumed or products formed, we first need to understand Faraday's laws which state the following:

1. The mass of a substance (m) produced or consumed at an electrode is directly proportional ($\propto$) to the electric charge (Q) ($m \propto Q$).
2. The amounts, in moles, of different substances produced or consumed at electrodes by the passage of the same amount of electricity are inversely proportional to the charges on their ions ($n \propto \frac{1}{\text{ionic charge}}$).
3. **Electric charge** is measured in **coulombs** and is represented by the symbol, Q. The amount of charge that 1 mole of electrons has is 96 500 coulombs (C). This amount is known as **Faraday's constant**, F, and can be written as:

$$F = 96\,500 \text{ C mol}^{-1}$$

This relationship can be expressed through the equation:

$$Q = n(\text{e}^-) \times F$$

where:

Q = The electric charge (in coulombs)
$n(\text{e}^-)$ = The number of moles of electrons
F = Faraday's constant (96 500 C mol^{-1})

Electric charge the amount of energy electrons carry; symbol Q

Coulomb the unit used to measure the amount of electric charge something has

Faraday's constant the amount of charge that 1 mole of electrons carries (F = 96 500 C mol^{-1})

Current the rate at which electrons flow within a circuit

Ampere the unit used for measuring electric current; also known as amp

Current and time

Current (I) is the rate that electric charge flows through a circuit during a certain period of time and is measured in **amperes** or amps (A). One ampere is equal to one coulomb of charge per second:

$$1 \text{ ampere (A)} = 1 \text{ coulomb (C) per second (s)}$$
$$1 \text{ A} = 1 \text{ C s}^{-1}$$

The current flowing in an electrochemical cell will be directly proportional to the charge. Put simply, the higher the current running through the cell, the more electrons passing through the circuit, and the greater the amount of products formed. For example, if twice the current is produced over a certain amount of time, then twice as many moles of the products will be formed. Similarly, twice as much of the reactants will be consumed.

The time, t, for which a cell is operating is measured in seconds and is also directly proportional to the charge. Put simply, the longer a cell operates, the more electrons pass through the circuit and the greater the amount of products formed.

These factors are represented by the following relationship:

$$Q = It$$

where:

Q = The electric charge (in coulombs)
I = The current (in amperes)
t = The time (in seconds).

NOTE

There is often a need to convert units from seconds to other units of time, and vice versa. It is worth spending time familiarising yourself with the conversion steps needed for such calculations.

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Calculations using Faraday's laws and stoichiometry

For a galvanic or fuel cell, the chemical reactions that occur are spontaneous, so that once the cell is connected electrical current will travel through the external circuit. An ammeter can be used to measure the current over time and subsequently determine the total charge that flows through the external circuit. Once this is known, the moles of electrons can be calculated and using the half equations for the reactions taking place, it is possible to determine how many moles of reactants have been consumed and/or how many moles of product are formed.

Worked example 4B–1: Using Faraday's laws and stoichiometry

VIDEO
WORKED EXAMPLE 4B–1

A galvanic cell consists of two half-cells, one containing a nickel electrode and nickel ions, Ni^{2+}, the other with a silver electrode and silver ions, Ag^+.

a How much charge will flow through the cell if 3.50 g of nickel reacts?

Solution

	Logic	Process
Step 1	Identify the two half-equations occurring in the cell using the electrochemical series.	Reduction: $Ag^+(aq) + e^- \rightarrow Ag(s)$ Oxidation: $Ni(s) \rightarrow Ni^{2+}(aq) + 2e^-$
Step 2	Calculate the number of moles of nickel using $n = \frac{m}{M}$.	$n(Ni) = \frac{m}{M}$ $n(Ni) = \frac{3.5\text{ g}}{58.7\text{ g mol}^{-1}}$ $n(Ni) = 0.0596$ mol
Step 3	Determine the mole ratio of electrons to solid nickel.	$n(e^-) : n(Ni) = 2 : 1$
Step 4	Calculate the number of moles of electrons using the mole ratio.	$n(e^-) = n(Ni) \times 2$ $n(e^-) = 0.0596 \times 2$ $n(e^-) = 0.119$ mol
Step 5	Calculate the amount of charge using Faraday's constant.	$Q = n(e^-) \times F$ $Q = 0.119\text{ mol} \times 96\,500$ $Q = 11\,500$ C

b If a constant current of 4.2 amps is applied, how long would it take for 3.5 g of nickel to react (to the nearest minute)?

Solution

	Logic	Process
Step 1	Identify the key pieces of information in the question.	$I = 4.2$ amps $Q = 11\,500$ C (from part **a**)
Step 2	Rearrange $Q = It$ to solve for t.	$Q = It$ $t = \frac{Q}{I}$ $t = \frac{11500}{4.2}$ $t = 2738$ seconds
Step 3	Convert the answer into minutes.	$t = \frac{2738}{60}$ $t = 46$ minutes

Charge of the ion

Consider a galvanic cell with one half-cell containing Na^+ ions that will be reduced at the cathode to sodium metal, as follows:

$$Na^+(aq) + e^- \rightarrow Na(s)$$

For every 1 mole of electrons flowing though the cell, **1** mole of sodium metal is produced.

However, now consider a different galvanic cell with the half-cell containing Mg^{2+} ions reacting at the cathode as follows:

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

In this reaction, to produce 1 mole of magnesium metal, there are **2** moles of electrons required, twice as many as were needed for sodium.

Lastly, imagine a galvanic cell with a half-cell containing Al^{3+} ions reacting at the cathode as follows:

$$Al^{3+}(aq) + 3e^- \rightarrow Al(s)$$

In this reaction, to produce 1 mole of aluminium metal, there are **3** moles of electrons required, three times as many as were needed for sodium.

As mentioned earlier, this relationship can be represented by the following equation:

$$Q = n(e^-) \times F$$

Simply put, the larger the charge on the ion, the smaller the amount of that species will react or be produced during the reaction.

WORKSHEET 4B–1
CALCULATIONS USING FARADAY'S LAWS

NOTE

The amount of a substance that reacts or is produced at an electrode is proportional to both the current and time but is inversely proportional to the charge of the ion.

Check-in questions – Set 1

1 State whether making the following changes would result in an increase or a decrease of the amount of reactants used in galvanic cells and fuel cells.
  - a increasing the length of time that a cell is operating for
  - b increasing the ionic charge on the ion species being reduced at the cathode

2 When using the formulas for Faraday calculations, state the units needed for each variable below.
  - a current
  - b time
  - c electric charge

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Worked example 4B–2: Calculating the current in a cell

VIDEO
WORKED
EXAMPLE 4B–2

A galvanic cell is set up as shown below. After 15.00 minutes, there is an increase in mass at the cathode of 0.95 grams. Calculate the current running through the cell, assuming that it remains constant.

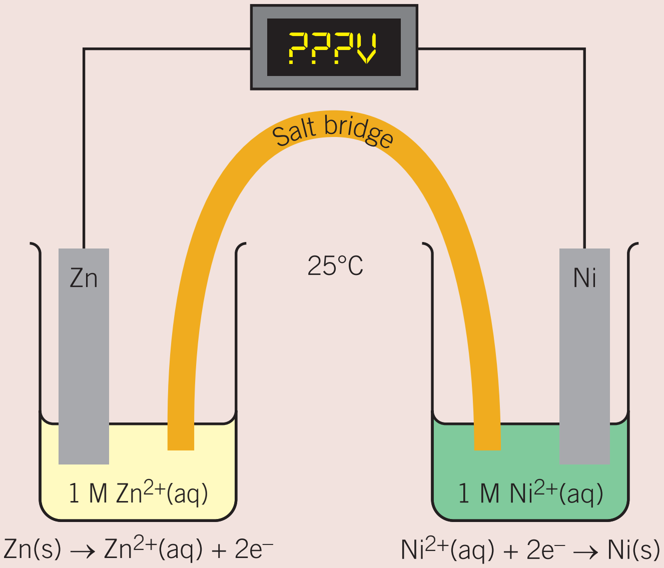

Figure 4B–2 A zinc–nickel cell

Solution

	Logic	Process
Step 1	Identify the reduction half-equation (as 0.95 grams are being deposited, not reacted), using the electrochemical series.	$Ni^{2+}(aq) + 2e^- \rightarrow Ni(s)$
Step 2	Calculate the moles of nickel using $n = \frac{m}{M}$	$n(Ni) = \frac{m}{M}$ $n(Ni) = \frac{0.95\text{ g}}{58.7\text{ g mol}^{-1}}$ $n(Ni) = 0.016$ mol
Step 3	Determine the mole ratio of electrons to solid nickel.	$n(e^-) : n(Ni) = 2:1$
Step 4	Calculate the moles of electrons using the mole ratio.	$n(e^-) = n(Ni) \times 2$ $n(e^-) = 0.016 \times 2$ $n(e^-) = 0.032$ mol
Step 5	Calculate the charge using Faraday's constant.	$Q = n(e^-) \times F$ $Q = 0.032\text{ mol} \times 96\,500$ $Q = 3124$ C
Step 6	Rearrange $Q = It$ to solve for I.	$Q = It$ $I = \frac{Q}{t}$ $I = \frac{3124}{(15 \times 60)}$ $I = 3.5$ amps

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4B SKILLS

Units and unit conversion

In this section, you have seen that in calculations you may be dealing with many different units: coulombs, amperes, grams, seconds, minutes, moles etc. It is important that you are confident with the unit that is associated with every aspect of your calculations, as you should make it a habit to include them in all your working-out steps and, even more importantly, in your final answer. An answer without units provided, assuming they are required, is meaningless and may not receive any marks.

In a similar fashion, it is also important to pay close attention to the units that are required for the answer. A common example of this is found when using the $Q = It$ equation, where the question may require you to provide an answer for the time in minutes. As you may remember, the expression involves time in seconds. Therefore, in questions such as this, you will need to divide the answer that you get by 60 to end up with an answer in the appropriate units.

Section 4B questions

1 Nickel ions undergo reduction to solid nickel at the cathode of a particular galvanic cell. Determine how long it will take to deposit 2.00 grams of nickel in a galvanic cell if a current of 1.85 amps is applied to the cell, to the nearest minute.

2 Solid copper undergoes oxidation to copper(II) ions at the anode in a galvanic cell. Determine the mass of copper lost if 1.2 amps of current is running through the cell for 12.0 minutes.

3 Determine the amount of current running through a fuel cell if 11.65 grams of silver at the cathode are deposited after 2.50 hours. The reaction occurring at the cathode is:

$$Ag^+(aq) + e^- \rightarrow Ag(s)$$

4 Hearing aids are often powered by alkaline batteries that last for 1200 hours. The half-reactions occurring in an alkaline battery are:

$$Zn(s) + 2OH^-(aq) \rightarrow ZnO(s) + H_2O(l) + 2e^-$$
$$2MnO_2(s) + H_2O(l) + 2e^- \rightarrow Mn_2O_3(s) + 2OH^-(aq)$$

If a hearing aid uses 1 mA of current, calculate the mass of zinc reacting during its lifetime. Assume the current remains constant.

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Chapter 4 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
4A.1	Compare the similarities and differences between galvanic cells and fuel cells	2☐, 11☐
4A.2	Identify and describe the common design features of fuel cells	6☐, 11☐, 14☐
4A.3	Explain the importance of key design features in terms of reaction efficiency	4☐, 11☐
4A.4	Describe green chemistry principles that enhance the sustainability of fuel cells, including the use of renewable feedstocks	5☐, 8☐, 11☐
4B.1	Determine the stoichiometric relationship between the quantity of reactant or product and electrons represented by half-equations in the electrochemical series	10☐
4B.2	Calculate the amount of current or time required for a galvanic or fuel cell to produce a given amount of electric charge using Faraday's laws equations	1☐, 3☐, 12☐, 13 ☐
4B.3	Calculate the amount of reactant used or product formed during reactions occurring in a galvanic or fuel cell using Faraday's laws equations	1☐, 7☐, 9☐, 10☐, 12☐, 13 ☐

Multiple-choice questions

1 What is the unit of electric charge used in Faraday's laws?

A ohm
B volt
C ampere
D coulomb

2 Which of the following best describes a fuel cell?

A a device that stores electrical energy in chemical form
B a device that generates mechanical energy from heat energy
C a device that converts chemical energy into electrical energy
D a device that converts electrical energy into chemical energy

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3 If a constant current of 2.6 amperes is applied, how long (in minutes) will it take to produce 9516 coulombs of electric charge?

A 6

B 61

C 410

D 3660

4 Which of the following statements is true regarding the advantages of fuel cells?

A Fuel cells require frequent recharging.

B Fuel cells have limited application areas.

C Fuel cells offer high energy-conversion efficiency.

D Fuel cells have high levels of carbon emissions.

5 Gasification is the process by which

A fuel cells release their waste products.

B biomass is converted to hydrogen gas.

C liquid hydrogen is converted to hydrogen gas.

D hydrogen gas is converted to electrical energy.

6 Which of the following combinations regarding fuel cell features and their roles is incorrect?

	Feature	Role
A	Anode	Site of oxidation
B	External circuit	Allows movement of electrons from the anode to the cathode
C	Catalyst	Increases the rate of the chemical reaction
D	Electrolyte	Allows movement of electrons from the cathode to the anode

7 Which of the following statements best represents Faraday's first law?

A The electric charge is directly proportional to the mass of substance consumed.

B The electric charge is inversely proportional to the mass of substance consumed.

C The electric charge is measured in amperes and is dependent on the length of time the cell is operating.

D The electric charge is measured in coulombs and is independent of the length of time the cell is operating.

8 Biogas can be re-formed into hydrogen to be used as a fuel in a fuel cell. Biogas can come from renewable feedstocks, which are thought to be more sustainable. A key advantage of renewable feedstocks is that they are

A expensive.

B energy rich.

C easily replenished.

D environmentally unfriendly.

9 Faraday's constant is the electric charge equivalent to

- **A** 1 mole of electrons.
- **B** 1 coulomb per second.
- **C** 96 500 Faraday.
- **D** 96 500 amperes.

10 How much charge would flow through a galvanic cell if 16.35 g of zinc reacts at the anode?

- **A** 12 063 C
- **B** 24 125 C
- **C** 48 250 C
- **D** 96 500 C

Short-answer questions

11 State whether the following statements are true or false. Justify your response.

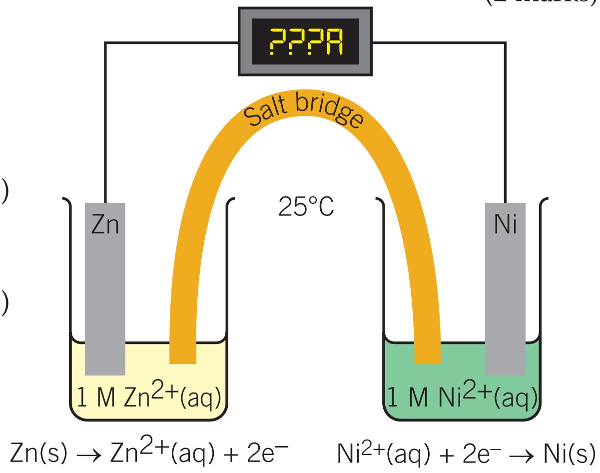
- **a** Fuel cells convert electrical energy into chemical energy. (1 mark)
- **b** Porous electrodes are used in fuel cells to allow gases to diffuse more easily. (1 mark)
- **c** Fuel cells can be recharged by connecting them to a power source. (1 mark)
- **d** Electrons travel from the anode to the cathode in fuel cells. (1 mark)
- **e** Fuel cells generate a lot of pollutants. (1 mark)
- **f** Renewable feedstocks can be used to source reactants used in fuel cells that are sustainable and minimise environmental impacts. (1 mark)

12 A galvanic cell consists of two half-cells, one containing a zinc electrode and zinc ions, Zn^{2+}, the other with a silver electrode and silver ions, Ag^{+}.

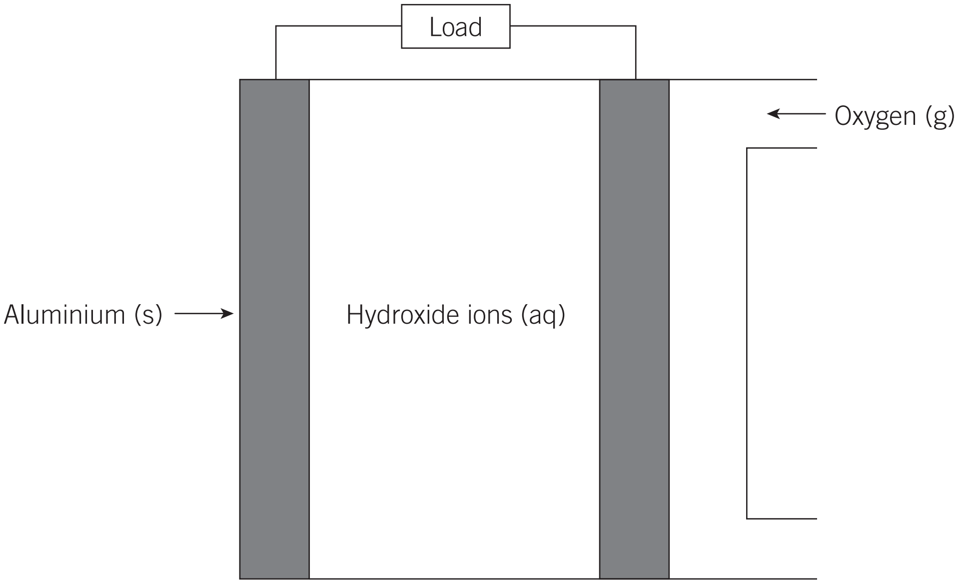
- **a** How much charge will flow through the cell if 3.50 grams of zinc react? (2 marks)
- **b** If a constant current of 2.50 amps is applied, how long, to the nearest minute, would it take for 3.50 grams of zinc to react? (2 marks)
- **c** When the cell is connected and allowed to react for five minutes, 1.95 grams of silver is deposited at the cathode. Assuming it is constant the entire time, calculate the amount of current running through the cell. (2 marks)
- **d** If the cell is left running for two hours, with a constant current of 0.30 amps, what is the expected decrease in mass of the anode? (2 marks)

13 Consider the galvanic cell shown on the right.

- **a** Calculate the length of time (in minutes) required to produce 0.40 grams at the cathode if this cell has a constant current of 3.0 amps. (2 marks)
- **b** Calculate the mass lost at the anode if this cell runs with a constant current of 6.0 amps for three minutes. (2 marks)



14 An alternative to hydrogen–oxygen fuel cells is the aluminium–oxygen battery, depicted in the image below.



The overall equation for the reaction in the aluminium–oxygen battery is:

$$4Al(s) + 3O_2(g) + 6H_2O(l) \rightarrow 4Al(OH)_3(s)$$

a Use oxidation numbers to demonstrate that a redox reaction has occurred. (2 marks)

b Which species undergoes oxidation? (1 mark)

c What is the oxidising agent? (1 mark)

d Write the half-equation for the oxidation reaction. (1 mark)

e Write the half-equation for the reduction reaction. (1 mark)

f The electrode in contact with oxygen is the focus of a lot of testing and trials. It is important that this electrode is both porous and coated with a catalyst. State why each of these features is crucial to the operation of the cell. (2 marks)

  i porous

  ii catalytic

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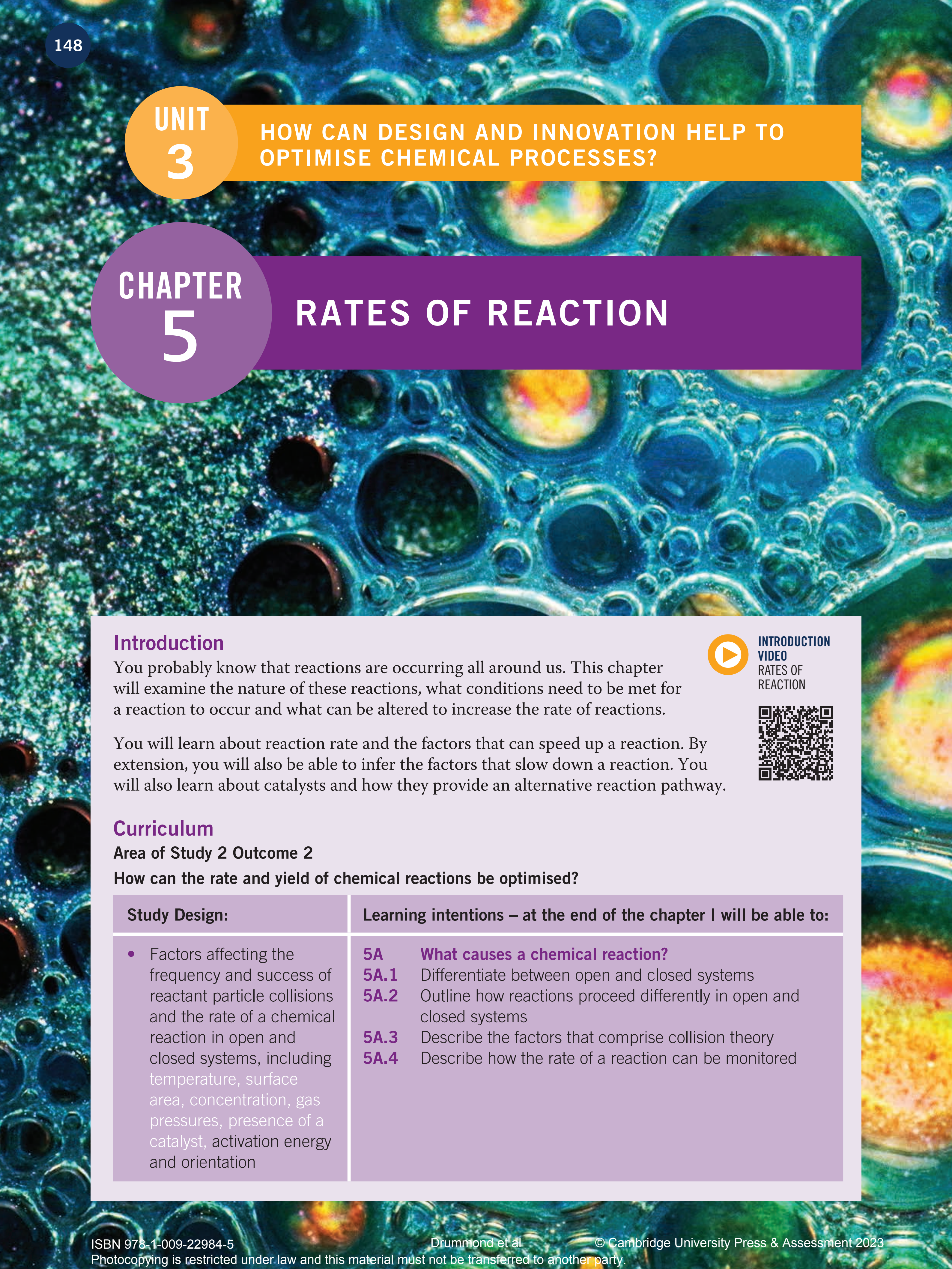


UNIT 3 HOW CAN DESIGN AND INNOVATION HELP TO OPTIMISE CHEMICAL PROCESSES?

CHAPTER 5 RATES OF REACTION

Introduction

You probably know that reactions are occurring all around us. This chapter will examine the nature of these reactions, what conditions need to be met for a reaction to occur and what can be altered to increase the rate of reactions.

You will learn about reaction rate and the factors that can speed up a reaction. By extension, you will also be able to infer the factors that slow down a reaction. You will also learn about catalysts and how they provide an alternative reaction pathway.

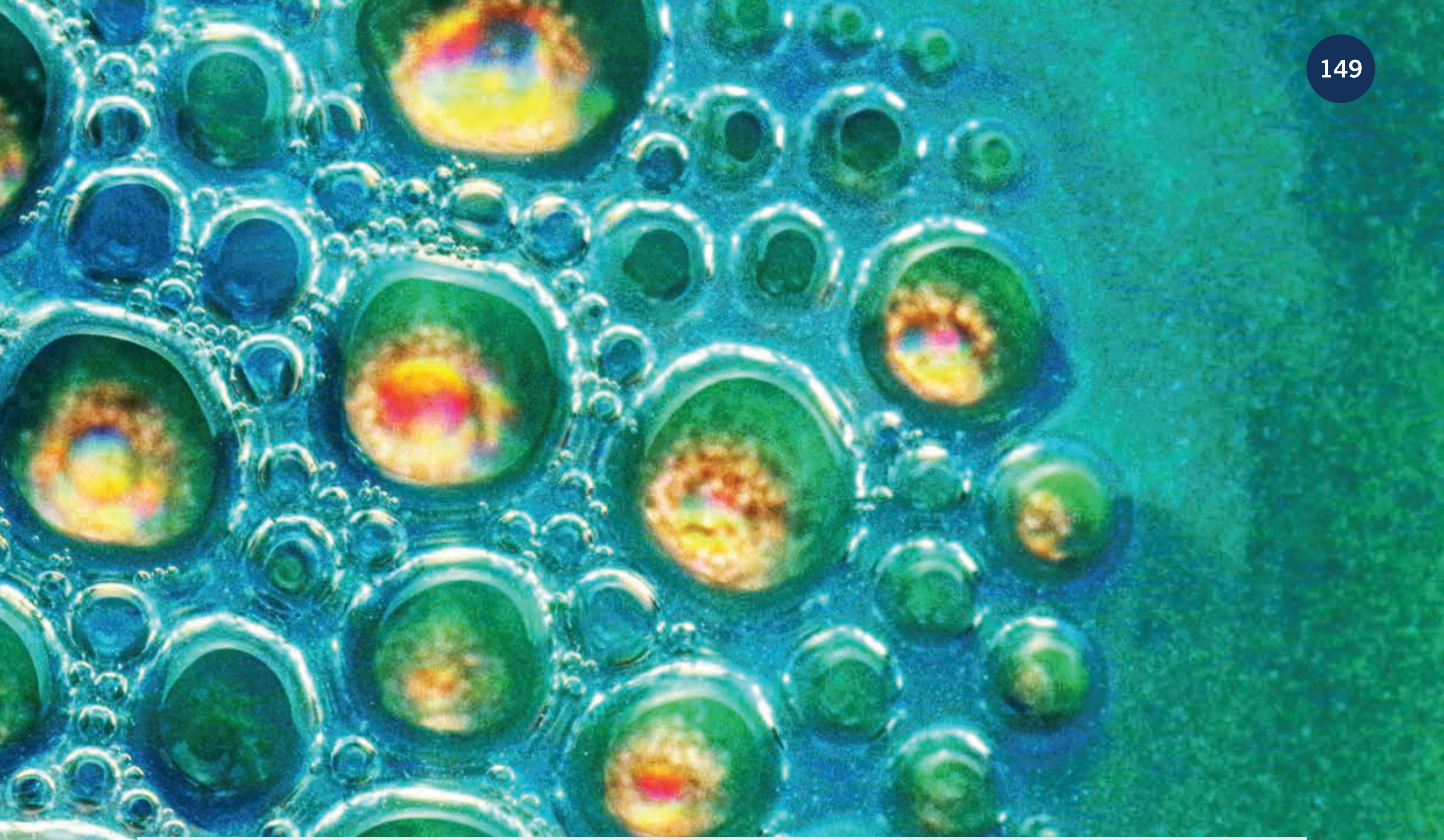
INTRODUCTION VIDEO
RATES OF REACTION

Curriculum

Area of Study 2 Outcome 2

How can the rate and yield of chemical reactions be optimised?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Factors affecting the frequency and success of reactant particle collisions and the rate of a chemical reaction in open and closed systems, including temperature, surface area, concentration, gas pressures, presence of a catalyst, activation energy and orientation	**5A What causes a chemical reaction?** 5A.1 Differentiate between open and closed systems 5A.2 Outline how reactions proceed differently in open and closed systems 5A.3 Describe the factors that comprise collision theory 5A.4 Describe how the rate of a reaction can be monitored



Study Design:	Learning intentions – at the end of the chapter I will be able to:
- Factors affecting the frequency and success of reactant particle collisions and the rate of a chemical reaction in open and closed systems, including temperature, surface area, concentration, gas pressures, presence of a catalyst, activation energy and orientation	**5B** **Factors affecting reaction rate** **5B.1** Explain the relationship between concentration and rate of reaction **5B.2** Explain the relationship between gas pressure and rate of reaction **5B.3** Explain the relationship between surface area and rate of reaction **5B.4** Explain the relationship between temperature and rate of reaction **5B.5** Outline the effect of temperature on the rate of reaction using a Maxwell–Boltzmann distribution curve
- The role of catalysts in increasing the rate of specific reactions with reference to alternative reaction pathways of lower activation energies, and represented using energy profile diagrams	**5B.6** Explain the relationship between the presence of a catalyst and rate of reaction **5B.7** Outline the effect of a catalyst on the rate of reaction using an energy profile diagram **5B.8** Outline the effect of a catalyst on the rate of reaction using a Maxwell–Boltzmann distribution curve

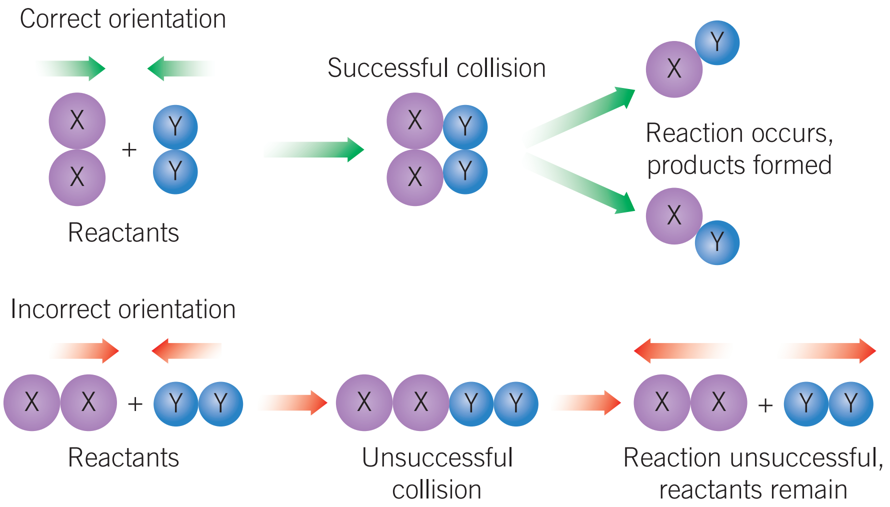
Glossary

Catalyst
Closed system
Collision theory
Heterogeneous
Homogeneous
Kinetic energy
Open system
Surface area

Concept map

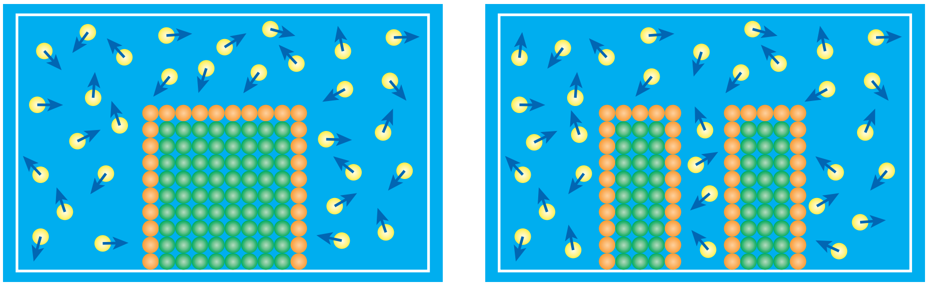
5A What causes a chemical reaction?

Exploring collision theory to understand what needs to happen for a successful reaction to occur



5B Factors affecting reaction rate

Exploring how factors, such as temperature and concentration, affect the rate of chemical reactions



See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

5A What causes a chemical reaction?

Study Design:
Factors affecting the frequency and success of reactant particle collisions and the rate of a chemical reaction in open and closed systems, including temperature, surface area, concentration, gas pressures, presence of a catalyst, activation energy and orientation

Glossary:
Closed system
Collision theory
Kinetic energy
Open system

ENGAGE

Laptops and limestone

The rate of a reaction is the speed that it goes from the starting reactants to the final products. Some reactions are very fast, on the scale of milliseconds or less, while others are so slow that it appears like nothing is happening. Consider a battery in your laptop – each second, the chemicals inside it are reacting millions of times to produce electrons and, in turn, electricity. The reactions are so fast that they cannot be seen, they can only be measured. Stalactites, however, are a great example of reactions that occur slowly. These structures in caves are a product of calcium reacting with carbon dioxide, but they take years to form. In fact, they can grow as little as 0.1 mm per year! Regardless of whether reactions are fast or slow, they all need to satisfy a number of conditions. In this section, we are going to discuss what has to happen for a reaction to occur and how the speed of a reaction can be monitored.

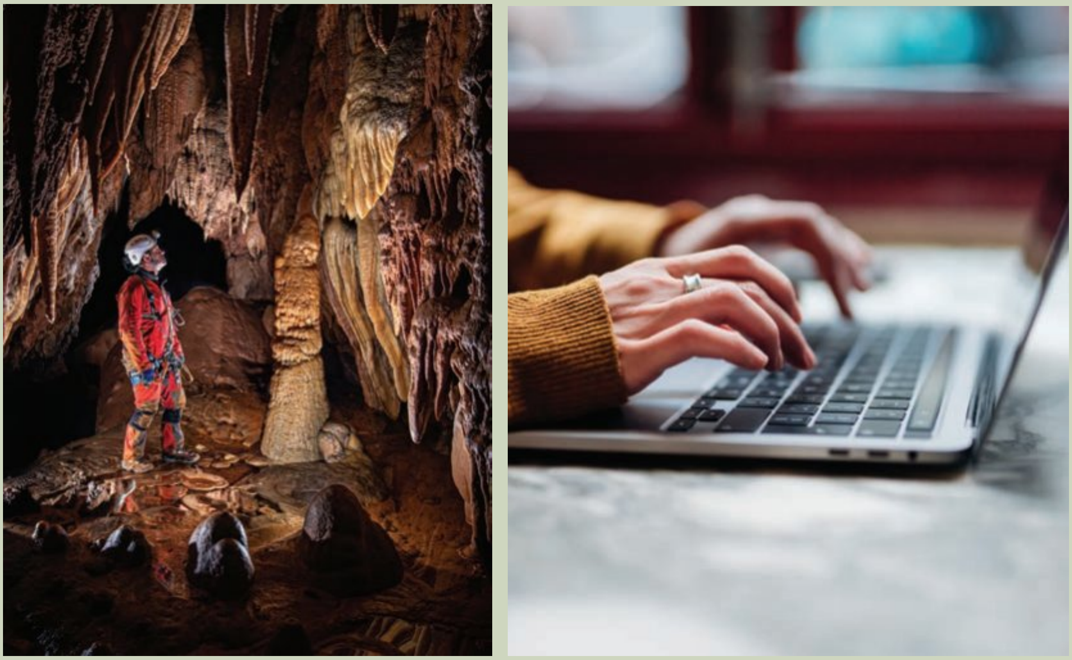


Figure 5A–1 The reactions that lead to the formation of stalactites take centuries (left), whereas the ones that produce electricity in a laptop battery are incredibly fast (right).

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EXPLAIN

Rates of reactions

Chemical reactions are occurring in our body and in nature all the time. Some of them are slow, others are fast. Similarly, reactions are also a major part of many of the industrial processes that help to produce important everyday products such as the following:

- Ammonia is formed from the reaction of hydrogen and nitrogen and is an important compound in the production of fertilisers commonly used in the farming industry.
- Sulfuric acid is produced from the reaction of sulfur, oxygen and water, and is also critical in the generation of fertilisers.
- Ethanol is produced from the fermentation of glucose, which is important in the production of wine and other alcoholic drinks.

When a reaction is occurring at an industrial level, it is particularly important that the rate of a reaction is fast enough that it allows products to be formed in a way that is cost effective, but not so fast that an explosion occurs. To achieve this balance and be able to control the reactions that are taking place, it is important to have a good understanding of the factors that determine the rate of a reaction. Reaction rate is very similar to speed and, like speed, the units of reaction rate are relative to time. Two ways that we can measure the rate of a reaction is by monitoring the decrease in the concentration of a reactant or the increase in the concentration of a product. We can visualise this graphically, as seen in Figure 5A–2. It is important to note that concentration is not always the easiest aspect of a reaction to measure, so other quantities can be measured. If a gas is produced as part of the reaction, the volume of this can be monitored over time to provide information about the rate of the reaction. Similarly, if a gas is produced and the reaction is taking place in an open system, the decrease in mass over time (as the gas moves to the surroundings) can be measured to calculate the reaction rate. Essentially, any aspect of a reaction that changes over time as a result of the reaction, and is measurable, can be used to calculate the rate of reaction.

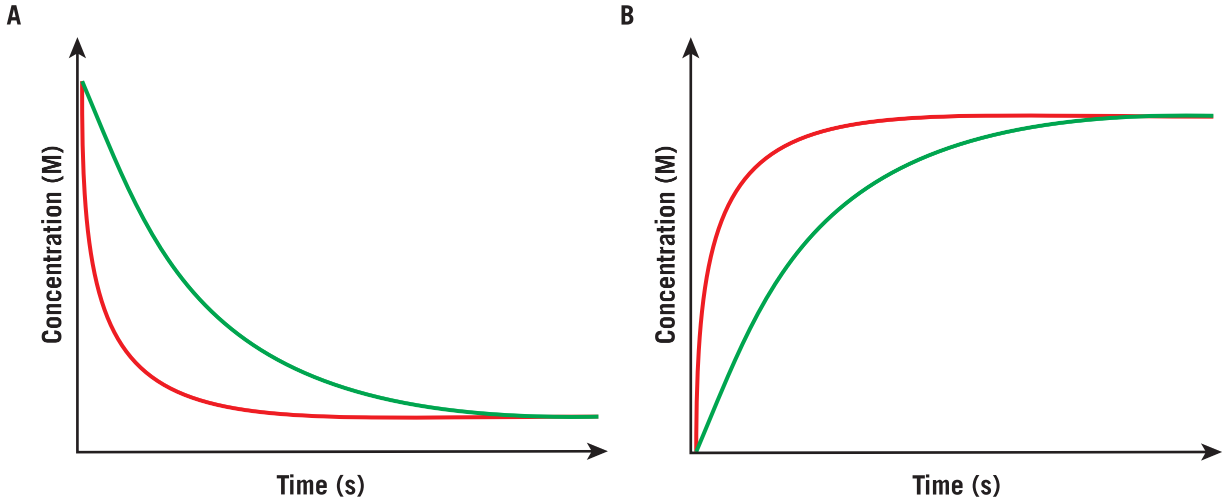

Figure 5A–2 Reaction rate can be measured by monitoring the decrease in concentration over time of a reactant (A) or increase in concentration over time of a product (B). In both instances, reaction rates can be relatively fast (red) or relatively slow (green).

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In the example shown in Figure 5A–2, the change in concentration of the reactants or products per unit of time is the way we measure the rate. As a reminder from Section 1C, a 'change' is shown by the Δ symbol, such that a change in concentration is shown as Δ*c*. This is shown mathematically below:

LINK **1C** EXOTHERMIC AND ENDOTHERMIC REACTIONS

$$\text{Rate} = \frac{\text{change in concentration}}{\text{change in time}} = \frac{\Delta c}{\Delta t}$$

It is important to note that while this equation represents the example shown in Figure 5A–2, you will likely come across other examples that require you to calculate change in mass or change in volume over time.

Open versus closed systems

When molecules react, we often think of them as two molecules existing in the absence of everything else and sitting right beside each other in space. This simple thought experiment helps us understand the atomic nature of molecules, but it is far from the reality of how reactions occur in real life.

Whether molecules come into contact to facilitate a reaction depends on the nature of the system they are in. Some molecules are in a system where they cannot escape; we call these **closed systems** (as represented in Figure 5A–3). A good example of this is a flask with a lid tightly screwed on. Some molecules are in a system where they can leave the area of the reaction; we call these **open systems**. A good example of an open system is the lungs, where molecules can be exhaled with an extremely high chance of never returning.

Closed system an environment where energy can be transferred between the reaction and the surroundings, but matter cannot

Open system an environment where both energy and matter can be transferred between the reaction and the surroundings

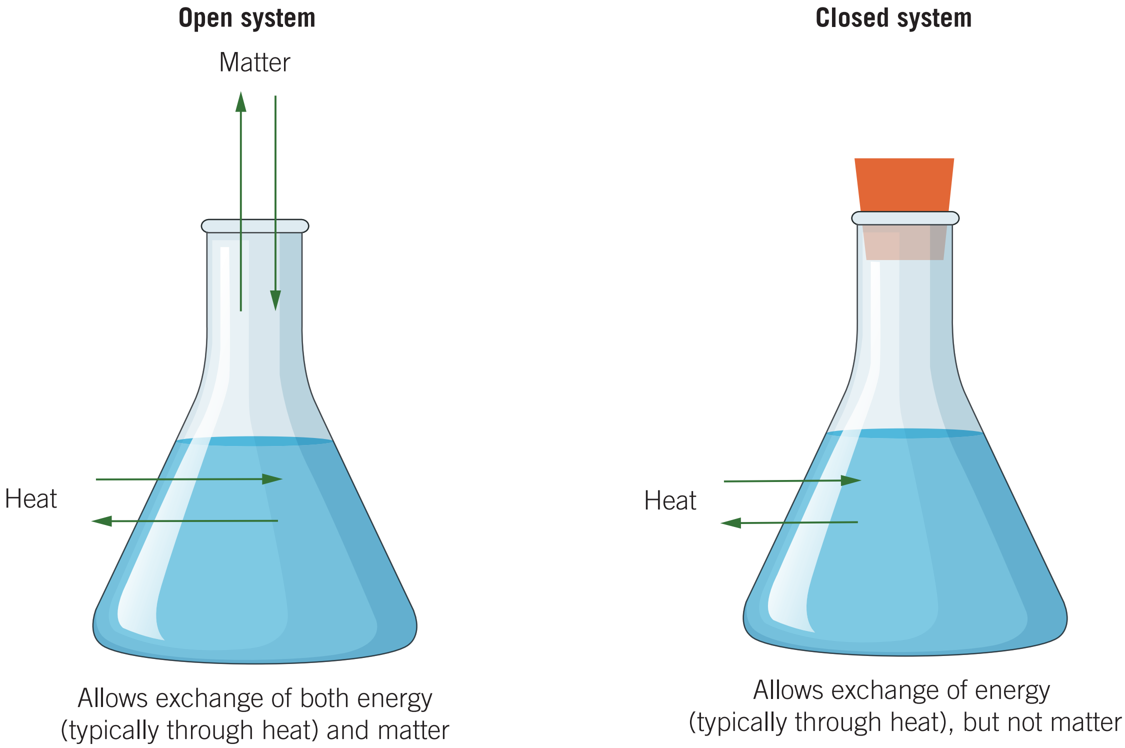

Figure 5A–3 Open systems (left) allow the transfer of energy and matter between the reaction and surroundings, whereas closed systems (right) hold the reactants and products within the system.

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Check-in questions – Set 1

1 In each of the following circumstances, describe how you would expect a concentration–time graph to change if the rate of reaction was increased.
   a Octane is undergoing combustion in a closed system and the rate of reaction is being monitored through measuring the volume of carbon dioxide produced.
   b Aspirin is reacting with water to form salicylic acid and acetic acid, and the rate of reaction is being monitored through measuring the concentration of aspirin.

2 For many reactions, it is important to know how fast or slow they are going.
   a What are two components of a reaction that can be monitored to measure the rate of a reaction?
   b Draw graphs to represent what you would expect to see for each answer given in part **a**, showing both a slow and a fast reaction for each.
   c Is it easier to monitor the rate of a reaction if it is in a closed or open system? Explain.

VIDEO 5A–1
UNDERSTANDING COLLISION THEORY

Collision theory

Collision theory the principle that allows for the prediction of the success and rate of a chemical reaction

Up until this point, we have discussed the fact that chemical reactions occur all the time around us and you may have the impression that this means that they happen easily. There is in fact a series of conditions that must be met for a reaction to take place, which is known as **collision theory**.

Three main points comprise collision theory.

1 Particles must collide.
As an example, the reaction to produce water involves oxygen reacting with hydrogen. The reaction can only occur if the hydrogen molecules collide with the oxygen molecules. However, this alone is not enough to ensure the reaction takes place.

Kinetic energy the energy an object or particle has due to its motion

1C EXOTHERMIC AND ENDOTHERMIC REACTIONS
LINK

2 Particles must collide with sufficient energy to react.
When reactions occur, the reactant molecules need to have enough energy to form the products of the reaction. Energy can come from a range of sources, but one of the most common forms is movement. This type of energy is called **kinetic energy**. Kinetic energy is one of the types of energy a molecule brings to a reaction when it collides with another molecule. A reaction can only be successful if the molecules reacting have sufficient kinetic energy to overcome the minimum energy requirements of the reaction (Figure 5A–4). The minimum energy is called activation energy, which you learned about in Section 1C.

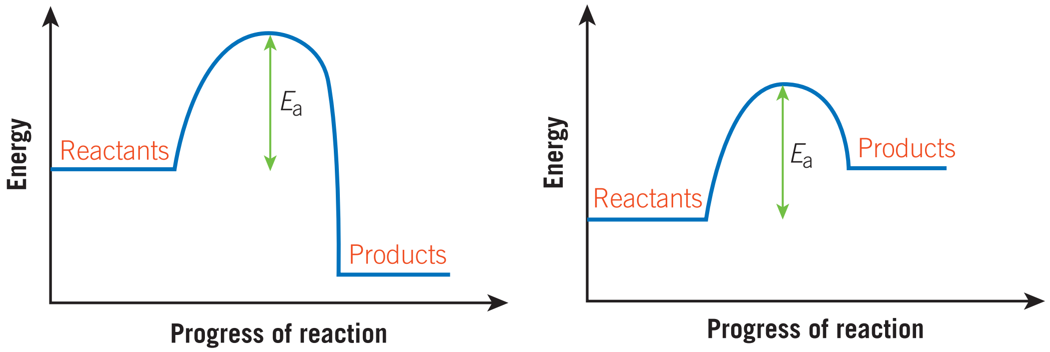


Figure 5A–4 For a reaction to occur, the reactant molecules must collide with sufficient energy; that is, energy greater than the activation energy. The activation energy (E_a) can be shown on an energy profile diagram, as shown by the green arrow.

3 Particles must collide in the correct orientation.
In the previous point, we considered successful reactions in terms of energy alone; however, when a collision occurs, it can be unsuccessful even if it has enough energy. This is because when molecules collide, they need to align in the right configuration to help form the products of the reaction. If not, the reaction will not proceed, and the molecules will simply bounce off one another. A good way to think of this is the 'lock-and-key' model. For a door to be successfully opened, not only do we need enough energy to insert the key in the lock, but we also need to have the key in the right alignment to fit into the keyhole. The concept of the lock-and-key model will be discussed in more detail when enzymes are introduced in Section 12B. This helps explain why some reactions may have low activation energies but still have a low percentage of reactants successfully forming products. Gases, for example, with such freedom to move, often collide in misaligned geometries, resulting in the molecules simply bouncing off one another (Figure 5A–5).

LINK **12B**
ENZYMES

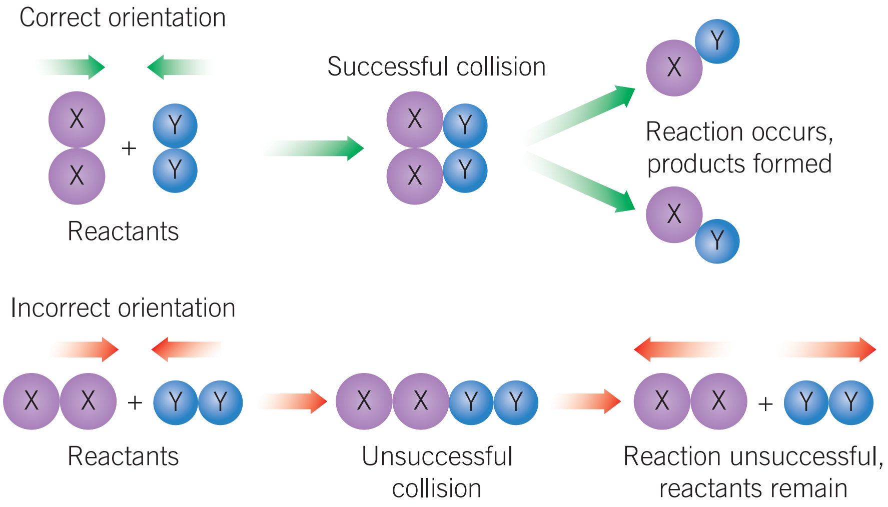
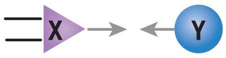
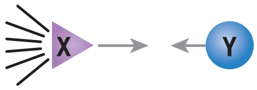
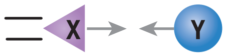
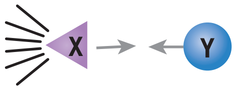


Figure 5A–5 Correct orientation (top diagram) allows the formation of products, whereas incorrect orientation (bottom diagram) leads to an unsuccessful reaction and the reactants bouncing off one another.

For a collision to be successful, two key factors are needed: correct orientation and sufficient energy to reach the activation energy of the reaction. This means that for any collision there are four possible scenarios (Table 5A–1).

Table 5A–1 Four possible outcomes of particle collisions

 Incorrect orientation, insufficient energy = no reaction	 Incorrect orientation, sufficient energy = no reaction
 Correct orientation, insufficient energy = no reaction	 Correct orientation, sufficient energy = reaction

WORKSHEET
5A–1
UNDERSTANDING
COLLISION
THEORY

VIDEO 5A–2
SKILLS:
USING GRAPHS IN
ANSWERS

5A SKILLS

Using graphs in answers

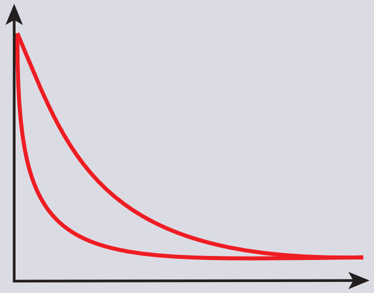
In some questions, you may be asked directly to draw a graph to form part of your answer. In other questions, while not specifically asked, you may find that using a graph as part of your response is a helpful way of illustrating your answer. In either case, there are a number of things that you have to remember to include with your diagram to ensure that you receive full marks.

Consider the following question and the answer provided for it.

Question:

Sodium ions can react with phosphate ions in solution to form sodium phosphate. Depending on the conditions, the rate of this reaction can be relatively fast or slow. Draw a graph showing the change in sodium ion concentration in solution over time for a fast and slow reaction.

Answer:

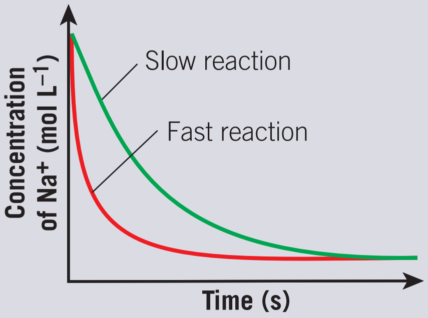


As an answer, the student has correctly identified that, as the question has asked for the change in concentration of a reactant, the curve should show a decrease over time. They have also provided two different curves, which do indicate different rates of reaction. However, there are a number of issues that would prevent this from gaining full marks, such as:

- The axes aren't labelled. These need information to show what is being represented on the graph. These should also be as specific as possible (e.g. the *y*-axis should show 'Concentration of Na^+', not just 'Concentration'. It is also important to include units, if applicable.
- The two curves aren't distinguished at all to indicate which is the fast reaction and which is the slow reaction. At a minimum, the curves need to be labelled in a way that highlights what curve represents what part of the answer. Ideally, you could also look to draw each one in a different colour to further differentiate the two.

Putting all of this together, a much better answer to this question would look like the following diagram.

Answer:



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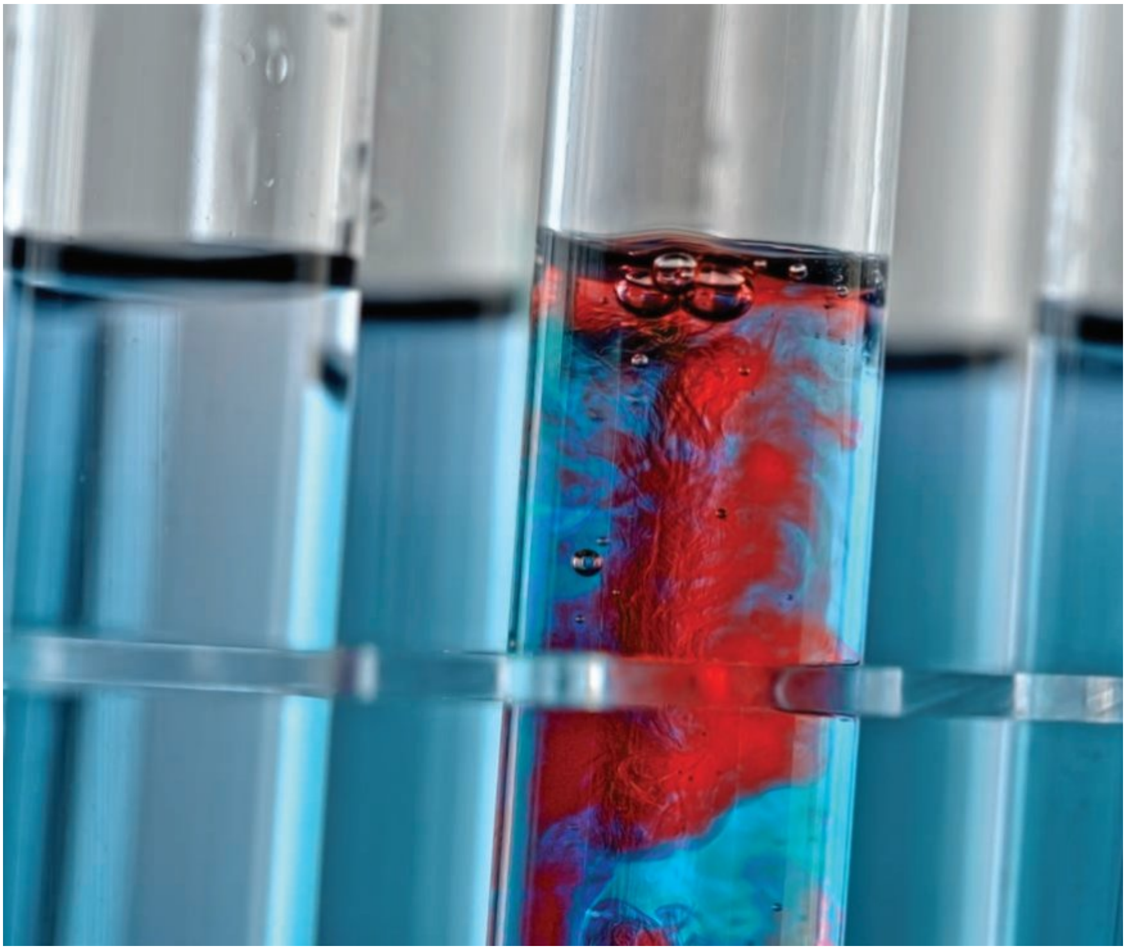
Section 5A questions

1 A scientist is observing a chemical reaction at a molecular level. They see a hydrogen molecule (H_2) and an oxygen molecule (O_2) collide, but no water is produced.
What are two reasons why a chemical reaction may not have eventuated from this collision?

2 Activation energy plays an important part in chemical reactions.
- a Draw an energy profile diagram for an exothermic reaction and clearly label the activation energy for the reaction.
- b How does the activation energy relate to collision theory?

3 A piece of solid magnesium metal is placed into a conical flask containing aqueous hydrochloric acid. A stopper is placed into the top of the flask after the reaction begins. The reaction produces aqueous magnesium chloride and hydrogen gas.
- a Write a balanced chemical equation for the reaction occurring in the flask.
- b Does the presence of a stopper suggest that this reaction is occurring in an open or closed system? Explain your choice by describing the parameters for the system you chose.
- c The reaction between magnesium and hydrochloric acid is exothermic. Based on your answer to part **b**, describe what would happen to the heat generated as part of this reaction.
- d Describe two approaches that you could take to monitor the rate of the reaction.



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5B Factors affecting reaction rate

- Factors affecting the frequency and success of reactant particle collisions and the rate of a chemical reaction in open and closed systems, including temperature, surface area, concentration, gas pressures, presence of a catalyst, activation energy and orientation
- The role of catalysts in increasing the rate of specific reactions with reference to alternative reaction pathways of lower activation energies, and represented using energy profile diagrams

Glossary:
Catalyst
Heterogeneous
Homogeneous
Surface area

ENGAGE

The chemistry of cooking

We control the rate of chemical reactions every day without even realising that we are doing it. Consider cooking yourself a steak for dinner – what happens if you cook the steak on a low heat compared to if you put it in a very hot frypan? You'll probably realise that the steak is going to cook much, much quicker when you have the stove up really high! While the same reaction is taking place in both situations, it is just happening at a much faster rate when the temperature of the frypan is higher. Understanding how different conditions and factors can impact on the rate of reaction is important, especially for those used in commercial and industrial settings. In this section, we are going to explore how concentration, gas pressure, temperature, surface area and catalysts impact on the rates of reactions.

EXPLAIN

Effects on reaction rates

In this section, we are going to be focusing on factors that affect the rate of reaction. For each one, it is important that you can do the following:

- State the relationship between the condition and the rate of reaction.
- Explain this relationship by referring to the relevant points in collision theory.

As we move through this section, we will discuss each factor individually and use this format to discuss their effect on the rate of reaction.

Concentration and rate of reaction

Relationship: An increased concentration leads to an increased rate of reaction.

Explanation: If we think back to Unit 2, concentration is a measurement of how many particles are in a given space or volume. This can be demonstrated in Figure 5B–1, which shows the concentration of a solution increasing from low to high.

LINK **UNIT 2**

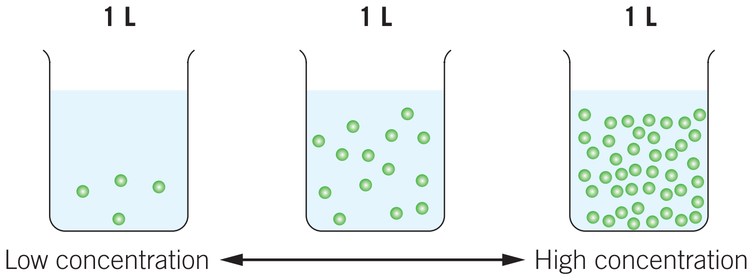

Figure 5B–1 In a high concentration solution, there are more particles in a given volume, so the probability of them colliding is higher than when the concentration is low.

LINK **5A** WHAT CAUSES A CHEMICAL REACTION?

So why does an increased concentration lead to an increased rate of reaction? To answer this, we must refer to collision theory. A summary of this is provided in Table 5B–1.

Table 5B–1 The effect of an increased concentration on the different aspects of collision theory

Collision theory	Effect of increased concentration
Particles must collide	Increased collision frequency
Particles must collide with sufficient energy	No effect
Particles must collide in the correct orientation	No effect

As Table 5B–1 illustrates, the main reason that an increased concentration leads to an increased rate of reaction is that there is an increased collision frequency. Put simply, when there are more particles in a given space, the probability of them colliding is much higher (Figure 5B–1).

If you think about this in a real-world scenario, imagine walking around your chemistry classroom when there are only five other people in the room. The likelihood that you will bump into one of them is low. However, if there were 50 people in the classroom, the chances of people running into each other while randomly moving around is much, much higher. We can think of particles colliding in low and high concentration solutions in the same way.

While an increased concentration doesn't affect the energy of the particles, nor the orientation that they collide in, the fact that there are more collisions (that is, a higher collision frequency) means that there are more chances for a successful reaction to occur.

Gas pressure and rate of reaction

Relationship: An increase in gas pressure leads to an increased rate of reaction.

Explanation: To understand the effect of gas pressure on the rate of reaction, we must understand the relationship between gas pressure and volume (generally this refers to the volume of the reaction vessel). As the volume decreases, the gas pressure increases. Conversely, as the volume increases, the gas pressure decreases. This is shown in Figure 5B–2, which shows two different-sized reaction vessels: they both contain the same number of particles but have different gas pressures.

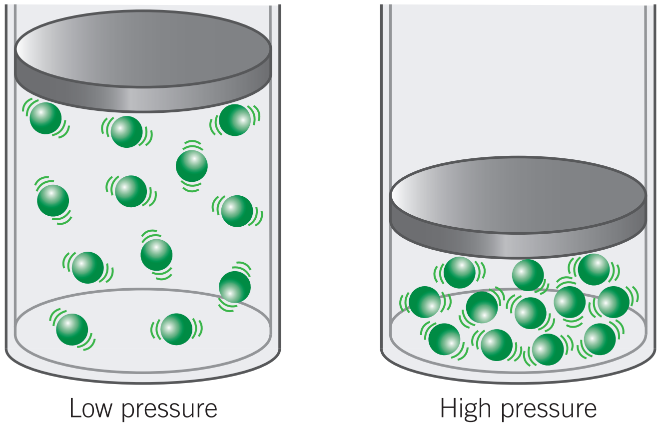

Figure 5B–2 The same amount of gas particles in a container with a greater volume (left) will have a lower gas pressure than if they were in a container with a smaller volume (right).

So why does an increased gas pressure lead to an increased rate of reaction? To answer this, we must refer to collision theory. A summary of this is provided in Table 5B–2.

Table 5B–2 The effect of increased gas pressure on the different aspects of collision theory

Collision theory	Effect of increased gas pressure
Particles must collide	Increased collision frequency
Particles must collide with sufficient energy	No effect
Particles must collide in the correct orientation	No effect

In closed systems, reactions are affected by the space they have available to operate in. According to collision theory, the more space available for molecules to occupy, the less likely they will collide (in correct alignment). If you had the same number of gas particles, one in a 1 L container (low pressure) and one in a 100 mL container (high pressure), we would expect more collisions when the pressure is higher (that is, in the 100 mL container).

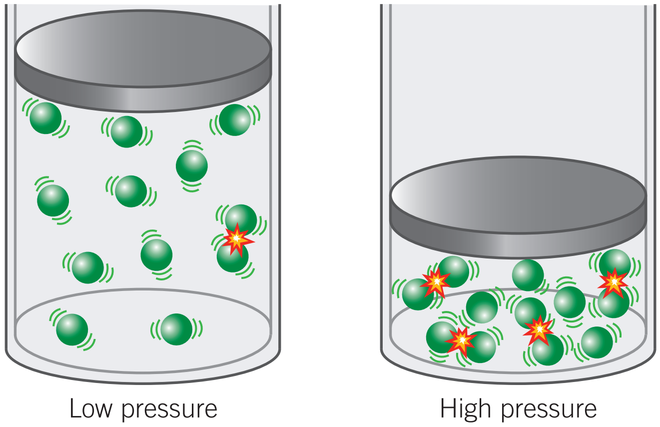

Figure 5B–3 Large volumes (left) have low pressures and the number of particle collisions is low; thus, the reaction rate is low. Small volumes (right) have high pressures and the number of particle collisions is high, thus the reaction rate is high.

As you can see, this is very similar to what was discussed for concentration. In this instance, instead of increasing the collision frequency by increasing the number of particles present in the space, we are decreasing the space that the particles are present in. To refer to our classroom analogy, this would be the equivalent of moving the five students from their chemistry classroom into a storage closet. As you can imagine, they are much more likely to bump into each other if they try and move around in that cramped space than they were in the large classroom.

Similar to concentration, an increased gas pressure does not affect the energy of the particles, nor the orientation that they collide in. However, once again, the fact that there are more collisions (that is, a higher collision frequency) means that there are more chances for a successful reaction to occur.

Check-in questions – Set 1

1 A chemical reaction between gases is occurring in a 250 mL container. The scientist wants to speed up the reaction and so decreases the volume of the container to 100 mL.
   a What will this change do to the pressure inside the container?
   b Will this change successfully increase the rate of the reaction? Explain why or why not.
2 State whether the following statements are true or false.
   a Decreasing the concentration of a solution leads to an increased collision frequency.
   b Increasing the concentration of a solution leads to an increase in the kinetic energy of the particles.
   c Increasing the concentration of a solution increases the rate of reaction by decreasing the activation energy.
   d Decreasing the concentration leads to a decreased rate of reaction.

Surface area and rate of reaction

Relationship: An increase in **surface area** leads to an increased rate of reaction. (Note: Sometimes you will see this described in terms of particle size. In this instance, the relationship is: An increase in particle size leads to a decreased rate of reaction.)

Surface area a measure of the area of a solid that is exposed and able to react

Explanation: When we talk about an increased surface area, it may be helpful to picture some examples. In Figure 5B–4, we can see an image of a solid piece of sodium metal (left) and sodium powder reacting (right). The solid sodium has a much lower surface area than the sodium powder, which is why the rate of reaction for the powder is so much greater (and explosive!).

Figure 5B–4 Solid sodium (left) is safe to have in the open as the surface area that can react with the atmosphere is a small proportion of the volume of the object, and thus the reaction rate is low. Powdered sodium (right), however, is made of many small particles, all of which can react with the atmosphere. Therefore, the reaction rate is fast (and the reaction is violent!).

So why does an increased surface area lead to an increased rate of reaction? To answer this, we must refer to collision theory again. A summary of this is provided in Table 5B–3.

Table 5B–3 The effect of an increased surface area on the different aspects of collision theory

Collision theory	Effect of increased surface area
Particles must collide	Increased collision frequency
Particles must collide with sufficient energy	No effect
Particles must collide in the correct orientation	No effect

To understand exactly why an increased surface area leads to an increased collision frequency, it can be helpful to visualise it (Figure 5B–5).

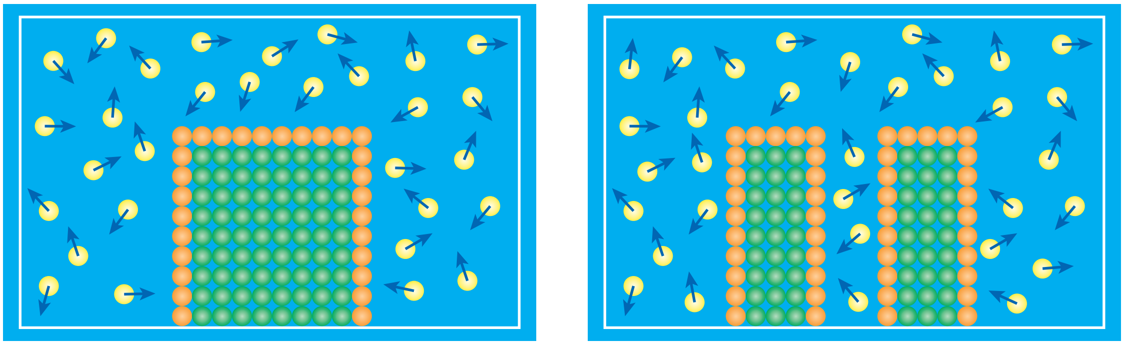

Figure 5B–5 Increasing the surface area of a reactant allows for an increased collision frequency. When there is a small surface area (left), there are fewer particles available to react (shown in orange) than when there is a larger surface area (right).

In Figure 5B–5, we can see clearly that it is just the particles on the outside that can collide with the other reactant in solution. However, as the surface area increases moving from left to right across the figure, the number of particles that are available to participate in collisions also increases.

Similar to concentration and gas pressure, an increased surface area doesn't affect the energy of the particles, nor the orientation that they collide in. However, once again, the fact that there are more collisions (that is, a higher collision frequency) means that there are more chances for a successful reaction to occur.

VIDEO 5B–1
HOW DOES TEMPERATURE AFFECT THE RATE OF A REACTION?

Temperature and rate of reaction

Relationship: An increase in temperature leads to an increased rate of reaction.

Explanation: Up until this point, the factors we have considered have affected the reaction rate by increasing the collision frequency. The effect of temperature requires us to understand an additional factor – the energy of collisions.

So why does an increased temperature lead to an increased rate of reaction? To answer this, we must refer to collision theory. A summary of this is provided in Table 5B–4.

Table 5B–4 The effect of an increased temperature on the different aspects of collision theory

Collision theory	Effect of increased temperature
Particles must collide	Increased collision frequency
Particles must collide with sufficient energy	Increased collisions with sufficient energy
Particles must collide in the correct orientation	No effect

For particles in a reaction mixture, as the temperature is increased, the added heat provides energy that they can use to move. This means that at higher temperatures, there are more particles that have higher amounts of kinetic energy. This can be represented through a graph known as a Maxwell–Boltzmann distribution curve (Figure 5B–6).

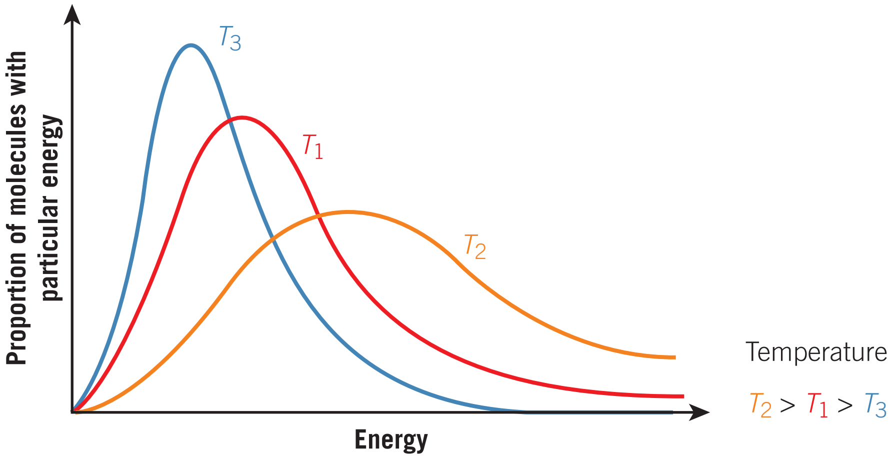

Figure 5B–6 A Maxwell–Boltzmann distribution curve showing that the proportion of molecules with higher energies increases as temperature increases

In Table 5B–4, we noted that this increase in kinetic energy of particles that results from an increase in temperature has two important outcomes on the rate of reaction.

1. As particles are moving around with greater energy, they are more likely to collide. This leads to an increased collision frequency.
2. As the particles that are colliding are likely to have greater energy due to the increase in temperature, these collisions are also more likely to be successful. This is because this increased energy means that a larger proportion of particles are colliding with energy greater than the activation energy. We can also represent this using a Maxwell–Boltzmann distribution curve (Figure 5B–7).

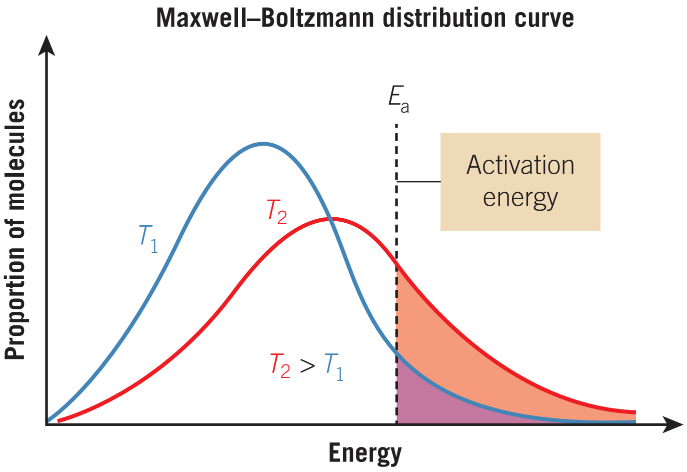

Figure 5B–7 At higher temperatures, there are more particles that have energy greater than the activation energy (E_a). At T_1, only particles in the purple shaded region would have sufficient energy to successfully react if they collided. However, at T_2, collisions between any of the particles in the purple and orange regions would have sufficient energy to react.This helps explain why higher temperatures result in an increased rate of reaction.

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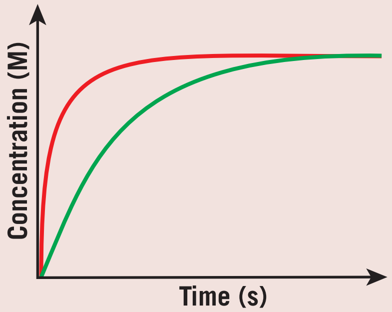
VIDEO
WORKED
EXAMPLE 5B–1

Worked example 5B–1: Comparing rate of reaction graphs

You are provided with a graph (on the right) that has two curves showing the rate of reaction at 10°C and 30°C. However, the curves are not labelled. Determine which curve corresponds to which experiment and explain your reasoning.



Solution

	Logic	Process
Step 1	Identify the factor that is being changed that will affect the rate of reaction.	In this experiment, the factor is temperature. Reactions are occurring at 10°C and 30°C.
Step 2	Recall the relationship between the factor and the rate of reaction.	An increase in temperature results in an increase in the rate of reaction.
Step 3	Identify which curve on the graph displays a greater rate of reaction.	The red curve represents a faster rate of reaction, as it has a steeper slope.
Step 4	Piece together Steps 1–3 to answer the question.	The red curve is the faster reaction, so it must be the one that occurs at 30°C, as a higher temperature leads to a higher rate of reaction. This means that the green curve is the reaction taking place at 10°C.

Catalysts and rate of reaction

Relationship: The presence of a catalyst leads to an increased rate of reaction.

Catalyst
a substance that increases the rate of a chemical reaction by lowering the activation energy by providing an alternative reaction pathway and is itself not consumed as part of the reaction

Explanation: **Catalysts** speed up the rate of a reaction by providing an alternative reaction pathway with a lower activation energy. This means that when the reaction occurs via the catalyst, the reactants need less energy for a successful reaction. This can be illustrated using an energy profile diagram (Figure 5B–8).

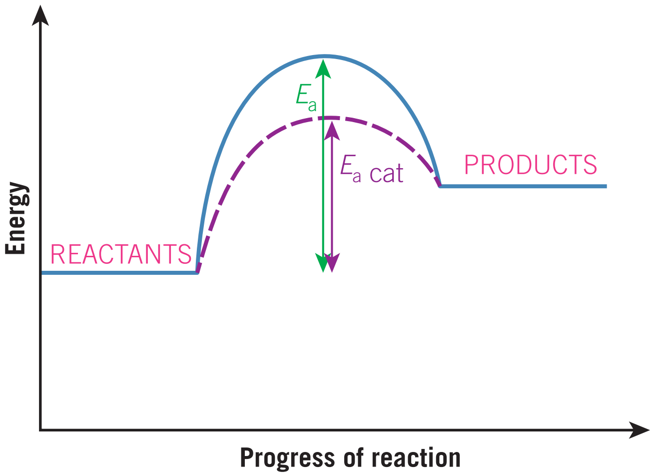


Figure 5B–8 A catalyst provides an alternative reaction pathway that lowers the activation energy of a reaction (purple dotted line) compared to the uncatalysed reaction (blue line).

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For all the other adjustable factors, we have explained their impact on the rate of reaction by linking them back to the factors that comprise collision theory. This is a little bit more difficult to do when discussing the effect that a catalyst has, as it potentially creates a situation that changes both the collision frequency and the number of collisions that have the correct orientation. However, the chemistry behind those two outcomes is beyond the scope of this course.

However, the one aspect of collision theory that is clearly altered as a result of including a catalyst in a chemical reaction is the number of collisions that have sufficient energy to react. Similar to temperature, this can be highlighted through using a Maxwell–Boltzmann distribution curve (Figure 5B–9).

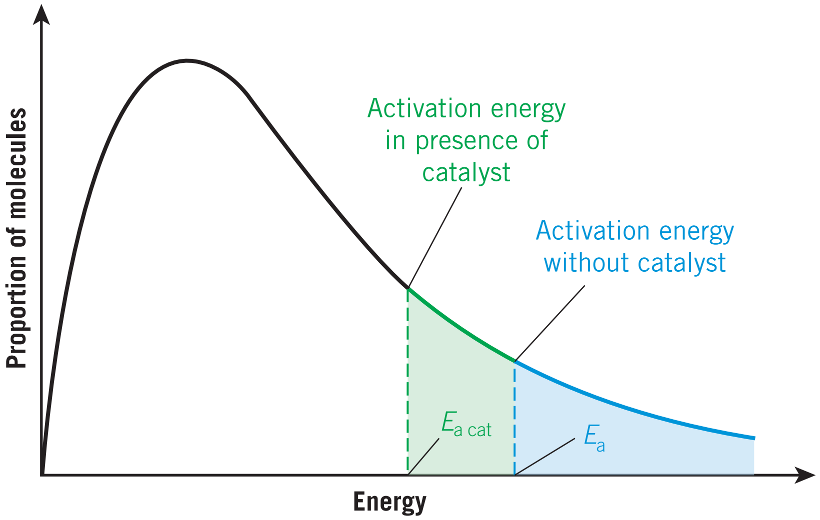


Figure 5B–9 Catalysed and uncatalysed activation energies on a Maxwell–Boltzmann distribution curve. Without a catalyst, only the particles in the blue shaded area will have sufficient energy to react. However, with a catalyst present, the particles in both the green and blue shaded areas will have sufficient energy to react.

In Figure 5B–9, without a catalyst, only the particles in the blue shaded area have sufficient energy to react. In the presence of a catalyst, all the particles in both the green and blue shaded areas would have sufficient energy to react.

This shows us that raising the temperature and including a catalyst both speed up the rate of a reaction by increasing the proportion of collisions that have sufficient energy to react (that is, energy greater than the activation energy). However, it is important to note the distinction between how they do this. This can be understood through the following simple analogy.

Let us assume that you have an upcoming chemistry test and the teachers have said that everyone who gets above 80% will be allowed to go on an excursion to the museum. A practice test is held the week before and only one student scores above 80%. Knowing that the school cannot run an excursion for just a single student, the teachers come up with two strategies to ensure that higher marks are achieved on the real test. These plans are:

1 Run after school tutorials on the test topic every day for the next week. With this extra help, more students should get above 80% on the test. This is the equivalent of raising the temperature of a reaction – it ensures that more particles have sufficient energy to overcome the activation energy.

2 Decide that a score of only 60% is required to go on the excursion, so that more students end up with a grade that allows them to go to the museum. This is the equivalent of using a catalyst – the activation energy is lower and so the threshold required for particles to react is also lower, which means that more particles have sufficient energy.

Heterogeneous a mixture composed of substances in different states or phases

Homogeneous a mixture composed of substances in the same state or phase

There are two types of catalysts – **heterogeneous** and **homogeneous** – and they differ based on their state compared with the reactants (Figure 5B–10). Zinc, for example, is the solid metal coating used in catalytic converters of cars and is considered a heterogeneous catalyst, as the reactants it facilitates are the gases emitted from fuel combustion. Adenosine triphosphate, or ATP, is considered a homogeneous catalyst in biological systems, as both it and the reactions it facilitates are aqueous in nature.

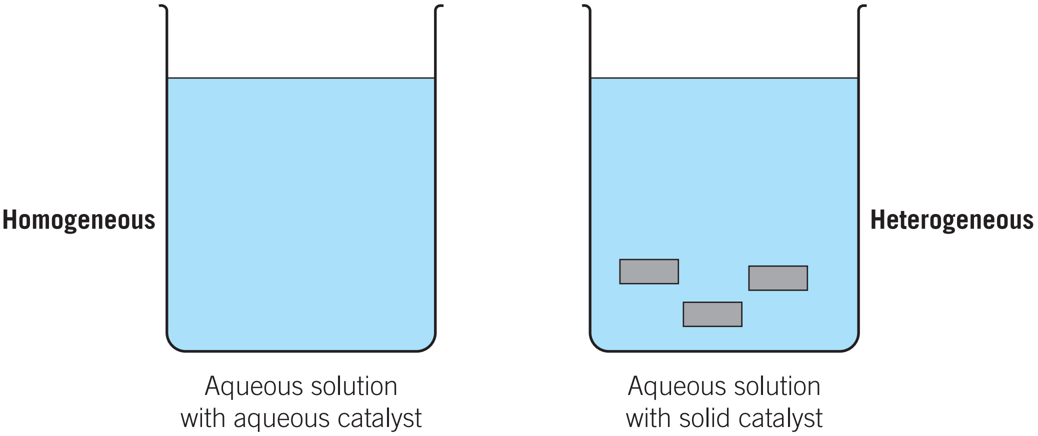


Figure 5B–10 Homogeneous catalysis occurs when both the catalyst and reactants are in the same phase (left), whereas heterogeneous catalysis occurs across different phases, such as aqueous reactants and a solid catalyst (right).

WORKSHEET 5B–1 ANALYSING RATES OF REACTION DATA

12B ENZYMES LINK

Catalysts, like the reactions they facilitate, can also be limited in their ability to work. Anything that alters the state of the catalyst affects it negatively (for example, rust affecting the surface area of a catalyst in a car catalytic converter). What this means is that all catalysts, both chemical and biological, have optimum conditions under which they work. These conditions include temperature, pH and oxidative state, to name a few. When we hear of a reaction that uses a catalyst, we should also consider the optimum conditions for the catalyst so it can have its effect. This will be discussed in more detail in Section 12B.

5B SKILLS

Structuring answers to questions
You will have noticed throughout this section that there was a clear emphasis placed on how to explain the relationship between different reaction conditions and their effect on the rate of a given reaction. While adopting a clear process like this should be beneficial for your understanding, it is also a helpful method to use for structuring your responses to questions.

This can be clearer by looking at a question and two potential answers for it.

Question:
Describe and explain the relationship between temperature and rate of reaction.

Answer 1:
Temperature impacts on the rate of reaction. If the temperature is higher, the rate of reaction will change and become faster. When the temperature is higher, more particles will have sufficient energy to react. This will increase the rate of reaction. Also, there will be an increased collision frequency, which will also cause the rate of reaction to increase. At higher temperatures, more particles will have greater kinetic energy. This means they will collide more often and with more energy.

Answer 2:
An increase in temperature leads to an increase in the rate of reaction. At higher temperatures, more particles will have greater kinetic energy. This results in an increase in reaction rate for two reasons. Firstly, as particles are moving more rapidly, they will collide more often. This results in an increased collision frequency and so more chances for a successful reaction to occur. Secondly, as particles have greater kinetic energy, this means that there will be more particles that have sufficient energy to react (that is, energy greater than the activation energy of the reaction). Both of these factors combine to contribute to the increased rate of reaction seen at higher temperatures.

While you can see that both answer 1 and answer 2 contain quite similar information regarding the relationship between temperature and rate of reaction, there is a clear difference in terms of how well they are structured. Answer 2 contains a much clearer structure, which effectively links all of the concepts together in an ordered fashion. Having your answers well structured like this makes it much easier for anyone assessing your work to see your understanding of the topic and provide you with full marks for the question.

Section 5B questions

1 List the reaction conditions that affect the following aspects of collision theory.
  a collision frequency
  b collisions with energy greater than the activation energy

2 For the following pairs, identify which would result in a faster reaction (assuming all other conditions were constant).
  a a large block of aluminium versus aluminium ‘chips’
  b room temperature versus in the fridge
  c 0.01 M sodium hydroxide versus 100 mM sodium hydroxide
  d 25 mL container versus 0.25 L container

3 Cellular respiration involves the breakdown of glucose to produce carbon dioxide, water and energy in the form of ATP. To test different reaction conditions on the cellular respiration of yeast, an experiment is set up to capture the carbon dioxide that is released.

The data recorded from this experiment is as follows.

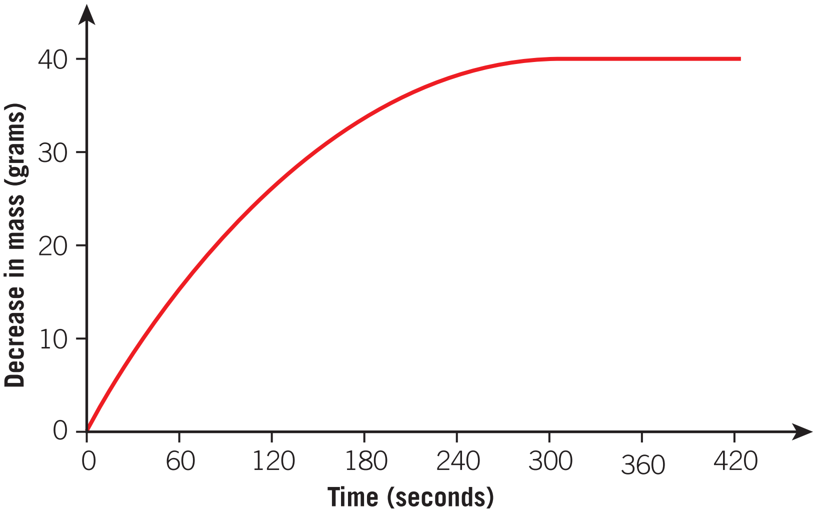
	0 mins	2 mins	4 mins	6 mins	8 mins	10 mins
Exp #1	0.00 mL	2.87 mL	5.05 mL	6.15 mL	6.45 mL	6.5 mL
Exp #2	0.00 mL	2.92 mL	5.01 mL	6.18 mL	6.45 mL	6.52 mL
Exp #3	0.00 mL	2.91 mL	4.99 mL	6.16 mL	6.48 mL	6.49 mL

- **a** Draw a graph that represents these data.
- **b** On your graph, draw and label the result you would expect to observe if the experiment was repeated with yeast that were missing the enzyme that acts as a catalyst for this reaction. You can assume that the reaction can still occur without the enzyme present.
- **c** Describe the difference between a homogeneous and heterogeneous catalyst.

4 Calcium carbonate reacts with hydrochloric acid according to the following equation:

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

The graph below shows the reaction that occurs when 500 mL of 3.64 M hydrochloric acid is added to 385 g of powdered calcium carbonate at room temperature.



Copy the graph above and sketch the graph that you would expect if each of the following changes were made.

- **a** A catalyst is added.
- **b** The HCl is heated to 50°C before it is used.
- **c** 4.50 M HCl is used.
- **d** 0.50 M HCl is used.
- **e** 500 g of $CaCO_3$ is used.

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Chapter 5 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
5A.1	Differentiate between open and closed systems	1☐
5A.2	Outline how reactions proceed differently in open and closed systems	3☐, 13☐
5A.3	Describe the factors that comprise collision theory	2☐, 10☐, 12☐
5A.4	Describe how the rate of a reaction can be monitored	8☐, 13☐
5B.1	Explain the relationship between concentration and rate of reaction	13☐
5B.2	Explain the relationship between gas pressure and rate of reaction	3☐, 12☐
5B.3	Explain the relationship between surface area and rate of reaction	7☐, 12☐
5B.4	Explain the relationship between temperature and rate of reaction	3☐, 6☐, 11☐, 12☐, 13☐
5B.5	Outline the effect of temperature on the rate of reaction using a Maxwell–Boltzmann distribution curve	4☐, 11☐
5B.6	Explain the relationship between the presence of a catalyst and rate of reaction	3☐, 5☐, 11☐, 13☐
5B.7	Outline the effect of a catalyst on the rate of reaction using an energy profile diagram	11☐
5B.8	Outline the effect of a catalyst on the rate of reaction using a Maxwell–Boltzmann distribution curve	9☐, 11☐

Multiple-choice questions

1 The biggest difference between an open and a closed system is that

A an open system lets in heat, whereas a closed system does not.

B a closed system lets in heat, whereas an open system does not.

C compounds produced in an open system can be released into the surroundings.

D compounds produced in a closed system can be released into the surroundings.

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2 Which of the following is **not** a requirement for a reaction to occur?

A reactant particles colliding

B reactant particles colliding in the correct orientation

C reactant particles colliding with energy greater than the enthalpy

D reactant particles colliding with energy greater than the activation energy

3 In the below equation, monitoring the production of carbon dioxide is a valid way to measure the rate of reaction.

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

Which of the following would make this difficult?

A performing the reaction using a catalyst

B performing the reaction at room temperature

C performing the reaction at low gas pressures

D performing the reaction in an open system

4 You are provided with a Maxwell–Boltzmann distribution curve that shows the distributions of particles at 4°C and 25°C. Which statement is most accurate about the 4°C peak compared to the 25°C peak?

A It will be lower and shifted to the left.

B It will be lower and shifted to the right.

C It will be higher and shifted to the left.

D It will be higher and shifted to the right.

5 Which of the following combinations is true for a reaction in the presence of a catalyst?

	Reaction rate	Activation energy
A	Lower	Lower
B	Higher	Higher
C	Higher	Lower
D	Lower	Higher

6 Which of the following statements is true regarding the behaviour of particles that are moved from a high temperature to a low temperature?

A Their average kinetic energy will increase.

B Their frequency of collisions will increase.

C Their Maxwell–Boltzmann distribution curve will flatten out.

D Their collisions are less likely to lead to a successful reaction.

7 You perform an experiment in which three beakers are set up with 50 mL of an aqueous solution of 0.1 M hydrochloric acid. Into beaker 1, you add magnesium powder. Into beaker 2, you add magnesium ribbon. Into beaker 3, you add a single block of magnesium. The mass of magnesium in all beakers is the same.

Which beaker would have the fastest rate of reaction?

A beaker 1

B beaker 2

C beaker 3

D The rate would be equal in all beakers.

8 You perform an experiment in which the reaction creates hydrogen gas as a product. To monitor the rate, you measure the volume of gas that is produced and record it after the reaction is completed. The best reason that this is not an effective way to measure reaction rate is because

A a gas product cannot be used to calculate rate.

B the measurements were not taken over time.

C it does not take into account the temperature of the room.

D the volume of hydrogen at the end of the reaction would be too small to measure accurately.

9 On a Maxwell–Boltzmann distribution curve, in relation to an uncatalysed activation energy, a catalysed activation energy would appear

A to the left on the x-axis.

B to the right on the x-axis.

C lower on the y-axis.

D higher on the y-axis.

10 Which of the following statements regarding collision theory is correct?

A Particles colliding with sufficient energy and an incorrect orientation will result in a successful reaction.

B Particles colliding with energy lower than the activation energy and the correct orientation will result in a successful reaction.

C Particles colliding with energy greater than the activation energy and the incorrect orientation will result in a successful reaction.

D Particles colliding with sufficient energy and the correct orientation will result in a successful reaction.

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Short-answer questions

11 A chemical reaction was performed that resulted in an aqueous solution going from colourless to dark blue. Your lab partner performed the experiment at two different temperatures to observe the effect that this had on the rate of reaction. All other variables were kept constant. Your partner produced the data table below, which shows their observation of the colour change every minute for 10 minutes (+ = colourless, +++++ = dark blue).

	0 min	1 min	2 min	3 min	4 min	5 min	6 min	7 min	8 min	9 min	10 min
T1	+	+	++	+++	+++	++++	+++++	+++++	+++++	+++++	+++++
T2	+	+	+	+	++	++	++	++	+++	+++	+++

a Unfortunately, your lab partner didn't note what sample was at what temperature and only recorded T1 and T2. Based on the data, state what you can say about the two temperatures and justify your answer. (2 marks)

b Draw a fully labelled Maxwell–Boltzmann distribution curve for the reacting particles in the samples at T1 and T2. (3 marks)

c Using your diagram from part **b**, explain the results observed in the experiment. (4 marks)

d You perform the same experiment as your partner; however, you decide to add a catalyst and observe the results. A colourless aqueous catalyst is added to beaker 2, while the same volume of water is added to beaker 1. Describe what you would observe in both beakers. (1 mark)

e Draw an energy profile diagram that illustrates the effect that the presence of a catalyst has on this reaction. It is known that the reaction is endothermic. (3 marks)

f Describe the effect that a catalyst has on the rate of a reaction. (2 marks)

g Using a Maxwell–Boltzmann distribution curve, explain how a catalyst has the effect described in part **f**. (4 marks)

12 One of the most fundamental chemical reactions in nature is the one that produces water, shown by the equation below.

$$2H_2(g) + O_2(g) \rightarrow 2H_2O(l)$$

a Using collision theory, describe what must happen for water to be produced. (3 marks)

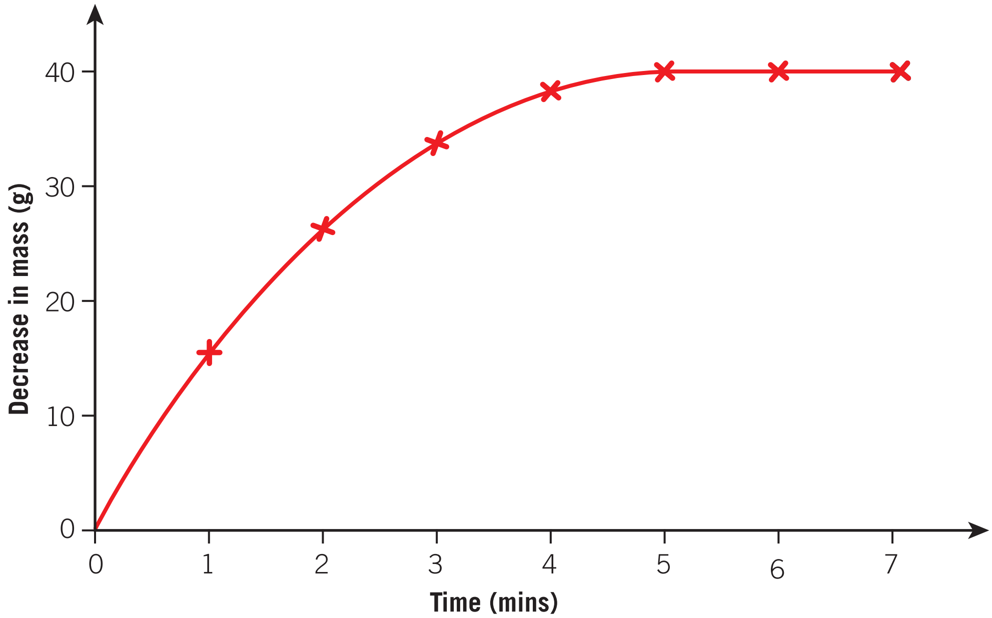
b State two ways that you could increase the rate of this reaction by increasing the collision frequency. (2 marks)

c Explain why increasing the surface area is not a viable way to increase the rate of this reaction. (2 marks)

13 Solid calcium carbonate reacts with aqueous solutions of hydrochloric acid to produce calcium chloride, water and carbon dioxide.

a Write a balanced equation for this reaction. (1 mark)

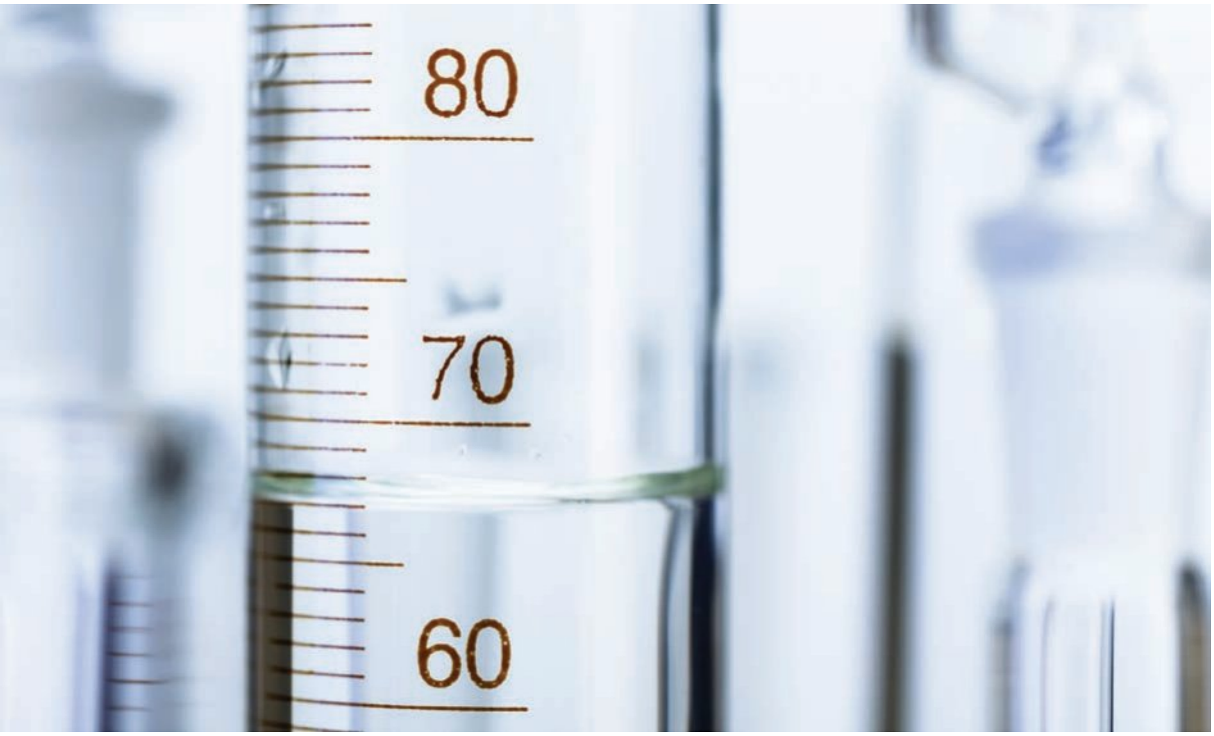
The graph on the following page shows the rate of the reaction, as measured by a loss of mass in grams recorded at 60 second intervals, when 500 mL of 3.64 M hydrochloric acid is added to 385 g of powdered calcium carbonate at room temperature.

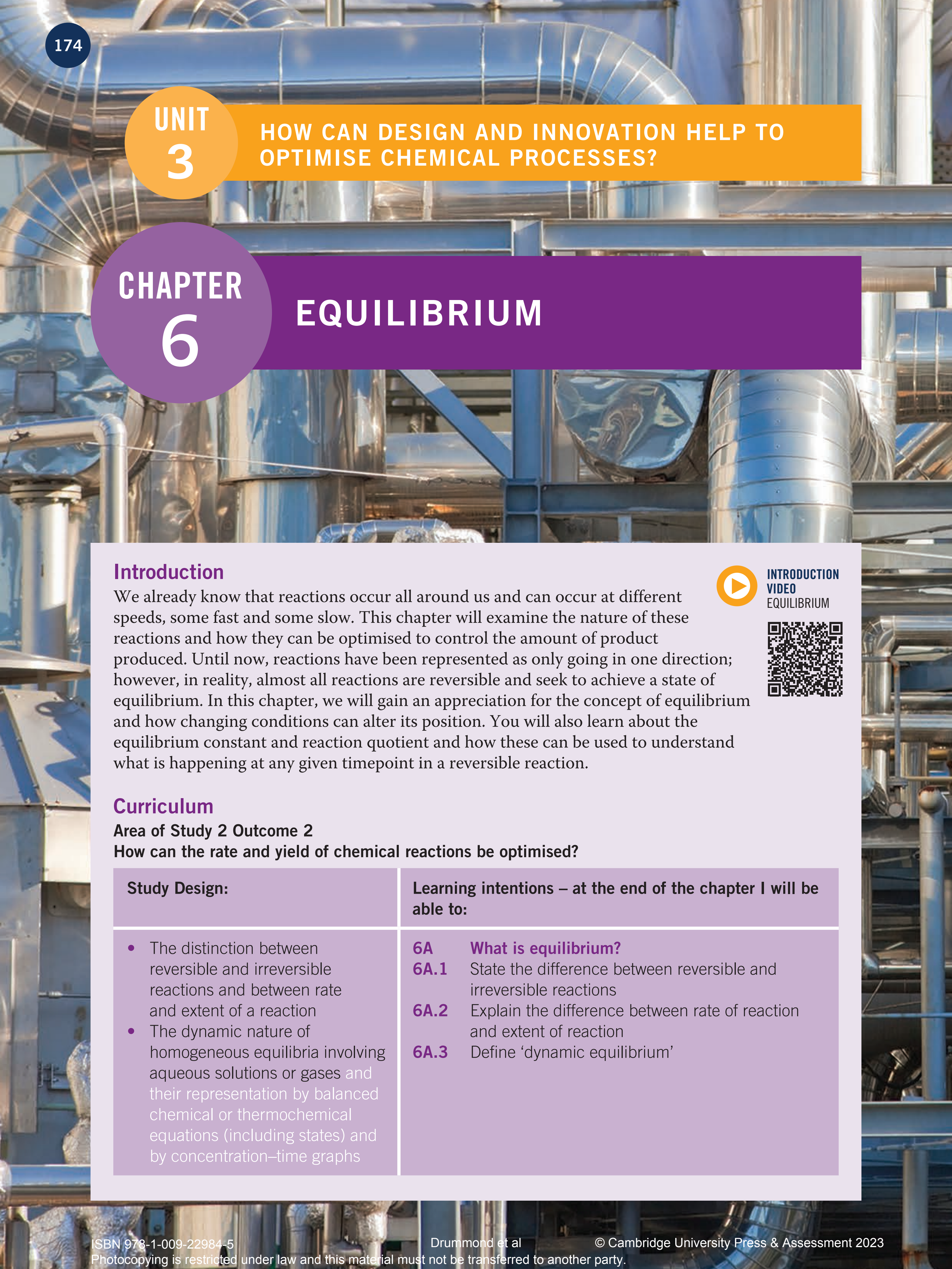


b What does the method of measurement for the rate of this reaction tell you about the system it must be occurring in? (2 marks)

c On a copy of the graph above, sketch what you expect to observe if the following changes were made.

- **i** A catalyst is added. (1 mark)
- **ii** The hydrochloric acid is heated to 50°C before it is used. (1 mark)
- **iii** 4.50 M hydrochloric acid is used. (1 mark)
- **iv** 0.50 M hydrochloric acid is used. (1 mark)
- **v** 500 g of calcium carbonate is used. (1 mark)





UNIT 3 HOW CAN DESIGN AND INNOVATION HELP TO OPTIMISE CHEMICAL PROCESSES?

CHAPTER 6 EQUILIBRIUM

Introduction

INTRODUCTION VIDEO
EQUILIBRIUM

We already know that reactions occur all around us and can occur at different speeds, some fast and some slow. This chapter will examine the nature of these reactions and how they can be optimised to control the amount of product produced. Until now, reactions have been represented as only going in one direction; however, in reality, almost all reactions are reversible and seek to achieve a state of equilibrium. In this chapter, we will gain an appreciation for the concept of equilibrium and how changing conditions can alter its position. You will also learn about the equilibrium constant and reaction quotient and how these can be used to understand what is happening at any given timepoint in a reversible reaction.

Curriculum

Area of Study 2 Outcome 2
How can the rate and yield of chemical reactions be optimised?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• The distinction between reversible and irreversible reactions and between rate and extent of a reaction • The dynamic nature of homogeneous equilibria involving aqueous solutions or gases and their representation by balanced chemical or thermochemical equations (including states) and by concentration–time graphs	**6A What is equilibrium?** **6A.1** State the difference between reversible and irreversible reactions **6A.2** Explain the difference between rate of reaction and extent of reaction **6A.3** Define ‘dynamic equilibrium’

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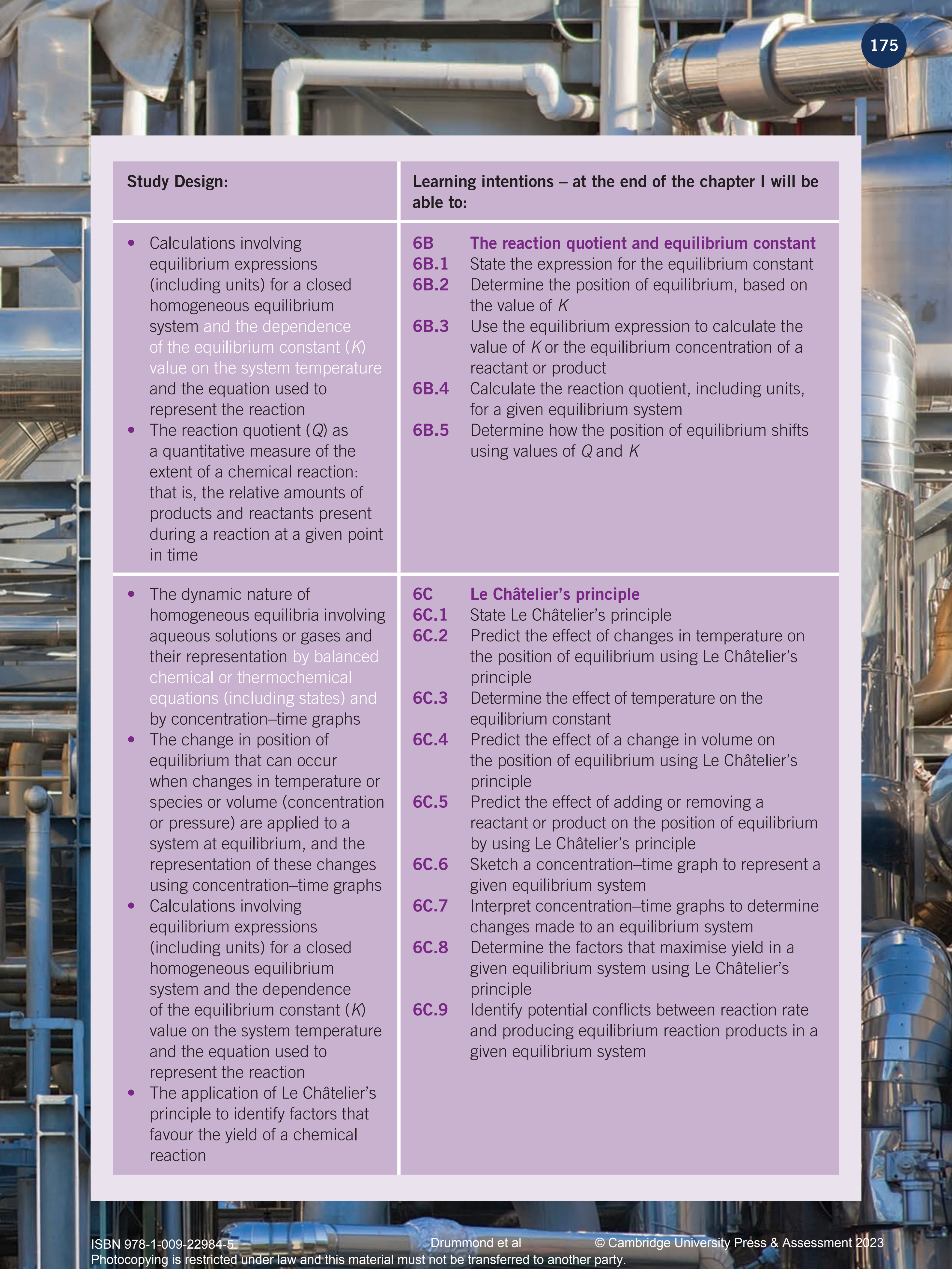

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Calculations involving equilibrium expressions (including units) for a closed homogeneous equilibrium system and the dependence of the equilibrium constant (K) value on the system temperature and the equation used to represent the reaction • The reaction quotient (Q) as a quantitative measure of the extent of a chemical reaction: that is, the relative amounts of products and reactants present during a reaction at a given point in time	**6B The reaction quotient and equilibrium constant** **6B.1** State the expression for the equilibrium constant **6B.2** Determine the position of equilibrium, based on the value of K **6B.3** Use the equilibrium expression to calculate the value of K or the equilibrium concentration of a reactant or product **6B.4** Calculate the reaction quotient, including units, for a given equilibrium system **6B.5** Determine how the position of equilibrium shifts using values of Q and K
• The dynamic nature of homogeneous equilibria involving aqueous solutions or gases and their representation by balanced chemical or thermochemical equations (including states) and by concentration–time graphs • The change in position of equilibrium that can occur when changes in temperature or species or volume (concentration or pressure) are applied to a system at equilibrium, and the representation of these changes using concentration–time graphs • Calculations involving equilibrium expressions (including units) for a closed homogeneous equilibrium system and the dependence of the equilibrium constant (K) value on the system temperature and the equation used to represent the reaction • The application of Le Châtelier's principle to identify factors that favour the yield of a chemical reaction	**6C Le Châtelier's principle** **6C.1** State Le Châtelier's principle **6C.2** Predict the effect of changes in temperature on the position of equilibrium using Le Châtelier's principle **6C.3** Determine the effect of temperature on the equilibrium constant **6C.4** Predict the effect of a change in volume on the position of equilibrium using Le Châtelier's principle **6C.5** Predict the effect of adding or removing a reactant or product on the position of equilibrium by using Le Châtelier's principle **6C.6** Sketch a concentration–time graph to represent a given equilibrium system **6C.7** Interpret concentration–time graphs to determine changes made to an equilibrium system **6C.8** Determine the factors that maximise yield in a given equilibrium system using Le Châtelier's principle **6C.9** Identify potential conflicts between reaction rate and producing equilibrium reaction products in a given equilibrium system

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Responses to the conflict between optimal rate and temperature considerations in producing equilibrium reaction products, with reference to the green chemistry principles of catalysis and designing for energy efficiency	**6C.10** Describe the green chemistry principle of catalysis **6C.11** Describe the green chemistry principle of designing for energy efficiency **6C.12** Explain how the green chemistry principles of catalysis and designing for energy efficiency can solve conflicts between optimal reaction rate and producing equilibrium reaction products in equilibrium systems

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Glossary

Dynamic equilibrium
Equilibrium
Equilibrium constant
Extent of reaction
Homogeneous equilibrium
Irreversible reaction
Le Châtelier’s principle
Position of equilibrium
Reaction quotient
Reversible reaction

Concept map

6A What is equilibrium?

Understanding the concept of reversible chemical reactions

Forward reaction $A + B \longrightarrow C + D$

Reverse reaction $C + D \longrightarrow A + B$

Reversible reaction $A + B \rightleftharpoons C + D$

6B The reaction quotient and equilibrium constant

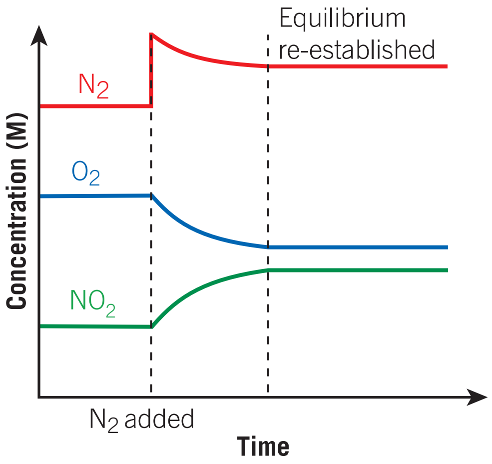
Calculations to determine the position of a reversible reaction at any given moment

$$aA + bB \rightleftharpoons cC + dD$$

$$K = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

6C Le Châtelier's principle

Understanding how a change in reaction conditions, such as temperature and pressure, impact the position of equilibrium



See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

6A What is equilibrium?

Study Design:

- The distinction between reversible and irreversible reactions and between rate and extent of a reaction
- The dynamic nature of homogenous equilibria involving aqueous solutions or gases and their representation by balanced chemical or thermochemical equations (including states) and by concentration–time graphs

Glossary:

Dynamic equilibrium
Equilibrium
Extent of reaction
Homogeneous equilibrium
Irreversible reaction
Position of equilibrium
Reversible reaction

ENGAGE

Cooking – an irreversible reaction

Cooking food is a great everyday example of chemical reactions taking place. When you place an egg in boiling water, for example, reactions are taking place that convert the runny, raw egg into the cooked version that you see here. Importantly, once you have cooked the egg, you can't turn it back into a raw egg and undo that process by placing it in the fridge or freezer. Initially, scientists believed that this was the only way reactions worked – reactants were turned into products and this process was final. However, in this section, you are going to learn that many chemical reactions are in fact reversible. You will learn the difference between reversible and irreversible reactions, as well as begin to understand that reversible reactions seek a balanced outcome, known as equilibrium.

EXPLAIN

Reversible and irreversible reactions

When we have looked at chemical equations and reactions so far, they have operated from left to right: reactants are used up and products are formed. However, in many situations the products of a reaction can also interact and form the original reactants. When a reaction can proceed in either direction, it is called a **reversible reaction**. In reversible reactions, the formation of products is called the forward reaction and the formation of the initial reactants is called the reverse, or backwards, reaction. To express the simultaneous reactions occurring forwards and backwards, two half-arrows are used rather than a single arrow.

Reversible reaction
a reaction that can proceed in both directions: from reactants to products and products to reactants

Forward reaction $A + B \longrightarrow C + D$

Reverse reaction $C + D \longrightarrow A + B$

Reversible reaction $A + B \rightleftharpoons C + D$

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In a closed system (so no reactants or products enter or escape), reversible reactions reach a state known as **equilibrium**. This is where the concentrations of reactants and products do not change. However, this does not mean there is no movement in the reaction. In equilibrium systems, there is still movement but the forward and reverse reactions are occurring at the same rate. This state of constant, equal movement is known as **dynamic equilibrium**.

Equilibrium the state in which the concentration of reactants and products does not change

Dynamic equilibrium when the forward and reverse reactions are occurring at the same non-zero rate

Many equilibrium systems in chemistry are dynamic, which means the following occur:

- All equilibrium reactions are incomplete, as both reactants and products are present at equilibrium.
- Bonds are constantly being made and broken – for both products and reactants.
- Energy is being transformed and used in the making and breaking of bonds.

This doesn't mean that **irreversible reactions** do not exist. There are lots of examples where reactions occur and their reverse reaction does not, such as the combustion of fossil fuels. Similarly, burning wood is impossible to 'un-burn'.

Irreversible reaction a unidirectional reaction where the reactants are converted to products, which cannot react further to produce the starting compounds again

Figure 6A–1 Rechargeable batteries and maintaining swimming pools both rely on reversible chemical reactions.

Extent of reaction versus rate of reaction

LINK CHAPTER 5

As we saw in Chapter 5, the rate of a chemical reaction represents the speed at which reactants are consumed and products are formed. It describes how quickly the concentrations of reactants and products change over time. Factors such as temperature, concentration, surface area and catalysts can influence the rate of a reaction. It is commonly expressed as the change in concentration of a reactant or product per unit of time.

The **extent of reaction**, however, refers to the degree to which the reaction proceeds towards completion. It tells us the amount of reactants that have been converted into products at a particular point in time.

To assess the extent of the reaction, we need to examine the relative concentrations of the reactants and products. If the concentrations of reactants are high and the concentrations of products are low, it suggests that the reaction has not proceeded significantly towards the product side. Conversely, if the concentrations of reactants are low and the concentrations of products are high, it indicates that the reaction has proceeded significantly towards the product side. Performing this assessment allows us to determine the **position of equilibrium** of a reaction and whether reactants or products are favoured at a given moment or concentration.

Extent of reaction the degree to which a reaction goes to completion

Position of equilibrium a quantitative measure of the relative amounts of reactants and products in an equilibrium system

Characteristics of an equilibrium system

There are five main characteristics of an equilibrium system:

- The reaction occurs in a closed system.
- The rate of forward and reverse reactions are equal.
- At equilibrium, there is a mixture of reactants and products.
- The concentrations of reactants and products are constant.
- The macroscopic properties appear constant.

Homogeneous equilibria

Equilibrium reactions can occur in many ways. In this chapter, we are going to focus on **homogeneous equilibrium**, which occurs between reactants and products that are in the same phase. In all of the equilibrium systems that you encounter in this course, the reactions will be homogeneous.

Homogeneous equilibrium an equilibrium system where all of the reactants and products are in the same phase

6A SKILLS

Precise language

One of the things that will be incredibly important throughout this chapter is making sure that you always use precise and correct language. As you will have seen through the listed characteristics of a system at dynamic equilibrium, there are very specific criteria that must be met. Considering this, you also must be very particular about how you describe them. Let's look at the following two statements that may be used to describe a system at equilibrium:

1 At equilibrium, the concentration of reactants and products are the same.
2 At equilibrium, the concentration of reactants and products are constant.

While these two statements seem very similar, only one of them is correct. Indeed, the only difference between them is that one says the concentrations are 'the same' and the other says they are 'constant'. While you might argue that if things stay the same, they stay constant … that is not what the sentences say! With this wording, statement 1 is incorrect and statement 2 is correct.

A good way to ensure that you word answers correctly is to consistently use the appropriate terminology whenever you are writing about equilibrium. This includes writing notes, flash cards and practice answers. As the old saying goes, 'practice makes perfect'!

Section 6A questions

1 Provide two differences between reversible and irreversible reactions.
2 Using an example, explain how the extent of a reaction is apparent.
3 Explain the difference between rate of reaction and extent of reaction.
4 What is meant by the term 'homogeneous equilibrium'?
5 Are the following statements regarding a system at dynamic equilibrium true or false?
   a The reactions have stopped.
   b The concentration of reactants and products are always equal.
   c The rate of the forward and reverse reactions are equal.
   d The equilibrium only ends once all the reactants have been used up.
   e If the reaction resulted in a colour change, the colour would remain constant while at equilibrium.
6 For the homogeneous equilibrium reaction: $2NO_2(g) \rightleftharpoons N_2O_4(g)$, describe what is happening at the molecular level when the system is at dynamic equilibrium.

6B The reaction quotient and equilibrium constant

Study Design:

- Calculations involving equilibrium expressions (including units) for a closed homogeneous equilibrium system and the dependence of the equilibrium constant (*K*) value on the system temperature and the equation used to represent the reaction
- The reaction quotient (*Q*) as a quantitative measure of the extent of a chemical reaction: that is, the relative amounts of products and reactants present during a reaction at a given point in time

Glossary:

Equilibrium constant
Reaction quotient

ENGAGE

From salt lakes to drug development

The concept of equilibrium was first raised in 1803 by a French chemist, Claude Louis Berthollet, after observations he made while studying sodium carbonate formation at the edge of salt lakes. However, it wasn't until 1864 that these findings were advanced into a mathematical relationship by Cato Guldberg and Peter Waage, who proposed the 'law of mass action'. In equilibrium reactions, this law encompasses the equilibrium expression, which is the topic of this section. This expression has been critically important in pharmacology, as it is used routinely to investigate the physiological impacts of medications, by looking at factors like dose–response curves or the rate at which a drug may bind to a receptor in the body. In this section, you will learn more about the equilibrium constant, *K*, as well as the reaction quotient, *Q*, how they relate to each other and how you can perform calculations for both.

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EXPLAIN

Locating equilibrium

CHAPTER 5 LINK

In Chapter 5, you learned that reactions have rates. For reactions that have reached equilibrium, they appear to have ‘no rate’ because the rates of the forward and reverse reactions are equal. This doesn’t mean that the concentrations of products and reactants are equal – the extent of the reaction gives us the final position of the reaction once it has reached equilibrium.

The easiest way to view this is by observing the concentration versus time graph for a given reaction. Let’s consider the reaction between N_2 and O_2 as they form NO_2. As mentioned in the previous section, a two-directional arrow indicates that the reaction is reversible.

$$N_2(g) + 2O_2(g) \rightleftharpoons 2NO_2(g)$$

The reaction between N_2 and O_2 to form NO_2 can be measured graphically by plotting the concentration of the different species over time, as in Figure 6B–1. As time increases, the concentrations reach a constant level; at this point the reaction has reached equilibrium.

Another way this can be considered is by viewing the rate of the forward and backward reactions side by side, as in Figure 6B–2.

Here, we can see the initial rate of the forward reaction is very high, as there are only reactants, but this decreases over time. However, once products are formed, the rate of the reverse reaction increases and eventually plateaus. At the point where both rates are equal and constant, equilibrium is reached.

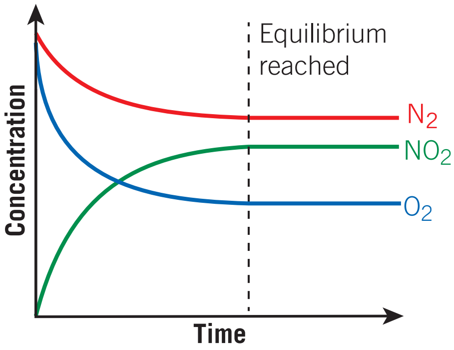

Figure 6B–1 A concentration–time graph of the reaction $N_2 + 2O_2 \rightleftharpoons 2NO_2$

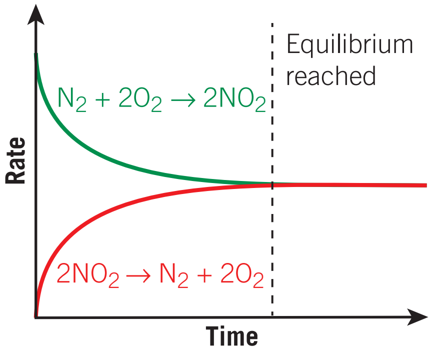

Figure 6B–2 A rate–time graph of the forward (green) and backward (red) reactions for the equilibrium system $N_2 + 2O_2 \rightleftharpoons 2NO_2$

The reaction quotient, *Q*

Reaction quotient the measurement of the relative amounts of products and reactants in a given reaction; symbol *Q*

The **reaction quotient** represents the ratio of molecules participating in a reaction at any given timepoint. We can think about a generalised chemical equation being represented as:

$$aA + bB \rightleftharpoons cC + dD$$

where A and B are the reactants, C and D are the products and the lower case letters represent their coefficients in a balanced equation.

The reaction quotient, represented by the symbol Q, for this reaction can be expressed as:

$$Q = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

As you can see from this expression, the reaction quotient is the concentrations of the products raised to the powers of their coefficients, divided by the concentrations of the reactants raised to the power of their coefficients.

As an example, if we have the reaction between nitrogen gas and oxygen gas to produce NO_2:

$$N_2(g) + 2O_2(g) \rightleftharpoons 2NO_2(g)$$

The reaction quotient for this reaction will be expressed as:

$$Q = \frac{[NO_2]^2}{[N_2][O_2]^2}$$

Note that powers in the expression match the stoichiometries of the initial reaction. The value of Q for this reaction, based on reactant and product concentrations at different timepoints, is calculated in Table 6B–1.

Table 6B–1 Calculating the reaction quotient from the stoichiometries of the reaction

Time (s)	$[N_2]$	$[O_2]$	$[NO_2]$	Q
1	0.05	0.10	0.00001	2×10^{-7}
10	0.02	0.04	0.06	1.13×10^{2}
20	0.01	0.02	0.13	4.23×10^{3}

Notice how at different timepoints within the reaction, the reaction quotient can give different values. This is because the reaction hasn't yet reached equilibrium. Once the system does reach equilibrium, Q becomes constant. To differentiate between a system in dynamic equilibrium and one that is not, this constant is referred to as the equilibrium constant.

The equilibrium constant, K

The **equilibrium constant,** K (sometimes also expressed as K_c), is expressed in exactly the same way as the reaction quotient. The only difference is, because the reaction has reached equilibrium, the value is a constant and always applies for that particular reaction under the given conditions. However, it is important to note that changing the temperature will change the value of the equilibrium constant. You will learn more about this in Section 6C.

Equilibrium constant the value of the reaction quotient at equilibrium; symbol K

LINK **6C** LE CHÂTELIER'S PRINCIPLE

Let us reconsider what we know about equilibrium thus far:

- It occurs when the rates of the forward and reverse reactions are equal.
- The observed concentrations of reactants and products are constant.
- It represents a macroscopically unchanging system, despite the system being dynamic at the atomic level.

Using the concentrations of the reactants and products at equilibrium, we can calculate the equilibrium constant by using the same generalised equation as for the reaction quotient. This is shown by the following expression:

$$aA + bB \rightleftharpoons cC + dD$$

$$K = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

For example, given the equation below:

$$N_2(g) + 2O_2(g) \rightleftharpoons 2NO_2(g)$$

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We can determine K for known concentrations of reactants and products using the following expression:

$$K = \frac{[NO_2]^2}{[N_2][O_2]^2}$$

We can also see how prior to reaching the equilibrium point, we can calculate the reaction quotient using the same formula. This is why data collection of reactant and product concentrations with time is a common way to measure both Q and K.

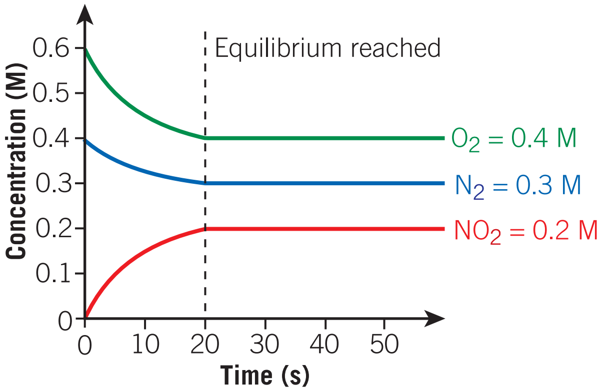

Figure 6B–3 This graph of concentration versus time for the reaction between N_2 and O_2 to form NO_2 allows for the calculation of K, as the values of each concentration are known.

Units of the reaction quotient and equilibrium constant

Previously, we have discussed most measurements as having definitive units. We measure concentration in moles per litre, temperature in degrees Celsius or Kelvin and pressure in kilopascals or atmospheres. However, the units of the reaction quotient and equilibrium constant are dependent on the specific reaction that they are representing. This is because the units for Q and K are products of the stoichiometry of the reactants and the products and their ratio. It is even possible to have a unitless value of K. To determine the correct units, it is important to understand the laws of indices (which you may have learned previously in maths). There are two rules you need to remember:

- When dividing indices with the same base, subtract the powers.
- When multiplying indices with the same base, add the powers.

Check-in questions – Set 1

1 Write the expression for the equilibrium constant and reaction quotient.
2 What is the difference between the equilibrium constant and the reaction quotient?

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Calculating the equilibrium constant

The equilibrium constant can be calculated for almost any reaction if the concentration of the species can be measured within the reaction. Worked examples 6B–1 and 6B–2 show two calculation methods.

Worked example 6B–1: Calculating the equilibrium constant using concentrations

VIDEO
WORKED
EXAMPLE 6B–1

When the conditions are right, such as when there is lightning, nitrogen and oxygen gas can react to form nitrogen dioxide – a toxic gas in the upper atmosphere. If an experiment is performed in a closed system where the energy of lightning is supplied, calculate the value of the equilibrium constant if the equilibrium concentrations of nitrogen, oxygen and nitrogen dioxide are 0.30 M, 0.40 M and 0.20 M respectively.

$$N_2(g) + 2O_2(g) \rightleftharpoons 2NO_2(g)$$

Solution

	Logic	Process
Step 1	Write out the relevant information from the question.	$[N_2] = 0.30\text{ M}$ $[O_2] = 0.40\text{ M}$ $[NO_2] = 0.20\text{ M}$
Step 2	Write out the equilibrium constant expression.	$K = \frac{[NO_2]^2}{[N_2][O_2]^2}$
Step 3	Substitute values into the equilibrium constant expression.	$K = \frac{(0.20\text{ M})^2}{0.30\text{ M} \times (0.40\text{ M})^2}$
Step 4	Solve for *K*, ensuring that units are correct by applying index laws.	$K_c = \frac{0.040\text{ M}^2}{0.048\text{ M}^3}$ $= 0.80\text{ M}^{-1}$

Calculations involving equilibrium

Now that we understand how *K* is calculated and its meaning, we need to consider what we need to calculate *K* and how to derive it, based on knowledge from previous chapters on stoichiometry and concentration. In Worked example 6B–1, the concentrations of all reactants and products at equilibrium were provided. However, you will also need to be able to solve problems in which these concentrations are not directly given. In these circumstances, you are usually provided with a mixture of initial concentrations and equilibrium concentrations. To be able to determine *K* in these types of questions, you need to use your knowledge of stoichiometry. To help organise the different parts of information, it is useful to use a technique known as an **ICE** (**I**nitial, **C**hange, **E**quilibrium) table. Table 6B–2 shows an example of an ICE table for the following reaction:

$$A + 2B \rightleftharpoons 2C + D$$

Table 6B–2 Example ICE table

	A	2*B*	2*C*	*D*
Initial				
Change				
Equilibrium				

This table would then be populated with the information given in the question, which you can then use to fill in the blank squares. It is important to remember that to calculate K, you need the equilibrium concentrations. Occasionally, you will be provided with values that relate to another quantity, such as the amount in moles. In these instances, you will need to convert them to molar concentrations. The following worked example shows the use of an ICE table in a specific scenario.

VIDEO
WORKED
EXAMPLE 6B–2

Worked example 6B–2: Using stoichiometry to calculate *K*

Two gases, NO_2 and N_2O_4, establish an equilibrium in a closed system at a specified temperature, according to the following equation:

$$N_2O_4(g) \rightleftharpoons 2NO_2(g)$$

A 0.27 mol sample of N_2O_4 was placed in a 1.0 L vessel. At equilibrium, there was only 0.14 mol of N_2O_4 remaining. Calculate the K for this reaction.

Solution

	Logic	Process	
Step 1	Write the reaction and create an ICE table.	$N_2O_4(g) \rightleftharpoons 2NO_2(g)$	
Step 2	Construct your ICE table and fill in the given information.	I = 0.27 mol	I = 0.00 mol
		C = ?	C = ?
		E = 0.14 mol	E = ?
Step 3	Convert all values to concentrations using $c = \frac{n}{V}$.	$I = \frac{0.27\text{ mol}}{1.0\text{ L}}$ $= 0.27\text{ M}$	$I = \frac{0.00\text{ mol}}{1.0\text{ L}}$ $= 0.00\text{ M}$
		C = ?	C = ?
		$E = \frac{0.14\text{ mol}}{1.0\text{ L}}$ $= 0.14\text{ M}$	E = ?
Step 4	Determine the change in concentration of the substance for which the equilibrium concentration is known.	I = 0.27 M	I = 0.00 M
		C = I – E = 0.27 M – 0.14 M = 0.13 M	C = ?
		E = 0.14 M	E = ?
Step 5	Use molar ratios to determine the change in concentration of the other substance(s), ensuring that the sign changes if it is on the other side of the equation.	I = 0.27 M	I = 0.00 M
		C = –0.13 M	C = 2 × 0.13 M = 0.26 M
		E = 0.14 M	E = ?
Step 6	Use the change in concentration values to calculate any unknown equilibrium concentrations.	I = 0.27 M	I = 0.00 M
		C = –0.13 M	C = 0.26 M
		E = 0.14 M	E = I + C E = 0.00 M + 0.26 M E = 0.26 M
Step 7	Substitute values into the equilibrium constant expression to solve for K, including units.	$K = \frac{[NO_2]^2}{[N_2O_4]} = \frac{(0.26\text{ M})^2}{0.14\text{ M}}$ $= 0.48\text{ M}$	

Relationship between *Q* and *K*

In this section, we have looked at calculations involving *Q* and *K* separately. However, it is important to note that we can relate the values obtained for these two terms to gain an understanding of what is happening at any given moment in a reaction. This is based on the following two aspects.

1. When a system involving a reversible reaction is not at equilibrium, we can only calculate the reaction quotient, *Q*.
2. The equilibrium constant for a given equilibrium system at a given temperature does not change, regardless of whether that system is currently at equilibrium or not.

Let's think about an example of an equilibrium system, for which we know the equilibrium constant. The system is not currently at equilibrium, which means that the rates of the forward and reverse reactions are not equal. Considering this, at this given point in time, one must be favoured … but which one? As the system is not at equilibrium, we can calculate the reaction quotient, *Q*, using provided values for the concentration of the reactants and products at that moment. Once we have the value for *Q*, we can compare it to *K* and our outcomes would be:

- $Q < K$ – in this instance, the forward reaction is currently being favoured. As the value of *Q* is less than *K*, the reaction needs to produce more products to reach equilibrium.
- $Q > K$ – in this instance, the reverse reaction is currently being favoured. As the value of *Q* is more than *K*, the reaction needs to produce more reactants to reach equilibrium.

A way of remembering this is explored in the following Skills section.

6B SKILLS

Memory tools

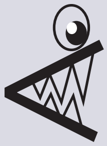
In this section, we have discussed how the reaction quotient, *Q*, relates to the equilibrium constant, *K*. One of the important things to learn from this is understanding that when a reaction is not at equilibrium, the value of *Q* can be used to determine which reaction is being favoured.

While the section has explained this from a theory point of view, there are also memory techniques that you can employ to help you remember. A common one is called 'follow the crocodile', which goes like this:

If $Q < K$, then the forward reaction is being favoured.

If $Q > K$, then the reverse reaction is being favoured.

At this point, it probably isn't apparent why it is called 'follow the crocodile'. To understand that, we just have to make some small additions to our < and > signs to make them look like this:



By turning the sign into a crocodile by adding an eye and teeth, we can see that in this case, the crocodile is moving to the right. If the opposite sign was used, the crocodile would be moving to the left. This can be a really handy memory tip to help you remember this relationship. However, it is important to note that this only works if you always write *Q* first!

Section 6B questions

1 X reacts with Y according to the following equation:

$$X(aq) + 2Y(aq) \rightleftharpoons 3XY(aq)$$

Using this equation, find:

a the expression for K.

b the units for K.

Another equilibrium system involves the reaction to form hydrogen fluoride gas according to the following equation:

$$H_2(g) + F_2(g) \rightleftharpoons 2HF(g)$$

The initial concentrations of hydrogen and fluorine, respectively, were 0.32 M and 0.080 M and the amount of hydrogen fluoride formed was 0.12 M. Given this:

c find the value for K.

d state whether the equilibrium favours the reactants or products and why.

2 The following reaction has an equilibrium constant of 0.200 M.

$$H_2CO_3(aq) \rightleftharpoons H^+(aq) + HCO_3^-(aq)$$

At equilibrium, the mixture contains 0.001 M H_2CO_3, 0.005 M HCO_3^- and an unknown amount of H^+. Find the concentration of H^+ in this mixture.

3 Carbonic acid dissociates to form a bicarbonate ion and a hydrogen ion, as in the equation below. If 1.0 M hydrogen carbonate, 0.8 M hydrogen ions and 0.8 M carbonic acid are present at equilibrium, determine the value of the equilibrium constant.

$$H_2CO_3(aq) \rightleftharpoons H^+(aq) + HCO_3^-(aq)$$

4 A 1.0 L container holds a mixture of 0.043 mol of H_2 gas, 0.062 mol of I_2 gas and 0.358 mol of HI gas at equilibrium at 440°C. The reaction is:

$$H_2(g) + I_2(g) \rightleftharpoons 2HI(g)$$

Calculate K.

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6C Le Châtelier's principle

Study Design:

- The dynamic nature of homogenous equilibria involving aqueous solutions or gases and their representation by balanced chemical or thermochemical equations (including states) and by concentration–time graphs
- The change in position of equilibrium that can occur when changes in temperature or species or volume (concentration or pressure) are applied to a system at equilibrium, and the representation of these changes using concentration–time graphs
- Calculations involving equilibrium expressions (including units) for a closed homogeneous equilibrium system and the dependence of the equilibrium constant (K) value on the system temperature and the equation used to represent the reaction
- The application of Le Châtelier's principle to identify factors that favour the yield of a chemical reaction
- Responses to the conflict between optimal rate and temperature considerations in producing equilibrium reaction products, with reference to the green chemistry principles of catalysis and designing for energy efficiency

Glossary:
Le Châtelier's principle

ENGAGE

A miner who made a major finding

Henry Louis Le Châtelier, a French chemist of the nineteenth century, made one of the most significant contributions to our understanding of chemistry through his work on equilibrium. He actually began his career as a mining engineer but then shifted to work as a laboratory chemist after a few years. His principle on equilibrium systems, Le Châtelier's principle, is the focus of this section. After he developed this theory, he spent a lot of time thinking about how it could be adapted to improve industrial processes, which led to him suggesting the most appropriate parameters for the production of ammonia. During the time when he was particularly interested in industrial chemistry, he also managed to perfect the oxyacetylene torch, which is a highly effective tool for cutting metals and welding. In this section, you will learn more about Le Châtelier's Principle and how it helps predict how changes to equilibrium systems alter the position of equilibrium. You will also explore how industrial processes sometimes need to find a balance between the rate of a reaction and the production of equilibrium reaction products and how green chemistry principles are being used to overcome these challenges.

EXPLAIN

Le Châtelier’s principle

In this section, we will explore what happens to systems at equilibrium when certain factors are changed. Our understanding of what happens in these situations is governed by **Le Châtelier’s principle**, which states that:

> ‘If an equilibrium system is subjected to a change, the system will adjust itself to partially oppose that change and restore equilibrium.’

Le Châtelier’s principle
If an equilibrium system is subjected to a change, the system will adjust itself to partially oppose that change and restore equilibrium

This section of the chapter examines how specific changes affect equilibrium systems, the value of *K* and how we can logically infer the consequences of these changes.

For each of the changes described in this section, there are essentially three steps that you need to follow to understand what effect it will have. These steps are summarised in the flow chart below.

Figure 6C–1 Henry Louis Le Châtelier extended our understanding of equilibrium through his work on the topic, which is summarised as Le Châtelier’s principle.

STEP 1:
Identify the condition that has changed

STEP 2:
Determine how that change can be opposed

STEP 3:
Determine whether opposing the change involves favouring the forward or reverse reaction

An important point regarding step 3 is that a number of different phrases can be used to describe the process that occurs to restore equilibrium. The statements below both describe the same thing and either would be equally valid to say in a given scenario.

- The forward reaction is favoured OR the position of equilibrium shifts to the right.
- The reverse reaction is favoured OR the position of equilibrium shifts to the left.

Adding reactant or product

For a closed system, adding a reactant or a product alters the concentration of that given species and thus, the equilibrium system. If a reactant is added, then the concentration of that reactant is higher than it should be, and as such, the system needs to respond to lower the concentration of reactants to restore equilibrium, as the example in Figure 6C–2 shows. For this to happen, the forward reaction is favoured.

Equally, if product is added to the system, the concentration of products is higher than it should be and the system opposes this change by favouring the reverse reaction.

These effects on equilibrium are summarised in the example system in Figure 6C–3.

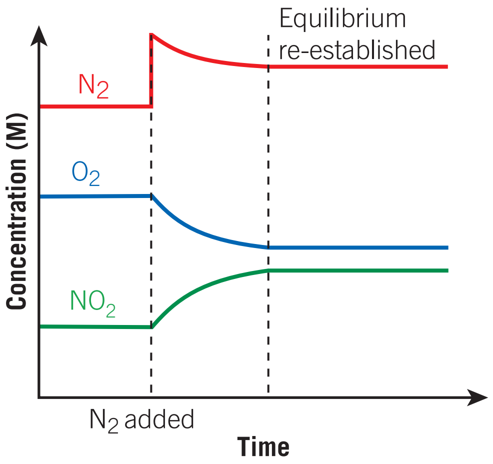
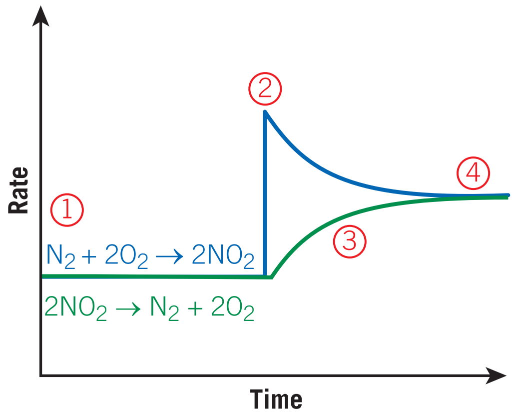


Figure 6C–2 The effect of adding N_2 to the $N_2 + 2O_2 \rightarrow 2NO_2$ equilibrium system



1 System at equilibrium – forward and reverse reaction rates are constant, non-zero and the same.
2 Nitrogen is added, and the rate of the forward reaction increases dramatically due to increased number of collisions.
3 As more products are produced, there is a slight increase in the reverse reaction rate, again due to more collisions.
4 Forward and reverse rates plateau and equilibrium is re-established.

Figure 6C–3 The step-by-step effect of adding a reactant to a system

It is important to understand that when there is a change in concentration, which is then opposed by the equilibrium system, the value of the equilibrium constant remains the same throughout. In fact, the only change that also results in a changed value for *K* is a change in temperature. This is a key feature of *K* values – they are specific for a given system under certain conditions.

Temperature, enthalpy and equilibrium

The effect of temperature on an equilibrium reaction depends on whether the reaction is endothermic or exothermic. Endothermic reactions use heat, whereas exothermic reactions release heat. Using our NO_2 example, we can now describe the reaction fully as an exothermic reaction. Given that the forward reaction produces heat, we know that the reverse reaction consumes heat. Therefore, the forward reaction is exothermic, and the reverse reaction is endothermic.

LINK **1C** EXOTHERMIC AND ENDOTHERMIC REACTIONS

A simple strategy for understanding the effect of changing the temperature of an equilibrium system involves writing 'heat' as part of the reaction. In an endothermic reaction, heat is used as part of the reaction process and so would be written on the side of the reactants. In an exothermic reaction, heat is released as part of the reaction process and so would be written on the side of the products; that is:

$$\begin{aligned}&\text{Endothermic: } A + B + \text{heat} \rightleftharpoons C + D\\&\text{Exothermic: } A + B \rightleftharpoons C + D + \text{heat}\end{aligned}$$

Using this strategy, we can then consider this condition change identically to how we thought about adding or removing a reactant or product. If we increase the temperature of an equilibrium system for an endothermic reaction, this increases the 'heat', which is on the reactants side of the equation. From our previous understanding, we can then determine that the system will oppose this change by favouring the forward reaction. Similarly, if we were to increase the temperature of an equilibrium system for an exothermic reaction, this increases the 'heat', which is on the products side of the equation. This would result in the reverse reaction being favoured.

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Changing the temperature will result in a changed value of *K*. Temperature is the only condition that you need to know about that changes the value of *K* for a reaction, and indeed a reaction will have a range of different *K* values and equilibrium positions for a range of different temperatures. Essentially, if the change in temperature results in the forward reaction being favoured (that is, a decreased temperature for an exothermic reaction or an increased temperature for an endothermic reaction), then the concentration of products will increase and so will the value of *K*. The opposite is true if the reverse reaction is favoured and the value of *K* will decrease. This is summarised in Table 6C–1 below and Figure 6C–4 on the right.

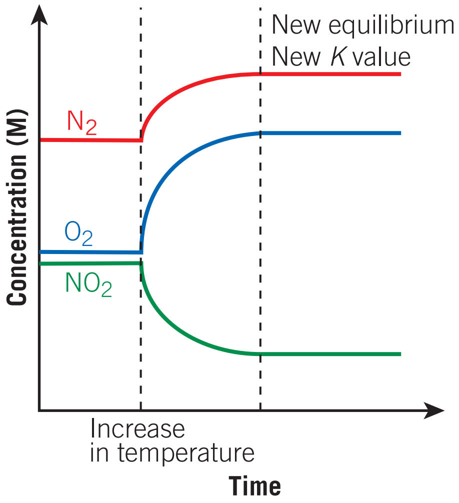

Figure 6C–4 The effect of a temperature change on the concentrations of different compounds in an equilibrium system

Table 6C–1 The effect of temperature on *K* for endothermic and exothermic reactions

Temperature	ΔH	*K*
Increase	Endothermic	Increase
	Exothermic	Decrease
Decrease	Endothermic	Decrease
	Exothermic	Increase

Pressure, volume and equilibrium

As you have learned before, volume and pressure are inversely related – that is, if you decrease the volume of a reaction vessel containing gases, the pressure will increase (assuming that the temperature and amount of gas are kept constant). In an equilibrium system, this will impact on the position of equilibrium, as it is equivalent to changing the concentration of the molecules in the system (that is, an increased pressure is due to a higher number of particles per unit of area). As such, based on Le Châtelier's principle, we should expect a change in the system to restore the equilibrium position. The rules for this are as follows.

- If pressure is increased, the equilibrium system will oppose the change by favouring the reaction that produces the least moles of gas.
- If the pressure is decreased, the equilibrium system will oppose the change by favouring the reaction that produces the most moles of gas.

For example, when compressed, the reaction between O_2 and N_2 that produces NO_2 experiences a shift away from equilibrium, as seen in Figure 6C–5 on the following page.

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As we can see through this example, there are three moles of gas on the reactants side of the equation, but only two moles on the products side. As the pressure was increased when the reaction volume was decreased, this led to the reaction that produced the least moles of gas being favoured – the forward reaction. Unlike temperature, changing the pressure/volume of a reaction doesn't change the value of K as the system can restore the original concentration ratio.

Occasionally, problems will involve the addition of an inert gas to an equilibrium system. While this will increase the overall pressure of the container, it does not change the partial pressures of any of the gases involved in the equilibrium system (assuming the volume and temperature of the system are kept constant), as represented in Figure 6C–6. Therefore, the addition of an inert gas does not change the position of equilibrium, nor does it change the value of K.

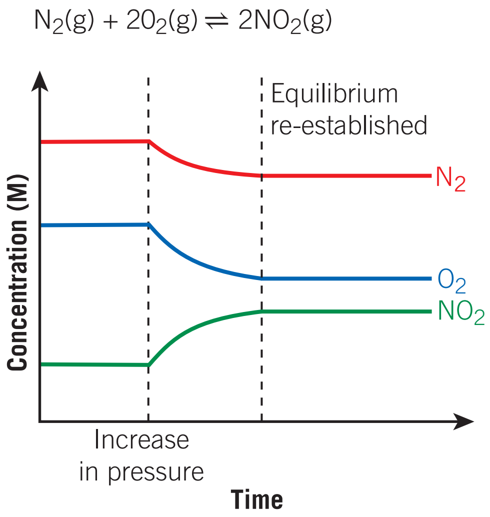

Figure 6C–5 Increasing the pressure of an equilibrium system results in the reaction producing the least moles of gas being favoured.

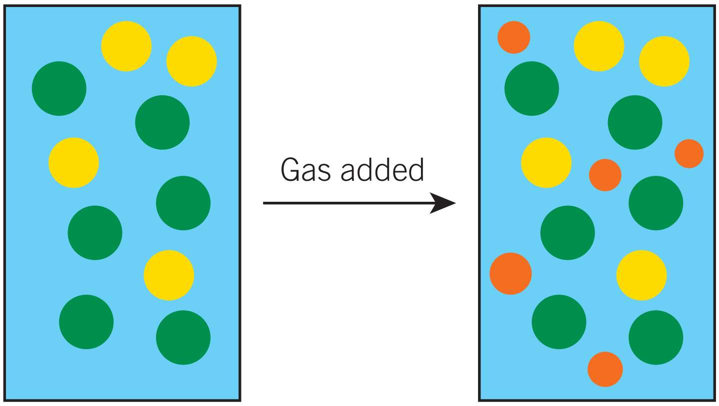

Figure 6C–6 Addition of inert gas (orange) has no effect as the overall concentrations of both reacting gases remain the same.

Dilution and equilibrium

Dilution of an aqueous equilibrium system, achieved through the addition of an unreactive solvent, also affects the position of equilibrium by decreasing the concentrations of the reactants and products. As such, the system will favour the reaction that produces more particles. If both sides of the reaction contain the same number of particles, then the position of equilibrium will be unchanged (as illustrated in Figure 6C–7). As with changes in pressure and volume, dilution does not change the value of K, just the equilibrium position.

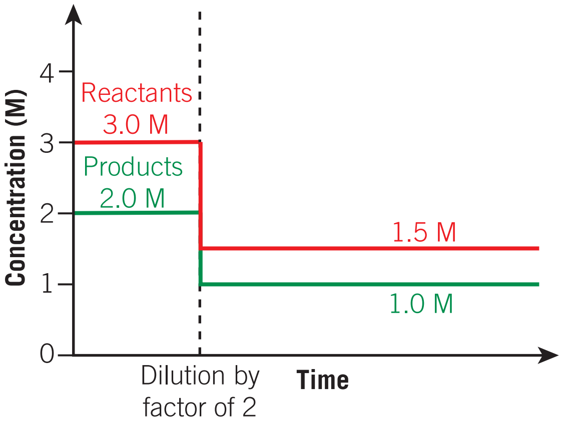

Figure 6C–7 Dilution of an aqueous mixture at equilibrium has no effect on equilibrium position if both sides of the equation have the same number of particles.

Catalysts and equilibrium

CHAPTER 5 LINK

As you learned in Chapter 5, catalysts alter the rate of reaction by decreasing the activation energy of a given reaction. What we didn't learn, however, is that the activation energy is lowered for both the forward and the reverse reactions. Therefore, the concentrations of the products and reactants don't change – just the speed at which they are formed. Thus, the value of *K* isn't changed, nor is the position of the equilibrium. Essentially, we just reach equilibrium faster if we use a catalyst (Figure 6C–8).

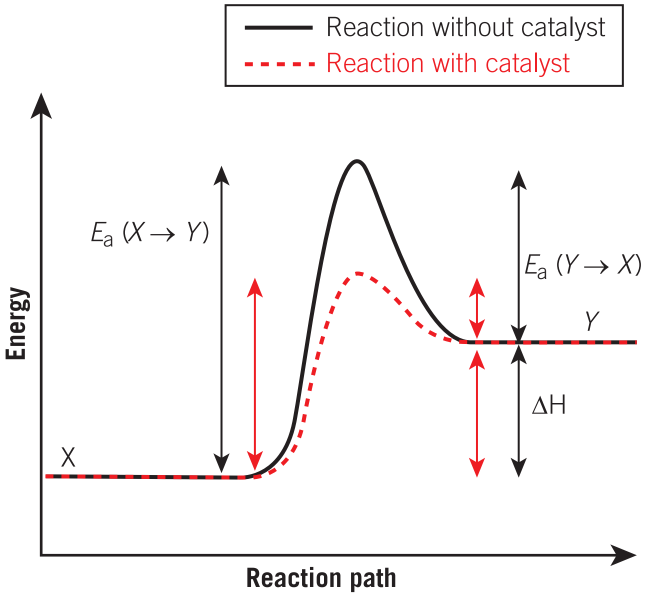

Figure 6C–8 The effect of a catalyst on activation energy

Using *K* to predict changes in equilibrium position

In the examples on the previous pages, we have discussed the rationale from a reaction perspective to predict the effect of changing concentration and temperature on the position of equilibrium. However, it is also possible to use the equilibrium constant to predict which reaction will be favoured to re-establish equilibrium.

Firstly, remember that temperature is the only condition that affects the value of the equilibrium constant. Therefore, in every other instance where a change is made, the system must oppose that change in a way that keeps the value of *K* constant.

Let's look at this using the formation of ammonia as an example. The equilibrium reaction that is occurring is:

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

Therefore, the equilibrium expression for this reaction is:

$$K = \frac{[NH_3]^2}{[N_2][H_2]^3}$$

Consider an example where equilibrium is disrupted through the addition of more nitrogen gas. When this happens, we can see that the denominator in our equilibrium expression will have increased. For *K* to remain constant, the numerator must also increase to balance this change. As the numerator is represented by the products in the reaction, for this to increase, the forward reaction must be favoured. This illustrates that the equilibrium expression can also be used as a way of predicting shifts in the position of equilibrium due to changes in reaction conditions.

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Table 6C–2 Summarising the effect of all external variables on an equilibrium system in light of Le Châtelier's principle

Condition change	Le Châtelier's response	Reaction favoured	Position of equilibrium	Does K change?
Adding reactant	Decrease concentration of reactants	Forward reaction	Shifts right	No
Adding product	Decrease concentration of products	Reverse reaction	Shifts left	No
Increasing temperature	Decrease temperature	Endothermic reaction	Depends on system	Yes
Decreasing temperature	Increase temperature	Exothermic reaction	Depends on system	Yes
Increasing pressure	Decrease pressure	Reaction that produces less particles	Depends on system	No
Decreasing pressure	Increase pressure	Reaction that produces more particles	Depends on system	No
Diluting reaction	Increase concentration	Reaction that produces more particles	Depends on system	No
Add a catalyst	None	Neither	No change	No

Competing factors in equilibrium

In Chapter 5, you looked at how reaction rate can be altered by a range of factors. In this chapter, you've learned how equilibrium will be reached regardless of speed, and that the equilibrium position is final for a given set of conditions. However, you also learned that by Le Châtelier's principle, reaction conditions can be altered to favour the reactants or products. Thus, to optimise a reaction, both rate and equilibrium effects must be considered.

LINK CHAPTER 5

For example, we know that higher temperatures result in faster reaction rates. However, we also know that for exothermic reactions, this will favour the reverse reaction and so will decrease the yield of products. For this reason, a compromise often needs to be found between achieving the optimal reaction rate and maximising the yield of a desired product.

We can consider both effects side by side and, for a given reaction, optimise the yield of the reaction (Table 6C–3).

Table 6C–3 Optimal conditions for high rate and high yield

Improve rate	Improve yield
Increase concentration	Add excess reactant
Increase temperature	Low temperature for exothermic reactions, high temperature for endothermic reactions
Increase pressure	Low or high pressure depending on the number of reactant/product particles in the system
Add appropriate catalyst	Removal of product as it is formed

Figure 6C–9 Reactions being conducted on a laboratory scale or an industrial scale will have different priorities for factors affecting reaction rate and yield.

Check-in questions – Set 1

1 What is Le Châtelier's principle and how does it relate to chemical equilibrium?

2 Consider the exothermic reaction, $2NO_2(g) \rightleftharpoons N_2O_4(g)$. If the system is at equilibrium and the temperature is increased, what will happen to the position of equilibrium and why?

3 Consider a homogeneous equilibrium system involving gaseous reactants and products. The volume of the container that the reaction is taking place in is halved. Describe the outcome of this change and explain what it will depend on.

Using graphical and thermochemical information to determine optimal conditions

It is important to understand how to use a range of different information to determine the optimal conditions to improve the yield of a chemical process. Three pieces of information are required to get a complete picture of how to optimise a reaction:

- the thermochemical equation, including the enthalpy
- the value of *K* so that we can determine where the equilibrium position lies
- a graph of the yield depending on temperature.

With this information, the optimum conditions for a reaction to occur and how these changes will affect the percentage yield can be determined.

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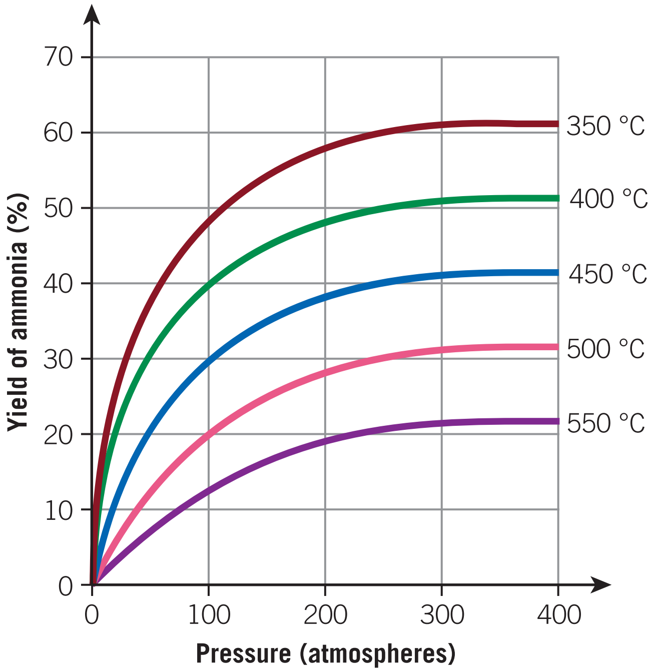

Figure 6C–10 Graph of ammonia yield versus pressure at different temperatures. Clearly, lower temperatures favour higher yields.

You can see from the graphical information in Figure 6C–10 that lower temperatures favour ammonia production. Looking at the thermochemical equation below, can you think why?

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g) \qquad \Delta H = -92 \text{ kJ mol}^{-1}$$

The reaction is exothermic, so high temperatures will favour the reverse reaction. On the other hand, low temperatures will favour the forward reaction. We can also see that on the reactants side there are four particles, whereas on the products side there are two particles. Therefore, increasing the pressure will favour the forward reaction. Adding a catalyst to achieve the optimal rate of reaction, without altering the position of equilibrium, might be a good idea. The Haber process to produce ammonia industrially does indeed use high pressure, a metal catalyst and medium to low temperatures to optimise yield.

Optimising reactions using green chemical principles

While optimising yield and rate is important in ensuring we get the most products formed, we can, inadvertently, produce an excessive amount of waste products or pollution when focused solely on these parameters. When the concept of green chemical principles was introduced, it required a shift in thinking from one of a traditional 'maximising yield' mindset to a more modern one of 'valuing waste elimination and avoiding toxic/hazardous materials'.

One way to do this is to use catalysts that are non-toxic to optimise the chemical reactions. Better yet, catalysts that are biodegradable and prefer milder reaction conditions favour greener outcomes. This has led to the expansion of the area of biocatalysis in recent years, as enzymes are starting to gain use industrially in place of traditional oxidants, reductants, acids and bases. Biocatalysts can also be produced sustainably using bacteria.

An example is the pharmaceutical industry, which traditionally produced an excess of waste materials by up to two orders of magnitude and 10^3 tonnes of waste per tonne of product. This industry has shifted more towards green chemical principles recently. The molecule sertraline, the active ingredient in an antidepressant produced by the pharmaceutical company Pfizer, is now synthesised in three steps instead of more than ten. This reduction in the number of steps, which is made possible by using a more selective catalyst, a more environmentally friendly solvent and knowledge of equilibrium to maximise product yield, results in a significant reduction in the amount of waste products generated from the process. In this way, the pharmaceutical production of sertraline illustrates how improving the design efficiency of reaction pathways and utilising catalysts can significantly reduce the environmental impact of chemical reactions required for the generation of consumer products.

Figure 6C–11 Sertraline is commonly used as an antidepressant.

VIDEO 6C–1 SKILLS: LOGICAL REASONING

6C SKILLS

Logical reasoning

You will have seen in this section that you will be expected to understand how a number of factors impact on the position of equilibrium. While this in itself is challenging enough, it would have also become apparent that the outcome it not always straightforward. As an example, we can't simply state how a change in temperature affects the position of equilibrium – it depends on whether the temperature is increased or decreased and also whether the reaction is exothermic or endothermic. When you consider all of this, there are a lot of things to remember!

However, it is important to note that if you understand and remember one thing, it is often possible to work out the other related situations by logical reasoning alone. Let's look at this using the example of changing concentration. In terms of changing concentration, there are four scenarios that we could be assessing, which are:

1. increasing the concentration of a reactant
2. decreasing the concentration of a reactant
3. increasing the concentration of a product
4. decreasing the concentration of a product

From this list, let's imagine that we could only remember the affect that change number 1 has – increasing the concentration of a reactant leads to the forward reaction being favoured. How does this help us solve the rest?

Well, 1 and 2 are the opposite of each other. So if 1 favours the forward reaction, 2 must favour the reverse reaction.

Similarly, 1 and 3 are also opposites of each other. So if 1 favours the forward reaction, 3 must favour the reverse reaction.

We can use this information to then solve for 4. Changes 3 and 4 are opposites of each other; so if 3 favours the reverse reaction, 4 must favour the forward reaction.

It can initially seem confusing to set it out as shown above, so you may prefer to look at it in a more visual fashion by constructing a grid like the one shown on the following page.

Increasing [reactant] Favours forward reaction	**Increasing [product]**
Decreasing [reactant]	**Decreasing [product]**

By setting the grid up like this, the boxes that are adjacent will always be the opposite and the one at a diagonal will always be the same. Copy the grid above and try filling it in to see it working.

Section 6C questions

1 Define 'Le Châtelier's principle'.

2 For the reactions below, indicate how the following changes will affect the equilibrium position:

- i adding reactant
- ii decreasing the temperature
- iii adding a catalyst
- iv decreasing the volume of the container

a $N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g) \qquad \Delta H = -92\ \text{kJ mol}^{-1}$

b $Fe(NO_3)_3(aq) + KNCS(aq) \rightleftharpoons FeNCS^{2+}(aq) + KNO_3(aq) + 2NO_3^{-}(aq)$

Exothermic reaction

3 Using an example, explain how dilution affects equilibrium position.

4 Draw the concentration–time graph that would be expected for nitrogen reacting with oxygen to form nitrogen dioxide that has reached equilibrium and is then moved to a larger container. What happens to the value of *K* for this reaction?

5 Discuss how rate and equilibrium affect reaction yield.

6 What information is required to assess the yield of a reaction?

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Chapter 6 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
6A.1	State the difference between reversible and irreversible reactions	4☐
6A.2	Explain the difference between rate of reaction and extent of reaction	11☐
6A.3	Define ‘dynamic equilibrium’	6☐
6B.1	State the expression for the equilibrium constant	12☐, 14☐
6B.2	Determine the position of equilibrium, based on the value of K	14☐
6B.3	Use the equilibrium expression to calculate the value of K or the equilibrium concentration of a reactant or product	5☐, 12☐, 14☐
6B.4	Calculate the reaction quotient, including units, for a given equilibrium system	14☐
6B.5	Determine how the position of equilibrium shifts using values of Q and K	1☐, 14☐
6C.1	State Le Châtelier’s principle	7☐
6C.2	Predict the effect of changes in temperature on the position of equilibrium using Le Châtelier’s principle	3☐, 12☐
6C.3	Determine the effect of temperature on the equilibrium constant	12☐
6C.4	Predict the effect of a change in volume on the position of equilibrium using Le Châtelier’s principle	10☐, 12☐
6C.5	Predict the effect of adding or removing a reactant or product on the position of equilibrium using Le Châtelier’s principle	13☐
6C.6	Sketch a concentration–time graph to represent a given equilibrium system	12☐
6C.7	Interpret concentration–time graphs to determine changes made to an equilibrium system	13☐
6C.8	Determine the factors that maximise yield in a given equilibrium system using Le Châtelier’s principle	2☐
6C.9	Identify potential conflicts between reaction rate and producing equilibrium reaction products in a given equilibrium system	8☐, 11☐
6C.10	Describe the green chemistry principle of catalysis	9☐
6C.11	Describe the green chemistry principle of designing for energy efficiency	11☐
6C.12	Explain how the green chemistry principles of catalysis and designing for energy efficiency can solve conflicts between optimal reaction rate and producing equilibrium reaction products in equilibrium systems	11☐

Multiple-choice questions

1 A change is made to a reaction at equilibrium. Just after this change is made, it is found that the reaction quotient is smaller than the equilibrium constant. At this time, the

A forward reaction is being favoured.

B reverse reaction is being favoured.

C reaction has re-established equilibrium.

D concentration of the products is greater than the concentration of the reactants.

2 Ammonia is produced via the following chemical reaction:

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g) \qquad \Delta H = -92 \text{ kJ mol}^{-1}$$

Which of the following changes to the reaction conditions will increase the yield of ammonia?

A increasing the volume

B removing hydrogen gas

C decreasing the pressure

D decreasing the temperature

3 Which of the following combinations of statements regarding the effect of an increase in temperature on an equilibrium system is true?

	Exothermic or endothermic	Effect on position of equilibrium
A	Exothermic	Equilibrium shifts to the right
B	Endothermic	Forward reaction is favoured
C	Exothermic	Forward reaction is favoured
D	Endothermic	Equilibrium shifts to the left

4 Which of the following best describes the difference between reversible and irreversible chemical reactions?

A Reversible reactions are those that can be undone by adding heat, while irreversible reactions cannot be undone by any means.

B Reversible reactions can proceed in either direction, while irreversible reactions can only proceed in one direction.

C Reversible reactions are those that can be reversed by adding a catalyst, while irreversible reactions cannot be reversed with a catalyst.

D Reversible reactions occur quickly, while irreversible reactions occur slowly.

5 Sulfur dioxide and oxygen react to form sulfur trioxide, which is an important step in the synthesis of sulfuric acid. The reaction for this is:

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

At equilibrium, the concentrations of SO_2, O_2 and SO_3 are found to be 0.03 M, 0.16 M and 0.54 M respectively. The value of K is

A 112.5 M^{-1}

B 112.5 M

C 2025 M^{-1}

D 2025 M

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6 Which of the following is statements about a reaction system at dynamic equilibrium is incorrect?

A The reaction is still occurring.

B The concentrations of the reactants and products are constant.

C The rate of the forward reaction is equal to the rate of the reverse reaction.

D The concentration of the products is equal to the concentration of the reactants.

7 According to Le Châtelier's principle, which of the following statements is true?

A An increase in temperature will result in an increased rate of reaction.

B A change in reaction conditions will result in an increased rate of the forward and reverse reactions.

C A change in reaction conditions will result in the position of equilibrium shifting to restore equilibrium.

D The reaction quotient will always be greater than the equilibrium constant directly after a change is made to the reaction conditions of a dynamic equilibrium.

8 For the production of ammonia according to the reaction shown below, which change in condition would lead to an increased rate of reaction but decreased yield of ammonia?

$$N_2(g) + 3H_2(g) \rightleftharpoons 2NH_3(g) \qquad \Delta H = -92 \text{ kJ mol}^{-1}$$

A introducing a catalyst

B increasing the pressure

C adding more nitrogen gas

D increasing the temperature

9 Catalysts allow for equilibrium systems to follow green chemistry principles because they

A increase the yield of the desired product.

B allow for the reaction to be conducted at higher pressures.

C allow for the reaction to be conducted at a lower temperature.

D increase the rate of the reaction and increase the value of the equilibrium constant.

10 A dynamic equilibrium has been established for the following chemical reaction:

$$Fe(NO_3)_3(aq) + KSCN(aq) \rightleftharpoons FeSCN^{2+}(aq) + KNO_3(aq) + 2NO_3^-(aq)$$

A 150 mL aliquot of water is added to a 50 mL solution of this reaction. What best describes what happens to the position of equilibrium for the reaction above?

A The position of equilibrium will not shift.

B The position of equilibrium will shift to the left.

C The position of equilibrium will shift to the right.

D The rate of the reaction will decrease due to a lower collision frequency.

Short-answer questions

11 Samantha is a chemical engineer working for a large ammonia production company. The company uses the Haber–Bosch process, a crucial industrial method for nitrogen fixation, to convert nitrogen (N_2) and hydrogen (H_2) into ammonia (NH_3), as shown below.

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

She has been assigned the task of optimising the conditions for the Haber–Bosch process to minimise cost and maximise output.

a Describe the difference between the rate of reaction and extent of reaction. (1 mark)

b For the equilibrium system described on the previous page, identify a reaction condition that would lead to an optimal rate of reaction but not produce the greatest amount of reaction products and explain why this is the case. (3 marks)

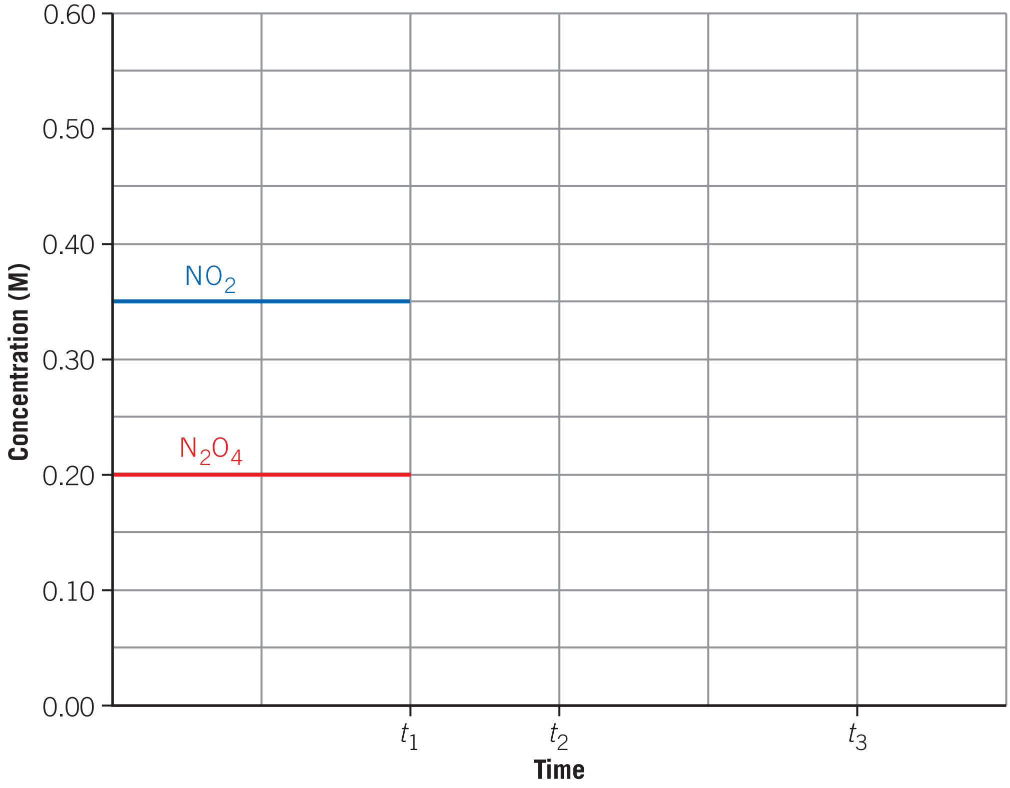
c Describe how two green energy principles are being used to overcome these issues in equilibrium systems. (4 marks)

12 A group of students has conducted experiments to investigate the equilibrium mixture given below:

$$2NO_2(g) \rightleftharpoons N_2O_4(g) \qquad \Delta H = -57 \text{ kJ mol}^{-1}$$

brown colourless

a An equilibrium mixture is prepared when a quantity of nitrogen dioxide is added to a large test tube and sealed securely. At t_1, the temperature of the equilibrium mixture at 25°C is increased to 100°C. Equilibrium is re-established at t_2. Copy and complete the concentration–time graph below to show the concentration of both species between t_1 and t_3. (2 marks)



b Write an expression for the equilibrium constant, K, for the reaction:

$$2NO_2(g) \rightleftharpoons N_2O_4(g)$$ (1 mark)

c i Use data from the graph to determine the magnitude of K at 25°C for:

$$2NO_2(g) \rightleftharpoons N_2O_4(g)$$ (2 marks)

ii Determine the value of K at 25°C for the reaction:

$$N_2O_4(g) \rightleftharpoons 2NO_2(g)$$

Include units with your answer. (1 mark)

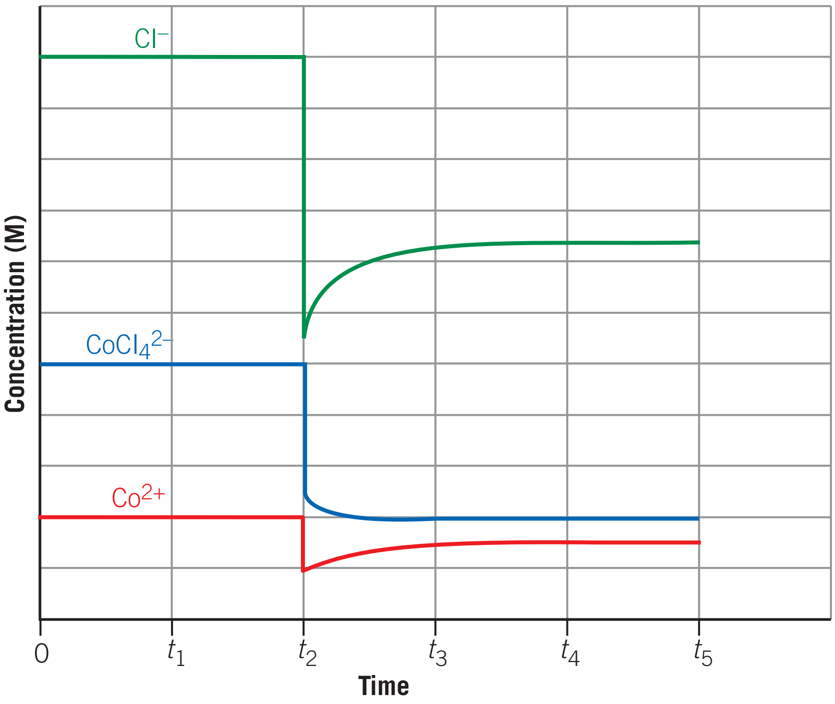
d The temperature of a system at 25°C is increased to 100°C. Choose from the options lower/no change/higher to indicate how the following would be affected. (5 marks)

- **i** the magnitude of the equilibrium constant, K
- **ii** the intensity of the brown colour of the mixture
- **iii** the rate of the reverse reaction
- **iv** the total mass of the two gases
- **v** the total number of gas molecules in the test tube

13 Another group of students conduct a different experiment, which is shown by the following reaction:

$$\underset{\text{pink}}{Co^{2+}(aq)} + 4Cl^-(aq) \rightleftharpoons \underset{\text{blue}}{CoCl_4^{2-}(aq)} \qquad \Delta H > 0$$

Shown below is a concentration–time graph for this equilibrium system. The graph shows the effect of a dilution at time t_2.



a During what time period(s) was the system at equilibrium? (1 mark)

b What colour change would have been observed with the dilution at t_2? (1 mark)

c Choose from the options lower/the same/higher to complete the following questions. Compared to the value at t_1, at t_4 the (3 marks)

- **i** value of K will be __________.
- **ii** concentration of $Co^{2+}(aq)$ will be __________.
- **iii** concentration of $CoCl_4^{2-}(aq)$ will be __________.

d At t_5, $CoCl_4^{2-}$ is added to the equilibrium mixture. Copy the graph and sketch the change that you would expect to see (assume that equilibrium is established again by t_6). Explain, using Le Châtelier's principle, what would happen to the position of equilibrium and the colour of the equilibrium mixture. (3 marks)

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14 Iron(III) ions react with thiocyanate to form iron(III) thiocyanate, according to the equation:

$$Fe^{3+}(aq) + SCN^{-}(aq) \rightleftharpoons FeSCN^{2+}(aq)$$

a What is the equilibrium expression for this reaction? (1 mark)

b The equilibrium constant for the above reaction is 7.89×10^2 at 25°C. If the equilibrium concentrations of Fe^{3+} and SCN^- are 0.005 M and 0.01 M, respectively, what is the concentration of $FeSCN^{2+}$ at equilibrium? (2 marks)

c The value of the equilibrium constant for this reaction is relatively large. What does this tell us about the extent of the reaction? (2 marks)

d If at a certain point in time during the reaction, the concentrations of Fe^{3+}, SCN^-, and $FeSCN^{2+}$ are 0.002 M, 0.015 M and 0.01 M, respectively, what is the reaction quotient (Q) for the reaction? (1 mark)

e Based on the values of K and Q, what is the direction of the reaction at this point and why? (2 marks)

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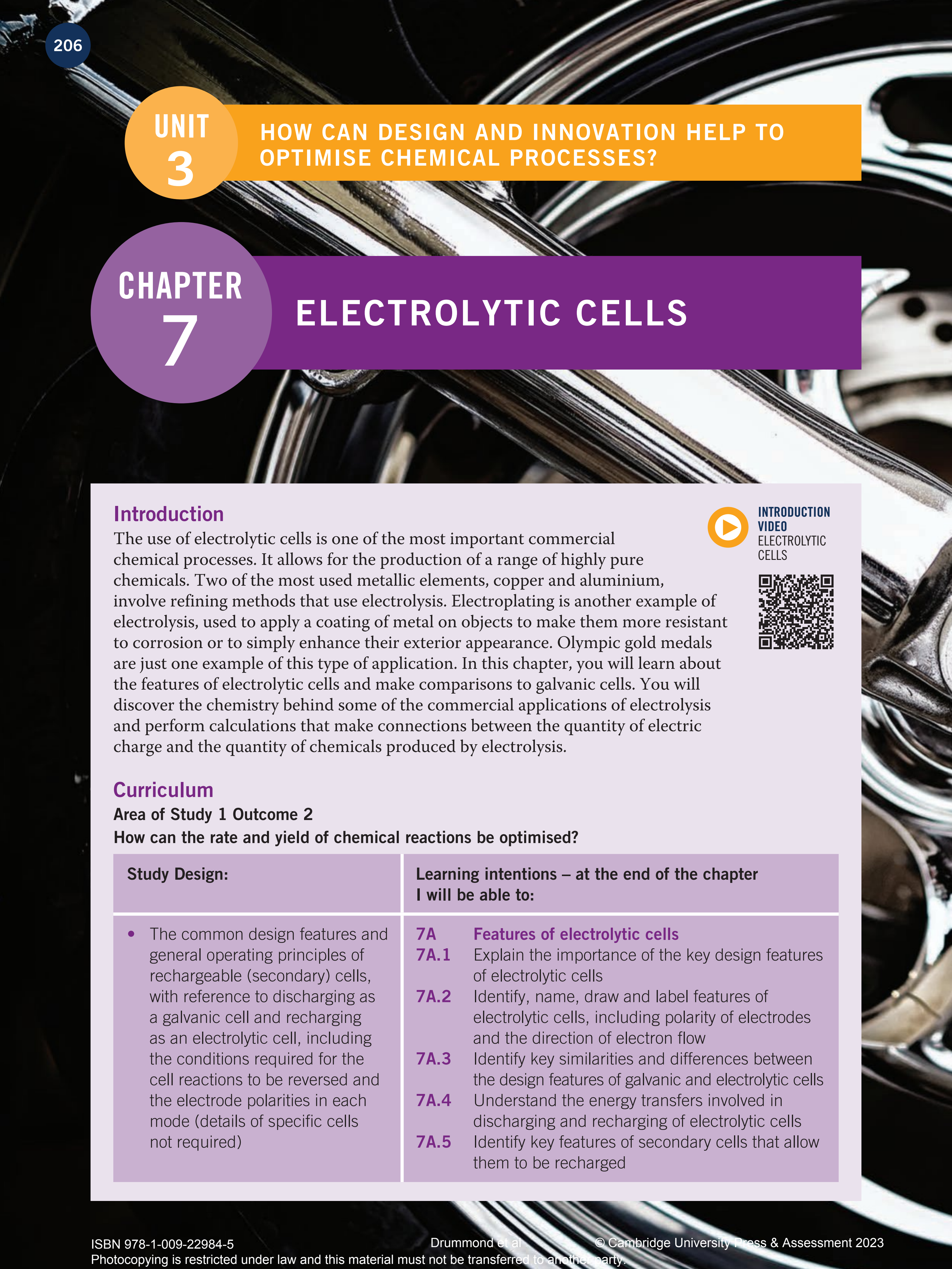

UNIT 3 HOW CAN DESIGN AND INNOVATION HELP TO OPTIMISE CHEMICAL PROCESSES?

CHAPTER 7 ELECTROLYTIC CELLS

Introduction

INTRODUCTION VIDEO
ELECTROLYTIC CELLS

The use of electrolytic cells is one of the most important commercial chemical processes. It allows for the production of a range of highly pure chemicals. Two of the most used metallic elements, copper and aluminium, involve refining methods that use electrolysis. Electroplating is another example of electrolysis, used to apply a coating of metal on objects to make them more resistant to corrosion or to simply enhance their exterior appearance. Olympic gold medals are just one example of this type of application. In this chapter, you will learn about the features of electrolytic cells and make comparisons to galvanic cells. You will discover the chemistry behind some of the commercial applications of electrolysis and perform calculations that make connections between the quantity of electric charge and the quantity of chemicals produced by electrolysis.

Curriculum

Area of Study 1 Outcome 2

How can the rate and yield of chemical reactions be optimised?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• The common design features and general operating principles of rechargeable (secondary) cells, with reference to discharging as a galvanic cell and recharging as an electrolytic cell, including the conditions required for the cell reactions to be reversed and the electrode polarities in each mode (details of specific cells not required)	**7A Features of electrolytic cells** **7A.1** Explain the importance of the key design features of electrolytic cells **7A.2** Identify, name, draw and label features of electrolytic cells, including polarity of electrodes and the direction of electron flow **7A.3** Identify key similarities and differences between the design features of galvanic and electrolytic cells **7A.4** Understand the energy transfers involved in discharging and recharging of electrolytic cells **7A.5** Identify key features of secondary cells that allow them to be recharged

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Study Design:	Learning intentions – at the end of the chapter I will be able to:
• The use and limitations of the electrochemical series to explain or predict the products of the electrolysis of particular chemicals, given their state (molten liquid or in aqueous solution) and the electrode materials used, including the writing of balanced equations (with states) for the reactions occurring at the anode and cathode and the overall redox reaction for the cell	**7B Predicting the products of electrolysis** **7B.1** Predict and compare the products of electrolysis when using molten and aqueous electrolytes **7B.2** Predict and compare the products of electrolysis when using different electrodes, including inert electrodes **7B.3** Predict and compare the products of electrolysis using the electrochemical series, including situations where there is competition at the electrodes **7B.4** Understand the effect of electrolyte concentration on the products at the electrodes **7B.5** Write balanced half-equations and balanced overall equations for specific electrolytic cells
• The common design features and general operating principles of commercial electrolytic cells (including, where practicable, the removal of products as they form), and the selection of suitable electrode materials, the electrolyte (including its state) and any chemical additives that result in a desired electrolysis product (details of specific cells not required) • The role of innovation in designing cells to meet society's energy needs in terms of producing 'green' hydrogen (including equations in acidic conditions) using the following methods: – polymer electrolyte membrane electrolysis powered by either photovoltaic (solar) or wind energy – artificial photosynthesis using a water oxidation and proton reduction catalyst system	**7C Commercial electrolytic cells** **7C.1** Identify key design features of commercial electrolytic cells that make them suitable to produce specific chemicals **7C.2** Explain how the selection of both the electrolyte and the type of electrodes used will influence the products generated by commercial electrolytic cells **7C.3** Describe ways that cells can be designed to enhance energy efficiency **7C.4** Describe ways that green chemistry principles can be applied to make the use of electrochemical cells more sustainable and environmentally friendly **7C.5** Describe how the electrolysis of water and artificial photosynthesis can be adapted to produce 'green' hydrogen

Study Design:	Learning intentions – at the end of the chapter I will be able to:
- The application of Faraday's laws and stoichiometry to determine the quantity of electrolytic reactant and product, and the current or time required to either use a particular quantity of reactant or produce a particular quantity of product	**7D** **Faraday's laws of electrolysis** **7D.1** Understand the stoichiometric relationship between the quantity of metal and electrons represented by half-equations in the electrochemical series **7D.2** Apply Faraday's laws to calculate the quantity of product, current or time required for an electrolytic cell

Glossary

Discharge cycle
Electrolysis
Electrolytic cell
Electroplating
Green hydrogen
Inert
Molten electrolyte
Non-spontaneous redox reaction
Recharge cycle
Secondary cell

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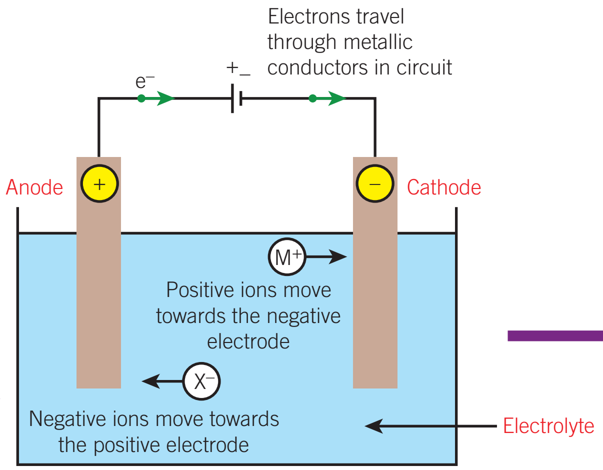
Concept map

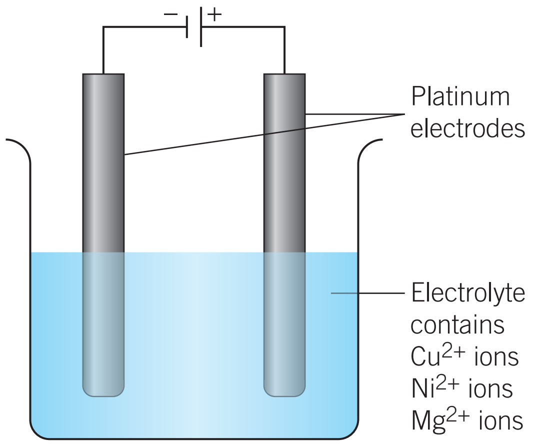
7A Features of electrolytic cells

Features of these cells as secondary cells



7B Predicting the products of electrolysis

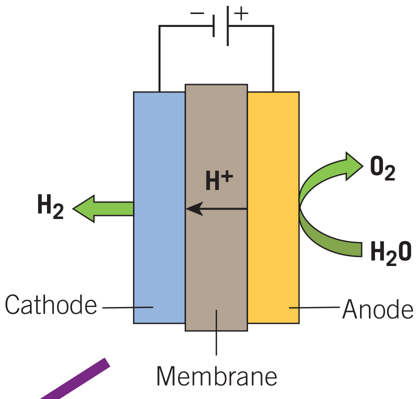
Effects of the choice of components and conditions



7C Commercial electrolytic cells

Design and innovation in commercial electrolytic cells with a focus on sustainability

PEM electrolysis



7D Faraday's laws of electrolysis

Calculations using these laws and stoichiometry

Four key steps to solving Faraday's laws of electrolysis questions

1 Determine number of moles of metal (using $n = \frac{m}{M}$).
2 Determine number of moles of electrons (using the relevant half-equation).
3 Determine the charge, Q, using $Q = n(e^-) \times F$.
4 Determine current (amps) or time (seconds), using $Q = It$.

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

7A Features of electrolytic cells

Study Design:

- The common design features and general operating principles of rechargeable (secondary) cells, with reference to discharging as a galvanic cell and recharging as an electrolytic cell, including the conditions required for the cell reactions to be reversed and the electrode polarities in each mode (details of specific cells not required)

Glossary:

Discharge cycle
Electrolysis
Electrolytic cell
Non-spontaneous redox reaction
Recharge cycle
Secondary cell

ENGAGE

Cell-ebrating batteries!

Have you ever forgotten to recharge the battery in your laptop, your tablet or your mobile phone? If so, you will know how annoying it can be when these devices run out of power! As the world shifts to a more mobile society, centred around having access to these essential devices for our day-to-day lives, it is important to recognise what features of rechargeable batteries make them so convenient and understand how they differ from single-use batteries.

There are many types of rechargeable batteries that combine different electrodes and electrolytes, including, among others, the lithium–ion (Li–ion), nickel–cadmium (Ni–Cd) and lead–acid batteries. This section will help you discover more about the important design aspects of such batteries.

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EXPLAIN

Electrolytic cells

Electrolytic cells are examples of electrochemical cells, which use electrical energy provided by an external power supply (for example, a battery) to force **non-spontaneous redox reactions** that would not normally occur to take place. This process is called **electrolysis** and involves the conversion of electrical energy into chemical energy. In a simplistic way, this can be thought of as the opposite of what occurs in galvanic cells, which involve spontaneous redox reactions that convert chemical energy into electrical energy.

Electrolytic cell a system in which electrical energy is converted to chemical energy

Non-spontaneous redox reaction a reaction that transforms electrical energy into chemical potential energy and has a negative cell potential (i.e. $E < 0$)

Electrolysis the process of forcing a redox reaction to occur by passing an electric current through an electrolyte

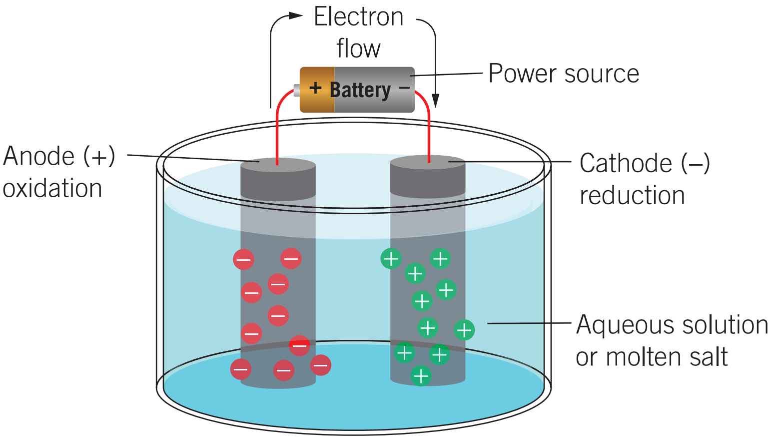


Figure 7A–1 Electrolysis involves a power source forcing electrons through the cell, resulting in reduction occurring at the cathode and oxidation occurring at the anode simultaneously. Cations and anions migrate from the electrolyte to the cathode and anode, respectively.

Features of electrolytic cells

Electrolytic cells, like galvanic cells, must contain two electrodes and an electrolyte. Energy from an external power source is required to drive the reactions. An oxidation reaction occurs at the anode at the same time that a reduction reaction occurs at the cathode. However, because the reactions are non-spontaneous, the reactants do not need to be separated in electrolytic cells and can be placed together into the same container. Although the reactants will not react spontaneously, one important design aspect of electrolytic cells is to ensure the separation of products to prevent them from prematurely reacting spontaneously.

Electrolysis

Through the internal circuit (the electrolyte), the current is carried by ions. In general, anions migrate to the anode and cations migrate to the cathode.

As electrolysis requires energy to force non-spontaneous reactions to take place, a potential greater than the cell potential for the spontaneous redox reaction must be supplied. Free-moving ions must be present in the electrolyte, which means that the electrolyte may be an aqueous solution, or it may be a molten salt consisting of mobile ions. Just like in galvanic cells, the strongest reducing agent present at the anode will undergo oxidation and the strongest oxidising agent present at the cathode will undergo reduction.

3C FEATURES OF GALVANIC CELLS LINK

Comparing galvanic cells with electrolytic cells

It is useful to remember that reduction always occurs at the cathode, regardless of the type of electrochemical cell. You should recall the mnemonic used for galvanic cells, the **Happy Red Cat**, to help identify the polarity and reactions occurring at each electrode. In electrolysis, there is an input of electrical energy, which changes the polarity of the electrode, but not the fact that reduction still occurs at the cathode. For our mnemonic, this means the *cat*hode is still the site of *red*uction, however it will now have a negative polarity. So rather than happy, for electrolytic cells we have a **Sad Red Cat**. This is an important difference between galvanic and electrolytic cells. A further summary and comparison of galvanic cells and electrolytic cells is provided in Table 7A–1.

Table 7A–1 A comparison of galvanic and electrolytic cells

Galvanic cell	Electrolytic cell
Requires two half-cells to separate the reactants	Only one container is required, but products must be separated.
Spontaneous reactions	Non-spontaneous reactions
Chemical energy is converted into electrical energy.	Electrical energy is converted into chemical energy.
The polarity of electrodes is determined by the reactions occurring in the cell.	The polarity of electrodes is determined by the external power source.
Cathode is positive	Cathode is negative
Anode is negative	Anode is positive
Reduction occurs at the cathode.	Reduction occurs at the cathode.
Oxidation occurs at the anode.	Oxidation occurs at the anode.
The strongest reducing agent undergoes oxidation and the strongest oxidising agent undergoes reduction.	The strongest reducing agent present at the anode undergoes oxidation and the strongest oxidising agent present at the cathode undergoes reduction.
Electrons flow through the external circuit from the anode to the cathode.	Electrons flow through the external circuit from the anode to the cathode.
From the salt bridge, anions migrate to the anode, cations migrate to the cathode.	From the electrolyte, anions migrate to the anode, cations migrate to the cathode.

General features of electrolytic cells

In electrolysis the reactions are non-spontaneous, which means that there must be energy from an external power source used to drive the reactions. Provided sufficient voltage is applied, electrons will be pushed from the negative terminal of the battery or power source towards the cathode, giving it a negative charge. Cations in the electrolyte will be attracted to the cathode, where reduction will occur. At the positive anode, anions from the electrolyte will be attracted and undergo oxidation on the surface of the electrode.

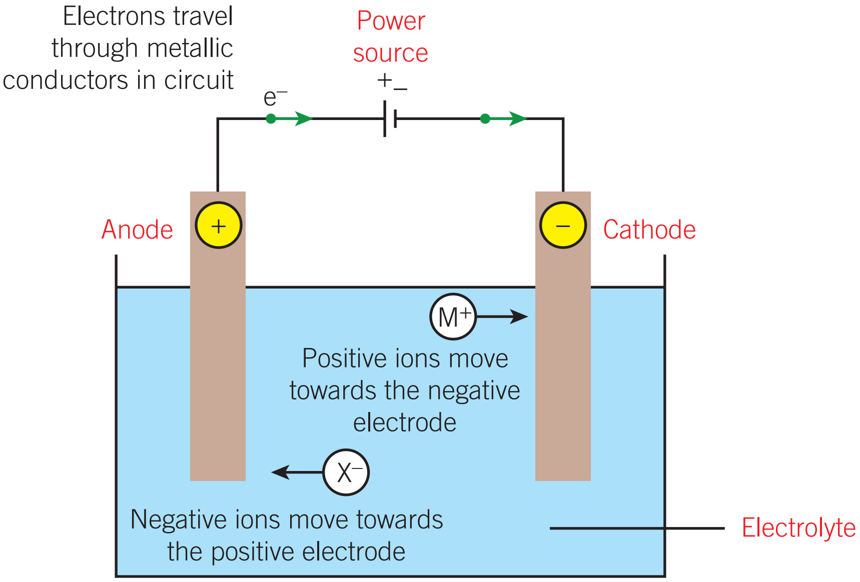
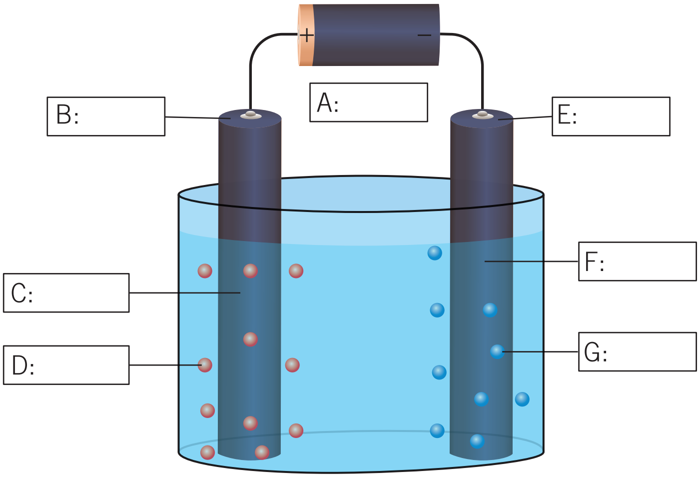


Figure 7A–2 Key components and movement of charged particles within an electrolytic cell

Check-in questions – Set 1

1 Copy the diagram of the electrolytic cell below and label the missing features, A–G. Include:
- direction of electron flow
- name of each electrode (anode or cathode)
- polarity of each electrode
- movement of anions and cations in the electrolyte.



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Secondary cells

LINK **CHAPTER 3**

Secondary cell a type of electrochemical cell that can undergo charge and discharge cycles; therefore, it can be recharged and reused

Discharge cycle when spontaneous chemical reactions occur converting chemical energy into electrical energy

Recharge cycle when electrical energy is used to force a non-spontaneous redox reaction that converts electrical energy into chemical energy

You should recall from Chapter 3 that primary cells include non-rechargeable batteries that spontaneously convert chemical energy into electrical energy. **Secondary cells** include *rechargeable* batteries that can undergo both a **discharge cycle** and **recharge cycle**, allowing them to be reused many times. The discharge process is exactly like that which occurs in a galvanic or primary cell. However, a secondary cell can be connected to a source of electrical energy that is used to force non-spontaneous reactions, converting the products of the discharge cycle back into the initial reactants again. Some examples of secondary cells include the lead–acid (car) battery, the lithium–ion battery and the nickel–cadmium battery.

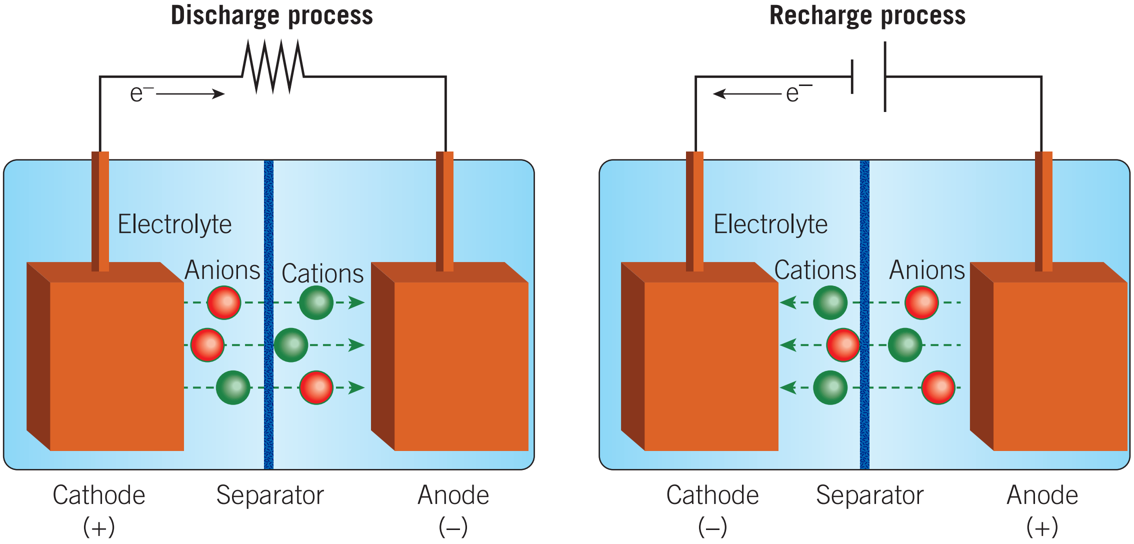

Figure 7A–3 The discharge and recharge processes of secondary cells

Recharging a secondary cell

When a secondary cell is discharging, it behaves just like a galvanic cell. However, recharging a secondary cell involves electrical energy being converted into chemical energy. This means the cell is behaving like an electrolytic cell. During recharge, the redox reactions that were occurring during discharge typically get reversed and the polarities of the electrodes swap. During discharge, the cathode is positive and the anode is negative. However, during recharge, the cathode is negative and the anode is positive. Although these polarities change when the reactions are reversed, reduction still *always* occurs at the cathode and oxidation at the anode.

One of the conditions necessary for recharging to be possible is that the products of the discharge reactions must remain in contact with the electrodes. This is essential, as it means that they will then be present on the electrode for the reverse reaction to occur when discharging resumes. For this to happen, the products are often solids that adhere to the electrodes. Furthermore, to recharge successfully, the amount of electrical energy put into the system must be greater than the potential difference of the cell. For example, the nickel–cadmium battery is a rechargeable battery that has a cell potential of 1.2 volts. Therefore, to recharge this battery, a voltage greater than 1.2 volts must be applied.

Worked example 7A–1: Recharging a secondary cell

VIDEO
WORKED EXAMPLE 7A–1

A zinc–cerium cell is a rechargeable secondary cell. It contains a membrane that separates the zinc anode from the carbon cathode, and the electrolyte is an acidic solution containing a mixture of cerium ions, Ce^{3+} and Ce^{4+}, and zinc ions, Zn^{2+}.

The half-equations occurring during discharge in the cell can be simplified as:

$$\text{Anode:} \quad Zn(s) \rightarrow Zn^{2+}(aq) + 2e^-$$

$$\text{Cathode:} \quad Ce^{4+}(aq) + e^- \rightarrow Ce^{3+}(aq)$$

a Write the overall balanced reaction for the discharge cycle.

b If the standard electrode potential ($E°$ value) for the cerium half-reaction shown is 1.65 V, calculate the voltage required to recharge the cell.

c Write the equation for the reaction occurring at the negative electrode during recharging.

Solution

	Logic	Process
Step 1	The discharge cycle occurs spontaneously according to the half-equations provided. Before adding the half-equations together, they must be balanced so that the number of electrons in each half-equation is equal. This can be done by multiplying the second half-equation by two.	$Zn(s) \rightarrow Zn^{2+}(aq) + 2e^-$ $2 \times (Ce^{4+}(aq) + e^- \rightarrow Ce^{3+}(aq))$ $= 2Ce^{4+}(aq) + 2e^- \rightarrow 2Ce^{3+}(aq)$
Step 2	Now that the number of electrons shown in each half-equation is the same, combine half-equations together (electrons cancel on each side).	**a** $2Ce^{4+}(aq) + Zn(s) \rightarrow 2Ce^{3+}(aq) + Zn^{2+}(aq)$
Step 3	By referring to the electrochemical series in the appendix of this book, find the $E°$ value for the zinc half-reaction. Use this to calculate the cell potential.	**b** $E° = -0.76$ Cell potential $= E°$ (oxidation) – $E°$ (reduction) $= 1.65 - (-0.76)$ $= 2.61$ V. To recharge the cell, a voltage of more than 2.61 V is required.
Step 4	The positive electrode during *discharge* is the cathode, but during *recharge* (during electrolysis) the polarities swap, so the positive electrode will be the anode.	**c** The recharge reaction will be the reverse of the discharge reaction, hence: $Zn^{2+}(aq) + 2e^- \rightarrow Zn(s)$

7A SKILLS

Identifying differences – need two to tango!

When writing answers to 'compare and contrast' questions, it's important to thoroughly describe the characteristics that distinguish each of the two items being compared. Simply outlining the attributes of one item won't provide a complete answer, as it doesn't establish a comparison between the two. The aim of these questions is to highlight both similarities and differences between two or more subjects. Therefore, effective responses should pinpoint a feature, describe how it functions or is manifested in one item and then describe how it functions or is manifested differently in the other item. This way, you not only point out the differences, but also clarify how these differences affect the nature or behaviour of the items in question.

For instance, consider the question: 'What are the differences between galvanic cells and electrolytic cells?' An incomplete answer might just say, 'Galvanic cells are spontaneous and convert chemical energy to electrical energy.' While this is accurate, it doesn't address how these attributes contrast with those of electrolytic cells. A better, more complete answer would be:

'Galvanic cells and electrolytic cells differ primarily in their spontaneity and energy conversion. Galvanic cells undergo spontaneous redox reactions and function to convert chemical energy to electrical energy. They operate by driving an electric current through an external circuit from the anode to the cathode. On the other hand, electrolytic cells require an external power source to drive non-spontaneous redox reactions, thus converting electrical energy into chemical energy. Their electric current is driven through the cell from the cathode to the anode.'

This response distinctly describes both galvanic and electrolytic cells, emphasising their contrasting features.

Section 7A questions

1 State whether the following statements are true or false for electrolytic cells, and justify your response.
   - a Electrons flow from the anode to the cathode.
   - b Oxidation occurs at the cathode.
   - c Electrical energy is converted to chemical energy.
   - d The polarity of the anode is negative.
   - e The cathode can show an increase in mass during a reaction.

2 State two similarities and two differences between galvanic cells and electrolytic cells.

3 Draw a fully labelled electrolytic cell.

4 What is the difference between a spontaneous redox reaction and a non-spontaneous redox reaction?

7B

Predicting the products of electrolysis

Study Design:
- The use and limitations of the electrochemical series to explain or predict the products of the electrolysis of particular chemicals, given their state (molten liquid or in aqueous solution) and the electrode materials used, including the writing of balanced equations (with states) for the reactions occurring at the anode and cathode and the overall redox reaction for the cell

Glossary:
Inert
Molten electrolyte

ENGAGE

Pipe dreams: fuelling progress ahead!

Extensive pipeline networks are now used around the world to transport water, oil, gas and other compounds between cities, countries and sometimes even continents. These pipelines have a huge impact on the economy of countries, as their ability to efficiently import and export natural resources is critical. However, these pipelines are not perfect and can often be plagued by issues, including corrosion of the metal pipes. The global cost of corrosion was estimated to be almost US$3 trillion in 2018! Therefore, finding the best solutions to avoid corrosion has become a significant area of research. One method that has been successfully applied in many locations is through the use of an electric current, which works by ensuring that the metal in the pipe acts as the cathode and so cannot undergo oxidation. In this section, you are going to learn about how we can use experimental data to predict electrolysis reactions.

EXPLAIN

Using the electrochemical series to predict which reactions will occur

The ability to predict which reactions are going to occur in an electrolytic cell is similar in many ways to the way we predict reactions in galvanic cells. In an electrolytic cell, two of the more important factors to consider are:

- the state of the electrolyte
- the material used for the electrodes.

It is convenient that regardless of whether we are dealing with a galvanic or electrolytic cell, the strongest oxidising agent present at the cathode will always undergo reduction and that the strongest reducing agent present at the anode will always undergo oxidation. Knowing this fact makes it possible to then predict which reactions are occurring within a particular electrolytic cell.

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Electrolytes

Some electrolytic cells will contain species in aqueous solutions, meaning that they also contain liquid water, $H_2O(l)$. Liquid water is listed multiple times on the electrochemical series and given that it can undergo both reduction and oxidation reactions, it is important to include it when considering the reactions that may take place. Other electrochemical cells may contain **molten electrolytes**, which are usually salts that get heated to temperatures above their melting point. The temperatures of these molten electrolytes are much higher than 100°C, meaning that no liquid water would be present, and so it can be excluded from being a potential reactant.

Molten electrolyte a chemical substance made from a hot liquified salt heated to over 100°C

NOTE

It is important to remember to write any redox equations with liquid states (l) for ions and metals whenever a molten electrolyte is being used. This is different to how they appear on the electrochemical series, where they are written with standard state symbols, so be careful when copying across equations under such circumstances. Note that gases (g) will remain the same.

Electrodes

The type of electrodes used must always be considered when predicting the reactions of electrolytic cells. Often electrodes are made from species that can take part in a reaction, for example, solid copper or zinc electrodes. Where this is the case, these species must always be considered when predicting reactions. However, sometimes non-reactive or **inert** materials, such as platinum or carbon, are used for electrodes in cells. Only species present in the electrolyte itself should be considered when predicting the reactions occurring in electrolytic cells containing inert electrodes.

Inert largely non-reactive; does not take part in a reaction

Competition at the electrodes

Electrolytic cells can have several chemical species that have the potential to react at each electrode, so it is vital to make sure you consider all of those present when predicting the reactions that will take place. Knowing that oxidation will always occur at the anode and reduction will always occur at the cathode, we can predict the electrode half-reactions that will occur for a given electrolytic cell at standard conditions.

NOTE

Some species appear more than once on the electrochemical series on both the left-hand *and* right-hand sides of the series. Liquid water is a good example of this. When predicting reactions, *all* relevant occurrences of each species must be considered to accurately identify the strongest reducing agent and strongest oxidising agent.

3D USING THE ELECTROCHEMICAL SERIES LINK

Predicting the products of electrolysis

The electrochemical series (in the appendix, on page 542) can be used to help predict which reactions are most likely to take place at the anode and cathode of an electrolytic cell.
The steps used to identify and predict the reactions occurring in an electrolytic cell are as follows:

1 Identify all the species present at *each* electrode. The list may be different for the anode and the cathode, depending on the material that the electrode is composed of and whether the cell has different, separated electrolyte sections. Be sure to look carefully at states and ionic charges. Be sure to include the electrodes if they are made of a reactive material. Be sure to include or exclude liquid water, depending on the type of electrolyte present in the cell.

2 Use the electrochemical series and highlight each of the locations where any species present appear.

3 For the cathode, identify the strongest oxidising agent, which will be reduced. The reduction half-equation can now be written, as it appears in the electrochemical series.

4 For the anode, identify the strongest reducing agent, which will be oxidised. The half-equation can now be written but must be *reversed* from the way that it appears in the electrochemical series to make it the oxidation half-equation.

5 Write the overall redox equation, if required, by balancing the number of electrons in each half-equation.

6 Sometimes you may have polyatomic anions present, such as sulfate ions, SO_4^{2-}, or nitrate ions, NO_3^-. These, along with any other polyatomic anions, do not take part in the redox reactions studied as part of this course, so even though they may be present, they can be excluded from the list of species that have the potential to react.

VIDEO
WORKED
EXAMPLE 7B–1

Worked example 7B–1: Comparing the products of electrolysis at each electrode

An aqueous solution of copper(II) ions is blue in colour. Compare the products of electrolysis of a 1 M copper sulfate aqueous solution using copper electrodes with those produced using inert platinum electrodes. Write the overall redox equation for each electrolytic cell and describe any qualitative observations you might expect to see while the cells are operating.

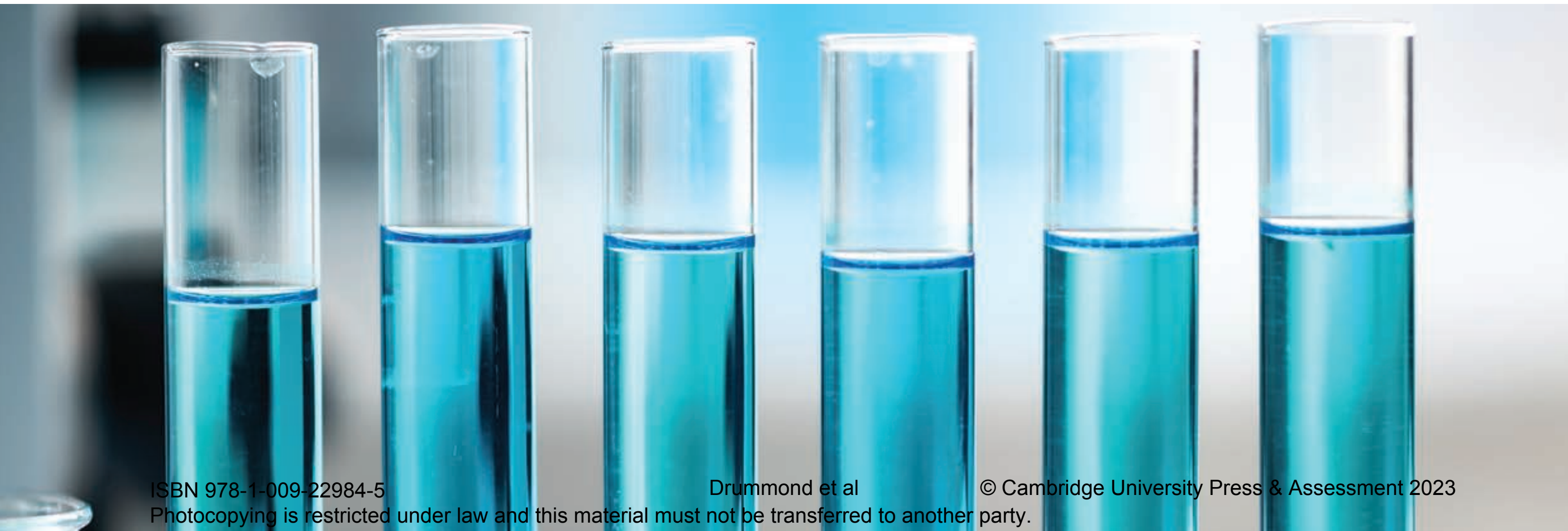
Solution

	Logic	Process
Step 1	List all species present that could react at the cathode and anode. Remember that the platinum electrodes are inert.	For the copper electrodes: at the cathode: $H_2O(l)$, $Cu(s)$, $Cu^{2+}(aq)$ at the anode: $H_2O(l)$, $Cu(s)$, $Cu^{2+}(aq)$ For the platinum electrode: at the cathode: $H_2O(l)$, $Cu^{2+}(aq)$ at the anode: $H_2O(l)$, $Cu^{2+}(aq)$
Step 2	Refer to the electrochemical series and identify the strongest oxidising agent (highest species on the left-hand side of the reaction arrow).	For both electrodes: $Cu^{2+}(aq)$ will undergo reduction at the cathode. $Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)$
Step 3	Refer to the electrochemical series and identify the strongest reducing agent (lowest species on the right-hand side of the reaction arrow).	For the copper electrodes: $Cu(s)$, which will undergo oxidation at the anode. Use the electrochemical series to identify the half-equation. $Cu(s) \rightarrow Cu^{2+}(aq) + 2e^-$ For the platinum electrodes: $H_2O(l)$ will undergo oxidation at the anode. In this example, water is the *only* species that is on the right-hand side, therefore the only species that can be oxidised. Use the electrochemical series to identify the half-equation. $2H_2O(l) \rightarrow O_2(g) + 4H^+(aq) + 4e^-$

Step 4	Use the half-equations to predict the products at each electrode.	For the copper electrodes: Solid copper will be produced at the cathode and copper ions, Cu^{2+}, will be produced at the anode. For the platinum electrodes: Solid copper will still be produced at the cathode; however, instead of copper ions, oxygen gas and hydrogen ions, H^+, will be produced at the anode.
Step 5	Combine the half-equations to give the full overall redox equation, ensuring electrons are equal in each half-equation before cancelling and adding the half-equations together.	For the copper electrodes: $Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)$ $Cu(s) \rightarrow Cu^{2+}(aq) + 2e^-$ $Cu(s) + Cu^{2+}(aq) + \cancel{2e^-} \rightarrow Cu(s) + Cu^{2+}(aq) + \cancel{2e^-}$ $Cu(s) + Cu^{2+}(aq) \rightarrow Cu(s) + Cu^{2+}(aq)$ For the platinum electrodes: $2 \times (Cu^{2+}(aq) + 2e^- \rightarrow Cu(s))$ $2Cu^{2+}(aq) + 4e^- \rightarrow 2Cu(s)$ $2H_2O(l) \rightarrow O_2(g) + 4H^+(aq) + 4e^-$ $2H_2O(l) + Cu^{2+}(aq) + \cancel{4e^-} \rightarrow 2Cu(s) + O_2(g) + 4H^+(aq) + \cancel{4e^-}$ $2H_2O(l) + Cu^{2+}(aq) \rightarrow 2Cu(s) + O_2(g) + 4H^+(aq)$
Step 6	Write your qualitative observations.	In the copper electrode system, there would be an increase in mass at the cathode and a decrease in mass at the anode. In the platinum electrode system, oxygen would be seen as bubbles of gas forming; however, it is also important to note that the production of hydrogen ions would decrease the pH of the electrolyte solution. The cathode in both systems would also end up with a coating of copper, and as the copper ions, $Cu^{2+}(aq)$, are consumed in the reaction, the electrolyte solution would show a decrease in the intensity of the blue colour associated with these ions.

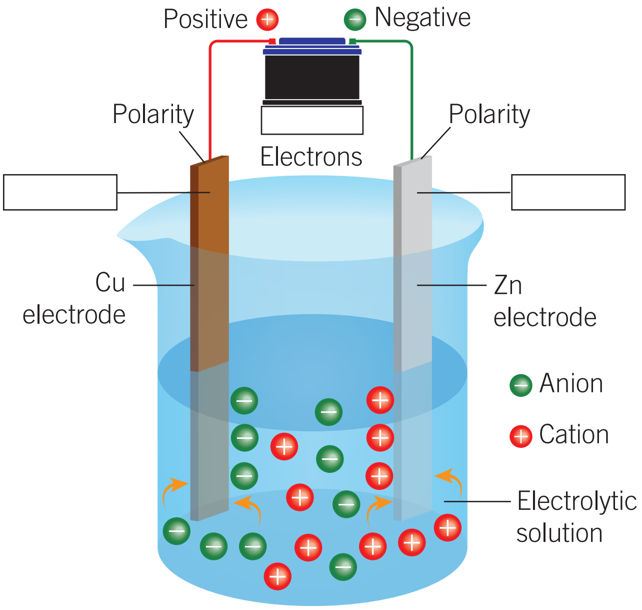
NOTE

Even though the electrochemical series lists the reactions as reversible reactions using equilibrium arrows, remember to always use a solid forward arrow to represent each half-equation occurring.



Check-in questions – Set 1

1 The electrolytic cell shown contains copper and zinc electrodes in a 1 M aqueous copper(II) sulfate solution.
  a Copy and complete the diagram by labelling the direction of electron flow, the anode and cathode, and the polarity of each electrode.
  b Write the half-reaction (reduction or oxidation) occurring at each electrode.
  c State one observation that is likely while the cell is operating.



Electrolysis

Non-standard conditions

Although the electrochemical series is useful in predicting redox reactions, one limitation is that it is only valid for use at standard conditions (1 M, 25°C and 100 kPa).

Despite its convenience as a tool to predict the redox reactions taking place in a cell, because cells rarely operate under standard conditions, it is only through experiments that we can be certain about which reactions will proceed. There are several factors that will affect electrolytic reactions, including:

- the concentration of the electrolyte
- gas pressures
- temperature
- current
- voltage
- the nature of the electrodes.

The effect of electrolyte concentration

When a standard solution of sodium chloride is electrolysed, there are two species present that can be oxidised at the anode: chloride ions, $Cl^-(aq)$, and water, $H_2O(l)$. By referring to the electrochemical series, the two half-equations, together with their electrode potential values, are:

$$2Cl^-(aq) \rightarrow Cl_2(g) + 2e^- \qquad E^\circ = -1.36\text{ V}$$

$$2H_2O(l) \rightarrow O_2(g) + 4H^+(aq) + 4e^- \qquad E^\circ = -1.23\text{ V}$$

The strongest reducing agent is water, H_2O, since it is listed higher on the right-hand side. As such, we would predict that water will undergo oxidation at the anode, as follows:

$$2H_2O(l) \rightarrow O_2(g) + 4H^+(aq) + 4e^-$$

This prediction would generally hold true, especially for low concentrations of sodium chloride solution, meaning that oxygen gas is the major product at the anode.

However, one limitation of using the electrochemical series to predict reactions is that it is based on solution concentrations of 1 M. As the standard electrode potential values are so close, if the concentration of the sodium chloride solution is increased beyond 1 M, the second reaction will occur more readily:

$$2Cl^-(aq) \rightarrow Cl_2(g) + 2e^-$$

This results in chlorine gas being the major product of the reaction at the anode.

NOTE

It pays to carefully check the concentrations of the solutions stated in a question. Using solutions that have a concentration other than 1 M may result in different reactions taking place to those predicted using the electrochemical series. Having an *increased* concentration of one species may mean that it reacts instead of another species predicted using the electrochemical series. This is often observed when the electrode potential values, E^0, are close together.

Exhausting the supply of reactants

Some consideration should also be given to what happens in an electrochemical cell if one of the species is completely exhausted. If one completely reacts, the next strongest species will start to react, provided there is another species available. For example, if the strongest reducing agent is completely exhausted during the reaction, the next strongest reducing agent present will then go on to react. However, it is also possible that a cell may stop reacting. This would occur if there were no more reducing agents present in the cell, despite a supply of oxidising agents or vice versa.

Check-in questions – Set 2

1 An electrolytic cell consists of inert graphite electrodes with a solution containing 1.00 M concentrations of lead ions, $Pb^{2+}(aq)$, cadmium ions, $Cd^{2+}(aq)$, cobalt ions, $Co^{2+}(aq)$, and nitrate ions, NO_3^- (aq).
   - a Identify the strongest reducing agent and strongest oxidising agent.
   - b Write the half-reactions occurring initially at the anode and cathode.
   - c Calculate the initial voltage required for the cell to operate.
   - d Predict what you will observe at the cathode over time. Justify your response.
   - e Predict what you will observe at the anode over time. Justify your response.
   - f Using equations, explain what would happen if the cell was initially set up using solid tin electrodes instead of inert graphite electrodes.

Molten electrolytes

If you look closely at the position of water on the left-hand side of the electrochemical series, you will notice that water is a stronger oxidising agent than many of the metal ions: manganese, aluminium, magnesium, sodium, calcium, potassium and lithium. This means it will be reduced at the cathode in preference to these metal ions. It is useful to recognise that to produce any of the metals whose ions are weaker oxidising agents than water, it must be done using a molten electrolyte, so that no water is present in the electrochemical cell.

Worked example 7B–2: Determining half-reactions in an electrolytic cell with a molten electrolyte

VIDEO
WORKED EXAMPLE 7B–2

An electrolytic cell with an aqueous 1 M magnesium chloride solution, $MgCl_2(aq)$, is set up using platinum electrodes. Initially, the reactions occurring at each electrode are:

$$\text{Anode: } 2H_2O(l) \rightarrow O_2(g) + 4H^+(aq) + 4e^-$$

$$\text{Cathode: } 2H_2O(l) + 2e^- \rightarrow H_2(g) + 2OH^-(aq)$$

State the reactions that would occur at each electrode if the electrolyte solution was changed to *molten* magnesium chloride, $MgCl_2(l)$.

Solution

	Logic	Process
Step 1	List the species present at each electrode.	Molten electrolytes are at such high temperatures that there would no longer be any water in the cell. Anode: $Cl^-(l)$ Cathode: $Mg^{2+}(l)$
Step 2	Write the reactions occurring at each electrode (remembering to use liquid for the state of any molten species involved).	Cathode: $Mg^{2+}(l) + 2e^- \rightarrow Mg(l)$ Anode: $2Cl^-(l) \rightarrow Cl_2(g) + 2e^-$

7B SKILLS

Significant figures – adding and subtracting

In performing addition and subtraction operations, the rule for significant figures states that the answer should not have more decimal places than the least accurate number in the problem. This means that the precision of the result should match the least precise measurement. For instance, if one number has a decimal place up to the tenths (like 7.6) and another goes up to the hundredths (like 3.34), your final answer should only have its decimal place up to the tenths, reflecting the least precise measurement.

For example, consider a scenario in which we are measuring cell potentials from two separate half-cell reactions in an electrolysis set-up. The first cell potential is 1.35 V (measured to the hundredths place) and the second cell potential is 0.8 V (measured to the tenths place). If we are to add these two potentials together, the correct result should only have its decimal place up to the tenths place because the least precise measurement has only one decimal place.

Incorrectly applying significant figures might yield a result like 2.15 V. Here, the result is precise up to the hundredths place, which violates the rule. The correct application of significant figures would give us a result of 2.2 V, properly rounded to the tenths place. Thus, it's crucial to identify the least precise measurement and adjust your result to match its level of precision to correctly apply significant figures in addition or subtraction.

Section 7B questions

1 An electrolytic cell consists of carbon electrodes immersed in an aqueous 1 M NaCl solution.

- a Write the reduction and oxidation half-equations that would take place in the cell.
- b Write the overall cell equation.
- c Explain what would happen if the aqueous 1 M NaCl solution was replaced with a molten NaCl electrolyte.
- d Describe what would happen if the aqueous 1 M NaCl solution was replaced with a concentrated aqueous 5 M NaCl solution.

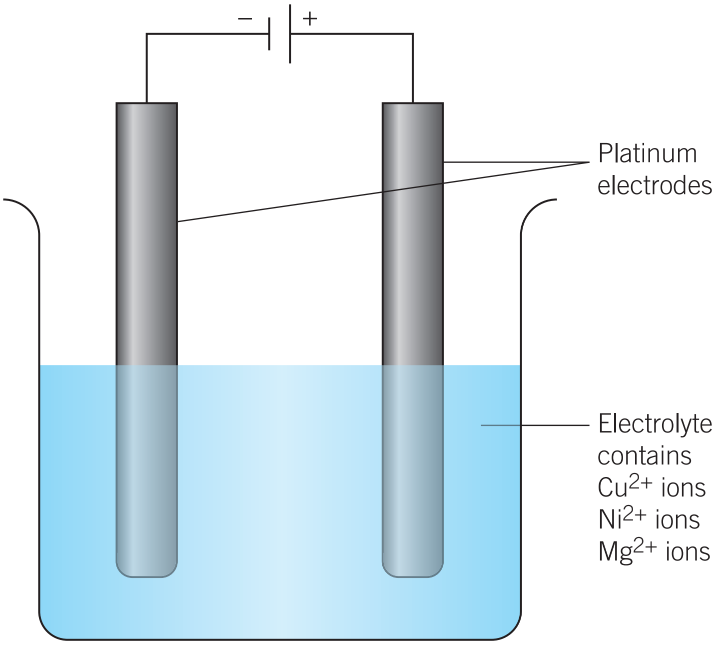
2 Draw a labelled diagram of an electrolytic cell made with a zinc cathode, an inert carbon anode and an electrolyte solution containing 1 M zinc nitrate, $Zn(NO_3)_2$.
Include:

- polarity of each electrode
- direction of electron flow
- half-reactions occurring at each electrode
- overall reaction
- voltage required to force reactions to proceed (to two decimal places).

3 An electrolytic cell is set up containing a mixture of 1 M copper nitrate, 1 M nickel nitrate and 1 M magnesium nitrate, and is electrolysed using platinum electrodes. Initially, the reactions occurring at each electrode are:

Anode: $2H_2O(l) \rightarrow O_2(g) + 4H^+(aq) + 4e^-$
Cathode: $Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)$

- a Redraw the diagram below and label the anode and cathode, including their polarity.
- b Show the direction of electron flow by adding an arrow to the diagram.
- c Using relevant chemical equations, explain what you would expect to happen over a long period of time.



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Commercial electrolytic cells

Study Design:

- The common design features and general operating principles of commercial electrolytic cells (including, where practicable, the removal of products as they form), and the selection of suitable electrode materials, the electrolyte (including its state) and any chemical additives that result in a desired electrolysis product (details of specific cells not required)
- The role of innovation in designing cells to meet society's energy needs in terms of producing 'green' hydrogen (including equations in acidic conditions) using the following methods:
  - polymer electrolyte membrane electrolysis powered by either photovoltaic (solar) or wind energy
  - artificial photosynthesis using a water oxidation and proton reduction catalyst system

Glossary:
Electroplating
Green hydrogen

ENGAGE

Fuel for thought in the future

For a few years now, there has been strong impetus for hydrogen gas to be considered as a future fuel. One significant factor is that hydrogen fuel cells only produce water (and heat), so they are seen as an environmentally friendly option as society moves to phase out the use of fossil fuels.

Hydrogen gas can be produced in several ways, including processes that use renewable wind or solar power. So why haven't we seen hydrogen fuel cells used more broadly in society? There is a high cost associated with the production processes, as well as the difficulty with storing and transporting hydrogen gas safely, as it is extremely flammable. Perhaps once improvements and advances are made in the infrastructure required, the use of hydrogen as a fuel will explode … metaphorically speaking!

Figure 7C–1 A hydrogen-powered bus being refuelled (left). A hydrogen gas production facility, powered by wind energy (right)

EXPLAIN

Commercial applications of electrolysis

Electroplating an application of electrolysis, whereby electrical energy is used to deposit a coating of one metal onto the surface of another substance

Electrolysis is used to commercially prepare many chemicals used in society and requires large amounts of electrical energy. As well as the cost associated with electrical energy supply, the use of electrolysis is also influenced by the availability of suitable electrolytes and electrodes to be used in cells. Often electrolysis is used to prevent corrosion or to improve the aesthetics of an object. For example, **electroplating** is used to produce Olympic gold medals. It is often used as the preferred method to produce chemical species on a large scale for other applications.

7B PREDICTING THE PRODUCTS OF ELECTROLYSIS LINK

In Section 7B, we explored how changing the state of the electrolyte and changing conditions, such as the materials electrodes are made from, can affect the products of the reactions taking place in an electrolytic cell. For commercial cells, these factors remain crucial to ensure that the desired electrolysis product is achieved. For some cells, it may be better to use reactive electrodes, whereas for others it may be beneficial to use inert electrodes made from carbon or platinum. Similarly, the use of concentrated aqueous electrolytes or molten electrolytes will potentially alter the reactions taking place in an electrolytic cell.

Because the products of electrolysis are often more reactive than the reactants in the cell, they must be kept separated once produced to prevent them from reacting spontaneously. This, as well as the ability to quickly remove and capture the desirable products of the reactions, are key design aspects for electrolytic cells.

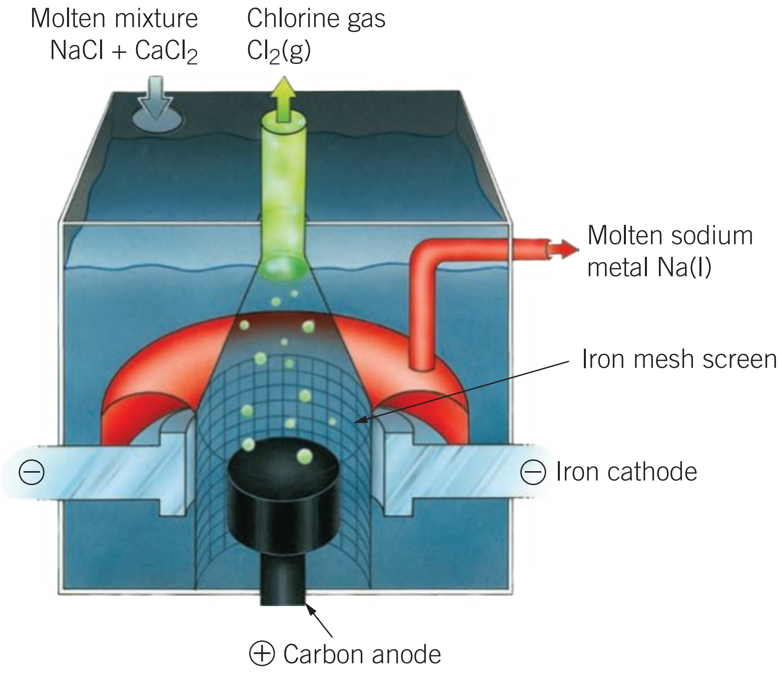


Figure 7C–2 Cross-sectional diagram of the Downs cell

The Downs cell shown in Figure 7C–2 is used commercially to produce both sodium metal and chlorine gas. The cell consists of a positive carbon anode in the centre, surrounded by a negative iron cathode. The electrolyte is a mixture of molten sodium chloride and calcium chloride. Aqueous sodium chloride cannot be used, as water is a stronger oxidising agent than sodium ions and so would react preferentially at the cathode. Notice the iron mesh screen that separates the chlorine gas produced at the anode from the sodium metal formed at the cathode. Should these species come into contact, they would spontaneously react together, meaning neither product could be captured for use. This separation of products is crucial in the design of electrolytic cells.

Another key design feature for the safe operation of these cells is to store the sodium metal produced in a way that prevents its contact with oxygen or water. The selection of an inert carbon anode will also ensure the desired reaction to produce chlorine gas takes place. This minimises the need to replace the electrode as often as would be required if using a reactive metal, such as copper or nickel.

Many commercial electrolytic cells produce dangerous chemicals, so the safe collection and storage of these is an important consideration reflected in their design. The membrane cell (shown in Figure 7C–3), used to produce sodium hydroxide, NaOH, is one such example where there are products that pose a potential safety risk.

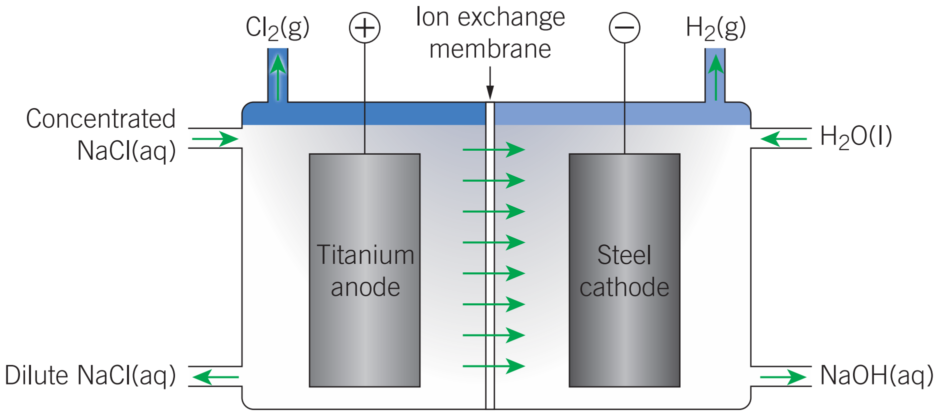


Figure 7C–3 A diagram of the membrane cell used in the production of sodium hydroxide

The membrane cell is an electrolytic cell used to produce sodium hydroxide, which also produces chlorine gas and hydrogen gas. Water molecules undergo reduction at the negative cathode (steel mesh), forming hydroxide ions and hydrogen gas, which because of its explosive and highly flammable properties is removed as it is produced. Chloride ions undergo oxidation at the positive anode, forming chlorine gas, which is also removed as it is produced. Chlorine is a toxic gas, so needs to be collected securely to ensure that no one operating the cell inhales it.

The membrane that separates the anode and cathode compartments in the cell also performs an important role. It selectively allows the sodium cations, Na^+, to pass through, but prevents the hydroxide ions and chloride ions from coming into contact, which would result in undesirable products forming.

Producing green hydrogen

Electrolysis of water

The process of electrolysing water efficiently and safely is at the forefront of current chemical research and development around the world. There is a desire to improve the design of electrolytic cells that can generate **green hydrogen** in an effort to help meet society's energy needs. The production of green hydrogen involves processes that use renewable and sustainable energy, such as wind and solar power.

Green hydrogen hydrogen generated by renewable energy with lower carbon emissions than other sources of hydrogen

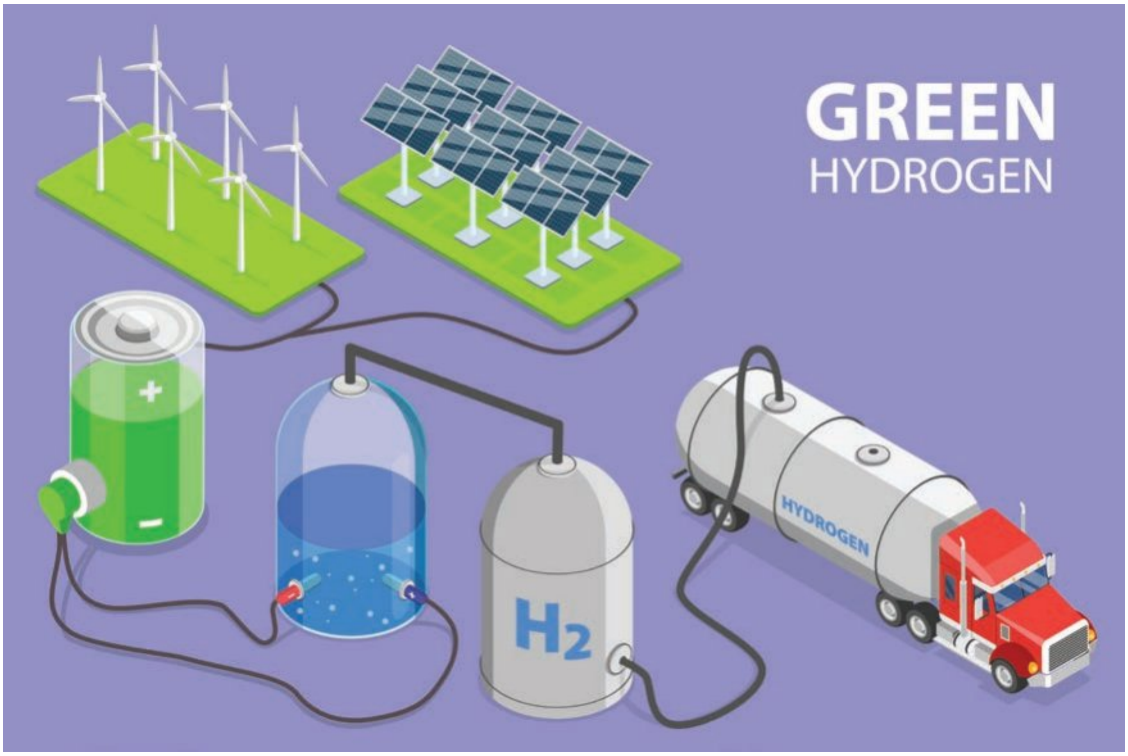


Figure 7C–4 Production of green hydrogen using renewable wind and solar energy

Before we look at some innovative ways this can be done, it is important to understand the fundamental chemistry involved in the electrolysis of water.

Water can be electrolysed to produce hydrogen gas (a useful fuel) and oxygen. However, pure water is a poor conductor of electricity, so in the laboratory process a small amount of sulfuric acid is added to enhance the conductivity. This is a great example of how the use of chemical additives improves the production of the desired species.

During the electrolysis of water, special collection chambers must be used for the gases that are produced. Important safety measures must be in place to ensure the safe operation of the electrolytic cell, but also for the storage and transport of hydrogen gas, which is highly flammable.

The reactions occurring in the cell are as follows:

Anode reaction: $2H_2O(l) \rightarrow O_2(g) + 4H^+(aq) + 4e^-$

Cathode reaction: $2H_2O(l) + 2e^- \rightarrow H_2(g) + 2OH^-(aq)$

At the anode, oxygen gas is produced as well as hydrogen ions, H^+, which results in a more acidic environment around the electrode. At the cathode, hydrogen gas is produced, as well as hydroxide ions, OH^-, resulting in a more alkaline environment around the electrode. Figure 7C–5 shows an illustration of what this may look like in the presence of universal indicator.

The hydrogen ions and hydroxide ions produced during the reactions at each electrode combine to form water, meaning that the overall reaction for the electrolysis of water can be represented as follows:

$$2H_2O(l) \rightarrow 2H_2(g) + O_2(g)$$

Figure 7C–5 Electrolysis of water into hydrogen and oxygen gas. In the schematic, a universal indicator has been added that turns red in the acidic environment generated around the anode and blue in the alkaline environment generated around the cathode.

The production of hydrogen and oxygen occurs in a 2-to-1 ratio, which means that twice as much gas by volume would be collected at the cathode as there would be at the anode. This is represented in Figure 7C–5, which shows the volume of gas forming at each electrode.

Check-in questions – Set 1

1 What useful fuel can be made from the electrolysis of water?
2 Why is sulfuric acid added to water before it undergoes electrolysis?
3 What is the purpose of the iron mesh screen in the Downs cell?

Polymer electrolyte membrane electrolysis

Polymer electrolyte membrane (PEM) electrolysis is a technology used to produce high purity ‘green’ hydrogen that can be powered by renewable energy supplies such as solar or wind energy. Solid polymers are used as the electrolyte, which increase conductivity and the ability to function at higher pressures. They are quite compact and operate at low temperatures up to around 80°C, although one downside is the requirement for expensive catalysts.

In PEM water electrolysis, water is electrochemically split into hydrogen and oxygen. The water at the anode is split into oxygen, O_2, protons, H^+, and electrons. The electrons travel through the external circuit to the cathode. The protons migrate through a proton-conducting membrane to the cathode side where they combine with the electrons and are reduced to hydrogen gas, H_2, as shown in Figure 7C–6.

Anode reaction: $2H_2O(l) \rightarrow 4H^+(aq) + O_2(g) + 4e^-$

Cathode reaction: $4H^+(aq) + 4e^- \rightarrow 2H_2(g)$

Overall reaction: $2H_2O(l) \rightarrow 2H_2(g) + O_2(g)$

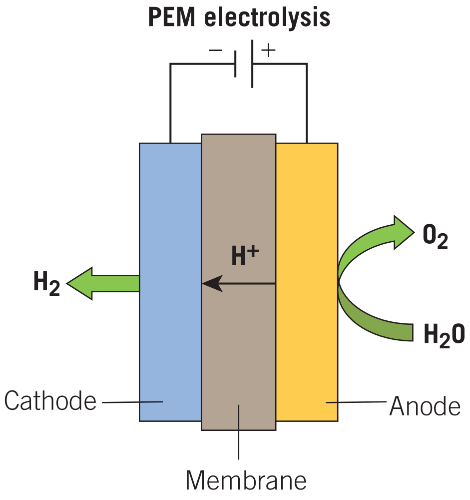


Figure 7C–6 Diagram of PEM electrolysis

1B PRODUCTION OF CHEMICAL ENERGY IN NATURE **LINK**

Artificial photosynthesis

Natural photosynthesis, which we examined in Section 1B, occurs in two stages: a light-dependent stage and a light-independent stage. In the light-dependent stage, energy from light is used to split water into oxygen and protons, and then in the light-independent stage, the protons are combined with carbon dioxide to create sugars that plants use for energy.

Scientists have worked on replicating this biological process through what is called artificial photosynthesis, taking inspiration from nature to convert sunlight into other forms of energy.

One method of artificial photosynthesis known as photocatalytic water splitting creates green hydrogen by mimicking the light-dependent stage, using visible light to create protons and oxygen. The produced protons must then be reduced to hydrogen molecules, but this is challenging as complete splitting is an energy-intensive, four-electron process:

Oxidation half-reaction: $2H_2O(l) \rightarrow 4H^+(aq) + O_2(g) + 4e^-$

Proton reduction half-reaction: $4H^+(aq) + 4e^- \rightarrow 2H_2(g)$

Overall reaction: $2H_2O(l) \rightarrow 2H_2(g) + O_2(g)$

To help overcome this high-energy requirement, catalysts are required to mediate the transfer of electrons. Some catalysts that have been explored include manganese, titanium dioxide and cobalt oxide.

One set-up of this system is detailed in Figure 7C–7 and uses two catalysts: a water-oxidation catalyst and a proton-reduction catalyst. When a photon of light hits the photosensitiser, it excites an electron, which is then donated to the semiconductor. This electron moves through the external circuit, where it is used by the proton-reduction catalyst to reduce hydrogen ions to hydrogen gas. To restore the charge balance in the photosensitiser, water is oxidised using the water-oxidation catalyst, which produces oxygen gas and electrons.

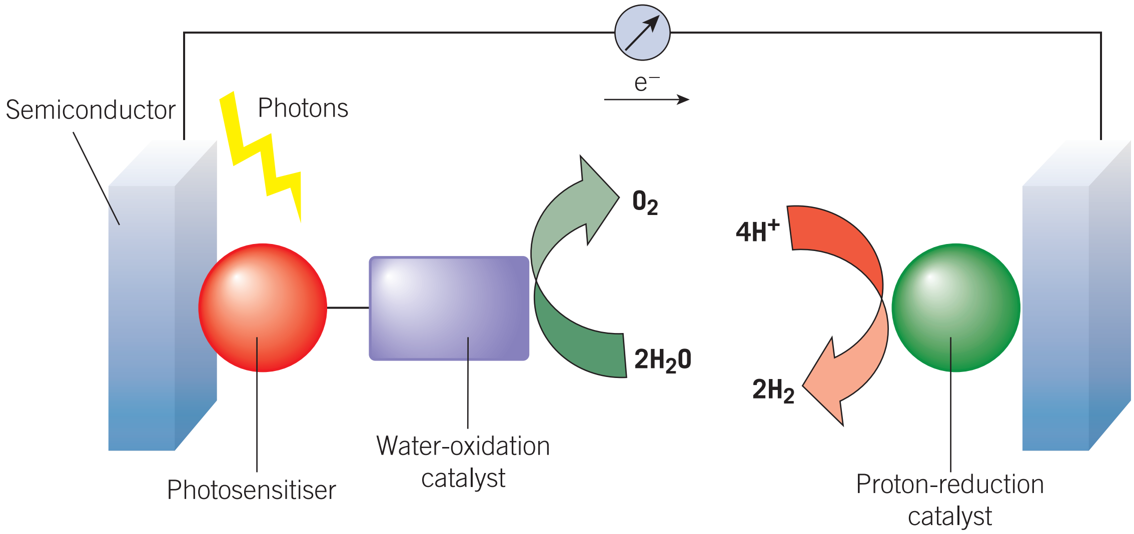


Figure 7C–7 Diagram of photocatalytic water splitting

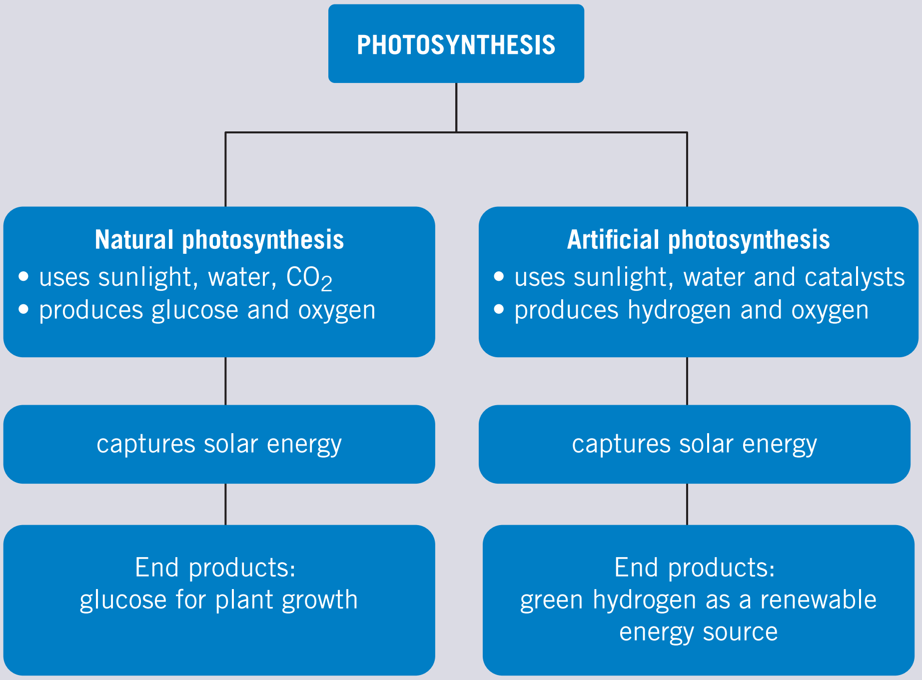
While this process appears simple in principle, there are several design problems that must be addressed if hydrogen is to be produced on a large scale in this manner. Catalysts can decompose and corrode during the process, and some catalysts will only function efficiently at certain temperatures and pressures. The hydrogen produced can mix with the oxygen, creating a risk of explosions.

VIDEO 7C–1
SKILLS: USING MIND MAPS TO MAKE CONNECTIONS

7C SKILLS

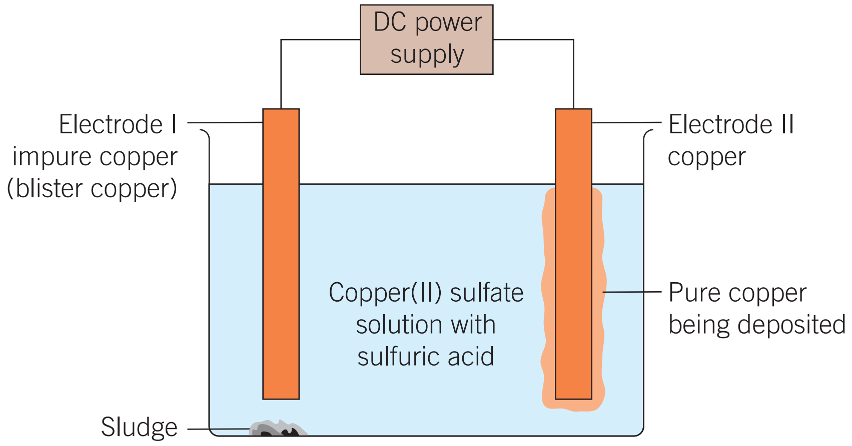
Using mind maps to make connections
Making connections between content significantly enhances memory retention and facilitates learning. This is largely due to the way our brains inherently seek and form patterns between information. Techniques like mind maps are valuable tools for visualising these connections and can significantly aid in the study process.

For example, if you're studying photosynthesis in plants and artificial photosynthesis for producing green hydrogen, a mind map can clarify these concepts. At the centre, you might put 'photosynthesis', with two branches for 'natural' and 'artificial'. Under 'natural photosynthesis', you could note 'uses sunlight, water, CO_2' and 'produces glucose and oxygen'. For 'artificial photosynthesis', you could specify 'uses sunlight, water and catalysts' and 'produces hydrogen and oxygen'. You might also create branches to note that both processes capture solar energy, but their end products and uses differ: glucose for plant growth in the case of natural photosynthesis, and green hydrogen as a renewable energy source in the case of artificial photosynthesis. By drawing these connections, you'll create a more comprehensive understanding of these processes.



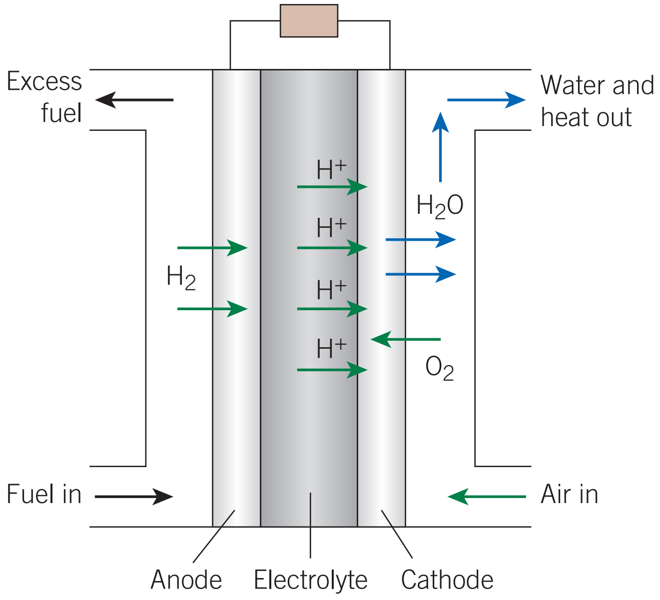
Section 7C questions

1 The electrolytic cell shown below is set up to yield pure copper from an impure piece of 'blister' copper. The electrolyte solution contains both copper(II) sulfate and sulfuric acid. The blister copper, Electrode I, contains a mixture of impurities, including cobalt, gold, iron, nickel, silver and zinc. The voltage applied is specifically adjusted so that only copper is deposited on Electrode II. During electrolysis, some ions remain in the solution, but other metal impurities form a 'sludge' beneath Electrode I.



- a State the name and polarity of Electrode I.
- b Write the equation for the reaction occurring at the cathode.
- c List the solid metal impurities that would be found in the sludge.

2 A proton-exchange membrane cell is shown below.



- a Write the overall reaction for the cell.
- b State the function of the electrolyte.
- c A membrane is used in this cell between the anode and cathode. What is the function of this membrane?

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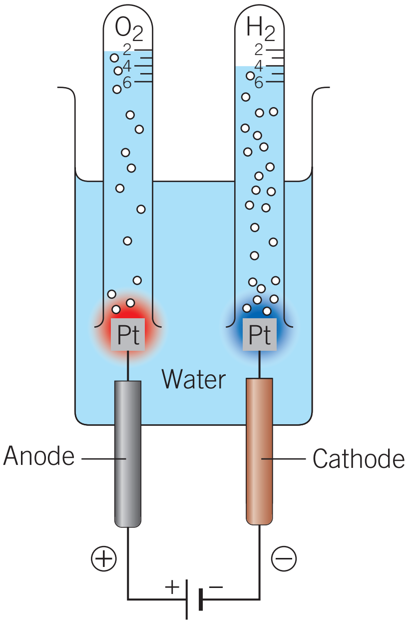
3 The apparatus for the electrolysis of water is shown below.



a Write the half-reactions occurring at each electrode.
b Write the overall reaction for the cell.
c If 4.5 moles of oxygen is produced at the anode, state how many moles of hydrogen would be produced at the cathode.

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7D

Faraday's laws of electrolysis

Study Design:

- The application of Faraday's laws and stoichiometry to determine the quantity of electrolytic reactant and product, and the current or time required to either use a particular quantity of reactant or produce a particular quantity of product

ENGAGE

Electroplating

Electroplating is one example of how electrolysis is used commercially. Car and motorcycle parts are commonly plated with chrome or nickel, which give a desirable shiny silver appearance. You may even have tapware or door handles in your house that are chrome plated. During the electroplating process, it is important to control the conditions to apply just the right quantity of metal coating. A layer too thin may expose the material underneath, but if it is too thick the object may lose its shape, as well as increasing the cost of materials unnecessarily. Chemists use Faraday's laws of electrolysis to help calculate the precise amounts needed for specific reactions, and in this section you will look at ways to perform these calculations yourself.

EXPLAIN

Faraday's laws of electrolysis

4B FARADAY'S LAWS LINK

You should recall looking at Faraday's laws in Section 4B, which are applied here to control and calculate the quantities involved in electrolytic cells. To refresh your memory, Faraday's two laws of electrolysis state that:

1. The mass of a substance produced or consumed at an electrode during electrolysis is directly proportional to the quantity of electricity passed ($m \propto Q$).
2. The amounts in moles of different substances produced or consumed at electrodes by the passage of the same amount of electricity are inversely proportional to the charges on their ions ($n \propto \frac{1}{\text{ionic charge}}$).

Essentially, there are *three* main factors that affect the amount of product formed at the cathode during electrolysis:

- the amount of current flowing through a cell
- the length of time current is applied
- the charge of the ion being reduced at the cathode.

Charge (quantity of electricity) has the symbol Q. It is measured in units of coulombs (C). The amount of charge that one mole of electrons has is 96 500 coulombs, which is Faraday's constant, F, and can be written as:

$$F = 96\,500\ \mathrm{C\,mol^{-1}}$$

The relationship between charge and the number of moles of electrons can be represented by the relationship:

$$Q = n(\mathrm{e^-}) \times F$$

where:

Q = The charge (in coulombs)
$n(\mathrm{e^-})$ = The amount, in moles, of electrons
F = Faraday's constant.

Current and time are represented by the relationship:

$$Q = It$$

where:

Q = The charge (in coulombs)
I = The current (in amperes)
t = The time (in seconds).

These relationships can be used for quantitative calculations involving electrolytic cells.

Theoretical yield versus actual yield

Often the amount predicted to be deposited at the cathode will differ from the actual amounts measured experimentally. This can be attributed to several factors, including contaminants in the solutions, variations in current, surface area and condition of the electrodes being used, temperature and pressure conditions, and some of the products flaking off the electrodes.

Calculations using Faraday's laws of electrolysis

In this section, we will look at how the two equations, $Q = It$ and $Q = n(\mathrm{e^-}) \times F$, can be used to quantify the process of electrolysis. The questions you are likely to see typically involve four steps, as outlined below.

Four key steps to solving Faraday's laws of electrolysis questions

1. Determine number of moles of metal (using $n = \frac{m}{M}$).
2. Determine number of moles of electrons (using the relevant half-equation).
3. Determine the charge, Q, using $Q = n(\mathrm{e^-}) \times F$.
4. Determine current (amps) or time (seconds), using $Q = It$.

NOTE

For some questions, you may have to apply the steps in reverse order. This will depend on what the question is asking. Worked example 7D–1 is one such example, where you are required to calculate the mass of the product at the cathode. It is worth paying extra attention to units also, particularly those involving time.

VIDEO
WORKED
EXAMPLE 7D–1

Worked example 7D–1: Calculating the mass of a product at an electrode

An electrolytic cell using a 1.0 M copper sulfate electrolyte solution is operating with a steady current of 5.0 amps for 30 minutes. Determine the mass of copper deposited, given that the reaction occurring at the cathode is:

$$\mathrm{Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)}$$

Solution

	Logic	Process
Step 1	Convert the given time to seconds.	$30 \times 60 = 1800$ seconds
Step 2	Calculate the charge using $Q = It$	$Q = 5.00\text{ A} \times 1800\text{ s} = 9000\text{ C}$
Step 3	Calculate the amount, in mol, of electrons with 9000 C of charge using $Q = n(\mathrm{e^-}) \times F$.	$n(\mathrm{e^-}) = \frac{Q}{F} = \frac{9000\text{ C}}{96\,500\text{ C mol}^{-1}}$ $= 0.0933$ mol
Step 4	Using the ratio shown in the half-equation, determine the amount, in mol, of metal being produced.	$\mathrm{Cu^{2+}(aq) + 2e^- \rightarrow Cu(s)}$ $n(\mathrm{Cu}) = \frac{1}{2} \times n(\mathrm{e^-})$ $= \frac{1}{2} \times 0.0933$ mol $= 0.0466$ mol
Step 5	Determine the mass of copper produced, using $n = \frac{m}{M}$.	$m(\mathrm{Cu}) = n \times M$ $M(\mathrm{Cu}) = 63.55\text{ g mol}^{-1}$ $m(\mathrm{Cu}) = 0.0466\text{ mol} \times 63.55\text{ g mol}^{-1} = 2.96\text{ g}$ Therefore, 3.0 grams of copper is deposited at the cathode.

VIDEO
WORKED
EXAMPLE 7D–2

Worked example 7D–2: Calculating the time to produce a product at an electrode

Aluminium metal is produced commercially by passing a current through a molten mixture of alumina and cryolite, using large carbon anodes. Calculate the length of time, to the nearest minute, a current of 45 000 A would need to be passed through the cell to generate 10.0 kg of aluminium if the reaction at the cathode is:

$$\mathrm{Al^{3+}(l) + 3e^- \rightarrow Al(l)}$$

Solution

	Logic	Process
Step 1	Determine the amount, in mol, of metal to be produced, using $n = \frac{m}{M}$. Note that the question provides a mass in kg, so that needs to first be converted to grams.	$10.0\text{ kg} \times 1000 = 10\,000$ grams $n(\mathrm{Al}) = \frac{m}{M}$ $= \frac{10\,000\text{ g}}{26.98\text{ g mol}^{-1}}$ $= 370.64$ mol
Step 2	Use the half-equation to determine the amount, in mol, of electrons required.	$\mathrm{Al^{3+}(l) + 3e^- \rightarrow Al(l)}$ $n(\mathrm{e^-}) = 3 \times n(\mathrm{Al})$ $= 3 \times 370.64\text{ g mol}^{-1}$ $= 1111.93$ mol

Step 3	Calculate the charge, using $Q = n(e^-) \times F$.	$Q = 1111.93 \text{ mol} \times 96\,500 \text{ C mol}^{-1}$ $= 107\,301\,704.97$ C needed.
Step 4	Calculate the time, using $Q = It$.	$t = \frac{Q}{I} = \frac{107\,301\,704.97 \text{ C}}{45\,000 \text{ A}}$ $= 2384.48$ seconds. Convert to minutes by dividing by 60. $\frac{2384.48 \text{ s}}{60} = 39.74$ minutes, rounded to the nearest minute $= 40.0$ minutes.

VIDEO 7D–1
SKILLS: PRESENTING YOUR CALCULATIONS

7D SKILLS

Presenting your calculations

To properly solve a calculation-based question in chemistry, there are a few critical steps. Firstly, it's crucial to identify the appropriate formula or equation and write it out. This serves as your calculation's framework, and you need to understand what each variable represents. Secondly, review all the provided values to determine if any unit conversions are required to maintain consistency in your equation.

Thirdly, substitute the relevant values into the equation, being cautious to align each value with its corresponding variable. Fourthly, perform the calculation, ideally using a calculator to ensure accuracy. Lastly, after completing the calculation, check the units of your final answer and adjust the number of significant figures to match the least precise measurement used in your calculation.

To illustrate, let's apply these steps in a Faraday's law problem in electrolysis. Suppose we need to find the mass of silver (Ag) deposited at the cathode when a current of 0.5 A is passed for 3 hours through a solution of silver ions. Given that silver ions gain one electron to become silver atoms, $Ag^+(aq) + e^- \rightarrow Ag(s)$, we can use the formulas:

$$Q = It \qquad n(e^-) = \frac{Q}{F} \qquad n = \frac{m}{M}$$

1. Firstly, we write out our formulas.
2. Secondly, we convert time from hours to seconds, getting 3 hours = 10 800 seconds.
3. Thirdly, we substitute our values into the first formula to calculate the total charge.

   $Q = 0.5 \text{ A} \times 10\,800 \text{ s} = 5400 \text{ C}$.

   Then, we substitute the calculated charge into the second formula to find the number of moles of electrons: $n(e^-) = \frac{5400 \text{ C}}{96485 \text{ C mol}^{-1}} = 0.0559$ mol.
4. Fourthly, we rearrange the third formula to solve for mass: $m = n \times M$. Substituting $n(e^-)$ and the molar mass of silver into this equation gives us: $m = 0.0559 \text{ mol} \times 107.87 \text{ g mol}^{-1} = 6.03$ g.
5. Lastly, after performing the calculation, we check our units (which are in grams) and adjust the number of significant figures to reflect the least precise measurement used in the calculation (which is the current, measured to the tenths place).

Therefore, the final answer is 6.0 g of Ag.

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Section 7D questions

1 To the nearest minute, determine how long it will take to deposit 20.0 grams of nickel in an electrolytic cell containing nickel sulfate, $NiSO_4$, if a current of 3.00 amps is applied to the cell.

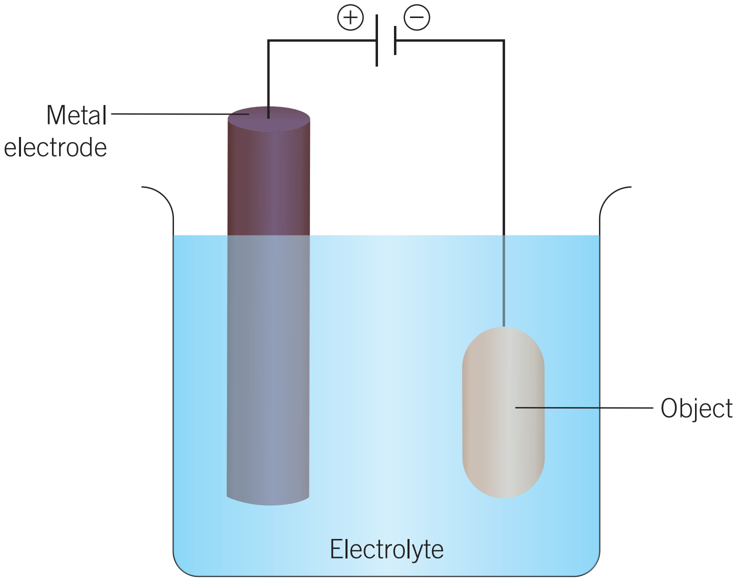
2 Determine the mass of copper deposited at the cathode when 2.0 amps of current is applied to a cell with an electrolyte containing Cu^{2+} for 7.0 minutes.

3 Determine the amount of current that was applied to an electrolytic cell, with an electrolyte containing $AgNO_3(aq)$, if 3.65 grams of silver is deposited after 1.5 hours.

4 Determine the mass of magnesium produced when a current of 1.8 A is passed through an electrolytic cell containing molten magnesium chloride, $MgCl_2$, for 100 minutes.

5 Calculate the amount of charge, in coulombs, required to deposit 50.0 grams of copper from a copper(II) sulfate solution, $CuSO_4(aq)$.

6 The diagram below shows an electrolytic cell containing an electrolyte. If the cell is run with 5 A for 30 minutes, which of the following electrolytes would result in the largest amount, in moles, deposited onto the object?



A 1 M $AgNO_3$
B 1 M $Cu(NO_3)_2$
C 1 M $Al(NO_3)_3$
D 1 M $Zn(NO_3)_2$

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Chapter 7 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
7A.1	Explain the importance of the key design features of electrolytic cells	13☐
7A.2	Identify, name, draw and label features of electrolytic cells, including polarity of electrodes and the direction of electron flow	3☐, 13☐
7A.3	Identify key similarities and differences between the design features of galvanic and electrolytic cells	2☐, 11☐
7A.4	Understand the energy transfers involved in discharging and recharging of electrolytic cells	11☐, 12☐
7A.5	Identify key features of secondary cells that allow them to be recharged	12☐
7B.1	Predict and compare the products of electrolysis when using molten and aqueous electrolytes	1☐, 4☐, 6☐, 13☐
7B.2	Predict and compare the products of electrolysis when using different electrodes, including inert electrodes	5☐, 13☐
7B.3	Predict and compare the products of electrolysis using the electrochemical series, including situations where there is competition at the electrodes	13☐
7B.4	Understand the effect of electrolyte concentration on the products at the electrodes	5☐
7B.5	Write balanced half-equations and balanced overall equations for specific electrolytic cells	12☐, 13☐
7C.1	Identify key design features of commercial electrolytic cells that make them suitable to produce specific chemicals	17☐
7C.2	Explain how the selection of both the electrolyte and the type of electrodes used will influence the products generated by commercial electrolytic cells	17☐
7C.3	Describe ways that cells can be designed to enhance energy efficiency	17☐
7C.4	Describe ways that green chemistry principles can be applied to make the use of electrochemical cells more sustainable and environmentally friendly	17☐
7C.5	Describe how the electrolysis of water and artificial photosynthesis can be adapted to produce 'green' hydrogen	17☐

7D.1	Understand the stoichiometric relationship between the quantity of metal and electrons represented by half-equations in the electrochemical series	15☐, 16☐
7D.2	Apply Faraday's laws to calculate the quantity of product, current or time required for an electrolytic cell	14☐

Multiple-choice questions

1 What are the products when molten potassium chloride undergoes electrolysis?

	Cathode	Anode
A	Cl	K
B	K	Cl_2
C	Cl_2	K
D	K	Cl

2 Identify the correct statement about electrolysis.

A Reduction occurs at the anode.
B Cations flow from the anode to the cathode.
C Electrons flow from the cathode to the anode.
D The polarity of the cathode is negative.

3 In an electrolytic cell, which of the following is true for the anode?

A It is the positive electrode, and it is the site of reduction.
B It is the positive electrode, and it is the site of oxidation.
C It is the negative electrode, and it is the site of reduction.
D It is the negative electrode, and it is the site of oxidation.

4 Which of the following combinations of products are correct for an electrolysis reaction at SLC using molten sodium chloride and inert electrodes?

	Cathode	Anode
A	Na	Cl_2
B	Cl_2	Na
C	H_2	Cl_2
D	Cl_2	H_2

5 Which of the following combinations of products are correct for an electrolysis reaction at SLC using concentrated aqueous sodium chloride solution and inert electrodes?

	Cathode	Anode
A	Na	Cl_2
B	Cl_2	Na
C	H_2	Cl_2
D	Cl_2	H_2

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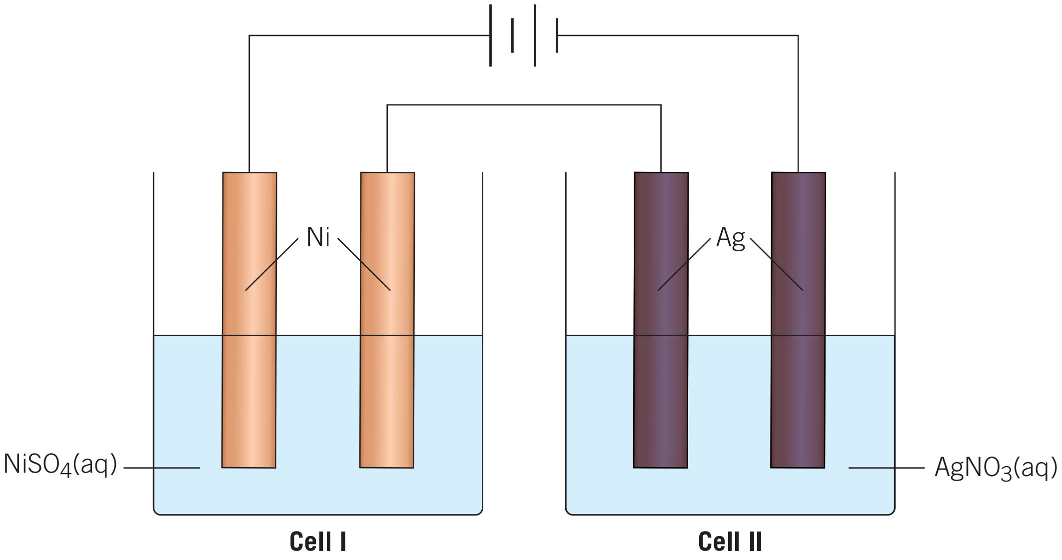
6 When molten lead(II) bromide is electrolysed
- **A** lead ions lose electrons at the cathode to form lead.
- **B** lead ions lose electrons at the anode to form lead.
- **C** lead ions gain electrons at the cathode to form lead.
- **D** lead ions gain electrons at the anode to form lead.

7 The electrolysis of which salt would result in the same products irrespective of whether it is an aqueous or molten electrolyte being used?
- **A** copper(II) bromide
- **B** copper(II) fluoride
- **C** magnesium bromide
- **D** magnesium fluoride

8 During the electrolysis of an aqueous metal salt, the metal is reduced and deposited at the cathode. Which one of the following would **not** affect the mass deposited at the cathode?
- **A** the amount of current passed through the cell
- **B** the amount of voltage passed through the cell
- **C** the charge on the metal ion
- **D** the molar mass of the metal

9 When 4.0 A of current is passed through an electrolytic cell containing a molten sodium chloride electrolyte for 30.0 minutes, the mass of sodium produced would be closest to
- **A** 1.72 grams.
- **B** 0.029 grams.
- **C** 3.43 grams.
- **D** 0.85 grams.

10 In the electrolysis apparatus shown below, 5.87 grams of nickel is deposited on the cathode of the Cell I. Determine the mass of silver, Ag, deposited at the cathode of Cell II.



- **A** 5.39 grams
- **B** 5.87 grams
- **C** 10.79 grams
- **D** 21.58 grams

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Short-answer questions

11 Galvanic and electrolytic cells are two types of electrochemical cells that share some similarities and differences. Indicate whether each of the statements below applies to galvanic cells only, electrolytic cells only, both galvanic and electrolytic cells, or neither galvanic nor electrolytic cells.

- **a** Electrical energy is converted to chemical energy. (1 mark)
- **b** Electrons flow from the cathode to the anode. (1 mark)
- **c** The polarity of the anode is negative. (1 mark)
- **d** A non-spontaneous redox reaction takes place. (1 mark)
- **e** Oxidation occurs at the anode. (1 mark)
- **f** Electrons flow through the conductive wire (external circuit). (1 mark)

12 Lead–acid batteries are a type of secondary cell commonly used in cars. A lead–acid battery consists of a spongy lead electrode and a lead dioxide electrode immersed in an electrolytic solution of sulfuric acid. The overall spontaneous chemical reaction is:

$$PbO_2(s) + Pb(s) + 2H_2SO_4(aq) \rightarrow 2PbSO_4(s) + 2H_2O(l)$$

- **a** What is a secondary cell and how does it differ from a primary cell? (1 mark)
- **b** What feature of the lead–acid battery enables it to be recharged? (1 mark)
- **c** Write balanced half-equations for the reactions occurring at each electrode during discharge. (2 marks)
  - **i** Anode:
  - **ii** Cathode:
- **d** Write balanced half-equations for the reactions occurring at each electrode during recharge. (2 marks)
  - **i** Anode:
  - **ii** Cathode:
- **e** What is the polarity of the lead dioxide electrode during discharge and recharge? (1 mark)
- **f** What energy transfers are involved during discharge and recharge? (1 mark)

13 Aluminium metal can be extracted from aluminium chloride, $AlCl_3$, via electrolysis, using graphite electrodes.

- **a** Draw a diagram of a molten aluminium chloride electrolytic cell. Include:
  - the polarity of each electrode
  - direction of electron flow
  - half-reactions occurring at each electrode
  - overall reaction
  - voltage required to force reactions to proceed (to two decimal places). (6 marks)
- **b** If the molten aluminium chloride electrolyte is replaced with an aqueous solution of aluminium chloride, the cell no longer functions to produce aluminium metal. Explain why this is the case with the use of balanced chemical equations. (2 marks)
- **c** The graphite anode is replaced with an aluminium electrode.
  - **i** What product would be formed at the anode? (1 mark)
  - **ii** Describe any observations you might expect to see on replacing the graphite electrode with aluminium. (1 mark)
- **d** A porous membrane is used in this cell between the anode and the cathode. What is the function of this membrane? (1 mark)

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14 How many minutes does it take to deposit 1.50 grams of copper from a copper(II) sulfate solution, $CuSO_4(aq)$, applying a current of 4.75 A? (2 marks)

15 An electrolytic cell produces 7.90 g of metal per hour when a current of 10.0 A is applied. If the cation in the salt has a 3+ charge, what is the metal? (2 marks)

16 Electrolysis of a molten iron compound with a current of 1.5 A for 30 minutes yields 0.52 g of iron metal at the cathode. Calculate the charge on the iron ions. (2 marks)

17 One of the biggest challenges currently being faced is how to improve industrial and commercial chemistry processes to make them more environmentally friendly.

- **a** Commercial electrolytic cells play a critical role in various industrial processes. Discuss two design enhancements that could be made to these cells to improve their efficiency. (2 marks)
- **b** Environmental sustainability is a growing concern in industrial practices. Suggest two modifications to the design or operation of commercial electrolytic cells that could make them more environmentally friendly. (2 marks)
- **c** Artificial photosynthesis is an emerging technology that mimics the natural process of photosynthesis in plants to produce green hydrogen. Briefly explain how this process works. (1 mark)
- **d** One of the key aspects of commercial electrolytic cells is the choice of electrolyte and electrodes. How do these choices impact the products formed in the cell? Provide an example to support your answer. (2 marks)
- **e** The production of green hydrogen through artificial photosynthesis has been hailed as a potential solution to energy storage issues associated with renewable energy sources. Explain why this is the case. (1 mark)

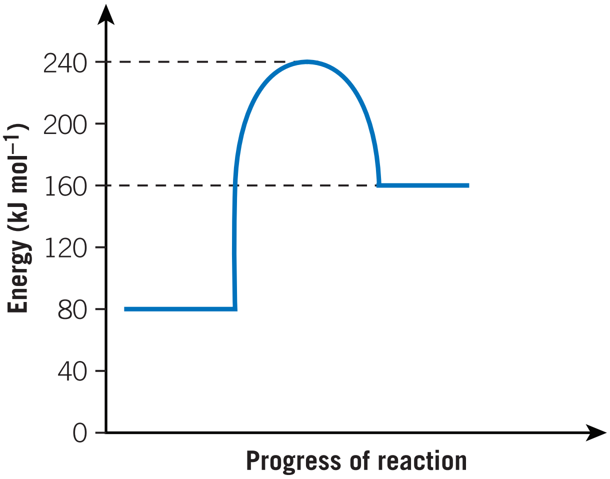
Unit 3 Revision exercise

Multiple-choice questions

1 Which one of the following statements about fossil fuels is correct?

- **A** Fossil fuels are primarily formed through the process of photosynthesis.
- **B** Fossil fuels are renewable resources that can be replenished within a short period of time.
- **C** Fossil fuels are non-renewable resources formed from the remains of plants and animals millions of years ago.
- **D** Fossil fuels are composed of hydrocarbons and impurities obtained through mining and drilling.

2 A reaction has the energy profile shown below.



Which of the following represents the energy profile of the reverse reaction?

	ΔH (kJ mol^{-1})	Activation energy (kJ mol^{-1})
A	+80	160
B	–80	160
C	+80	80
D	–80	80

3 Which of the following reactions would release the greatest mass of carbon dioxide gas?

- **A** complete combustion of 10 g of methane
- **B** complete combustion of 10 mole of methane
- **C** complete combustion of 10 g of ethane
- **D** complete combustion of 10 mole of ethane

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4 Equal amounts of warm ethanol (c(ethanol) = 2.46 J g^{-1} K^{-1}) at 60°C and cool water (c(H_2O) = 4.186 J g^{-1} K^{-1}) at 10°C are mixed in a beaker. Which of the following statements correctly describes the system?

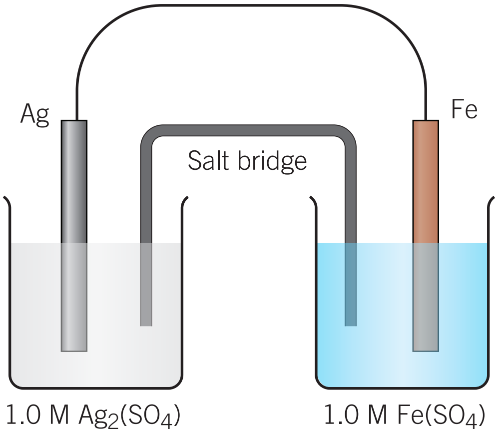
A Heat energy is transferred from the water to the ethanol as the specific heat capacity of water is higher than ethanol.

B Heat energy is transferred from the ethanol to the water until the average temperature of 45°C is reached.

C The final temperature of the solution will be closer to 60°C than 10°C, as the specific heat capacity of water is higher than ethanol.

D The final temperature of the solution will be closer to 10°C than 60°C, as the specific heat capacity of water is higher than ethanol.

5 A galvanic cell is set up as shown in the diagram below.



When the cell is operating

A electrons move from the Ag electrode to the Fe electrode.

B the mass of the Ag electrode increases.

C Fe^{2+} ions move toward the Ag electrode.

D the concentration of Ag^+ ions increases.

6 Some galvanic cells made up of three half-cells (Y^{3+}/Y^{2+}, X^+/X and Z^{2+}/Z^+) are set up under standard conditions. Using the information about the combinations shown, what is the correct order of increasing cell potential?

$$Y^{3+} + Z^+ \rightarrow Y^{2+} + Z^{2+}$$
$$X^+ + Z^+ \rightarrow X + Z^{2+}$$
$$X^+ + Y^{2+} \rightarrow \text{no reaction}$$
$$Z^{2+} + X \rightarrow \text{no reaction}$$

A $Z < X < Y$

B $Y < X < Z$

C $X < Y < Z$

D $Z < Y < X$

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7 The overall equation for a glucose fuel cell is

$$C_6H_{12}O_6(aq) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l)$$

The equation for the reaction that occurs at the anode in this fuel cell is

A $C_6H_{12}O_6(aq) + 6H_2O(l) \rightarrow 6O_2(g) + 24H^+(aq) + 24e^-$

B $6O_2(g) + 24H^+(aq) + 24e^- \rightarrow C_6H_{12}O_6(aq) + 6H_2O(l)$

C $2H_2O(l) \rightarrow O_2(g) + 4H^+(aq) + 4e^-$

D $O_2(g) + 4H^+(aq) + 4e^- \rightarrow 2H_2O(l)$

8 In a galvanic cell, a copper anode is used, and its mass decreases by 0.25 g during operating. The current passing through the cell is 0.4 A. What is the approximate time the cell was running for?

A 8 minutes

B 15 minutes

C 30 minutes

D 45 minutes

9 Which statements correctly describe the effect of increasing the temperature of a reaction?

I The activation energy is decreased, enabling more particles to react.

II The activation energy is unchanged but a higher proportion of particles have kinetic energy above this level.

III The average kinetic energy of particles is increased, allowing a higher proportion to collide successfully.

A I only

B II only

C III only

D II and III

Refer to the following information for Questions 10 and 11.

Nitrogen dioxide, NO_2, and nitrogen tetroxide, N_2O_4, form an equilibrium system, described by:

$$\underset{\text{brown}}{2NO_2(g)} \rightleftharpoons \underset{\text{colourless}}{N_2O_4(g)} \qquad \Delta H = -57.2\ \text{kJ mol}^{-1}$$

10 Which of the following would increase both the rate of the forward reaction and the yield of nitrogen tetroxide produced?

A decreasing the pressure

B increasing the pressure

C increasing the temperature

D adding a catalyst

11 Nitrogen tetroxide gas is injected into a sealed vessel (of fixed volume) containing an equilibrium mixture of nitrogen dioxide and nitrogen tetroxide. Which of the following correctly describes the changes that will occur as the system shifts towards a new equilibrium?

A The colour will become lighter.

B The temperature will increase.

C The proportion of N_2O_4 to NO_2 will decrease.

D The concentration of NO_2 will decrease.

12 If an equilibrium is established by initially adding equimolar amounts of A and B to a 1 L vessel, which of the following conditions must be true once the mixture achieves equilibrium?

$$2A + B \rightleftharpoons 2C \qquad K = 0.1$$

A [A] = [B]

B [A] = [C]

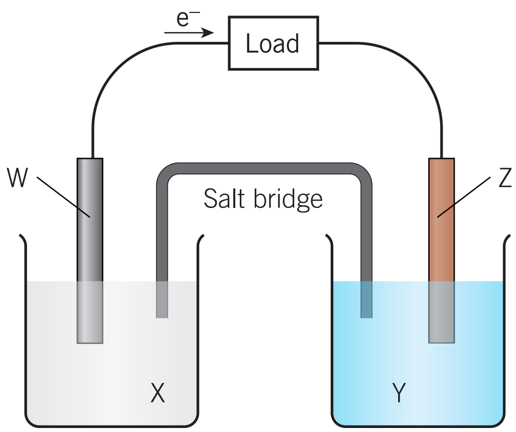
C [A] < [B]

D [A] > [B]

13 A diagram of an electrochemical cell is shown on the right.

Which of the following gives the correct combination of the anode and the electrolyte in the oxidation half-cell?

	Anode	Electrolyte (oxidation half-cell)
A	Z	X
B	Z	Y
C	W	Y
D	W	X



14 When molten potassium chloride, KCl(l), is electrolysed, the product formed at the cathode is

A potassium liquid, K(l).

B chorine gas, Cl_2(g).

C oxygen gas, O_2(g).

D potassium ions, K^+.

15 A current of 5.3 A is applied to an electrolytic cell for 305 minutes, resulting in the deposition of 0.5 mol of metal at the cathode. The metal is most likely to be

A lithium.

B aluminium.

C sodium.

C magnesium.

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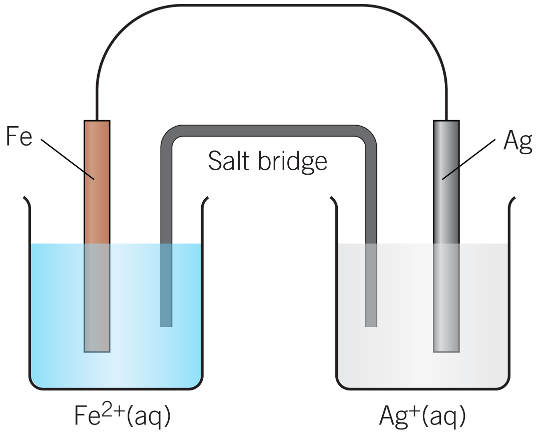
Short-answer questions

1 E10 fuel is a type of fuel that contains 10% ethanol and 90% petrol. Ethanol is derived from renewable sources such as corn or sugarcane. E10 fuel is commonly used as an alternative to regular petrol due to its potential environmental benefits and potential to reduce reliance on fossil fuels. The energy content of ethanol is approximately 23.4 MJ L^{-1}, while the energy content of petrol is approximately 34.2 MJ L^{-1}. (12 marks)

- **a** Explain why ethanol is considered a renewable fuel. (2 marks)
- **b** Explain, with the aid of a balanced chemical reaction, how ethanol is produced in plants such as corn and sugarcane. (2 marks)
- **c** Discuss two potential environmental benefits of using E10 fuel compared to regular petrol. (2 marks)
- **d** Explain why E10 is more viscous than regular petrol under the same conditions. (2 marks)
- **e** Calculate the energy content of 1 L of E10 fuel. (2 marks)
- **f** Calculate the number of litres of E10 fuel that are required to be burned to produce the same amount of energy as 2 L of petrol. (2 marks)

2 The following diagram shows a galvanic cell. (9 marks)



- **a** Write a balanced chemical equation to represent the spontaneous reaction occurring in the cell. (1 mark)
- **b** Identify the oxidant and the reductant. (1 mark)
- **c** Calculate the standard cell potential. (1 mark)
- **d** Draw arrows on the diagram to indicate the direction of electron flow. (1 mark)
- **e** A salt bridge connects the two sides of the galvanic cell.
  - **i** Suggest a suitable material for the salt bridge. (1 mark)
  - **ii** Provide two explanations why the material selected in part **i** is suitable. (2 marks)
- **f** Calculate the mass change of the anode if this cell runs with a constant current of 5.0 amps for four minutes. Indicate whether the mass decreases or increases. (2 marks)

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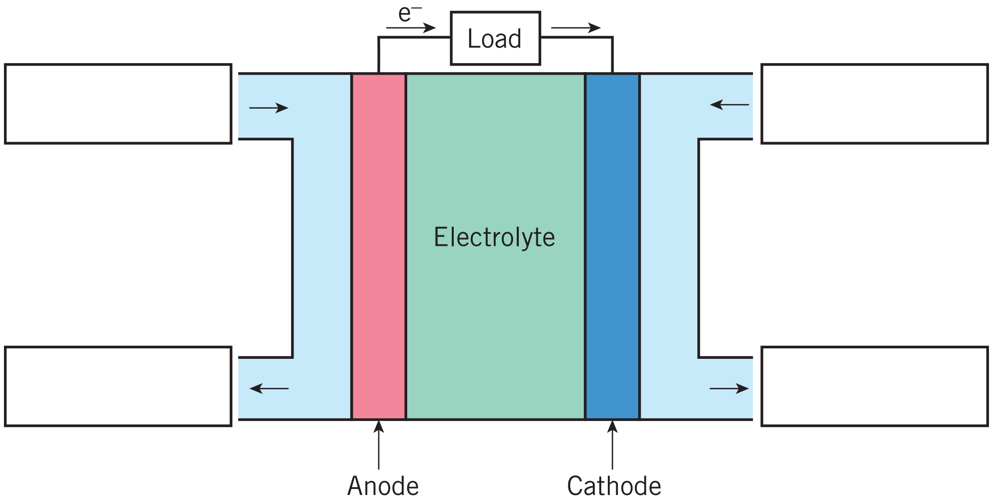
3 A methanol–oxygen acidic fuel cell, also known as a direct methanol fuel cell (DMFC), is an electrochemical device that generates electricity through the oxidation of methanol and the reduction of oxygen in an acidic environment. (13 marks)

a Fill in the empty boxes on the diagram below, indicating the materials entering and exiting the anode and cathode of the DMFC. (4 marks)



b **i** Write an equation for the balanced overall redox reaction that occurs in this cell. (1 mark)

ii Write the balanced half-cell equation that occurs at the anode. (1 mark)

iii Write the balanced half-cell equation that occurs at the cathode. (1 mark)

c Explain the role of the solid polymer electrolyte membrane in a methanol–oxygen acidic fuel cell. (2 marks)

d The fuel cell is operated at an average current of 6.2 A over a six-hour period.

i Calculate the amount, in mol, of CO_2 produced by the fuel cell. (2 marks)

ii Calculate the amount of energy, in kilojoules, that would be produced if the fuel cell operates at an efficiency of 65%. (2 marks)

4 The carbonic acid-bicarbonate buffer system is an essential equilibrium process that helps maintain the pH balance in the human body. (6 marks)

The first step of the equilibrium process involves the dissolution of carbon dioxide (CO_2) in water, forming carbonic acid (H_2CO_3):

$$CO_2(aq) + H_2O(l) \rightleftharpoons H_2CO_3(aq) \qquad K = 1.7 \times 10^{-3}$$

Carbonic acid can then dissociate into hydrogen ions (H^+) and bicarbonate ions (HCO_3^-) according to the second equilibrium:

$$H_2CO_3(aq) \rightleftharpoons H^+(aq) + HCO_3^-(aq) \qquad K = 2.5 \times 10^{-4}$$

a Write the equilibrium expression for the first equilibrium process. (1 mark)

b Calculate the ratio of bicarbonate ions (HCO_3^-) to carbonic acid (H_2CO_3), given a H^+ concentration of $10^{-7.4}$ M. (2 marks)

c Using Le Châtelier's principle, describe how an increase in CO_2 concentration in the human body would alter the concentration of H^+ ions. (3 marks)

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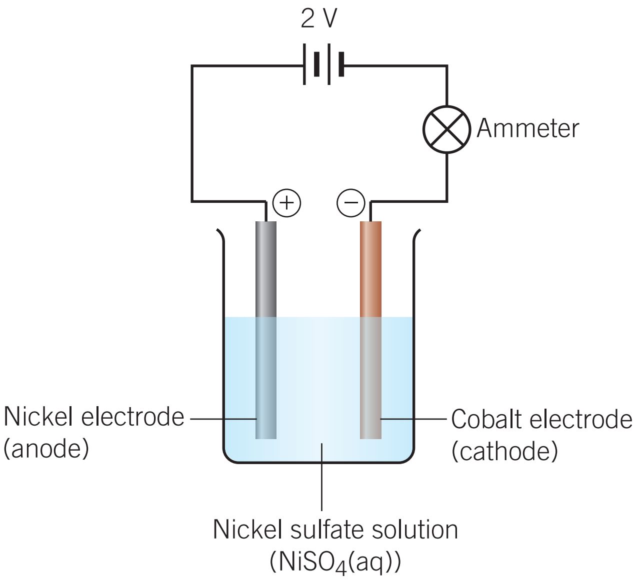
5 The information below relates to an experiment that a student conducted. You are provided with the aim, method and recorded results.

Aim: To investigate how the amount of charge passing through an electroplating cell affects the mass of metal deposited at the cathode.



Method:

1 Weigh and record the mass of the cobalt cathode.
2 Set up the cell as shown.
3 Turn the power on and start the timer at the same time.
4 Record the current as shown on the ammeter.
5 Turn the power off after 10.0 minutes.
6 Carefully remove the cobalt cathode, gently pat it dry and record the mass.

Results:

Current	1.20 A
Initial mass of cobalt cathode	2.023 g
Mass of cobalt cathode after 10.0 minutes	2.185 g

The following questions relate to the information regarding the student's experiment described above. (10 marks)

a Faraday's first law identifies the relationship between the amount of charge flowing through a circuit and the mass of metal deposited at the cathode. What is the predicted effect of doubling the charge flowing through an electroplating cell, on the mass of metal deposited at the cathode? (1 mark)

b Explain the advantage, in a nickel-plating cell, of using a nickel anode rather than an inert electrode such as graphite. (1 mark)

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c Write the ionic half-equation for the reduction reaction occurring in this cell. (1 mark)

d Use the student's results to answer the following questions.

  i Determine the amount of electrons, in mol, that flowed through the cell in the first 10.0 minutes. (2 marks)

  ii Calculate the theoretical mass of nickel that could be deposited at the cathode in the first 10.0 minutes. (2 marks)

  iii Compare the theoretical mass with the mass actually deposited and suggest one reason for the discrepancy. (1 mark)

e Suggest two modifications to the method that would improve the accuracy of the student's results. Justify each suggestion. (2 marks)

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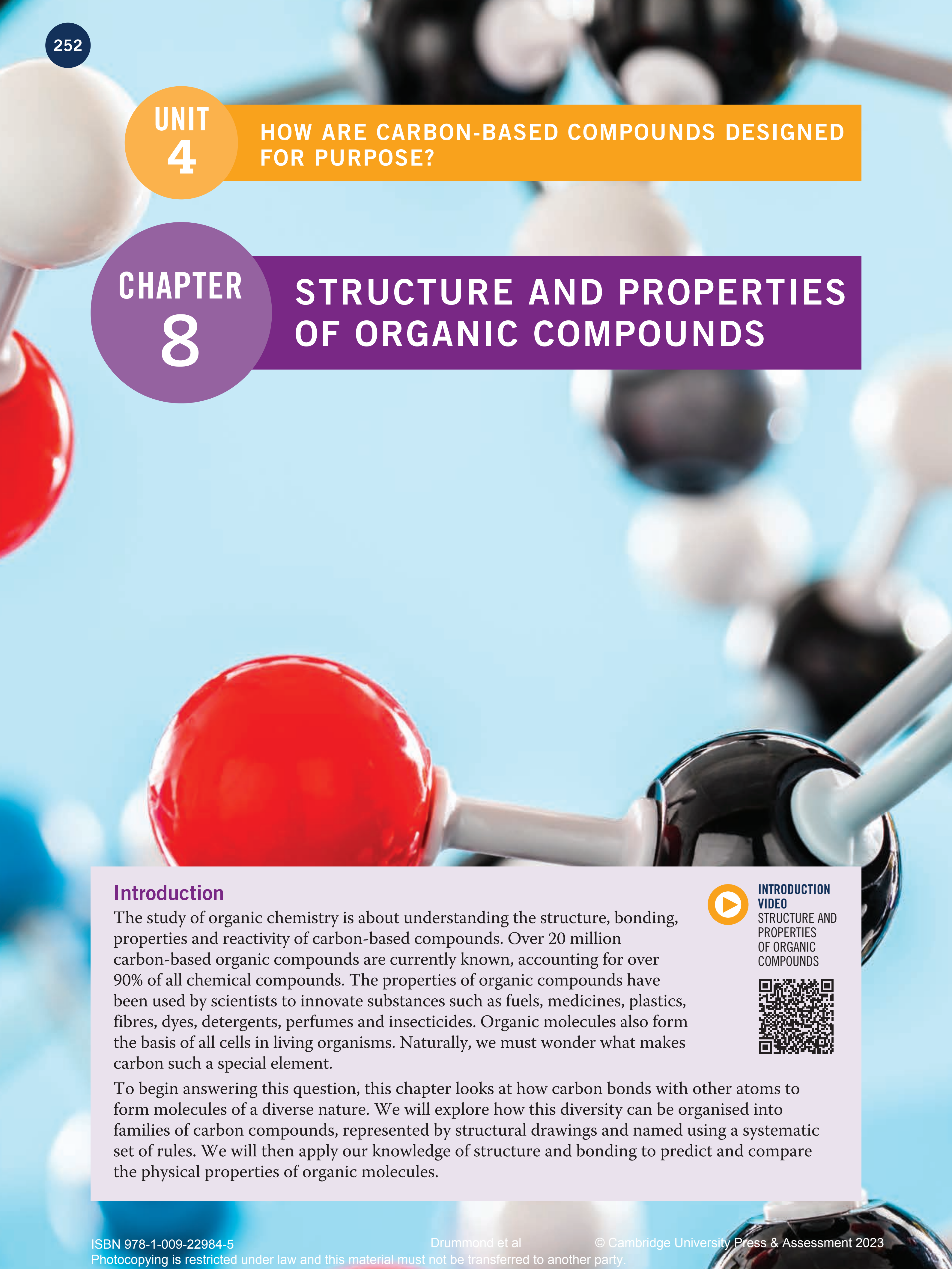

UNIT 4

HOW ARE CARBON-BASED COMPOUNDS DESIGNED FOR PURPOSE?

CHAPTER 8

STRUCTURE AND PROPERTIES OF ORGANIC COMPOUNDS

Introduction

INTRODUCTION VIDEO
STRUCTURE AND PROPERTIES OF ORGANIC COMPOUNDS

The study of organic chemistry is about understanding the structure, bonding, properties and reactivity of carbon-based compounds. Over 20 million carbon-based organic compounds are currently known, accounting for over 90% of all chemical compounds. The properties of organic compounds have been used by scientists to innovate substances such as fuels, medicines, plastics, fibres, dyes, detergents, perfumes and insecticides. Organic molecules also form the basis of all cells in living organisms. Naturally, we must wonder what makes carbon such a special element.

To begin answering this question, this chapter looks at how carbon bonds with other atoms to form molecules of a diverse nature. We will explore how this diversity can be organised into families of carbon compounds, represented by structural drawings and named using a systematic set of rules. We will then apply our knowledge of structure and bonding to predict and compare the physical properties of organic molecules.

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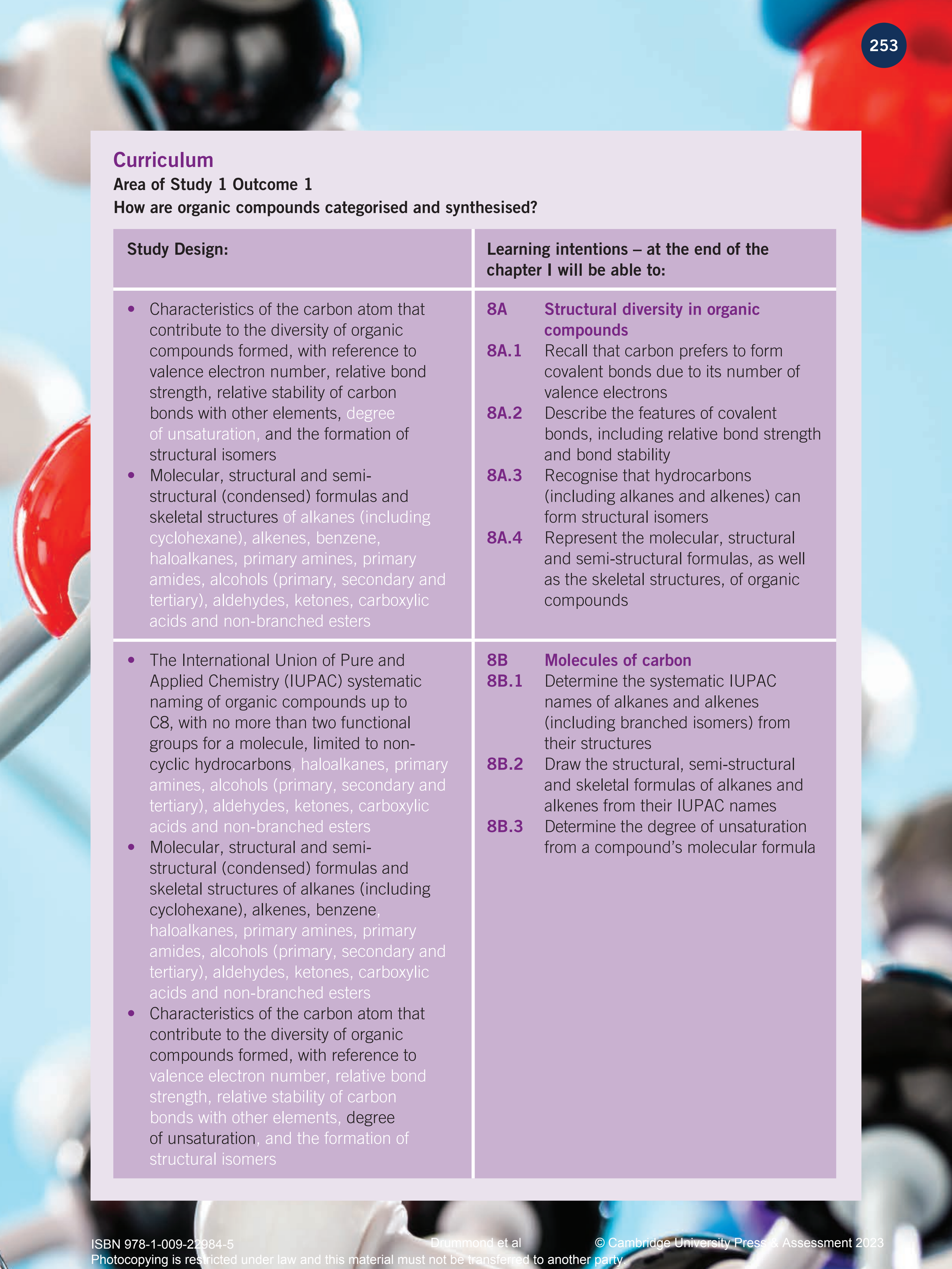

Curriculum

Area of Study 1 Outcome 1

How are organic compounds categorised and synthesised?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Characteristics of the carbon atom that contribute to the diversity of organic compounds formed, with reference to valence electron number, relative bond strength, relative stability of carbon bonds with other elements, degree of unsaturation, and the formation of structural isomers • Molecular, structural and semi-structural (condensed) formulas and skeletal structures of alkanes (including cyclohexane), alkenes, benzene, haloalkanes, primary amines, primary amides, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters	**8A Structural diversity in organic compounds** **8A.1** Recall that carbon prefers to form covalent bonds due to its number of valence electrons **8A.2** Describe the features of covalent bonds, including relative bond strength and bond stability **8A.3** Recognise that hydrocarbons (including alkanes and alkenes) can form structural isomers **8A.4** Represent the molecular, structural and semi-structural formulas, as well as the skeletal structures, of organic compounds
• The International Union of Pure and Applied Chemistry (IUPAC) systematic naming of organic compounds up to C8, with no more than two functional groups for a molecule, limited to non-cyclic hydrocarbons, haloalkanes, primary amines, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters • Molecular, structural and semi-structural (condensed) formulas and skeletal structures of alkanes (including cyclohexane), alkenes, benzene, haloalkanes, primary amines, primary amides, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters • Characteristics of the carbon atom that contribute to the diversity of organic compounds formed, with reference to valence electron number, relative bond strength, relative stability of carbon bonds with other elements, degree of unsaturation, and the formation of structural isomers	**8B Molecules of carbon** **8B.1** Determine the systematic IUPAC names of alkanes and alkenes (including branched isomers) from their structures **8B.2** Draw the structural, semi-structural and skeletal formulas of alkanes and alkenes from their IUPAC names **8B.3** Determine the degree of unsaturation from a compound's molecular formula

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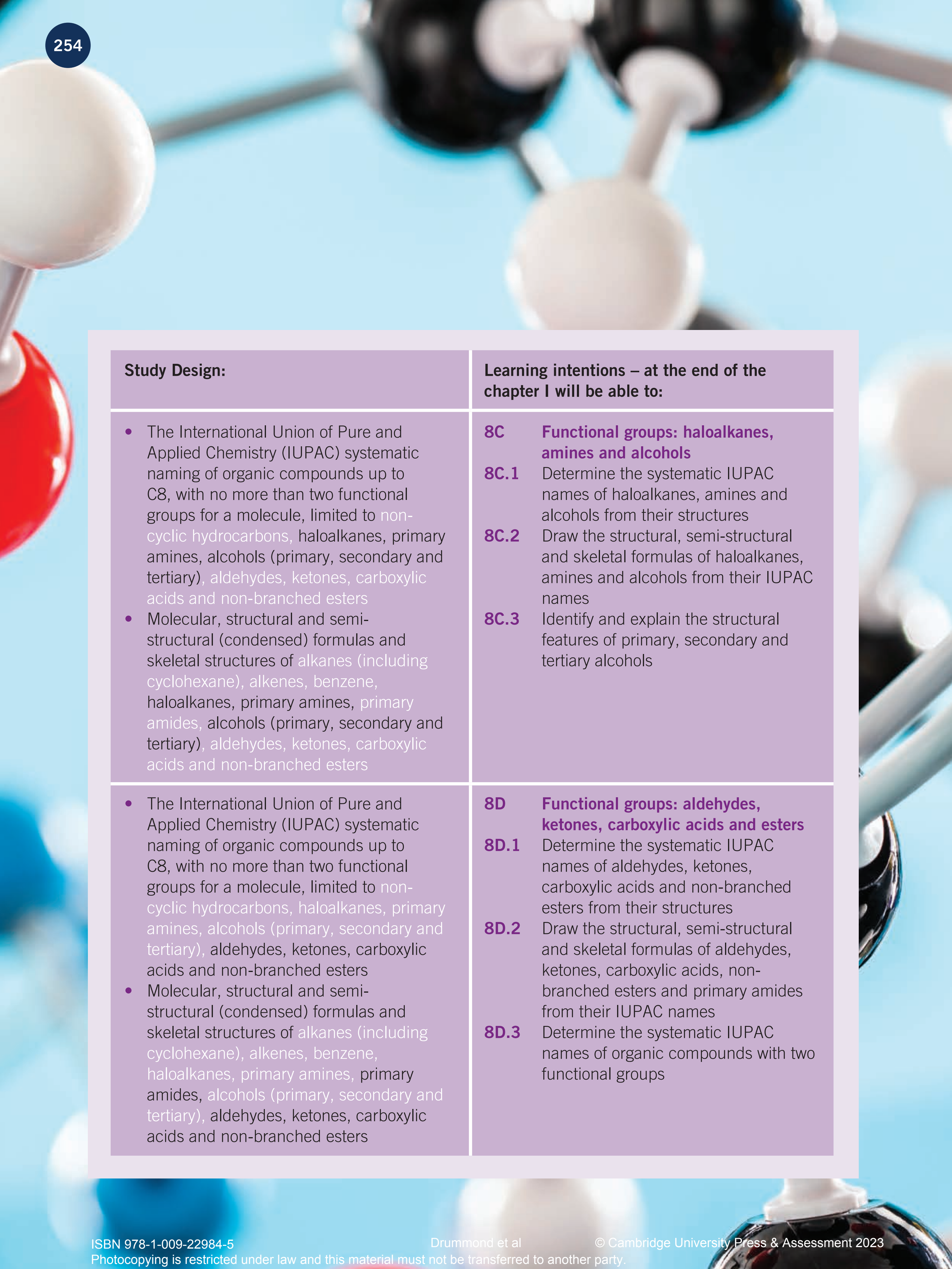

Study Design:	Learning intentions – at the end of the chapter I will be able to:
- The International Union of Pure and Applied Chemistry (IUPAC) systematic naming of organic compounds up to C8, with no more than two functional groups for a molecule, limited to non-cyclic hydrocarbons, haloalkanes, primary amines, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters - Molecular, structural and semi-structural (condensed) formulas and skeletal structures of alkanes (including cyclohexane), alkenes, benzene, haloalkanes, primary amines, primary amides, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters	**8C Functional groups: haloalkanes, amines and alcohols** **8C.1** Determine the systematic IUPAC names of haloalkanes, amines and alcohols from their structures **8C.2** Draw the structural, semi-structural and skeletal formulas of haloalkanes, amines and alcohols from their IUPAC names **8C.3** Identify and explain the structural features of primary, secondary and tertiary alcohols
- The International Union of Pure and Applied Chemistry (IUPAC) systematic naming of organic compounds up to C8, with no more than two functional groups for a molecule, limited to non-cyclic hydrocarbons, haloalkanes, primary amines, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters - Molecular, structural and semi-structural (condensed) formulas and skeletal structures of alkanes (including cyclohexane), alkenes, benzene, haloalkanes, primary amines, primary amides, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters	**8D Functional groups: aldehydes, ketones, carboxylic acids and esters** **8D.1** Determine the systematic IUPAC names of aldehydes, ketones, carboxylic acids and non-branched esters from their structures **8D.2** Draw the structural, semi-structural and skeletal formulas of aldehydes, ketones, carboxylic acids, non-branched esters and primary amides from their IUPAC names **8D.3** Determine the systematic IUPAC names of organic compounds with two functional groups

Study Design:	Learning intentions – at the end of the chapter I will be able to:
- Trends in physical properties within homologous series (boiling point and melting point, viscosity), with reference to structure and bonding	**8E** **Physical properties of organic compounds** **8E.1** Recall the key features of different types of intermolecular forces/bonding **8E.2** Identify the intermolecular forces/bonds present in different families of organic molecules **8E.3** Discuss the trends in physical properties (boiling point, melting point, viscosity) with reference to structure and bonding of molecules within a homologous series

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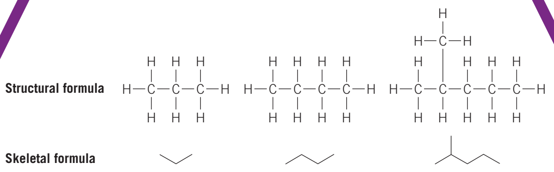
Glossary

Alcohol
Aldehyde
Alkanol
Alkyl group
Amide functional group
Amine
Amino functional group
Aromatic compound
Boiling point
Bond strength
Branched isomer
Carbonyl group
Carboxyl group
Carboxylic acid
Cyclic alkane
Cycloalkane
Degree of unsaturation
Delocalised electron
Dimer
Ester
Ester functional group
Fluid
Functional group
Functional group isomer
Haloalkane
Homologous series
Hydroxyl group
Ketone
Kinetic energy
Melting point
Molecular formula
n-Alkane
Parent hydrocarbon
Polyunsaturated
Positional isomer
Primary alcohol (1° alcohol)
Primary amide
Saturated
Secondary alcohol (2° alcohol)
Semi-structural formula
Skeletal formula
Skeletal isomer
Straight-chain alkane
Structural isomer
Structural formula
Tertiary alcohol (3° alcohol)
Unsaturated
Valence electron
Valence shell
Valence shell electron pair repulsion (VSEPR)
Vapour pressure
Viscosity

Concept map

8A Structural diversity in organic compounds

Molecular, structural, semi-structural and skeletal formulas

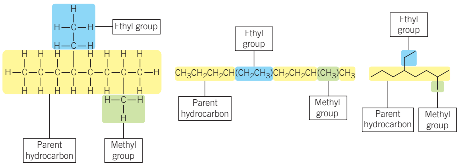


Alkanes
Alkenes
Benzene

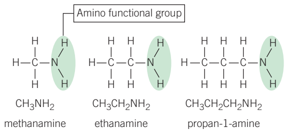
Haloalkanes
Primary amines
Alcohols

Primary amides
Aldehydes
Ketones
Carboxylic acids
Esters

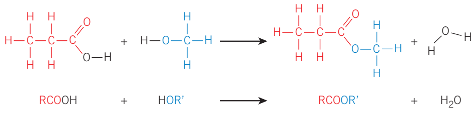
8B Molecules of carbon



8C Functional groups: haloalkanes, amines and alcohols

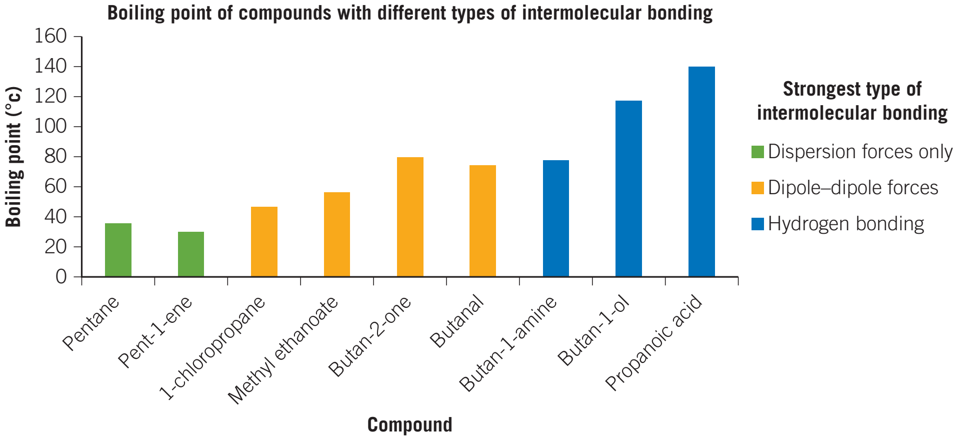


8D Functional groups: aldehydes, ketones, carboxylic acids and esters



Comparison of physical properties, like boiling point, melting point and viscosity, due to the organic compound's structure and bonding

8E Physical properties of organic compounds



See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

8A

Structural diversity in organic compounds

Study Design:

- Characteristics of the carbon atom that contribute to the diversity of organic compounds formed, with reference to valence electron number, relative bond strength, relative stability of carbon bonds with other elements, degree of unsaturation, and the formation of structural isomers
- Molecular, structural and semi-structural (condensed) formulas and skeletal structures of alkanes (including cyclohexane), alkenes, benzene, haloalkanes, primary amines, primary amides, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters

Glossary:

Alkyl group
Bond strength
Functional group
Functional group isomer
Molecular formula
Parent hydrocarbon
Positional isomer
Semi-structural formula
Skeletal formula
Skeletal isomer
Structural isomer
Structural formula
Valence electron
Valence shell
Valence shell electron pair repulsion (VSEPR)

ENGAGE

Origins of organic carbon

As you may be aware, the carbon cycle describes the journey of carbon atoms on our planet (Figure 8A–1). The processes in the carbon cycle directly relate to how we obtain food, energy and numerous other vital resources. In an ideal world, the processes that contribute to the atmospheric levels of carbon dioxide (CO_2) would be balanced by those that consume atmospheric CO_2.

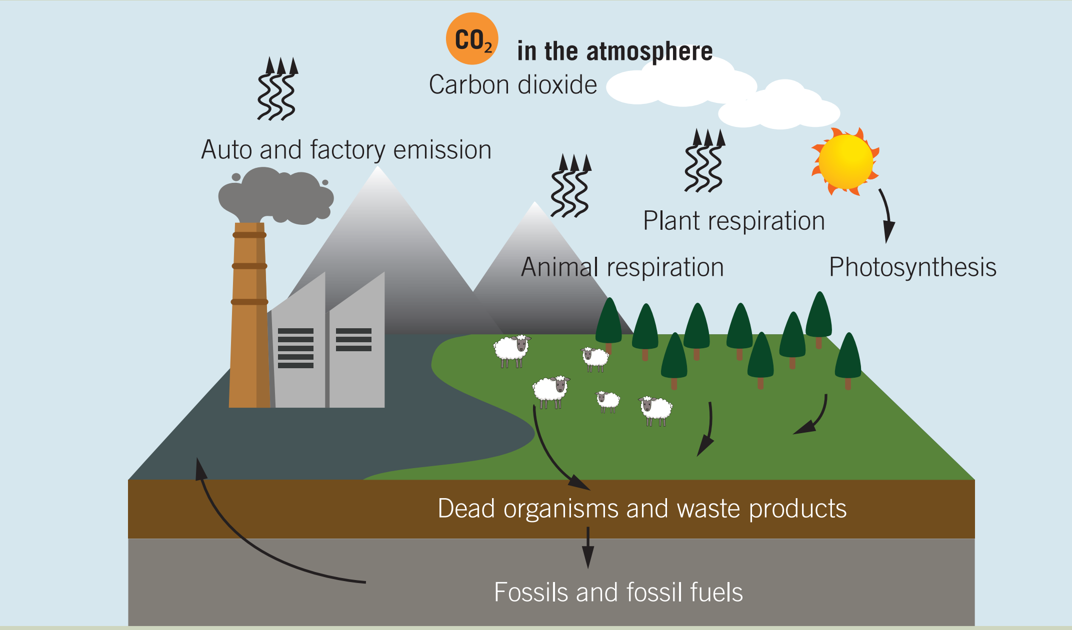


Figure 8A–1 The carbon cycle

1B
PRODUCTION OF CHEMICAL ENERGY IN NATURE
LINK

Now, we can view the carbon cycle with some fresh perspectives. The living organisms in the carbon cycle are mostly made up of organic forms of carbon (carbohydrate, protein and fats). Most sources of food are also made up of predominantly organic carbon. But where does all the organic carbon come from? The answer can be found on the carbon cycle in a vital process called photosynthesis. Using atmospheric CO_2, plants use the process of photosynthesis to convert inorganic carbon (CO_2) into organic carbon in the form of glucose ($C_6H_{12}O_6$). In fact, plants contribute over 90% of the organic carbon available in our biosphere. This organic carbon then becomes the sustenance for every other living organism on the planet.

EXPLAIN

Carbon is at the centre of organic chemistry

Studying organic chemistry gives us insights into life, medicine and materials. When we mention organic compounds, we are talking about carbon-based compounds. Carbon atoms, linked by single, double and triple covalent bonds, form the framework of all organic molecules while other elements like H, N and O complete the picture. In this section, we explore what makes carbon such a unique and versatile element. We begin with a fundamental assessment of carbon's electron configuration and how that relates to its properties in bonding.

Valence electron number

Valence electron an electron found in the outermost shell of an atom

Valence shell the outermost shell of an atom

Carbon occupies an interesting position in the periodic table (Figure 8A–2). Being in group 14, carbon has four **valence electrons** in its **valence shell**. During bonding, carbon prefers to share its four valance electrons to achieve stability. As a result, carbon usually forms four covalent bonds with up to four other non-metallic atoms. What makes carbon special in comparison to elements in other groups is that it can form bonds with one or more other carbon atoms, resulting in structures that resemble chains or rings. This feature means that carbon-based molecules can adopt a diverse range of possible structures.

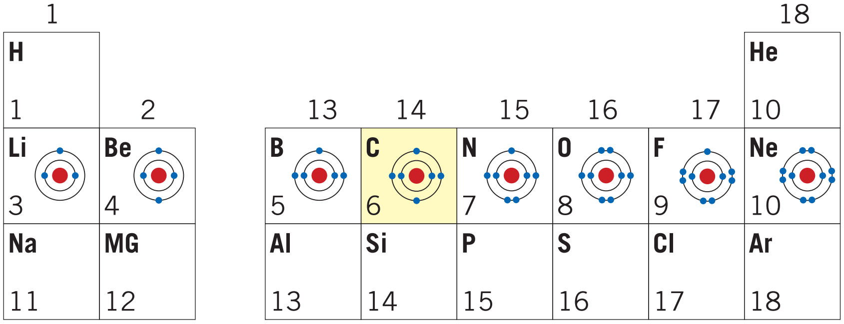


Figure 8A–2 Carbon's electron configuration and position on the periodic table

Diversity in molecular structures

Valence shell electron pair repulsion (VSEPR) a model used to predict the geometric shape of molecules based on the number of valence shell electron pairs surrounding the central atoms in molecules

An important feature of covalent molecules is the diversity of their structures. Consider a single carbon atom with its four valence electrons. For it to become stable, it shares its four valence electrons through covalent bonding with other non-metallic atoms. This means that each carbon atom forms four covalent bonds with up to four neighbouring atoms. These covalent bonds can range between single bonds, double bonds and triple bonds (not covered in this Study Design). The type of covalent bonds and number of neighbouring atoms around the central carbon influences the molecular shape according to **valence shell electron pair repulsion (VSEPR)** theory (Figure 8A–3).

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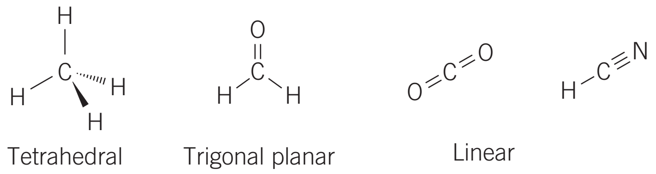
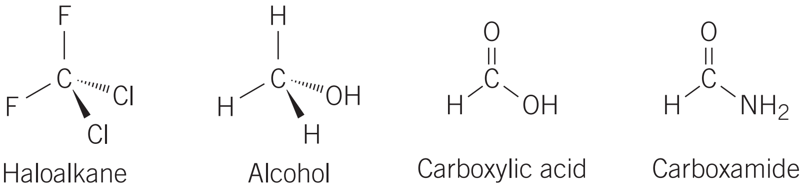


Tetrahedral Trigonal planar Linear

Figure 8A–3 Carbon-based molecules can adopt a diverse range of shapes.

Carbon's neighbouring atoms can range between H, C, N, O, P and S, and any of the group 17 halogens, to name only the common candidates (Figure 8A–4). Different **functional groups** arise depending on the types of atoms around the carbon atom, which influence the physical and chemical properties of the molecule.

Functional group an atom or a group of atoms in an organic molecule that largely determines the molecule's properties and reactions



Haloalkane Alcohol Carboxylic acid Carboxamide

Figure 8A–4 Carbon can bond to a diverse range of atoms.

LINK **8C** FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS

LINK **8D** FUNCTIONAL GROUPS: ALDEHYDES, KETONES, CARBOXYLIC ACIDS AND ESTERS

Finally, if any one or more of these neighbouring atoms is another C atom, the size of the molecule increases. Each new carbon added to the molecule brings further opportunity for diversity (Figure 8A–5).

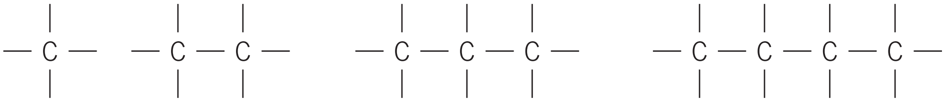


Figure 8A–5 Carbon-based molecules increase in size as the number of carbon atoms increases.

In summary, the vast structural diversity of carbon-based molecules is possible because countless variations in molecular shape, functional group and molecular size are possible. This structural diversity is what gives organic molecules their interesting and useful properties.

Bond strength and stability

When we envisage a covalent bond, we think of a model involving two atoms with shared electrons between them. The negative charge from the electrons electrostatically attracts the positive nuclei of the two atoms and thus results in the two atoms being covalently bonded.

However, not all covalent bonds are equal. For example, a C–H bond is different from a C–Br bond because hydrogen and bromine have different electronegativities and atomic radii. These differences in atomic properties influence the strength of the covalent bond. Physically, we can determine the strength of a covalent bond by measuring how much energy is required to break it (Figure 8A–6 on the following page). The energy (in kJ) required to break one mole (mol) of bonds between two specific atoms in the gaseous state is called its **bond strength** or average bond energy. Higher bond strength = stronger bond = more stable bond. Table 8A–1 on the following page gives the average bond energy for some common bonds found in organic chemistry.

LINK **UNIT 1**

Bond strength the amount of energy required to break apart one mole of a covalent bond in the gas state, measured in kJ mol^{-1}; also referred to as average bond energy

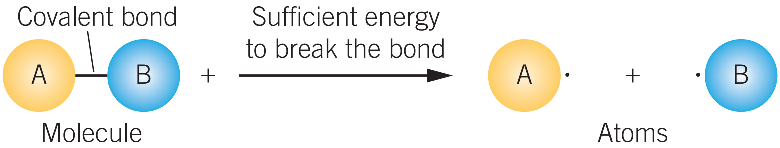


Figure 8A–6 Sufficient energy must be supplied to break a covalent bond between two atoms.

Table 8A–1 Average bond energies of different types of covalent bonds

Bond	Average bond energy (kJ mol^{-1})	Bond	Average bond energy (kJ mol^{-1})
C–H	413	C–F	485
C–C	347	C–Cl	339
C═C	614	C–Br	276
C≡C	839	C–I	240
C–O	358	O–H	467
C═O	745	N–H	391
C–N	305	H–H	432
C–S	259	O=O	495

Rather than trying to make sense of individual values in the above table, it is more important to be able to compare average bond energies of different types of bonds and draw valid conclusions from the data. For example, the average bond energy of a C–N bond (305 kJ mol^{-1}) is lower than a C–O bond (358 kJ mol^{-1}). Therefore, we can expect a C–N bond to be relatively weaker and relatively less stable than a C–O bond.

There are two trends in the average bond energy data above that are worth noting.

- **Average bond energy increases as the number of bonds between two atoms increases**. For example, a C═C double bond has a higher bond energy than a C–C single bond. Rationally, the more bonds there are, the more energy is required to break them.

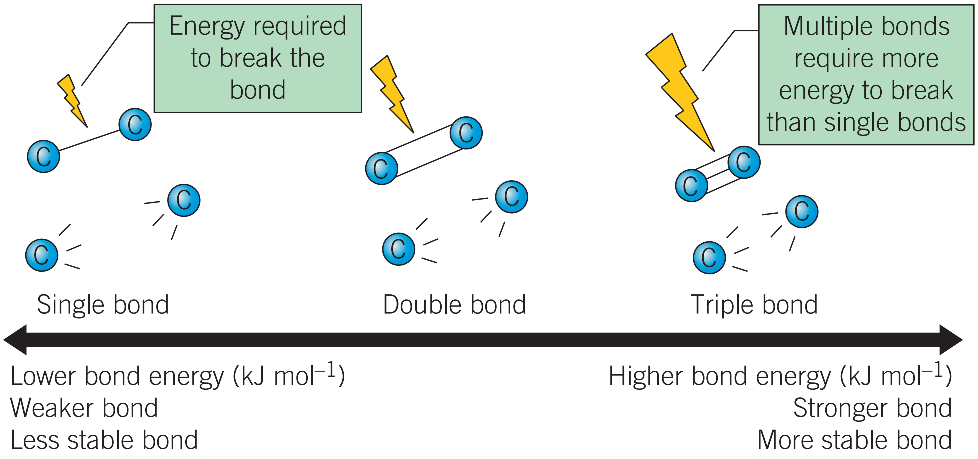


Figure 8A–7 Comparing single, double and triple bond energies

- When an atom is bonded to a series of atoms belonging to the same group, **the average bond energy typically decreases going down the group**. For example, the average bond energy decreases in the order: C–F > C–Cl > C–Br > C–I. This is because as the atomic radius increases, so does the length of the covalent bond. Longer bonds are usually weaker bonds and require less energy to break.

UNIT 1 LINK

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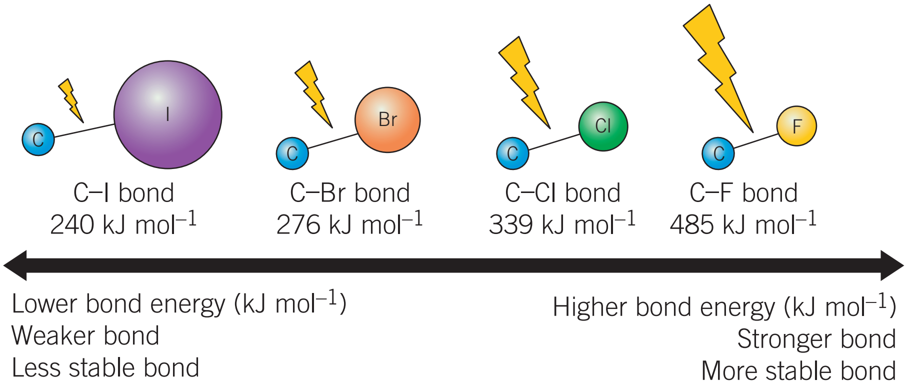


Figure 8A–8 Comparing carbon–halide bond energies

Check-in questions – Set 1

1 Determine which of the following bonds you expect to be more stable. Justify your response.
  - a C–S bond or C–O bond
  - b C–O bond or C═O bond

Representing organic compounds

To effectively communicate organic chemistry to a wide range of audiences, scientists have devised different ways to represent organic molecules. The most widely used representations are molecular formula, structural formula, semi-structural formula and skeletal formula. You have already encountered the first three of these representations in your previous studies. In this section, we will revise these already familiar representations and explore the key aspects of the skeletal formula. As you explore each of the following representations, think about their inherent advantages and disadvantages and the circumstances in which they are best used.

LINK UNIT 1

Molecular and structural formula

The **molecular formula** represents a list of elements and the number of atoms of each element in a molecule. The number of atoms is indicated as a subscript following each chemical symbol. No number is required when there is only one atom of the element. Carbon (C) always appears as the first element listed, followed by hydrogen (H). All other elements present are then listed alphabetically. The molecular formula is the simplest representation of an organic compound. However, its simplicity comes at the cost of not representing how the atoms are bonded. As a result, the molecular formula is unable to distinguish between isomers and often omits necessary information about functional groups within a molecule.

LINK CHAPTER 11

Molecular formula the chemical formula that gives the total number of atoms of each element within a compound

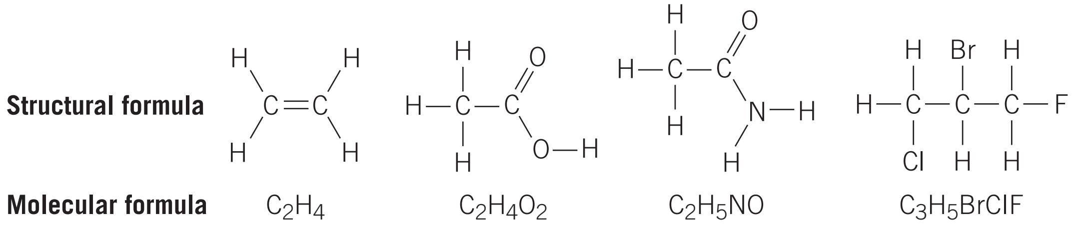


Figure 8A–9 Comparing the structural and molecular formulas of organic compounds

Structural formula a representation of how the individual atoms of the compound may be arranged in three-dimensional space

In contrast, the **structural formula** explicitly shows how all atoms in a molecule are connected. Every atom is represented by its chemical symbol and bonds are represented by lines (one line for a single bond and two lines for a double bond). While the structure and types of functional groups are clearly shown, drawing a structural formula can be tedious and repetitive. This is especially true for larger molecules where there is a high number of carbon and hydrogen atoms. Furthermore, showing every hydrogen atom in the molecule makes the representation unnecessarily large and may direct attention away from the important features or functional groups within the molecule. Yet, despite these drawbacks, the structural formula is a necessary representation for students at the beginning of their organic chemistry training and for scientific communication to the public because it is the simplest to comprehend.

Semi-structural formula

Semi-structural (condensed) formula a representation of organic molecules that shows the order in which atoms or groups of atoms are connected

The **semi-structural (or condensed) formula** usually omits the bonds within a molecule. While this representation uses less space than structural formula on paper, it is arguably more difficult to interpret. This is because it is further removed from the actual shape of the molecule. A lot of recognisable features of functional groups, including double bonds, are often condensed and therefore not immediately obvious.

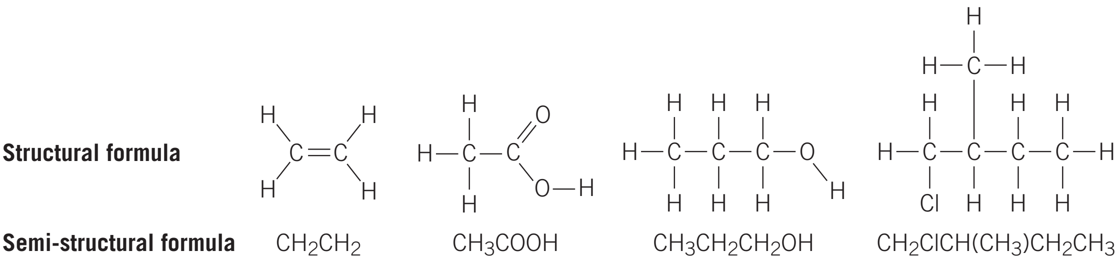


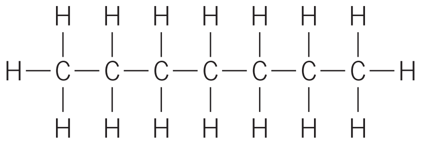
Figure 8A–10 Comparing the structural and semi-structural formulas of organic compounds

Alkyl group a group that is part of a larger molecule and is represented as an alkane minus a hydrogen atom, e.g. methyl ($-CH_3$)

Parent hydrocarbon the longest continuous carbon chain in a molecule

Brackets are often used in semi-structural formulas. There are two main reasons why brackets are used:

- Brackets are used to condense repeating units. In mathematics, we can write the expression 3 × 3 × 3 × 3 × 3 or we can condense it by using the index notation 3^5. The same idea can be applied to semi-structural formulas. For example, a molecule such as heptane contains five repeating CH_2 units in its structure. These CH_2 units can be written in brackets followed by a number in subscript indicating the number of repeats (e.g. $(CH_2)_5$).
- Brackets are used to highlight branched **alkyl groups**. In any semi-structural formula, branching alkyl groups need to be distinguished from the main hydrocarbon chain to avoid ambiguity. For example, 3-methylpentane has a methyl ($-CH_3$) branch on the third carbon. This methyl group must be written in brackets, so it does not get confused with the main pentane **parent hydrocarbon** (e.g. $CH_3CH(CH_3)CH_2CH_3$).

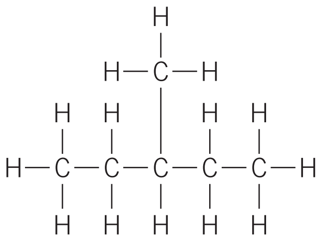


$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$ = $CH_3(CH_2)_5CH_3$

✓ **Correct** This semi-structure of heptane has not been condensed but would still be considered correct.

✓ **Correct** This semi-structure of heptane has been condensed by placing all repeating CH_2 units in brackets.

Figure 8A–11 Using brackets to condense multiple repeating units in a semi-structural formula



$CH_3CH_2CHCH_3CH_2CH_3$

✗

Incorrect
Brackets have not been used to indicate the methyl branch. It can easily be confused as being part of the parent hydrocarbon.

$CH_3CH_2CH(CH_3)CH_2CH_3$

✓

Correct
Brackets have been used to indicate the methyl branch, which makes it easy to distinguish from the parent hydrocarbon.

Figure 8A–12 Using brackets to highlight branching alkyl groups in a semi-structural formula

Skeletal formula

The **skeletal formula** or skeletal representation is a commonly used method to represent large or complex organic compounds. As shown in Figure 8A–13, it is a concise way to draw organic compounds using zigzag lines to outline the carbon structure. It might be helpful to think of skeletal representation as a shorthand version of the structural formula. Both skeletal and structural formulas use lines to represent bonds. The main difference is that the skeletal formula does not require the chemical symbols for carbon and hydrogen to be explicitly written in most cases. This circumvents the repetitive aspects of drawing a structural formula as discussed on the previous page. The skeletal formula is also quicker to draw and more space efficient than the structural formula.

Skeletal formula a representation of molecular structure in which covalent bonds are shown as zigzag lines. The symbol for all elements other than C and H are always drawn. Carbon and hydrogen are often omitted

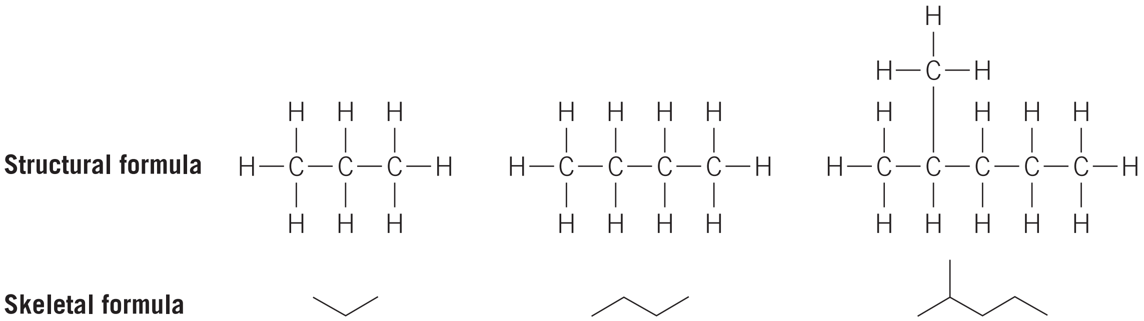


Figure 8A–13 Comparing the structural and skeletal formulas of organic compounds

To accurately draw skeletal representations, you need to observe the following conventions.

- Hydrocarbon chains are represented by zigzag lines. It does not matter if the zigzag line starts upwards or downwards.
- The ends and vertices (points when the line changes direction) represent carbon atoms.
- The lines represent covalent bonds.
- Hydrogen atoms that are bonded to carbons are not drawn. Recall that all carbons require exactly four bonds. In skeletal representations, it is assumed that all carbons meet this requirement. Therefore, any carbon showing fewer than four bonds in a skeletal formula would satisfy its bonding requirement with 'invisible' covalent bonds to hydrogen atoms.
- An alkyl group branched from the parent hydrocarbon points in the same direction as the vertex.

Figure 8A–14 below shows examples of the conventions from the previous page being applied.

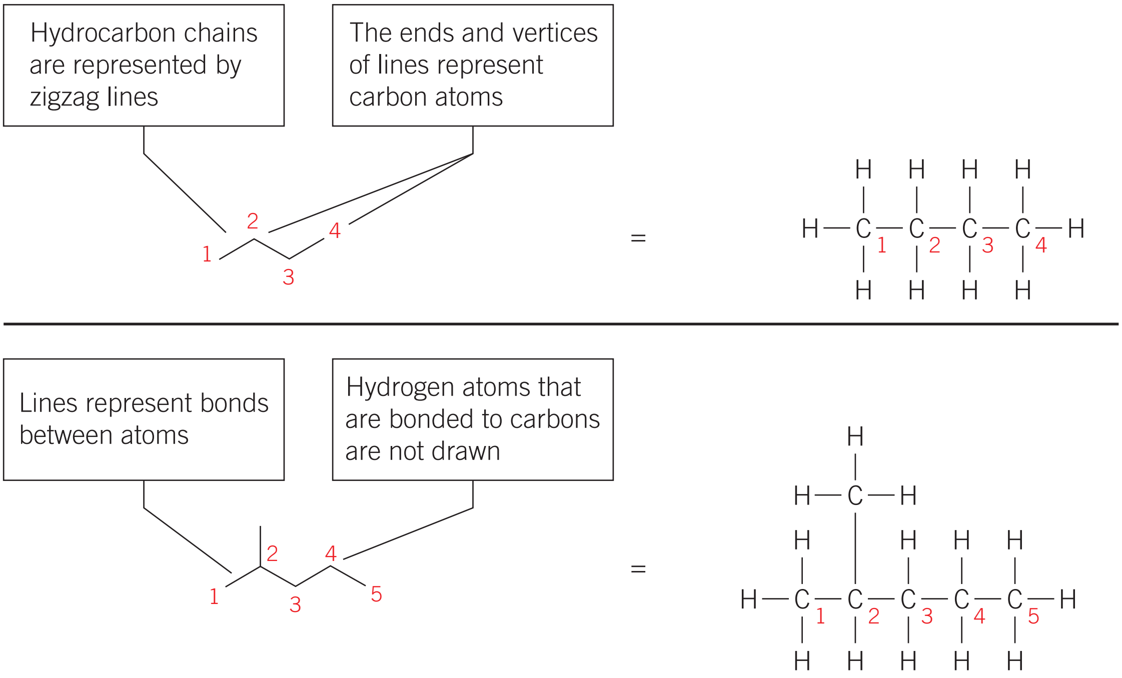


Figure 8A–14 Conventions for drawing skeletal formula of alkanes

In addition, the following conventions apply when there is a functional group present in the molecule:

- Double bonds are shown as two parallel lines.
- All other atoms (O, N, S, F, Cl, Br, I etc.) are represented by their chemical symbols.
- Hydrogen atoms (H) bonded to atoms other than carbon are always shown.
- When necessary, bonds can appear as solid or dashed wedges to indicate three-dimensional geometry.

UNIT 1 LINK

NOTE

As a reminder from Unit 1, below are the five shapes of molecules determined by VSEPR theory.

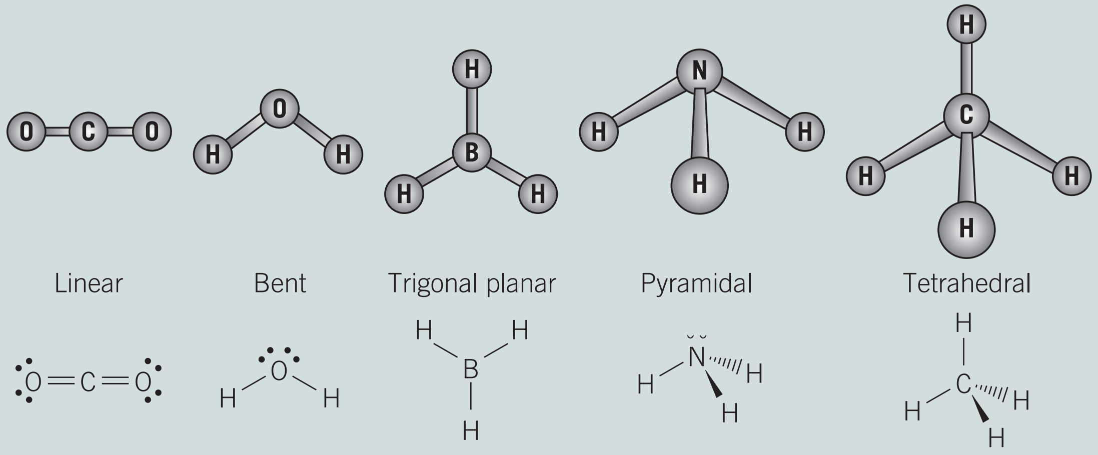


Figure 8A–15 shows examples of the listed conventions being applied.

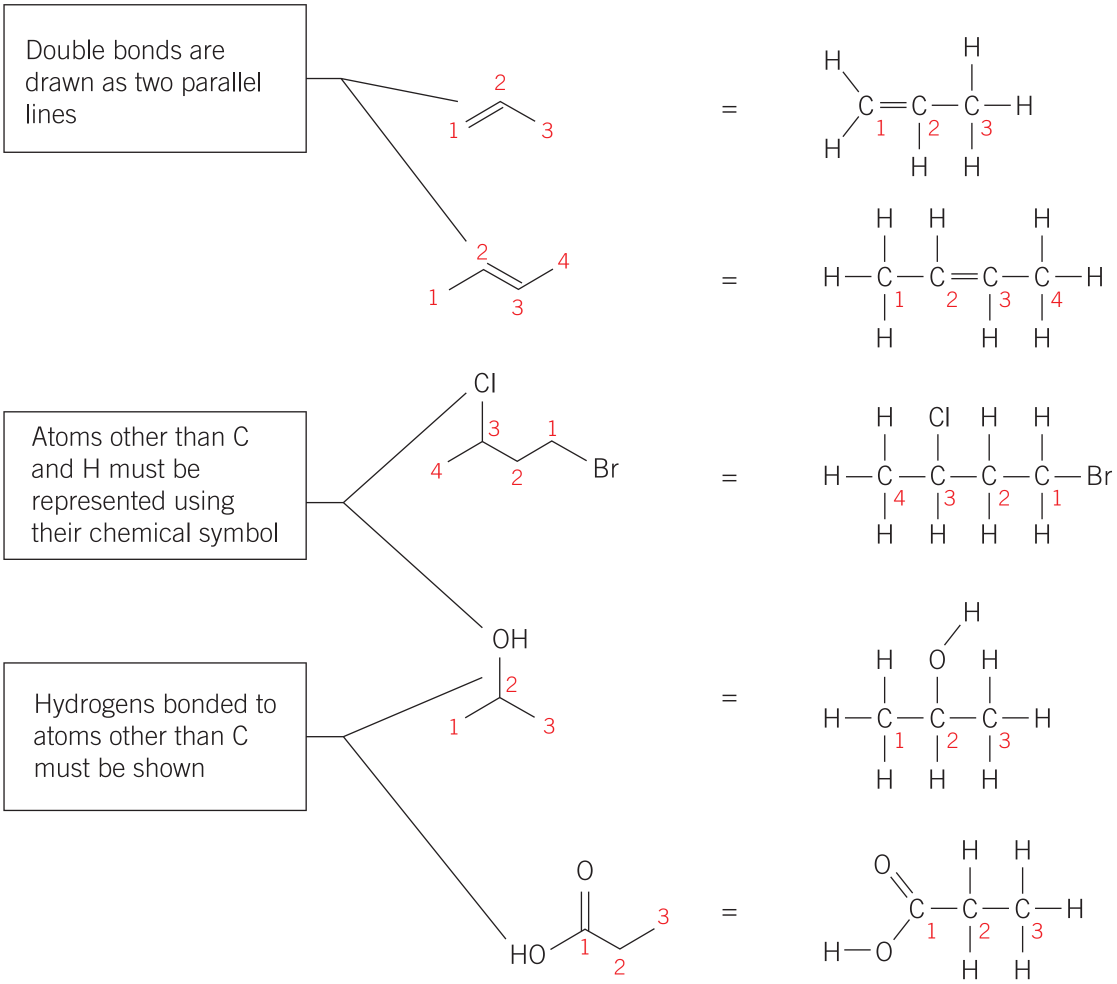


Figure 8A–15 Conventions for drawing skeletal formula of organic molecules

It is important to be able to recognise the number of implied hydrogens bonded to each carbon in a skeletal structure. Figure 8A–16 shows the number of hydrogens connected to each carbon indicated by the number in the boxes.

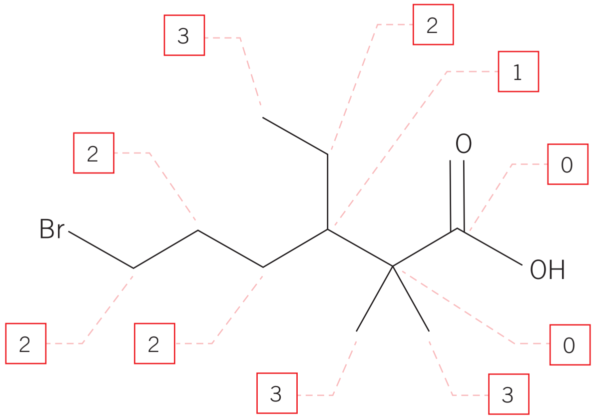


Figure 8A–16 The number of hydrogens connected to each carbon in a skeletal representation of a molecule

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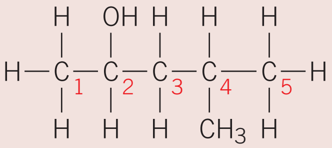
Worked example 8A–1 demonstrates a general procedure for converting a structural formula into its corresponding skeletal representation.

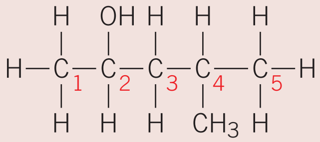
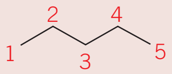
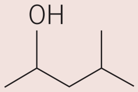
VIDEO
WORKED
EXAMPLE 8A–1

Worked example 8A–1: Drawing a skeletal formula of a molecule from its structural formula

Draw the following molecule using the skeletal representation.



Solution

	Logic	Process
Step 1	Identify and number the longest continuous carbon chain (parent hydrocarbon).	
Step 2	Represent the parent hydrocarbon using zigzag lines where the ends and vertices represent carbons.	
Step 3	Complete the skeletal representation by drawing any alkyl side chains and functional groups.	

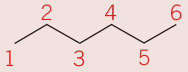
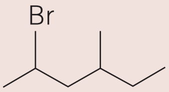
Worked example 8A–2 demonstrates a general procedure for converting a semi-structural formula into its corresponding skeletal representation.

VIDEO
WORKED
EXAMPLE 8A–2

Worked example 8A–2: Drawing a skeletal formula of a molecule from its semi-structural formula

Draw the skeletal representation of $CH_3CHBrCH_2CH(CH_3)CH_2CH_3$.

Solution

	Logic	Process
Step 1	Identify and number the longest continuous carbon chain (parent hydrocarbon).	$CH_3CHBrCH_2CH(CH_3)CH_2CH_3$ 1 2 3 4 5 6
Step 2	Represent the parent hydrocarbon using zigzag lines where the ends and vertices represent carbons.	
Step 3	Complete the skeletal representation by drawing any alkyl side chains and functional groups.	

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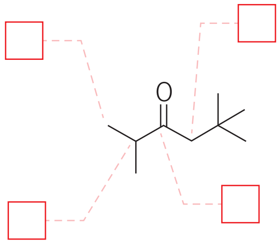
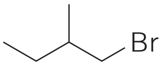
Check-in questions – Set 2

1 Redraw the structure in your workbook and determine the number of hydrogens connected to each carbon atom.

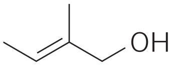


2 Write the molecular formula of each of the following compounds.

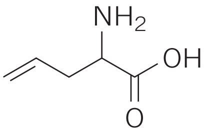
a



b



c



3 Draw the skeletal representation of each of the following molecules.

a $CH_3CH_2CH_2CH_2OH$

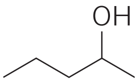
b $CH_3CH(CH_3)CH_2Cl$

c $CH_3CH_2CH_2CHCH_2$

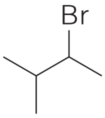
d $CH_3C(CH_3)_2CH_3$

4 Write the semi-structural formula of each of the following molecules.

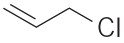
a



b



c



Structural (constitutional) isomers

Another way in which organic molecules can achieve diversity is by changing the way the atoms are bonded to each other. In chemistry, compounds that have the same molecular formula, but different arrangement of atoms and bonds are called **structural isomers** or constitutional isomers. As molecules become larger, a greater number of structural isomers become possible because there are more ways to arrange the atoms and bonds. Figure 8A–17 shows an example of how the atoms and bonds of C_4H_{10} can be arranged in two different ways to form two isomers.

Structural isomer
a molecule with the same molecular formula but different connectivity of atoms. Also referred to as a constitutional isomer


Butane Methylpropane

Figure 8A–17 Two structural isomers of C_4H_{10}

Skeletal isomer a molecule with the same molecular formula but differing in the arrangement of its carbon structure; also referred to as a chain isomer

There are three different types of structural isomers. The first is **skeletal isomers** or chain isomers. This is when molecules have the same molecular formula, but different carbon structures. For example, Figure 8A–18 shows three compounds of C_5H_{12} with different carbon structures. They represent an example of skeletal isomers.

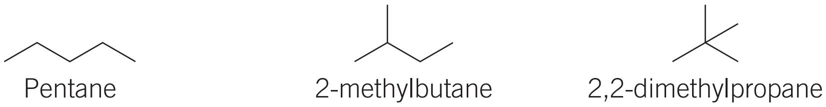


Figure 8A–18 Skeletal isomers of C_5H_{12}

Positional isomer a molecule with the same molecular formula and parent hydrocarbon but different positions of functional groups

8C FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS **LINK**

8D FUNCTIONAL GROUPS: ALDEHYDES, KETONES, CARBOXYLIC ACIDS AND ESTERS **LINK**

The second type is **positional isomers**. This is where molecules have the same molecular formula but different positions for their functional group(s). Figure 8A–19 shows three structures of $C_5H_{12}O$ with the hydroxyl functional group bonded to different carbons on each molecule. They represent an example of positional isomers.

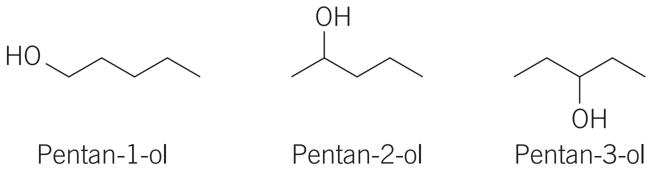


Figure 8A–19 Positional isomers of $C_5H_{12}O$

Functional group isomer a molecule with the same molecular formula and parent hydrocarbon but different types of functional groups

The third type is called **functional group isomers** or functional isomers. This is where molecules have the same molecular formula but different types of functional group. Figure 8A–20 shows two structures of $C_4H_8O_2$ where one has a carboxyl functional group and the other has an ester functional group.

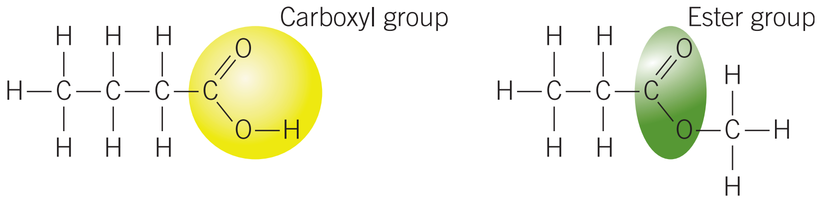
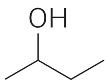


Figure 8A–20 Functional isomers of $C_4H_8O_2$

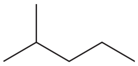
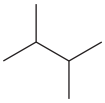
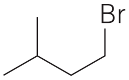
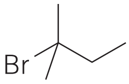
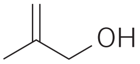
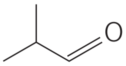
Check-in questions – Set 3

1 Draw a positional isomer of the following alcohol.



2 Draw all four structural isomers of C_4H_9Br.

3 Classify the following pairs of molecules as skeletal, positional or functional isomers.

	Molecules	Type of isomers
a	 	
b	  	
c	  	

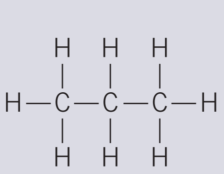
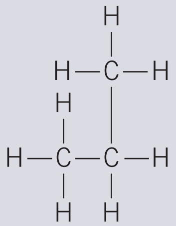
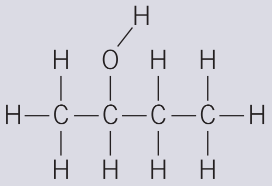
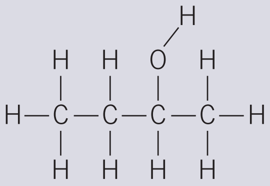
8A SKILLS

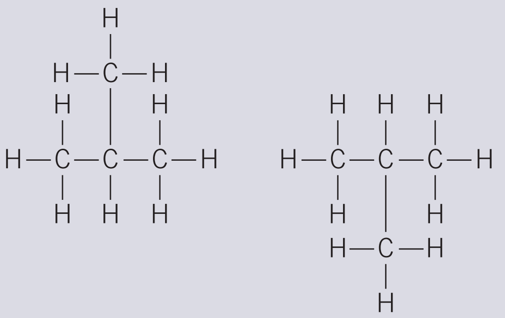
VIDEO 8A–1
SKILLS: DISTINGUISHING BETWEEN STRUCTURAL ISOMERS AND IDENTICAL STRUCTURES

Distinguishing between structural isomers and identical structures

There are times when the same molecule can be drawn in different perspectives by either rotating the structure, flipping the structure or drawing bonds at different angles. The same molecules drawn in different ways are **not** structural isomers. Table 8A–2 illustrates common cases where two different drawings of the same molecule may be mistaken as isomers. The skill you may need to practise is being able to identify whether two molecules, drawn in different ways, are structural isomers or identical structures.

Table 8A–2 Examples of structures that are easily mistaken as structural isomers

Molecular formula	Structural formulas	Explanation
C_3H_8	 	The two structures have the same arrangement of atoms and bonds but are drawn with different bond angles. They represent the same molecule and are not isomers.
$C_4H_{10}O$	 	The two molecules may appear as positional isomers, but they are the same molecule. The structure on the left is drawn as a flipped version of the structure on the right. The hydroxyl group is located on the same carbon in both molecules. Therefore, these two structures are not isomers.

C_4H_{10}		Single bonds are free to rotate so it does not matter whether the alkyl group is pointing up or down. These two structures are identical and do not represent isomers.

Section 8A questions

1 Carbon is an important element in organic chemistry. It has the electron configuration $1s^22s^22p^2$.
   a How many covalent bonds does a neutral carbon atom usually form?
   b Explain your answer to part **a** using carbon's electron configuration.

2 Define 'average bond energy'.

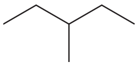
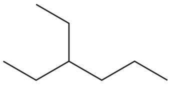
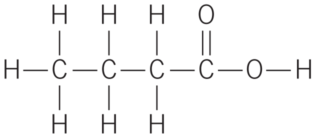
3 Rank the following from the lowest to highest bond strength.
   a C≡N, C–N, C═N
   b C–I, C–F, C–Br

4 Carbon can form bonds with many different elements. The average bond energy of C–Si is 301 kJ mol^{-1}, whereas the average bond energy of C–C is 347 kJ mol^{-1}. Which bond is more stable? Explain your answer.

5 The average bond energy of C═O is 745 k mol^{-1}. Determine the amount of energy required to completely convert 2.5 mol of $CO_2(g)$ into gaseous atoms of C and O.

6 Write the molecular formula of each of the following compounds.
   a $CH_2CHCH_2CH_2Cl$
   b $C_5H_{12}O$

7 Draw the skeletal formula of each of the following compounds.
   a $CH_3CHCHCH_3$
   b $CH_3CHOHCH_2CH_3$
   c $CH_3CH(CH_3)CH(CH_3)CH_2CH_3$
   d $CH_3(CH_2)_5CH_2Br$
   e $HOOCCH_2CH_2CH_3$

8 Write the semi-structural formula of each of the following compounds.
   a 
   b 
   c 

9 Draw three isomers of $CH_3CH_2CH_2CH_2OH$ using their structural formulas.

8B Molecules of carbon

Study Design:

- The International Union of Pure and Applied Chemistry (IUPAC) systematic naming of organic compounds up to C8, with no more than two functional groups for a molecule, limited to non-cyclic hydrocarbons, haloalkanes, primary amines, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters
- Molecular, structural and semi-structural (condensed) formulas and skeletal structures of alkanes (including cyclohexane), alkenes, benzene, haloalkanes, primary amines, primary amides, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters
- Characteristics of the carbon atom that contribute to the diversity of organic compounds formed, with reference to valence electron number, relative bond strength, relative stability of carbon bonds with other elements, degree of unsaturation, and the formation of structural isomers

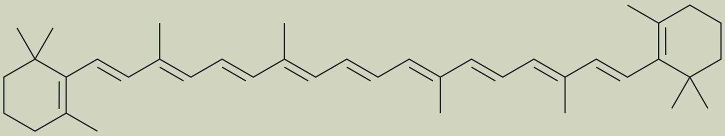
Glossary:

Aromatic compound
Branched isomer
Cyclic alkane
Cycloalkane
Degree of unsaturation
Delocalised electron
Homologous series
Polyunsaturated
Saturated
Straight-chain alkane
Unsaturated

ENGAGE

β-Carotene

Carrots, sweet potatoes, pumpkin, mangoes and apricots are just some of the delicious orange-coloured fruits and vegetables available from a grocery store. While they taste vastly different, they all contain the same pigment that gives them their rich orange colour – β-carotene. This compound is a hydrocarbon with many C=C double bonds. The electrons in the C=C double bonds interact with light, giving the compound its characteristic colour. The food industry adds β-carotene to margarine to give it a more appealing colour.



β-carotene

Figure 8B–1 The structure of β-carotene gives carrots their characteristic colour.

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EXPLAIN

Homologous series

UNIT 1 LINK

Homologous series
a sequence of compounds that have identical functional groups and similar chemical properties but differ by a $-CH_2-$ group in their structure

To simplify and organise our study of organic chemistry, we classify organic molecules into different families. Each family has a characteristic feature or functional group. The members within a family are organised into a **homologous series** where each member differs from the previous one by a $-CH_2-$ unit. Table 8B–1 gives a summary of the different homologous series you have encountered before. All members of the same homologous series have:

- the same general formula
- similar chemical properties
- a trend for their physical properties that is dependent on their molar mass.

Table 8B–1 Homologous series of different families of molecules

Family	Functional group	General formula	Homologous series
Alkane	–	C_nH_{2n+2}	CH_4 C_2H_6 C_3H_8 C_4H_{10} …
Alkene	C=C double bond	C_nH_{2n}	C_2H_4 C_3H_6 C_4H_8 C_5H_{10} …
Chloroalkane	Chloro	$C_nH_{2n+1}Cl$	CH_3Cl C_2H_5Cl C_3H_7Cl C_4H_9Cl …
Alcohol (alkanol)	Hydroxyl	$C_nH_{2n+1}OH$	CH_3OH C_2H_5OH C_3H_7OH C_4H_9OH …
Carboxylic acid	Carboxyl	$C_nH_{2n+1}COOH$	$HCOOH$ CH_3COOH C_2H_5COOH C_3H_7COOH …

The rest of this chapter explores the structural features of several different families of organic compounds, how to name the molecules within them and the trends in their physical properties.

Hydrocarbons

1A TYPES OF FUELS LINK

The most fundamental carbon compounds are the hydrocarbons. These are molecules made up of only carbon and hydrogen atoms. A combination of these two elements can form a wide variety of hydrocarbon structures with different physical and chemical properties. A common source of hydrocarbons in nature is crude oil, which is a natural resource used for energy generation and production of plastic goods. Hydrocarbon compounds can be further classified into different homologous series. This section explores the structural features and the systematic naming of two of these series: alkanes and alkenes.

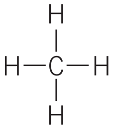
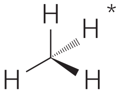
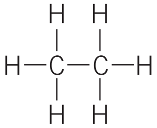
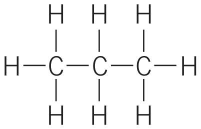
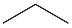
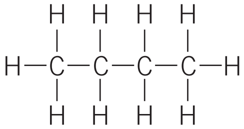
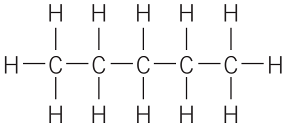
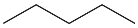
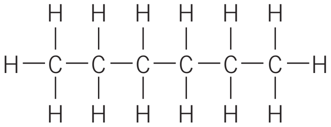
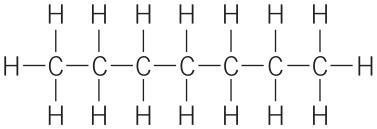
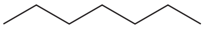
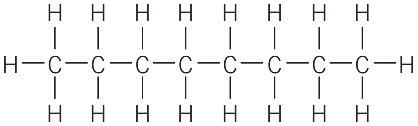
Alkanes

Alkanes are **saturated** hydrocarbons, meaning that only single bonds exist between their carbon atoms. Alkanes have the general formula C_nH_{2n+2}. The names and structures of a homologous series of eight **straight-chain alkanes** are shown in Table 8B–2. The 'ane' component found in all their names indicate that they are alkane molecules. Their molecular formulas show the incremental increase of a $–CH_2–$ unit from one member to the next within the homologous series. This is a feature that extends to all other homologous series.

Saturated
an organic molecule in which all C–C bonds are single bonds

Straight-chain alkane
an alkane consisting of a continuous chain of carbon atoms

Table 8B–2 Name and structure of the first eight straight-chain alkanes

Number of carbons	Name	Molecular formula	Semi-structural formula	Structural formula	Skeletal formula
1	Methane	CH_4	CH_4		 *
2	Ethane	C_2H_6	CH_3CH_3		 *
3	Propane	C_3H_8	$CH_3CH_2CH_3$		
4	Butane	C_4H_{10}	$CH_3CH_2CH_2CH_3$		
5	Pentane	C_5H_{12}	$CH_3(CH_2)_3CH_3$		
6	Hexane	C_6H_{14}	$CH_3(CH_2)_4CH_3$		
7	Heptane	C_7H_{16}	$CH_3(CH_2)_5CH_3$		
8	Octane	C_8H_{18}	$CH_3(CH_2)_6CH_3$		

* The hydrogens bonded to the carbon are shown in methane for the sake of clarity. The semi-structural formula is more commonly used to represent small molecules like methane and ethane.

Branched isomer a molecule with the same molecular formula but different arrangement of alkyl branches

Alkanes larger than C_3H_8 can form **branched isomers**. These skeletal isomers of straight-chain alkanes consist of alkyl groups branching from a parent hydrocarbon. Figure 8B–2 highlights the alkyl groups and parent hydrocarbon of the same branched-chain alkane using three different representations.

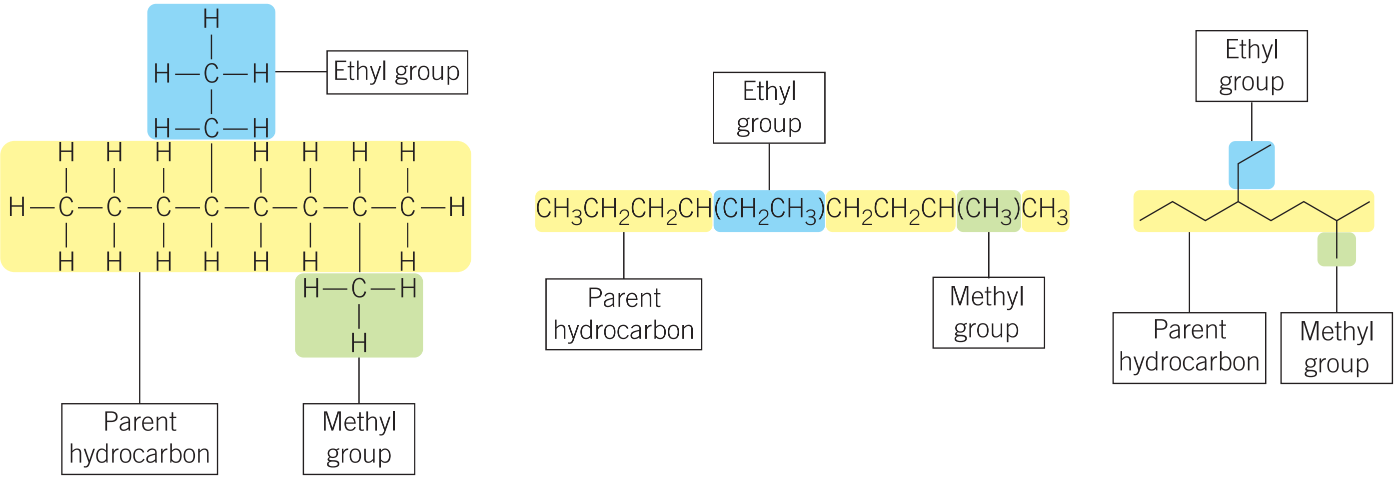


Figure 8B–2 A branched alkane involves alkyl groups connected to a main parent hydrocarbon

Alkyl groups have names based on the number of carbon atoms within them. For example, a $-CH_3$ branch is called a methyl group. The 'meth' component refers to one carbon and the 'yl' component indicates that it is an alkyl group. The names of the first four alkyl groups are listed in Table 8B–3.

Table 8B–3 Names of common alkyl groups

Name	Structure
Methyl	$-CH_3$
Ethyl	$-CH_2CH_3$
Propyl	$-CH_2CH_2CH_3$
Butyl	$-CH_2CH_2CH_2CH_3$

Nomenclature of alkanes

Names of all organic compounds are guided by a set of rules under the International Union of Pure and Applied Chemistry (IUPAC) systematic nomenclature. The utility of this nomenclature system is that the name of a molecule fully describes all aspects of its structure. A trained person, without using an external reference or database, should be able to analyse the name of any molecule and be able to draw the correct structure of that molecule. This naming system allows us to efficiently communicate organic chemistry.

All alkanes can be named using the steps from the flow chart below.

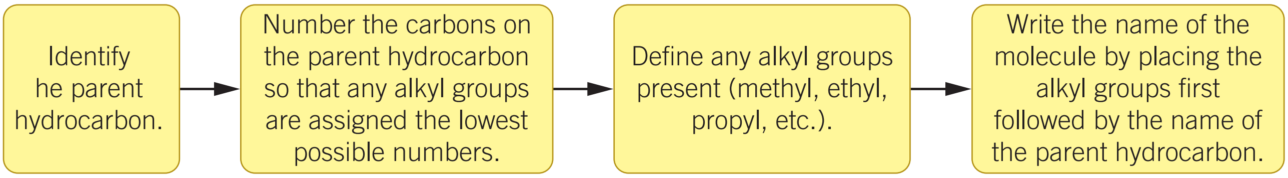
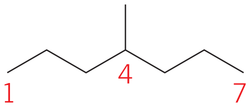


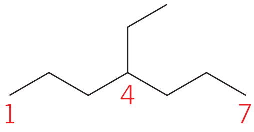
Figure 8B–3 Flow chart showing the general procedure for naming an alkane

The following rules apply when naming alkanes.

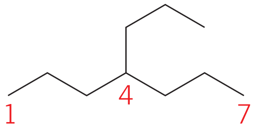
- The parent hydrocarbon is the longest continuous carbon chain.
- The names of all alkanes end in 'ane' (Table 8B–2 on page 273).
- The name(s) of the alkyl groups (Table 8B–3) are placed before the parent hydrocarbon in alphabetical order.
- A number, separated by a hyphen, is used before the alkyl group to represent the position on the parent hydrocarbon where the alkyl group is bonded.



4-methylheptane

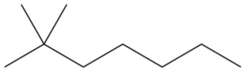


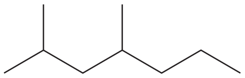
4-ethylheptane

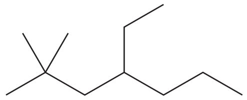


4-propylheptane

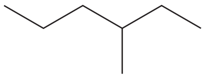
- Multipliers 'di', 'tri' or 'tetra' are used for multiple occurrences of the **same** alkyl group. The multipliers are not considered for alphabetical ordering.


2,2-dimethylheptane


2,4-dimethylheptane


4-ethyl-2,2-dimethylheptane

- Number the carbons in the parent hydrocarbon from the end that gives the alkyl groups the lowest possible numbers.



4-methylhexane

✗

Incorrect

Consider numbering the parent hydrocarbon from right to left. This would give the methyl group a lower number.

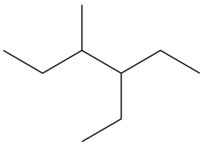
3-methylhexane

✓

Correct

This is the correct name for the molecule. The methyl group has been given the lowest possible number.

- If there is competition for the lower number, the group which is alphabetically first in the name receives it.



4-ethyl-3-methylhexane

✗

Incorrect

The same set of numbers is achieve by numbering the molecule from either end. To break the tie, the group that appears first (ethyl) should have the lower number.

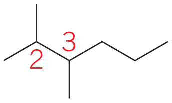
3-ethyl-4-methylhexane

✓

Correct

This is the correct name for the molecule.

- Do not use any spaces in the name.
- Use hyphens to separate numbers from words.
- Use commas to separate numbers.



2,3-dimethyl hexane ✗

2,3 dimethylhexane ✗

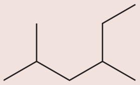
2 3-dimethylhexane ✗

2,3-dimethylhexane ✓

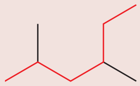
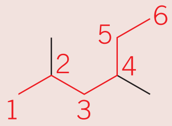
VIDEO WORKED EXAMPLE 8B–1

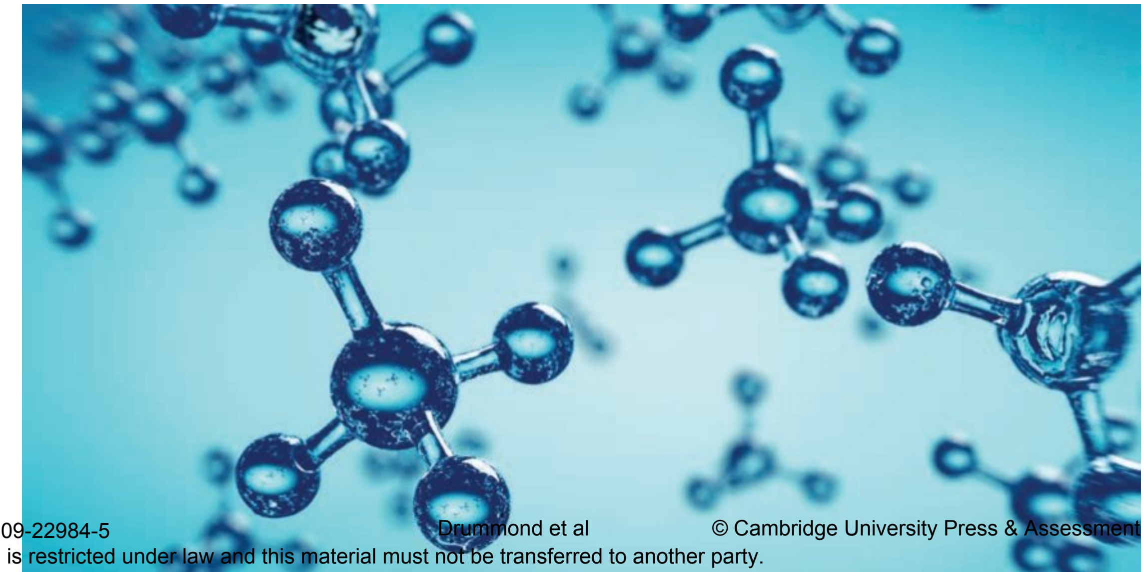
Worked example 8B–1: Naming an alkane molecule

Determine the name of the following alkane.



Solution

	Logic	Process
Step 1	Identify the parent hydrocarbon (longest continuous carbon chain, as shown in red).	
Step 2	Number the parent hydrocarbon so that any alkyl groups are assigned the lowest possible numbers.	
Step 3	Write the name of the parent hydrocarbon.	Hexane
Step 4	Identify and name the alkyl groups with their locations.	2-methyl and 4-methyl
Step 5	Write the full name of the molecule by combining the elements in steps 3 and 4. Alkyl groups appear as prefixes before the parent hydrocarbon. Don't forget to include multipliers if the same alkyl group is present more than once.	2,4-dimethylhexane

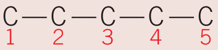
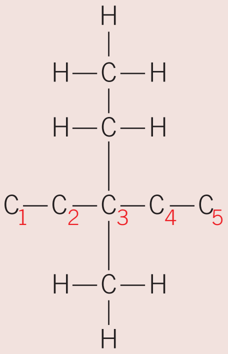
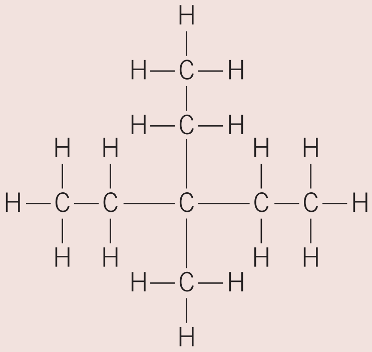


Worked example 8B–2: Drawing an alkane with alkyl groups

VIDEO
WORKED
EXAMPLE 8B–2

Draw the structural formula of 3-ethyl-3-methylpentane.

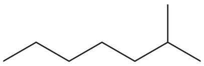
Solution

	Logic	Process
Step 1	Identify the parent hydrocarbon.	3-ethyl-3-methyl **pentane**
Step 2	Draw the carbon chain of the parent hydrocarbon. Number the carbons in the chain.	
Step 3	Draw the alkyl groups in the appropriate locations.	
Step 4	Draw the rest of the hydrogens on the parent hydrocarbon.	

Check-in questions – Set 1

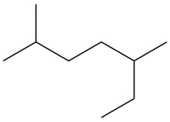
1 Name the following molecules.

a

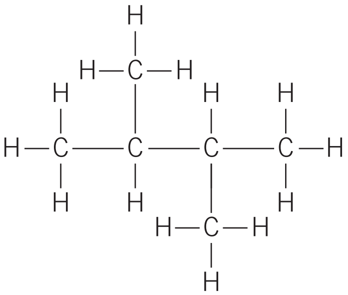


b $CH_3(CH_2)_3CH(CH_3)CH_2CH_3$

c



d



2 Write the semi-structural formula of the following molecules.

a heptane

b 3-ethylpentane

c 2,2-dimethylpentane

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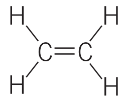
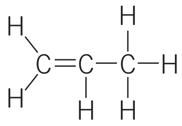
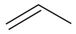
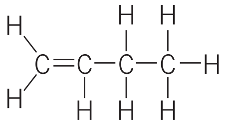
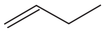
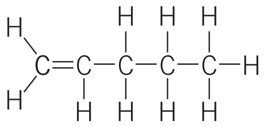
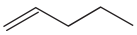
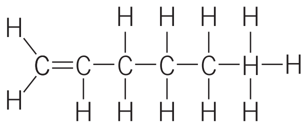
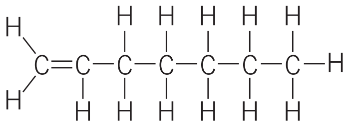
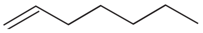
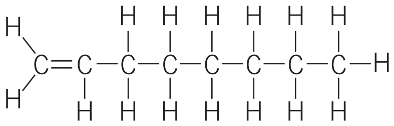
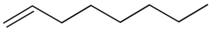
Alkenes

Alkenes are unsaturated hydrocarbons characterised by the presence of one or more C═C double bond(s). Alkenes with a single C═C double bond belong in the same homologous series. The smallest member of this homologous series is ethene. The names and structures of the first seven straight-chain alk-1-enes are shown in Table 8B–4. The general formula for alkenes with one C═C double bond is C_nH_{2n}.

Table 8B–4 Formulas of the first seven straight-chain alkanes

Number of carbons	Name	Molecular formula	Semi-structural formula	Structural formula	Skeletal formula
2	Ethene	C_2H_4	CH_2CH_2		
3	Propene	C_3H_6	CH_2CHCH_3		
4	But-1-ene	C_4H_8	$CH_2CHCH_2CH_3$		
5	Pent-1-ene	C_5H_{10}	$CH_2CHCH_2CH_2CH_3$		
6	Hex-1-ene	C_6H_{12}	$CH_2CH(CH_2)_3CH_3$		
7	Hept-1-ene	C_7H_{14}	$CH_2CH(CH_2)_4CH_3$		
8	Oct-1-ene	C_8H_{16}	$CH_2CH(CH_2)_5CH_3$		

UNIT 1 LINK

Alkenes are an important family of organic molecules. Alkenes are used to produce important plastics that we commonly use daily. For example, ethene is used to produce polyethylene (polyethene), the polymer used to make milk bottles, plastic cling wrap, plastic bags, plastic bottles and many other common objects (Figure 8B–4).

Figure 8B–4 Common household objects made from polyethene, a polymer of ethene

Nomenclature of alkenes

Like alkanes, straight chain alkenes use the same naming system based on the number of carbon atoms in the longest continuous chain as the parent hydrocarbon. Names of all alkenes end in 'ene' instead of 'ane' as for alkanes. The location of the C═C double bond needs to be specified in the name for alkenes larger than C_3H_6 due to possible isomers. Follow the general flow chart when naming alkenes (Figure 8B–5).

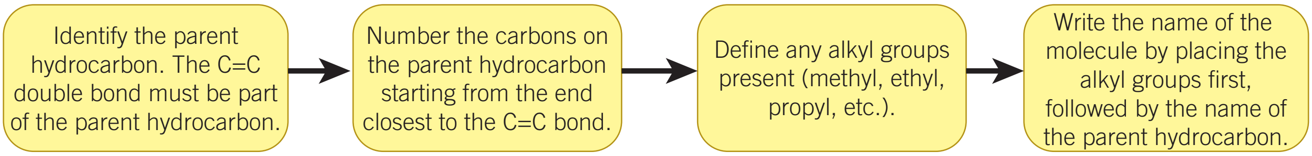
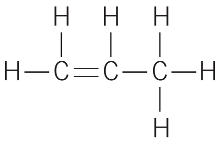


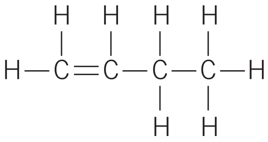
Figure 8B–5 Flow chart showing the general procedure for naming alkenes

In addition to the rules for alkanes, the following rules may need to be applied when naming alkenes.

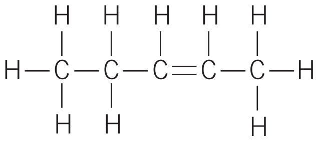
- Include the C═C double bond in the longest continuous carbon chain (parent hydrocarbon).
- Number the chain starting from the end closest to the C═C double bond. This ensures that the C═C double bond is assigned the lowest possible number.
- If positional isomers are possible, use numbers to indicate the first carbon of the C═C double bond.



Propene

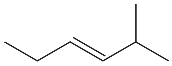


But-1-ene



Pent-2-ene

- If the C═C double bond is equidistant to both ends of the parent hydrocarbon, assign any alkyl group(s) the lowest possible number(s).



5-methylhex-3-ene

✗

Incorrect

Consider numbering the parent hydrocarbon from right to left. This would give the methyl group a lower number.

2-methylhex-3-ene

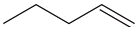
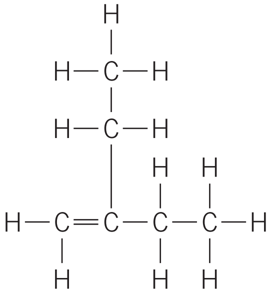
✓

Correct

This is the correct name for the molecule. The methyl group has been given the lowest possible number.

Check-in questions – Set 2

1 Write the name of each of the following molecules.

- **a** 
- **b** $CH_3CHCHCH(CH_3)CH_2CH_3$
- **c** $CH_2C(CH_3)CH_2CH_3$
- **d** 

2 Draw the skeletal structure of each of the following molecules.

- **a** hex-3-ene
- **b** 4-methylpent-1-ene
- **c** 2,3-dimethylbut-2-ene

Cyclic hydrocarbons

Cyclohexane

Cyclic alkane or cycloalkane a molecule with one or more rings of saturated carbons in its structure

Hydrocarbons can also adopt a cyclic or ring structure. Imagine a hexane molecule with an extra covalent bond connecting the first and last carbon atoms. Consequently, each of these carbons need to lose a hydrogen atom to maintain exactly four bonds. This molecule is called cyclohexane (C_6H_{12}) and is shown in Figure 8B–6. The ‘cyclo’ part of the name indicates a cyclic structure. The second part of the name describes the total number of carbons in the ring structure. Many other **cyclic alkanes** or **cycloalkanes** exist in nature or can be synthesised by chemists. These include cyclopropane (the smallest possible cyclic alkane), cyclobutane, cyclopentane, cyclooctane etc. Even though cyclohexane (C_6H_{12}) and hexane (C_6H_{14}) are both saturated molecules with six carbon atoms, they are not structural isomers because they have different molecular formulas. In fact, cycloalkanes are a separate homologous series from straight-chain alkanes.

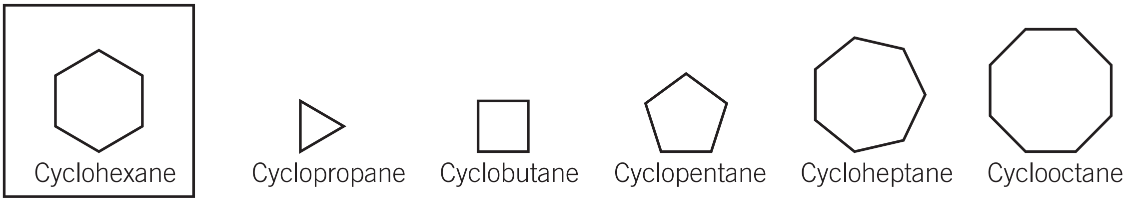


Figure 8B–6 Structures of cyclohexane and other members of the cycloalkane family

Benzene

Another cyclic hydrocarbon deserving a particular mention is benzene (C_6H_6), a molecule commonly found in petrochemicals. Its structure, as shown in Figure 8B–7, shares similarities with cyclohexane but each carbon atom is bonded to only one hydrogen atom. All six carbon atoms in benzene adopt a trigonal planar geometry, resulting in the entire molecule being planar or flat. This makes each carbon in benzene appear to only have three bonds. In fact, the last valance electron from each of the 6 carbon atoms form rings of **delocalised electrons** above and below the molecule. Benzene is often represented as a hexagon with a circle in the middle. This circle represents the delocalised electron ring.

Delocalised electron
an electron that is not associated with any particular atom and is free to move

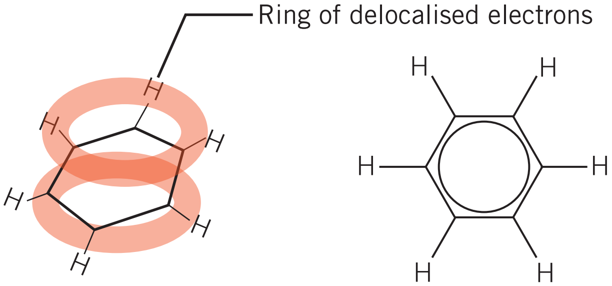


Figure 8B–7 Representations of benzene

Other representations of benzene include three alternating double bonds around a hexagon. While this is a less accurate representation of benzene, it does help us conceptualise the 'location' of the electrons around the cyclic molecule. This becomes useful when we need to explain how benzene and other similar molecules react in chemical reactions.

Figure 8B–8 Alternative representations of benzene

It should be noted that the ring of delocalised electrons gives benzene extra stability compared to a typical alkene. Benzene and many other planar cyclic compounds with a ring of delocalised electrons belong to a class of compounds called **aromatic compounds** (Figure 8B–9). These compounds have a wide variety of uses, including therapeutics, dyes and plastics.

Aromatic compound
a cyclic molecule with a ring of delocalised electrons

LINK **12A** ORGANIC COMPOUNDS AS MEDICINES

WORKSHEET 8B–1 NAMING ALKANES AND ALKENES

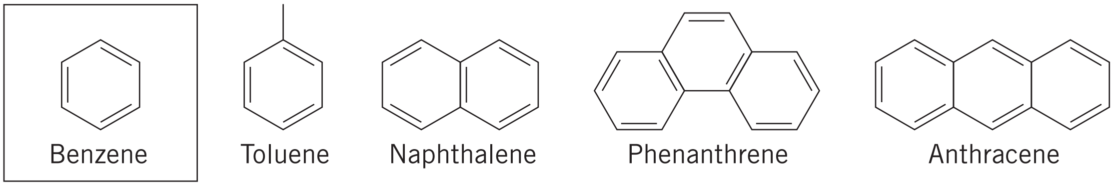


Figure 8B–9 Structures of benzene and other aromatic compounds

Degree of unsaturation

Molecules with at least one double bond (or triple bond) are described as **unsaturated**. The word 'unsaturated' is associated with the idea that the molecule is 'not full'. This is because one of the bonds from the double bond can break allowing the molecule to form new bonds to more atoms. For example, adding two hydrogen atoms to a molecule of but-1-ene gives the product butane, as shown in Figure 8B–10. In contrast to but-1-ene, butane does not have any double bonds. Therefore, it is considered saturated or 'full' because no more addition of atoms is possible. To extend on this idea, molecules with more than one double

Unsaturated
a molecule that has one or more $C{=}C$ double bonds or $C{\equiv}C$ triple bonds

bond are considered to have a higher degree of unsaturation because a greater number of H atoms could be added to them. Molecules with a higher degree of unsaturation are referred to as **polyunsaturated**. This leads to the idea that different molecules have a different **degree of unsaturation** (DoU).

Polyunsaturated an organic compound that has two or more C═C double bonds or C≡C triple bonds

Degree of unsaturation a calculation of the number of ring systems and double bonds (and triple bonds) in a molecule; can be shortened to DoU

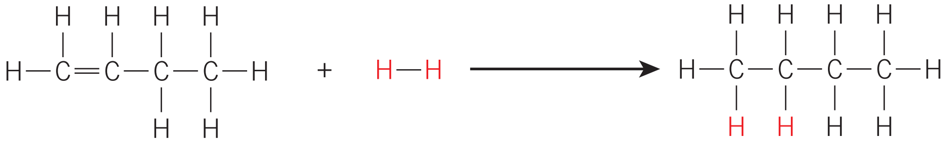


Figure 8B–10 Addition of hydrogen (H_2) to unsaturated but-1-ene gives the saturated product butane.

Counting the bonds

The degree of unsaturation of a molecule can be quantified by its total number of double bonds, triple bonds and cyclic structures. If the molecule's structure is known, we can determine the degree of unsaturation by simply counting the number of double bonds, triple bonds or cyclic structures that appear in the molecule. It is important to note that double bonds and triple bonds are **not** limited to C═C double bonds or C≡C triple bonds. A C═O would qualify as a double bond.

The following formula summarises this process. While triple bonds do affect the degree of unsaturation, they are not part of this Study Design and therefore have been excluded from this version of the formula.

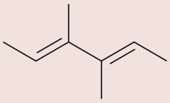
Degree of unsaturation (DoU) = number of double bonds + number of cyclic structures

The following examples demonstrate how this equation can be applied to different circumstances.

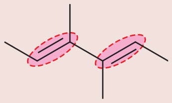
VIDEO WORKED EXAMPLE 8B–3

Worked example 8B–3: Determining the degree of unsaturation by counting the bonds (1)

Determine the degree of unsaturation of the following alkene.



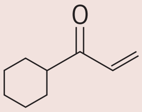
Solution

	Logic	Process
Step 1	Circle or highlight all double bonds and cyclic structures.	
Step 2	Apply the number of double bonds and cyclic structures to the DoU equation.	DoU = double bonds + cyclic structure DoU = 2 + 0
Step 3	Solve the equation.	DoU = 2

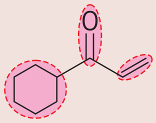
Worked example 8B–4: Determining the degree of unsaturation by counting the bonds (2)

VIDEO WORKED EXAMPLE 8B–4

Determine the degree of unsaturation of the following molecule.



Solution

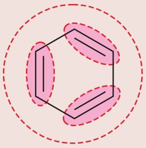
	Logic	Process
Step 1	Circle or highlight all double bonds and cyclic structures.	
Step 2	Apply the number of double bonds and cyclic structures to the DoU equation.	DoU = double bonds + cyclic structure DoU = 2 + 1
Step 3	Solve the equation.	DoU = 3

Worked example 8B–5: Determining the degree of unsaturation by counting the bonds (3)

VIDEO WORKED EXAMPLE 8B–5

Determine the degree of unsaturation of benzene.

Solution

	Logic	Process
Step 1	Circle or highlight all double bonds and cyclic structures.	
Step 2	Apply the number of double bonds and cyclic structures to the DoU equation.	DoU = 3 + 1
Step 3	Solve the equation.	DoU = 4

Using the molecular formula

The degree of unsaturation can also be determined using the molecular formula of a compound. The following equation applies when the molecular formula is known:

$$\text{DoU} = \frac{2\text{C}+2+\text{N}-\text{H}-\text{X}}{2}$$

where:
C = The number of carbon atoms
N = The number of nitrogen atoms
H = The number of hydrogen atoms
X = The number of halogen atoms (F, Cl, Br, I).

The following worked examples demonstrate how this equation can be applied to different circumstances.

ISBN 978-1-009-22984-5 Drummond et al

VIDEO
WORKED EXAMPLE 8B–6

Worked example 8B–6: Determining the degree of unsaturation using the molecular formula (1)

Calculate the degree of unsaturation of a compound with the molecular formula C_4H_6.

Solution

	Logic	Process
Step 1	Analyse the molecular formula for the terms that appear in the DoU equation.	C = 4 (4 carbon atoms) N = 0 (no nitrogen atoms) H = 6 (6 hydrogen atoms) X = 0 (no halogen atoms)
Step 2	Substitute the terms in the DoU equation for their respective numbers.	$\text{DoU} = \frac{2 \times 4 + 2 + 0 - 6 - 0}{2}$
Step 3	Solve the equation.	DoU = 2

VIDEO
WORKED EXAMPLE 8B–7

Worked example 8B–7: Determining the degree of unsaturation using the molecular formula (2)

Calculate the degree of unsaturation for the amino acid tyrosine, $C_9H_{11}NO_3$.

Solution

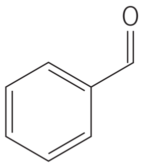
	Logic	Process
Step 1	Analyse the molecular formula for the terms that appear in the DoU equation.	C = 9 N = 1 H = 11 X = 0
Step 2	Substitute the terms in the DoU equation for their respective numbers.	$\text{DoU} = \frac{2 \times 9 + 2 + 1 - 11 - 0}{2}$
Step 3	Solve the equation.	DoU = 5

WORKSHEET 8B–2
CALCULATING DEGREE OF UNSATURATION

Check-in questions – Set 3

1 Calculate the degree of unsaturation in the following molecules.
  - a C_5H_8
  - b $C_7H_{14}O$
  - c $C_5H_9NO_4$

2 Determine the degree of unsaturation for benzaldehyde (shown below).



ISBN 978-1-009-22984-5 Drummond et al

VIDEO 8B–1
SKILLS: NAMING ORGANIC MOLECULES

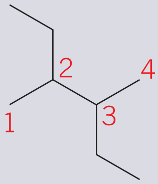
8B SKILLS

Naming organic molecules

The ability to rectify incorrect molecule names is a skill that shows your proficiency in applying the IUPAC rules that govern how molecules are named. Not following the exact rules for naming organic molecules may lead you to come up with incorrect names. For example, the name 2,3-diethylbutane is an incorrect name for the structure that it represents.

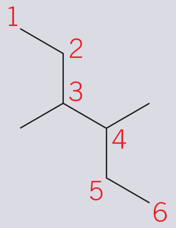
Question: Draw the structure of 2,3-diethylbutane, state the reason why it is incorrectly named and write the correct name of the molecule.

Solution: Draw a skeletal diagram of 2,3-diethylbutane.



2,3-diethylbutane

Reason: The parent hydrocarbon was not correctly identified because it was not the longest continuous carbon chain. The correct numbering system is shown below.



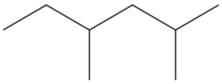
Correct name: 2,3-dimethylhexane

Individually, construct a similar type of question and model solution. Once complete, swap your question with a friend and turn this naming activity into a revision game.

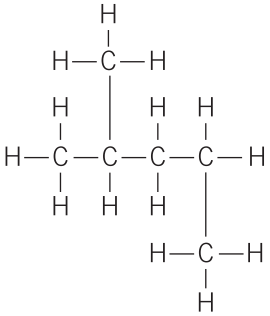
Section 8B questions

1 Write the IUPAC names of the following molecules.

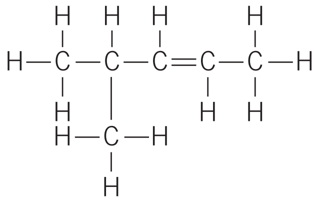
a



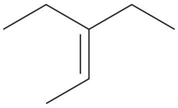
b



c



d



e $CH_3(CH_2)_3CHC(CH_3)_2$

2 Draw the structural formula of each of the following hydrocarbons.

a 2-methylbutane

b 2,4-dimethylpentane

c 4-ethylhex-2-ene

d 3,3-dimethylhex-1-ene

3 Which two compounds in Question **2** are structural isomers?

4 Define ‘homologous series’.

5 Using the skeletal formula, draw and name the structures of the following molecules.

a a saturated straight-chain hydrocarbon with five carbon atoms

b a branched alkane with four carbon atoms

c an unsaturated hydrocarbon with three carbon atoms

d two isomers of hex-1-ene, each having two alkyl groups

6 Calculate the degree of unsaturation of the following molecules.

a $C_{10}H_{16}$

b C_6H_{10}

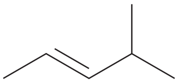
c C_2F_6

d $C_6H_9Cl_2NO$

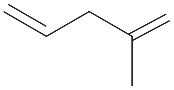
e $C_5H_5NO_3$

7 Determine the degree of unsaturation of the following molecules from their structures.

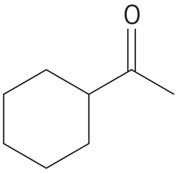
a



b



c



d $CH_2CHCH_2CH_2CH_3$

e $CH_3CH_2CHC(CH_3)CH_2CHCHCH_3$

8C Functional groups: haloalkanes, amines and alcohols

Study Design:

- The International Union of Pure and Applied Chemistry (IUPAC) systematic naming of organic compounds up to C8, with no more than two functional groups for a molecule, limited to non-cyclic hydrocarbons, haloalkanes, primary amines, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters
- Molecular, structural and semi-structural (condensed) formulas and skeletal structures of alkanes (including cyclohexane), alkenes, benzene, haloalkanes, primary amines, primary amides, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters

Glossary:

Alcohol
Alkanol
Amine
Amino functional group
Haloalkane
Hydroxyl group
Primary alcohol (1º alcohol)
Secondary alcohol (2º alcohol)
Tertiary alcohol (3º alcohol)

ENGAGE

Grain alcohol and wood alcohol

Alcohols such as methanol and ethanol are widely produced for their industrial and commercial significance. Methanol (also called wood alcohol because once upon a time it was produced by heating wood in the absence of oxygen) is highly toxic when consumed. Ingesting even a small amount of methanol can lead to blindness, organ failure and death. Illegally sourced alcohol (bootleg alcohol) can sometimes contain traces of methanol, which can cause severe harm if consumed.

In contrast, ethanol is a component of many alcoholic beverages. It is produced by fermentation of the glucose in grapes, potato, corn, rye, wheat and various other grains. It is given the name 'grain alcohol' because of its production method. The type of plant species used for the fermentation determines the type of beverage (red wine, white wine, beer, whiskey or bourbon etc.) produced (Figure 8C–1). While ethanol does not have the same severe effects as methanol, excess consumption can lead to loss of coordination, lowered inhibition, nausea, headache and loss of consciousness.

LINK 1B PRODUCTION OF CHEMICAL ENERGY IN NATURE

The ethanol content of alcoholic beverages is usually taxed by governments, making ethanol an expensive substance. However, because it is also an important substance for research and industry, any ethanol not intended for consumption is not taxed. This source of ethanol is often denatured, meaning that it is made undrinkable by mixing it with small quantities of methanol or other substances.

Figure 8C–1 Barley grains are fermented to produce beer.

EXPLAIN

What are functional groups?

8A STRUCTURAL DIVERSITY IN ORGANIC COMPOUNDS LINK

As we saw earlier in Section 8A, a way to achieve molecular diversity is by changing the elements bonded to the carbon chain in an organic molecule. Imagine substituting a hydrogen atom in an alkane with another atom or group of atoms. This modification generates a new derivative of the original alkane. For example, substituting a hydrogen on an alkane for a chlorine gives a chloroalkane (Figure 8C–2). Similarly, substituting a hydrogen on an alkane for a hydroxyl (–OH) group gives an alcohol.

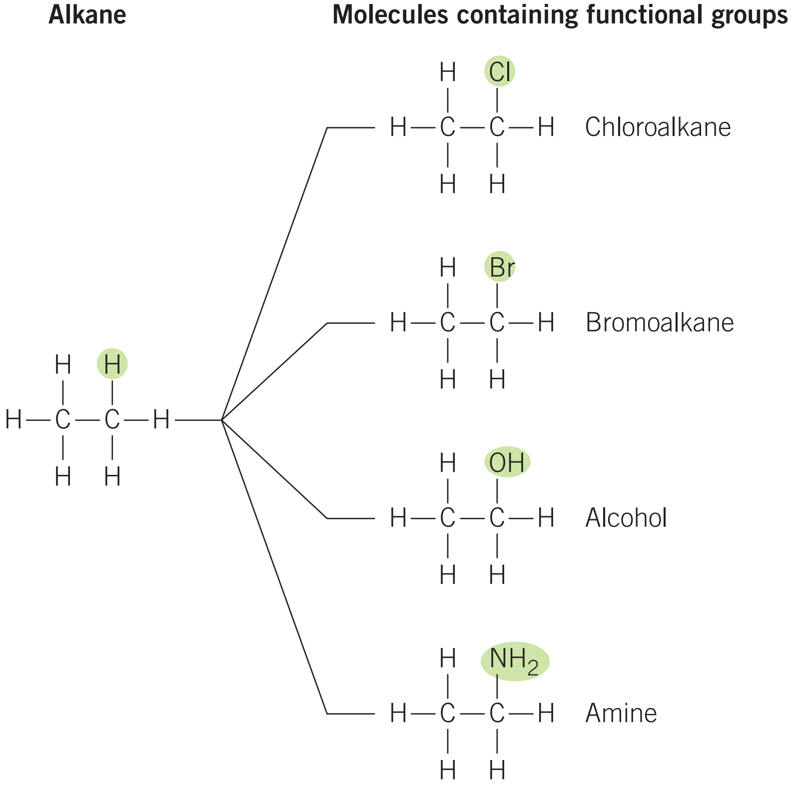


Figure 8C–2 Substituting a hydrogen on an alkane for other elements introduces functional groups to the molecule.

A functional group is a specific atom or group of atoms within a molecule that gives the molecule its own characteristic properties. In Figure 8C–2, the newly introduced atom or group of atoms are the functional groups of the molecules. Importantly, organic compounds are organised into families based on the type of functional group they possess. All molecules within the same family have the same functional group and exhibit similar chemical properties. For example, the molecules shown in Figure 8C–3 all have a chloro-functional group. Despite having a different number of carbon atoms, their identical functional group means that they have similar chemical properties. A chemist can expect that they would all behave in a very similar manner during a reaction. The organisation of organic compounds into families allows chemists to make predictions and generalisations about molecules they have never encountered before.

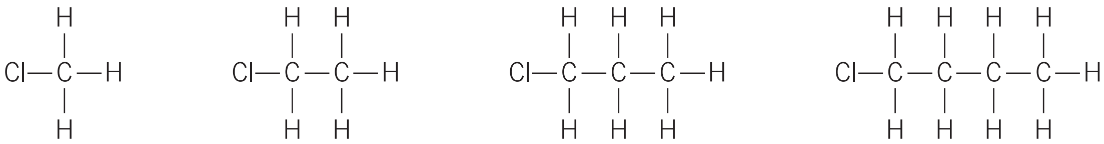


Figure 8C–3 A homologous series of chloroalkanes has identical functional groups and very similar chemical properties. They would all behave in a similar manner during a chemical reaction.

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This section explores the structural features and nomenclature of molecules bearing the following functional groups:

- halo functional group (a fluoro-, chloro-, bromo- or iodo- functional group)
- hydroxyl functional group
- amino functional group.

Haloalkanes

Haloalkanes are a family of molecules in which one or more of the hydrogens in an alkane is substituted for a halogen atom (F, Cl, Br or I). Each of the halogen atoms is given its own name when it is bonded to a molecule. These names are derived by removing the 'ine' from its elemental name and replacing it with an 'o'. So, a fluor**ine** atom in an organic molecule would be called a fluoro- functional group. The other groups are called chloro-, bromo- and iodo- (Figure 8C–4). The term 'halo functional group' is sometimes used to refer to them collectively.

Haloalkane
an alkane in which one or more halogen atoms has replaced a hydrogen atom or atoms

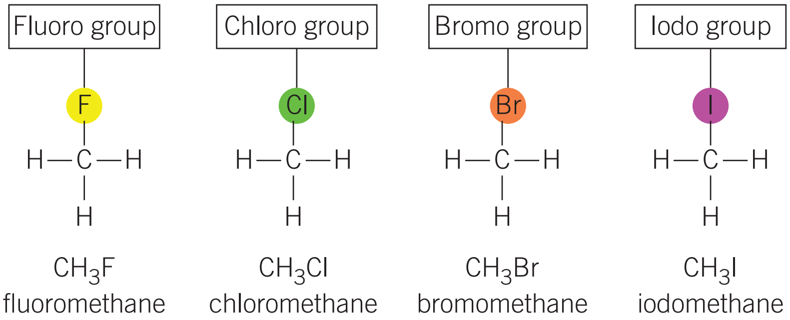


Figure 8C–4 Structures and functional groups of various halomethanes

Haloalkanes are found in a range of applications, including flame retardants, refrigerants, aerosols, solvents, pesticides and pharmaceuticals. Some haloalkanes have adverse effects on our environment. One example is Freon™, a commercial product consisting of a mixture of haloalkanes used in refrigeration, air conditioning and aerosol propellants. Unfortunately, Freon™ also causes ozone depletion and has been phased out of use.

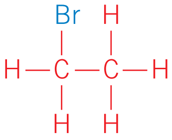
LINK 12A ORGANIC COMPOUNDS AS MEDICINES

Figure 8C–5 Haloalkanes traditionally used as aerosol propellants depleted the ozone layer in our atmosphere.

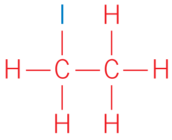
Nomenclature of haloalkanes

When naming haloalkanes, it is important to include the halogen atom in the longest parent hydrocarbon. Apply all the rules for naming alkanes along with the following additional rules specific to haloalkanes.

- The name of the halo functional group appears before the name of the parent hydrocarbon.

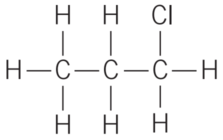


bromoethane



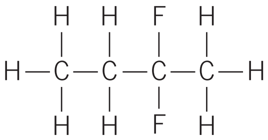
iodoethane

- If positional isomers are possible, use numbers to indicate the carbon to which the halo group is bonded.
- Assign the lowest possible number to the halo group. This involves numbering the parent hydrocarbon starting from the end closest to the functional group.



chloropropane	**3-chloropropane**	**1-chloropropane**
✗	✗	✓
Incorrect	**Incorrect**	**Correct**
Positional isomers are possible in this molecule. The name needs to specify the position of the functional group.	The chloro group has not been assigned the lowest possible number. Start numbering the parent hydrocarbon from the end closest to the chloro group.	This is the correct name for the molecule.

- Use prefixes ‘di’, ‘tri’ and ‘tetra’ if two, three or four, respectively, identical halo functional groups are present.
- Order the name alphabetically if more than one type of halo functional group is present or if an alkyl group is present.



2-fluoro-2-fluorobutane	**2-difluorobutane**	**2,2-difluorobutane**
✗	✗	✓
Incorrect	**Incorrect**	**Correct**
The two identical functional groups are condensed by using ‘di’ before the name.	The position of both fluoro groups needs to be specified in the name even if they are on the same carbon.	This is the correct name for the molecule.

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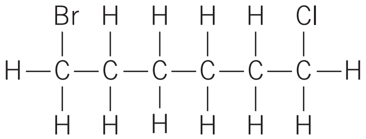
- In the case where there is a tie between two halo functional groups, the one that appears first (alphabetically) will get the lower number.



$$\mathrm{H{-}\underset{H}{\overset{Br}{C}}{-}\underset{H}{\overset{H}{C}}{-}\underset{H}{\overset{H}{C}}{-}\underset{H}{\overset{H}{C}}{-}\underset{H}{\overset{H}{C}}{-}\underset{H}{\overset{Cl}{C}}{-}H}$$

6-bromo-1-chlorohexane

✗

Incorrect

Numbering the molecule from either end results in a tie-break between the bromo and the chloro groups getting the lower number (1 and 6). In this case, the bromo group, which appears first in the name, gets the lower of the two numbers.

1-bromo-6-chlorohexane

✓

Correct

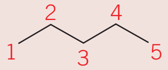
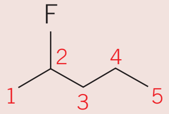
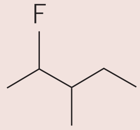
This is the correct name for the molecule.

Worked example 8C–1: Drawing the skeletal formula of a haloalkane

VIDEO
WORKED EXAMPLE 8C–1

Draw the structure of 2-fluoro-3-methylpentane using the skeletal formula.

Solution

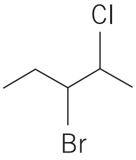
	Logic	Process
Step 1	Identify the parent hydrocarbon.	2-fluoro-3-methyl**pentane**
Step 2	Draw and number the parent hydrocarbon.	
Step 3	Draw the halo functional group in the location outlined by the name.	 **2-fluoro**-3-methyl**pentane**
Step 4	Draw the alkyl group in the location outlined by the name.	 **2-fluoro-3-methylpentane**

Check-in questions – Set 1

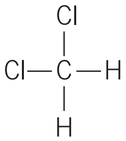
1 Write the systematic name of the following haloalkanes.

a $CH_3CH_2CHBrCH_3$

b



c



$$\mathrm{Cl{-}\underset{H}{\overset{Cl}{C}}{-}H}$$

2 Draw the following molecules using the skeletal formula.

a 2-bromobutane

b 1-chloro-1-fluoroethane

c 2,2-dibromo-1-chloropropane

d 1-fluoro-2-methylbutane

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Alcohols

Substituting a hydrogen of an alkane for a **hydroxyl group** (–OH) gives an **alkanol** or **alcohol**. For simplicity, the terms 'alkanol' and 'alcohol' are often used interchangeably. In a strict sense, 'alcohol' is a broader term referring to any molecule with a hydroxyl functional group, whereas 'alkanol' refers to saturated molecules bearing a hydroxyl group. The first three members of the alkanol homologous series are shown in Figure 8C–6.

Hydroxyl group a functional group characterised by –OH bonded to a carbon atom

Alkanol an alkane in which a hydroxyl group (–OH) has replaced a hydrogen atom

Alcohol a family of organic compounds characterised by a hydroxyl (–OH) functional group

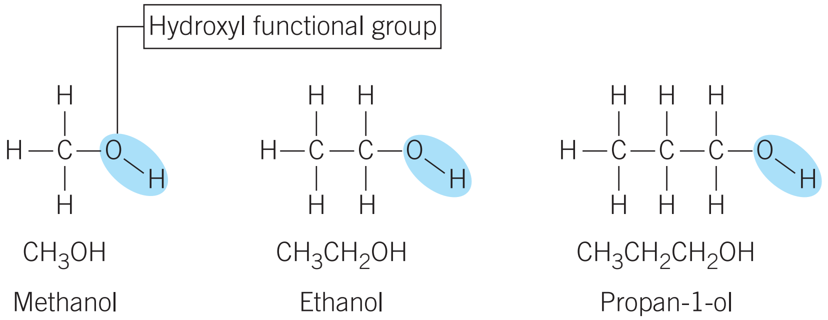


Figure 8C–6 First three members of the alkanol homologous series

Hydroxyl groups are polar functional groups due to oxygen having a higher electronegativity than its neighbouring atoms and the V-shaped bond arrangement around the oxygen atom. The two lone pairs on the oxygen atom are significant features because they allow the formation of intermolecular hydrogen bonds with another molecule (Figure 8C–7).

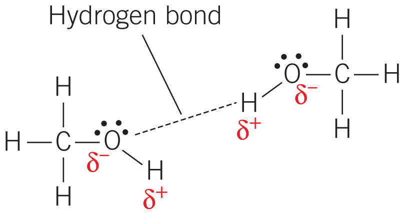


Figure 8C–7 Hydrogen bonding between two molecules of methanol

Types of alcohols

Alcohols can be further divided into three different types based on the structure of their carbon chain. The names of these three different types are:

- **primary alcohol (1° alcohol)**
- **secondary alcohol (2° alcohol)**
- **tertiary alcohol (3° alcohol)**.

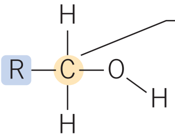
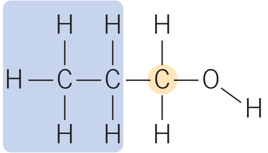
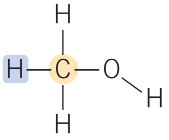
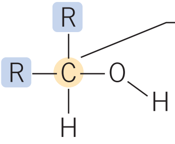
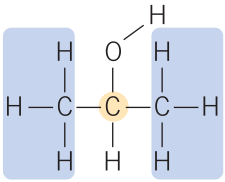
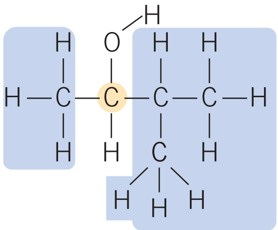
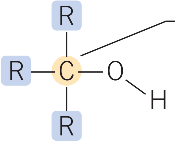
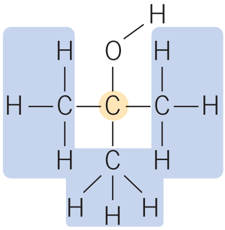
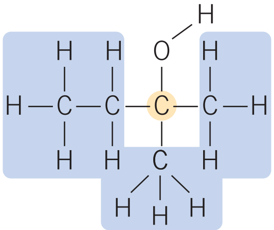
In a primary alcohol, the carbon bonded to the hydroxyl group has, at most, one alkyl group attached to it. An alkyl group (denoted by the symbol *R*) refers to any hydrocarbon chain. In a secondary alcohol, the hydroxyl carbon has two alkyl groups attached to it. In a tertiary alcohol, the hydroxyl carbon has three alkyl groups attached to it. Table 8C–1 shows these structural features along with examples of each type of alcohol.

Primary alcohol (1° alcohol) an alcohol molecule in which the carbon bonded to the hydroxyl group is also bonded to (at most) one alkyl group

Secondary alcohol (2° alcohol) an alcohol molecule in which the carbon bonded to the hydroxyl group is also bonded to two alkyl groups

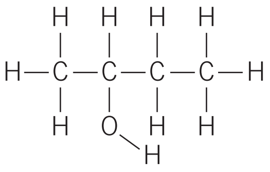
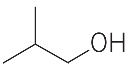
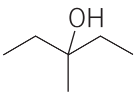
Tertiary alcohol (3° alcohol) an alcohol molecule in which the carbon bonded to the hydroxyl group is also bonded to three alkyl groups

Table 8C–1 Definition and examples of the three different types of alcohols

Alcohol type	Definition	Examples	
Primary alcohol (1° alcohol)	 In a **primary alcohol**, the carbon bonded to the hydroxyl group is bonded to (at most) one other alkyl group.		
Secondary alcohol (2° alcohol)	 In a **secondary alcohol**, the carbon bonded to the hydroxyl group is bonded to two other alkyl groups.		
Tertiary alcohol (3° alcohol)	 In a **tertiary alcohol**, the carbon bonded to the hydroxyl group is bonded to three other alkyl groups.		

Check-in questions – Set 2

1 Label the following alcohols as primary, secondary or tertiary.

Structure	Type of alcohol
	
$CH_3CHOHCH_2CH_2CH_3$	
	
	

2 Draw the structural formula of a tertiary alcohol with the molecular formula $C_4H_{10}O$.

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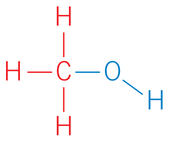
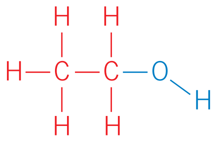
Nomenclature of alcohols

When naming an alcohol, it is important to first identify the longest parent hydrocarbon containing the hydroxyl group. Apply all the rules for naming alkanes along with the following additional rules specific to alcohols.

- The names of alcohols derived from alkanes are constructed by replacing the final ‘e’ in the name of the alkane with ‘ol’. For example, the alcohol derived from methane is called methan**ol**.

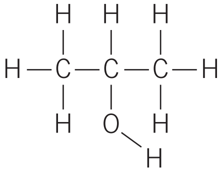


methanol



ethanol

- If positional isomers are possible, the location of the hydroxyl group must be specified in the name. This is done using a number, separated by hyphens, before the ‘ol’ part of the name. The number indicates the carbon to which the hydroxyl group is bonded.



propanol

✗

Incorrect

Positional isomers are possible in this molecule. The name needs to specify the position of the functional group.

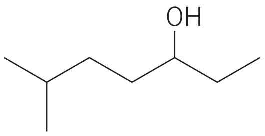
propan-2-ol

✓

Correct

This is the correct name for the molecule. There are positional isomers possible so the name needs to differentiate propan-2-ol from propan-1-ol.

- The parent hydrocarbon is numbered from the end closest to the hydroxyl group. This ensures that the hydroxyl group carbon is assigned the lowest possible number.



2-methylheptan-5-ol

✗

Incorrect

The hydroxyl group takes priority and should be given the lowest possible number.

6-methylheptan-3-ol

✓

Correct

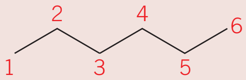
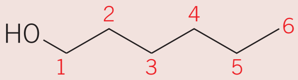
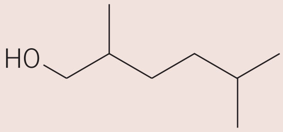
This is the correct name for the molecule. The molecule is numbered starting from the end closest to the hydroxyl group.

Worked example 8C–2: Drawing the skeletal formula of an alcohol

VIDEO
WORKED EXAMPLE 8C–2

Draw the structure of 2,5-dimethylhexan-1-ol using the skeletal formula.

Solution

	Logic	Process
Step 1	Identify and draw the parent hydrocarbon.	 2,5-dimethyl**hexan**-1-ol
Step 2	Number the parent hydrocarbon.	
Step 3	Draw the hydroxyl functional group in the location outlined by the name.	 2,5-dimethyl**hexan-1-ol**
Step 4	Draw any alkyl groups in the location outlined by the name.	 **2,5-dimethylhexan-1-ol**

Check-in questions – Set 3

1 Draw the following molecules using the structural formula.
  a pentan-3-ol
  b 3-ethylhexan-1-ol
  c 2,2-dimethylpropan-1-ol
2 Write the systematic name of the following alkanols.
  a $CH_2OHCH_2CH_2CH_3$
  b $CH_3CH_2CH(CH_2CH_3)CH_2CH_2OH$
  c $CH_3(CH_2)_3CHOHCH_2CH_3$

Primary amines

Substituting a hydrogen of an alkane for an **amino functional group** ($-NH_2$) gives an **amine**. Amines are another family of organic molecules. Amines are commonly found in household cleaning products, paints, dyes and various pharmaceutical products. The structure of the first three members of the amine homologous series is shown in Figure 8C–8 below. The scope of this course is limited to only primary amines.

LINK
12A
ORGANIC COMPOUNDS AS MEDICINES

Amino functional group
a functional group consisting of $-NH_2$

Amine
a family of organic compounds characterised by an amino ($-NH_2$) functional group

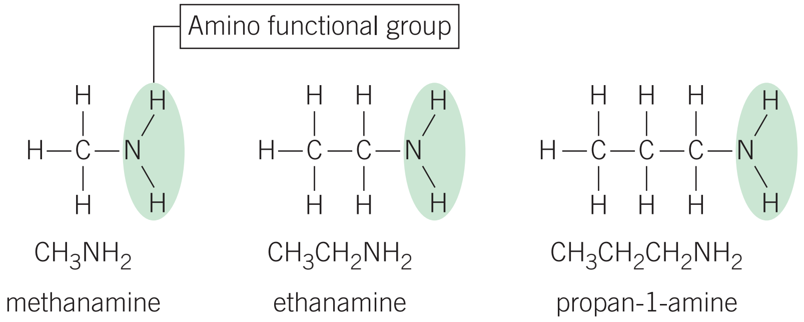


Figure 8C–8 First three members of the primary amine homologous series

The amino group adopts a trigonal pyramidal shape due to the lone pair of electrons on the nitrogen atom. This makes the amino group a polar functional group. Like hydroxyl groups, the lone pair on the nitrogen can form an intermolecular hydrogen bond with a hydrogen of another amino group.

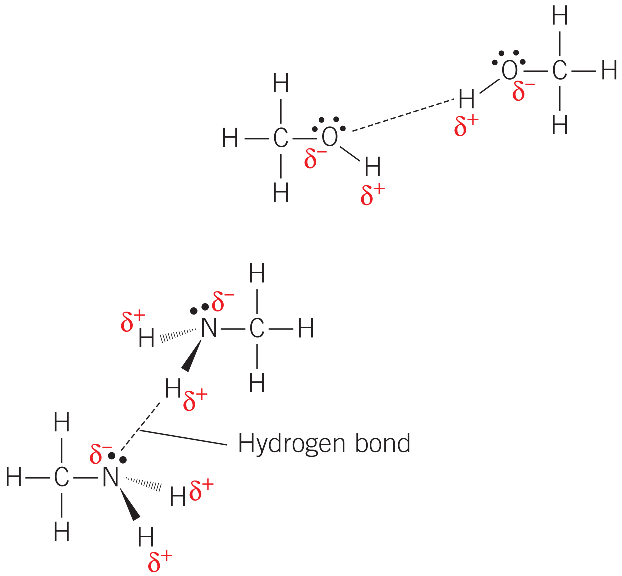


Figure 8C–9 Intermolecular hydrogen bonding between two primary amines and between two primary alcohols

UNIT 2 LINK

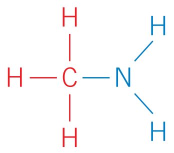
The amino group is an alkaline or basic functional group. This means that an aqueous solution of an amine has a pH greater than 7 at 25°C. In an acid–base reaction, the amino group accepts a hydrogen (H^+) ion to give an $-NH_3^+$ group (called an ammonium group). Alkyl ammoniums and amines are conjugate acid–base pairs.

Figure 8C–10 Propan-1-amine acting as a base in a reaction with H_2O

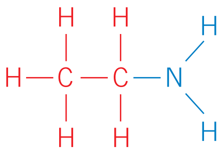
Nomenclature of primary amines

The nomenclature rules that apply to primary amines are very similar to those of alcohols mentioned previously. The first step is always to identify the longest continuous carbon chain with the amino functional group. The rules specific to primary amines are summarised below.

- The names of primary amines derived from alkanes are constructed by replacing the final ‘e’ in the name of the alkane with ‘amine’. For example, the primary amine derived from methane is called methan**amine**.



methanamine



ethanamine

- If positional isomers are possible, the location of the amino group must be specified in the name. This is done using a number, separated by hyphens, before the ‘amine’ part of the name. The number indicates the carbon to which the amino group is bonded.

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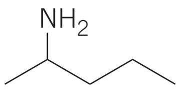


pentanamine

✗

Incorrect

Positional isomers are possible in this molecule. The name needs to specify the position of the functional group.

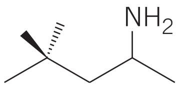
pentan-2-amine

✓

Correct

This is the correct name for the molecule. There are positional isomers possible so the name needs to differentiate pentan-1-amine, pentan-2-amine and pentan-3-amine.

- The parent hydrocarbon is numbered from the end closest to the amino group. This ensures that the amino group carbon is assigned the lowest possible number.



2,2-dimethylpentan-4-amine

✗

Incorrect

The amino group takes priority and should be given the lowest possible number.

4,4-dimethylpentan-2-amine

✓

Correct

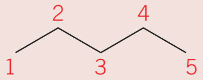
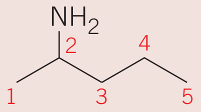
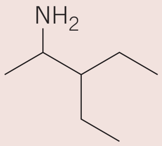
This is the correct name for the molecule. The molecule is numbered starting from the end closest to the amino group.

Worked example 8C–3: Drawing the skeletal formula of an amine

VIDEO
WORKED
EXAMPLE 8C–3

Draw the structure of 3-ethylpentan-2-amine using the skeletal formula.

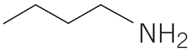
Solution

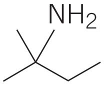
	Logic	Process
Step 1	Identify and draw the parent hydrocarbon.	 3-ethyl**pentan**-2-amine
Step 2	Number the parent hydrocarbon.	
Step 3	Draw the amino functional group in the location outlined by the name.	 3-ethyl**pentan-2-amine**
Step 4	Draw any alkyl groups in the location outlined by the name.	 **3-ethylpentan-2-amine**

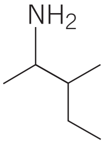
ISBN 978-1-009-22984-5

Check-in questions – Set 4

1 Write the systematic name of the following amines.

a


b


c


2 Write the semi-structural formula of the following molecules.

a propan-1-amine
b 4-methylhexan-2-amine
c 2-methylpentan-3-amine

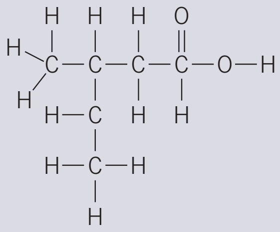
VIDEO 8C–1 SKILLS: DRAWING AND NAMING FUNCTIONAL GROUPS

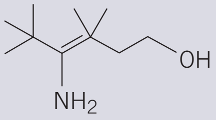
WORKSHEET 8C–1 DRAWING AND NAMING FUNCTIONAL GROUPS 1

8C SKILLS

Drawing and naming functional groups

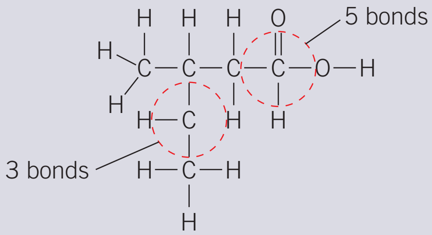
During an assessment, making a single mistake when drawing a structure usually leads to no marks being awarded for your work. Therefore, the skill of checking your drawings should be essential, if time permits. A simple way to check the structures you've drawn is to count the number of bonds to each carbon. Each carbon must always have exactly four bonds. In this course, this usually means either a carbon with four single bonds or one double bond and two single bonds. This is particularly useful for structural formulas, where a common mistake is to miss a hydrogen or draw an extra hydrogen atom. In a skeletal formula where hydrogens connected to carbons are usually not shown, you can still check for any carbons with more than four bonds. Try applying this skill by identifying all errors in the two structures below.

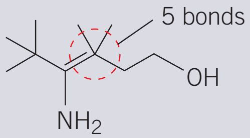




This same skill can also be applied to neutral oxygen and nitrogen atoms. A neutral oxygen atom must have exactly two bonds and a neutral nitrogen atom must have exactly three bonds.

Solutions to the above activity:





Section 8C questions

1 Draw the following alkanols and label them as primary, secondary or tertiary.
  - a butan-2-ol
  - b 3-methylpentan-3-ol
  - c 3,4-dimethylhexan-1-ol
  - d octan-3-ol

2 Write the IUPAC names of the following molecules.
  - a $CH_3CH_2CH_2CHOHCH_2CH_3$
  - b $CH_2ClCHClCH_2CH_2CH_3$
  - c $CH_2OHCH_2CH(CH_3)CH(CH_3)CH_3$
  - d $CH_3CH_2CH(CH_2CH_3)CH_2CH_2CH_2NH_2$

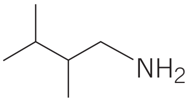
3 Draw the skeletal formulas of the following molecules.
  - a 2-bromoheptane
  - b 3-chloro-3-ethylpentane
  - c 3-methylbutan-2-ol
  - d 3-ethyl-2-methylhexan-2-ol
  - e 4-iodobutan-2-amine
  - f 5,5-dimethylhexan-1-amine

4 Which two molecules from Question **3** belong to the same homologous series?

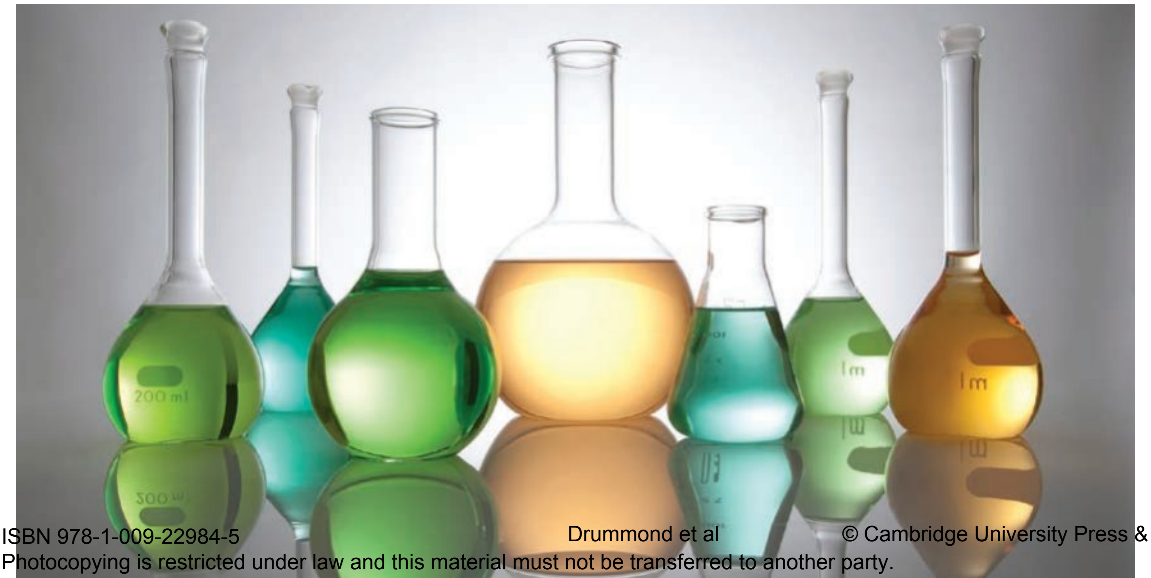
5 Draw the structural formula of the following **incorrect** names and then provide the correct IUPAC name.
  - a 3-methylhexan-4-ol
  - b 3-ethylbutan-2-amine
  - c 3-propylbutan-4-ol

6 Using the semi-structural formula, draw and name the following molecules.
  - a a branched chloroalkane with four carbon atoms
  - b a straight-chain amine with five carbons and the amino group on the third carbon
  - c an isomer of pentanol with two methyl groups attached to the parent chain

7 The structure of an amine is shown below.



  - a Write the IUPAC name of the amine.
  - b How many positional isomers does the amine have? Draw and name them all.



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8D Functional groups: aldehydes, ketones, carboxylic acids, esters and amides

Study Design:

- The International Union of Pure and Applied Chemistry (IUPAC) systematic naming of organic compounds up to C8, with no more than two functional groups for a molecule, limited to non-cyclic hydrocarbons, haloalkanes, primary amines, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters
- Molecular, structural and semi-structural (condensed) formulas and skeletal structures of alkanes (including cyclohexane), alkenes, benzene, haloalkanes, primary amines, primary amides, alcohols (primary, secondary and tertiary), aldehydes, ketones, carboxylic acids and non-branched esters

Glossary:

Aldehyde
Amide functional group
Carbonyl group
Carboxyl group
Carboxylic acid
Dimer
Ester
Ester functional group
Ketone
Primary amide

ENGAGE

The odour of butanedione

Fresh sweat excreted from our skin doesn't have a smell. The unpleasant smell that we associate with perspiration is due to bacterial activity. The bacteria that are always present on our skin convert the compounds in our sweat into odorous compounds that our nose can detect. One of these compounds is butanedione (Figure 8D–1). This compound features two carbonyl functional groups – the main topic of this section.

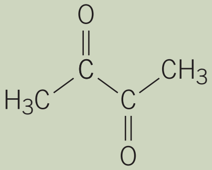

Figure 8D–1 Structure of butanedione, the compound we associate with body odour

EXPLAIN

Carbonyl functional group

8C FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS

LINK

The **carbonyl group** consists of a carbon atom double bonded to an oxygen atom: C═O. Drawing on the same concept from Section 8C, we can visualise a carbonyl group as a carbon from an alkane having two hydrogen atoms substituted for an oxygen atom (Figure 8D–2).

Carbonyl group a functional group consisting of –C═O

The carbonyl group is a common feature in all five families of organic molecules discussed in this section. It is the functional group that characterises aldehydes and ketones. In carboxylic acids, esters and amides, it forms part of a larger functional group (Figure 8D–3).

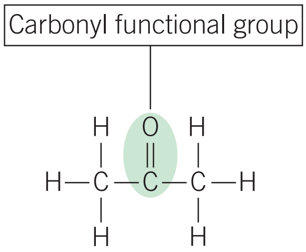

Figure 8D–2 The carbonyl functional group consists of a carbon double bonded to an oxygen.

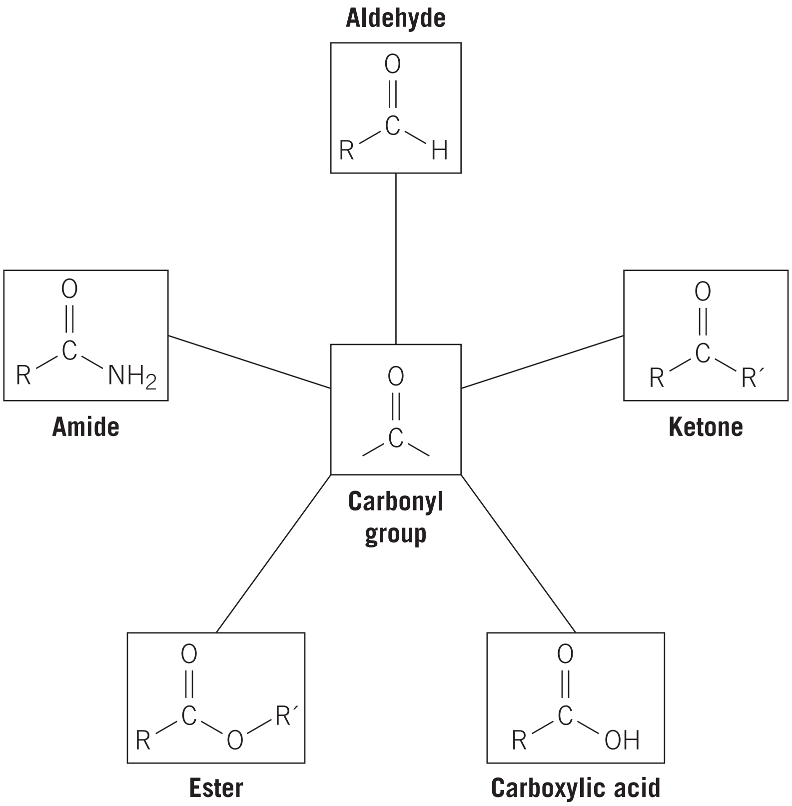

Figure 8D–3 The carbonyl functional group is a feature in many families of organic molecules.

Aldehyde
a molecule containing a carbonyl group where the carbon atom of the carbonyl group is bonded to a hydrogen atom. It has the general formula RCHO

Ketone
a molecule containing a carbonyl group where the carbon of the carbonyl group is bonded to two other carbon atoms. It has the general formula RCOR'

Aldehydes and ketones

Aldehydes and **ketones** are two families of organic compounds characterised by the presence of a carbonyl functional group. Both aldehydes and ketones have the general chemical formula $C_nH_{2n}O$. Aldehydes have a carbonyl group on the first carbon of the parent hydrocarbon. This means that the carbonyl carbon of an aldehyde is always bonded to a H, making the general structure of aldehydes RCHO, where R is either a hydrogen or an alkyl group. The first member of the aldehyde homologous series is methanal.

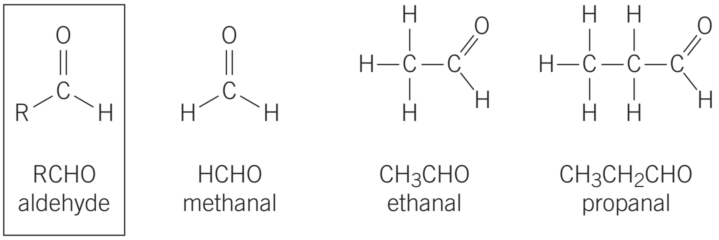

Figure 8D–4 General structure of aldehydes and the first three members of the homologous series

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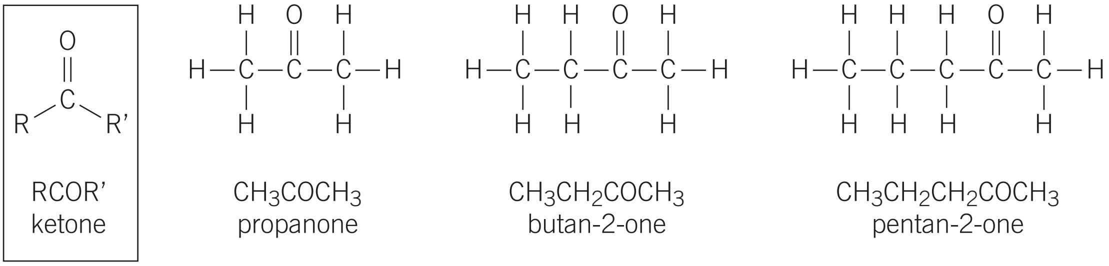
In contrast, the carbonyl group in ketones must be located somewhere in the middle of the carbon chain. In essence, aldehydes and ketones are positional isomers (compare the structures of propanal in Figure 8D–4 and propanone in Figure 8D–5). The general structure of ketones is RCOR' where R and R' represent two alkyl groups that may or may not be the same. Therefore, the first member of the ketone homologous series is propanone.



RCOR' ketone

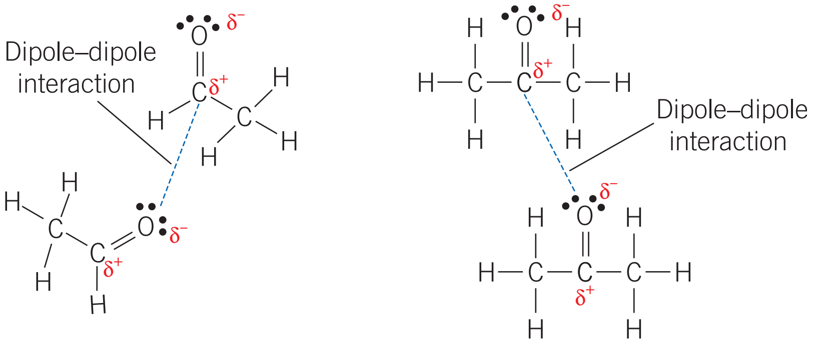
CH_3COCH_3 propanone

$CH_3CH_2COCH_3$ butan-2-one

$CH_3CH_2CH_2COCH_3$ pentan-2-one

Figure 8D–5 General structure of ketones and the first three members of the homologous series

The carbonyl functional group is polar due to oxygen being more electronegative than carbon. This means that the oxygen of the carbonyl group is partially negative, while the carbon is partially positive. Aldehydes and ketones are usually polar molecules. As a result, intermolecular dipole–dipole interactions can form between molecules of aldehydes and ketones as shown in Figure 8D–6.



Intermolecular dipole–dipole interaction between two ethanal molecules

Intermolecular dipole–dipole interaction between two propanone molecules

Figure 8D–6 Dipole–dipole interaction between molecules of ethanal and propanone

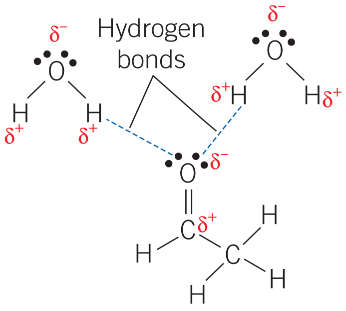


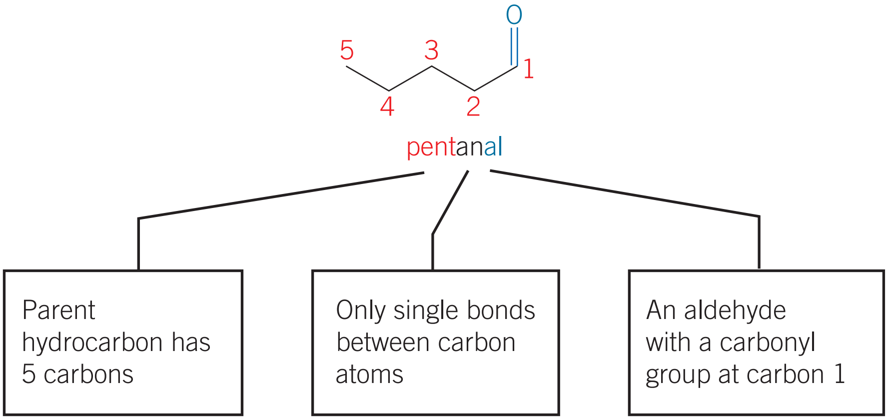
Figure 8D–7 Hydrogen bonding between ethanal and water molecules

The two lone pairs of electrons on the carbonyl oxygen also allows aldehydes and ketones to form intermolecular hydrogen bonds with another molecule with a H–F, H–O or H–N group. Two aldehyde or ketone molecules cannot form hydrogen bonds between themselves because they lack a H bonded to F, O or N. However, aldehydes and ketones can form hydrogen bonds with molecules like H_2O as shown in Figure 8D–7. This interaction explains why small aldehydes and ketones are soluble in water.

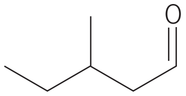
Nomenclature of aldehydes

When naming aldehydes, the rules for naming alkanes need to be applied along with the following rules specific to aldehydes.

- The names of aldehydes derived from alkanes are constructed by replacing the final 'e' in the name of the alkane with 'al'. For example, the aldehyde derived from pentan**e** is called pentan**al**.



- The parent hydrocarbon is numbered starting from the carbonyl carbon.
- There is no need to define the location of the carbonyl group in aldehydes since it is assigned as 1 by default. Locations of other groups need to be specified in the name accordingly.



3-methylbutan-1-al

✗

Incorrect

The carbonyl carbon in an aldehyde is the first carbon by default. Therefore, it is redundant to specify its position in the name.

3-methylbutanal

✓

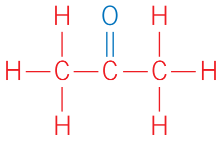
Correct

This is the correct name for the molecule.

Nomenclature of ketones

When naming ketones, the rules for naming alkanes need to be applied along with the following rules specific to ketones.

- The names of ketones derived from alkanes are constructed by replacing the final 'e' in the name of the alkane with 'one'. For example, the ketone derived from propan**e** is called propan**one**.



propanone

- Where positional isomers are possible, the location of the carbonyl must be stated in the name. This is done by using a number, separated by hyphens, positioned before the '-one'.

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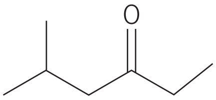
- The parent hydrocarbon is numbered from the end closest to the carbonyl group. This gives the carbonyl carbon the lowest possible number.



2-methylhexanone

✗

Incorrect

There are two errors in this name. The location of the carbonyl group is not stated, making the name ambiguous. In addition, the molecule has been numbered from left to right, which is incorrect. This does not give the carbonyl group the lowest possible number (if it were actually stated in the name).

5-methylhexan-3-one

✓

Correct

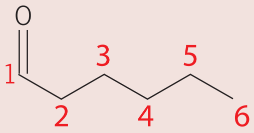
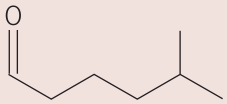
This is the correct name for the molecule.The carbonyl group has been assigned the lowest possible number and the location has been included in the name.

VIDEO WORKED EXAMPLE 8D–1

Worked example 8D–1: Drawing the skeletal structure of an aldehyde

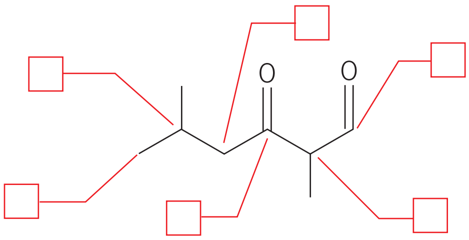
Draw the skeletal structure of 5-methylhexanal.

Solution

	Logic	Process
Step 1	Draw the carbons for the parent hydrocarbon. Number the carbons.	 5-methyl**hexan**al
Step 2	Add the functional group in the correct location on the parent chain.	 5-methyl**hexanal**
Step 3	Add the alkyl group(s) in the correct location(s) on the parent chain.	 **5-methylhexanal**

Check-in questions – Set 1

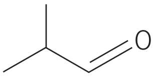
1 Copy the following diagram and write the number of hydrogen atoms connected to each carbon indicated by the boxes.



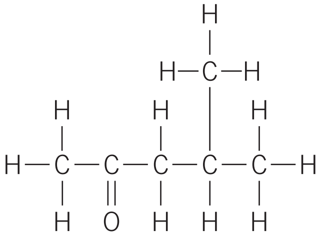
2 Write the names of the following molecules.

a $CH_3COCH_2CH_3$

b



c



3 Draw the structural formula of each of the following molecules.

a pentanal

b 2,4-dimethylpentan-3-one

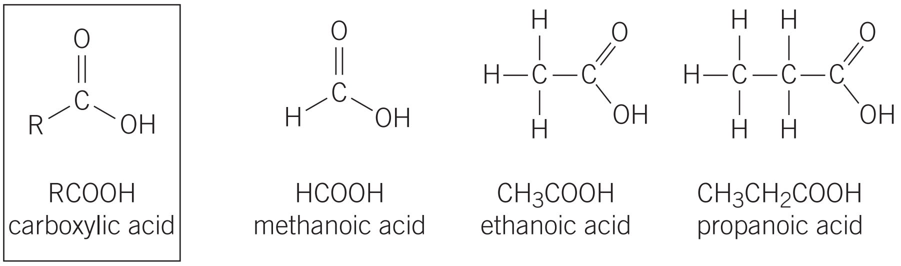
c 3-ethyl-4-methylhexanal

Carboxylic acids

Carboxylic acids are a family of molecules characterised by the presence of a **carboxyl group** (–COOH). The carboxyl group consists of a carbonyl group bonded to a hydroxyl group. In a carboxylic acid derived from an alkane, the carboxyl group is always located on the first carbon. Carboxylic acids derived from alkanes have the general formula $C_nH_{2n+1}COOH$. This can be further simplified to RCOOH, where R represents either a hydrogen or an alkyl group. The first three members of the carboxylic acid homologous series are shown in Figure 8D–8.

Carboxylic acid a family of organic molecules characterised by the presence of a carboxyl group

Carboxyl group a functional group consisting of –COOH. It consists of a carbonyl group bonded to a hydroxyl group.



RCOOH carboxylic acid

HCOOH methanoic acid

CH_3COOH ethanoic acid

CH_3CH_2COOH propanoic acid

Figure 8D–8 General structure and the first three members of the carboxylic acid homologous series

Carboxylic acids are weak organic acids that can donate the H from the carboxyl group. Some of these acids can be commonly found in nature or around the household. For example, methanoic acid is produced by species of ants as a self-defence chemical weapon and ethanoic acid is what gives vinegar its sour taste.

Figure 8D–9 (a) Ants release methanoic acid to ward off potential threats. (b) Household vinegar typically contains 4–8% ethanoic acid.

Dimer
a complex in which two identical or similar molecules are linked together

Carboxyl functional groups are polar. The C═O and O–H portions allow the functional group to form intermolecular hydrogen bonding between two molecules of carboxylic acids. The complementary arrangement of two carboxyl groups allows carboxylic acids to form **dimers** (Figure 8D–10). As a result, the intermolecular bonding between the two carboxylic acids in a dimer is stronger than a typical hydrogen bond.

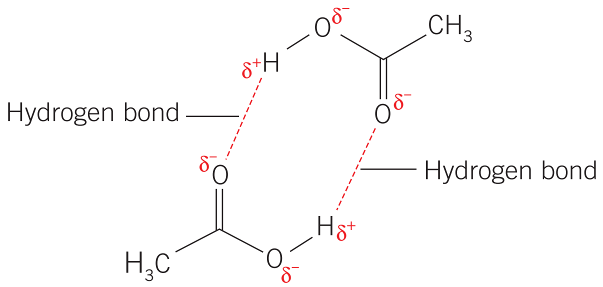
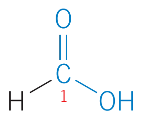


Figure 8D–10 Hydrogen bonding between two ethanoic acid molecules to form a dimer

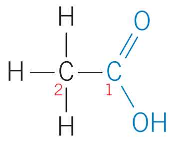
Nomenclature of carboxylic acids

When naming carboxylic acids, the rules for naming alkanes need to be applied along with the following rules specific for carboxylic acids.

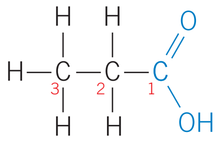
- The names of carboxylic acids derived from alkanes are constructed by replacing the last letter in the name of the alkane with 'oic acid'. For example, the carboxylic acid derived from ethan**e** is called ethan**oic acid**.



methanoic acid

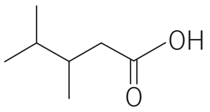


ethanoic acid



propanoic acid

- The parent hydrocarbon is numbered starting from the carboxyl group carbon. This means that the carboxyl group carbon is always assigned as 1.
- There is no need to specify the location of the carboxyl group since it is always the first carbon by default. The location of other groups, such as alkyl groups, needs to be specified in the name.



3,4-dimethylpentan-1-oic acid

✗

Incorrect
The carbon of the carboxyl group is the first carbon by default and therefore does not need to be included in the name.

3,4-dimethylpentanoic acid

✓

Correct
This is the correct name for the molecule.

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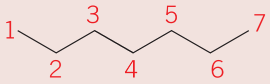
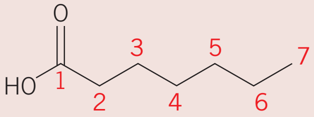
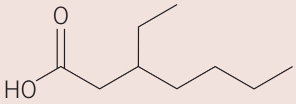
Worked example 8D–2: Drawing the skeletal structure of a carboxylic acid

VIDEO
WORKED
EXAMPLE 8D–2

Draw the skeletal structure of 3-ethylheptanoic acid.

Solution

	Logic	Process
Step 1	Draw the carbons for the parent hydrocarbon. Number the carbons.	 3-ethyl**heptan**oic acid
Step 2	Add the functional group in the correct location on the parent chain.	 3-ethyl**heptanoic acid**
Step 3	Add the alkyl group(s) in the correct location(s) on the parent chain.	 **3-ethylheptanoic acid**

Esters

Esters are a family of organic molecules characterised by the **ester functional group**. An ester is a derivative of a carboxylic acid in which the –OH portion of the carboxyl group is substituted for an OR’ group, where R’ is an alkyl group. The general structure of an ester is RCOOR’, as shown in Figure 8D–11.

Ester
a molecule containing the ester functional group with the general formula RCOOR’

Ester functional group
a functional group consisting of –COO–

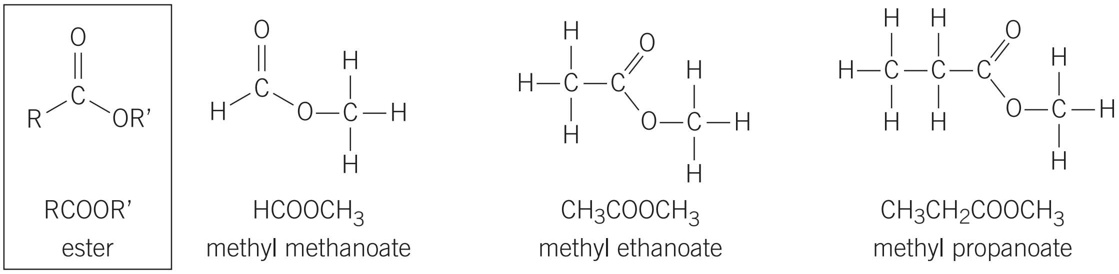
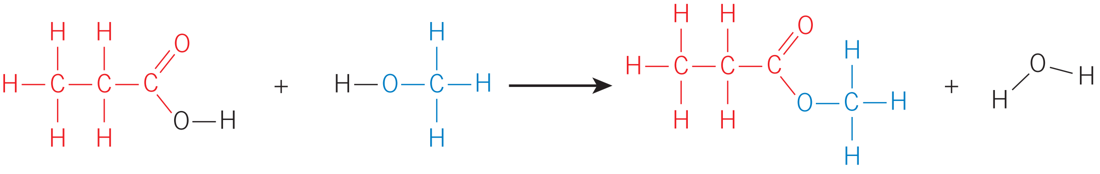


Figure 8D–11 General structures of the ester homologous series

The similarity between a carboxyl functional group and an ester functional group is not a coincidence. Esters are usually made by reacting a carboxylic acid with an alcohol. The carboxylic acid provides the RCO– portion of the ester and the alcohol provides the –OR’ portion. This is important when we discuss the nomenclature of esters. We will also discuss reactions that form esters in more detail in Section 9B.

LINK **9B**
ORGANIC
REACTIONS:
CONDENSATION
AND HYDROLYSIS



$$RCOOH + HOR' \longrightarrow RCOOR' + H_2O$$

Figure 8D–12 Esters are produced from a reaction between a carboxylic acid and an alcohol.

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Esters are often fragrant molecules. Many esters have a pleasant floral or fruity scent or flavour. Various naturally occurring esters contribute to the aroma of flowers and taste of fruits. Esters are also produced and added to many food products to complement their smell or taste. The artificial flavourings used in many food items are likely to be esters. Figure 8D–13 shows the scent created by various ester molecules.

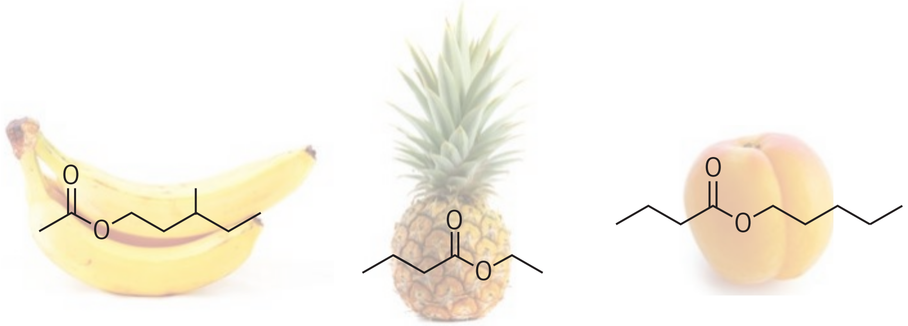

Figure 8D–13 Structures of esters with their associated scents: banana – 3-methylbutyl ethanoate; pineapple – ethyl butanoate; apricot – pentyl butanoate

Esters are polar due to the electronegativity difference between the carbonyl carbon and the oxygen atoms. The partially negative oxygen atoms of one ester molecule can form intermolecular dipole–dipole interactions with the partially positive carbonyl carbon of another ester, as shown in Figure 8D–14.

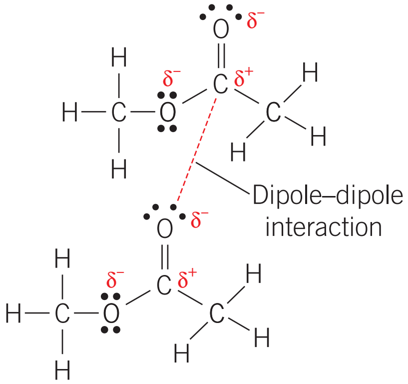

Figure 8D–14 Dipole–dipole interaction between two methyl ethanoate molecules

Like aldehydes and ketones, esters also lack the necessary hydrogen required to form hydrogen bonding with each other. However, the oxygen atoms in the functional group can form hydrogen bonds with other molecules like H_2O, as shown in Figure 8D–15.

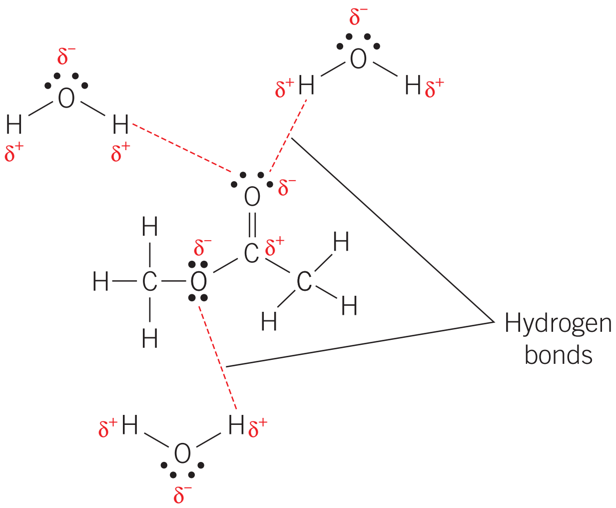

Figure 8D–15 Hydrogen bonding between methyl ethanoate and water

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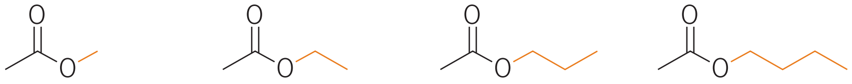
Nomenclature of esters

The names of straight chain esters are made up of two words. The first word describes the alcohol part of the molecule (Figure 8D–16). This portion of the molecule is named as an alkyl group ending in 'yl'.



methyl ethanoate **ethyl** ethanoate **propyl** ethanoate **butyl** ethanoate

Figure 8D–16 The first word in the name of an ester describes the alcohol part of the structure.

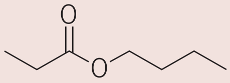
The second word describes the carboxylic acid part of the molecule (Figure 8D–17). The name of this portion of the molecule ends in 'oate'. The names of the alcohol part and the carboxylic acid part then combine to give the full name of the ester.

methyl **methanoate** methyl **ethanoate** methyl **propanoate** methyl **butanoate**

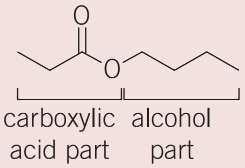
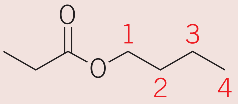
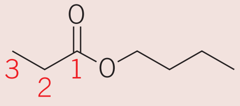
Figure 8D–17 The second word in the name of an ester describes the carboxylic acid part of the structure.

Worked example 8D–3: Naming an ester

Write the name of the following ester.



Solution

	Logic	Process
Step 1	Identify the carboxylic acid part and the alcohol part of the ester.	
Step 2	Number and write the name of the alcohol part first.	 **butyl**
Step 3	Number and write the name of the carboxylic acid part second.	 **butyl propanoate**

VIDEO
WORKED
EXAMPLE 8D–3

WORKSHEET
8D–1 DRAWING
AND NAMING
FUNCTIONAL
GROUPS 2

Primary amides

Primary amides are a family of organic molecules characterised by the **amide functional group**. Primary amides are derivatives of carboxylic acids where the hydroxyl (–OH) portion of the carboxyl group is substituted for an amino ($-NH_2$) group. Just like in carboxylic acids, the carbon of the amide functional group is always the first carbon of the chain. The general structure of primary amides is $RCONH_2$ where R is either H or an alkyl group (Figure 8D–18).

Primary amide a molecule containing an amide functional group with the general formula $RCONH_2$

Amide functional group a functional group consisting of $-CONH_2$

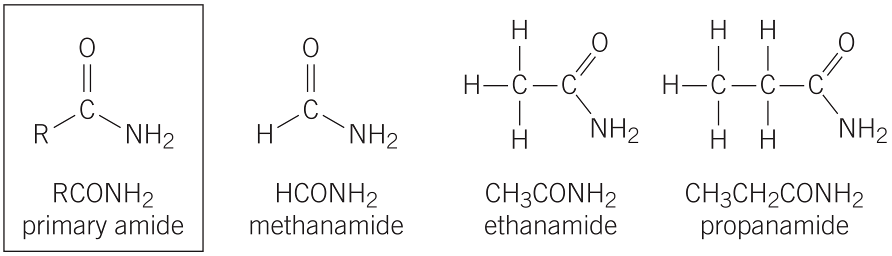


Figure 8D–18 General structure and the first three members of the primary amide homologous series

Primary amides can form intermolecular hydrogen bonding with each other as shown in Figure 8D–19. In addition, primary amides can also form hydrogen bonds with other molecules, like H_2O.

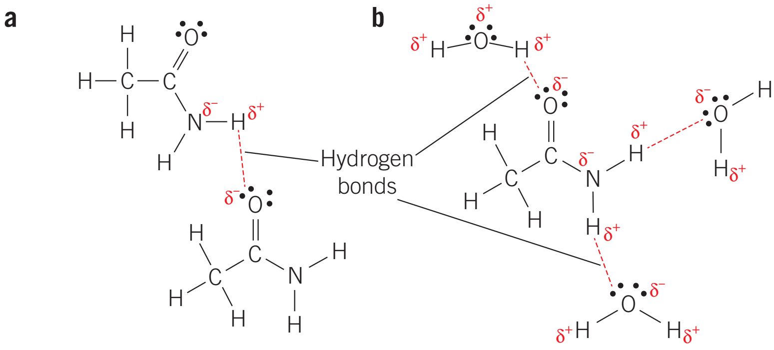


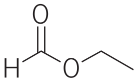
Figure 8D–19 (a) Hydrogen bond between two primary amides. (b) Hydrogen bonds between a primary amide and water

Check-in questions – Set 2

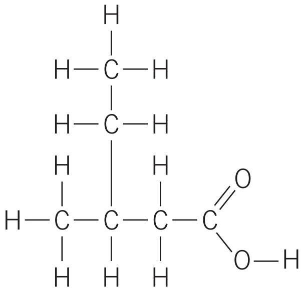
1 Write the names of the following molecules.

a $CH_3CH_2CH_2COOCH_3$

b



c



2 Draw the skeletal formulas of the following molecules.

a propyl propanoate

b 3-methylbutanoic acid

c ethyl butanoate

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Naming organic compounds with two functional groups

The diversity of organic molecules can be further expanded by having more than one functional group on a molecule. While this idea may seem daunting, we will limit our discussion to molecules with no more than two functional groups. These functional groups may be identical or different in nature.

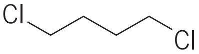
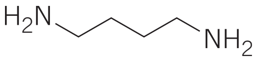
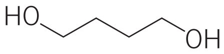
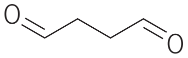
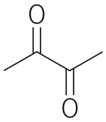
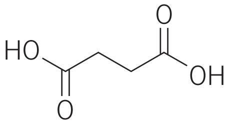
Naming molecules with two identical functional groups

The following rules need to be applied when naming a molecule with two identical functional groups.

- Add a 'di' before the part of the name relevant to the functional group; for example, CH_2Br_2 is called **di**bromomethane.
- The 'e' is returned if 'di' is used after the name of the hydrocarbon; for example, $CHOCH_2CHO$ is called propan**e**dial.
- If positional isomers are possible, then the location of both functional groups needs to be specified; for example, $CH_2OHCH_2CH_2OH$ is called propane-**1,3**-diol.
- An 'a' is added after the first part of the name for molecules with two C═C double bonds; for example, but**a**-1,3-diene instead of but-1,3-diene.

Table 8D–1 shows examples of molecules with two identical functional groups from each of the families we have discussed so far and how the rules are applied.

Table 8D–1 Names of molecules with two identical functional groups

Family	Structure	Name
Alkene		Buta-1,3-diene
Chloroalkane		1,4-dichlorobutane
Amine		Butane-1,4-diamine
Alkanol		Butane-1,4-diol
Aldehyde		Butanedial
Ketone		Butane-2,3-dione
Carboxylic acid		Butanedioic acid

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Naming molecules with two different functional groups

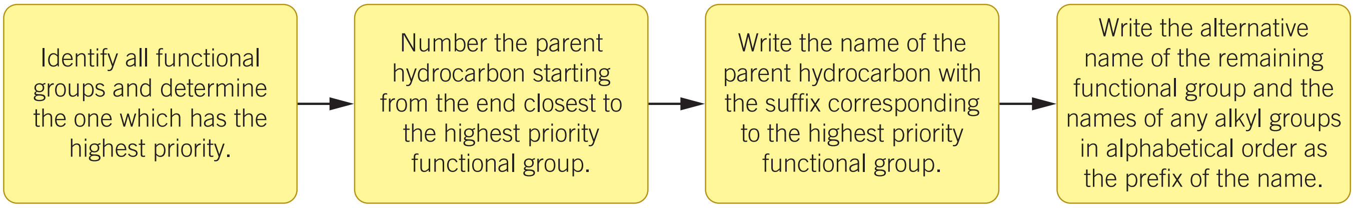
When naming molecules with two different functional groups, we must assess and rank the functional groups in terms of their priority. IUPAC has prioritised each functional group according to the rules in Table 8D–2.

Table 8D–2 IUPAC functional group priorities

Priority	Class	Functional group	Alternative name	Suffix
Highest	Carboxylic acids	–COOH	carboxy	-oic acid
	Aldehydes	–CHO	oxo	-al
	Ketones	–CO–	oxo	-one
	Alcohols	–OH	hydroxy	-ol
	Amines	$–NH_2$	amino	-amine
	Alkenes	C=C	–ene–	-ene
Lowest	Haloalkanes	–X	halo*	–

*Halo refers more specifically to fluoro-, chloro-, bromo- or iodo-

Once the group with the highest priority is identified, the parent hydrocarbon is numbered from the end closest to that group. This ensures that the highest priority functional group always gets the lowest possible number. The functional group with the highest priority forms the suffix (last) part of the name. The other functional group(s) use their alternative names and form the prefix or first part of the name. The flow chart in Figure 8D–20 outlines the general process for naming molecules with two (or more) functional groups.


Identify all functional groups and determine the one which has the highest priority.

Number the parent hydrocarbon starting from the end closest to the highest priority functional group.

Write the name of the parent hydrocarbon with the suffix corresponding to the highest priority functional group.

Write the alternative name of the remaining functional group and the names of any alkyl groups in alphabetical order as the prefix of the name.

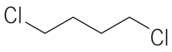
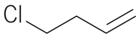
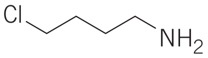
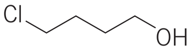
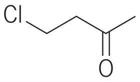
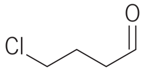
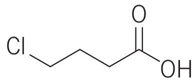
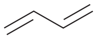
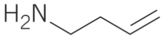
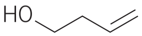
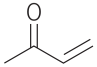
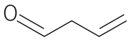
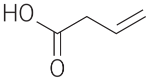
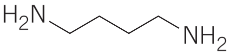
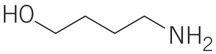
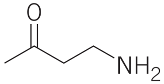
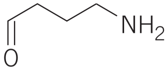
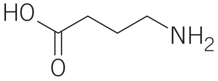
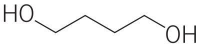
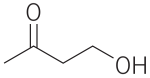
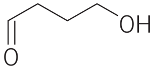
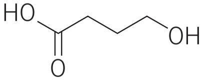
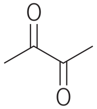
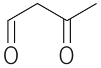
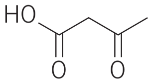
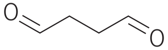
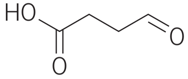
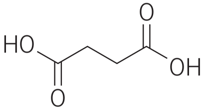
Figure 8D–20 Flow chart showing the general process for naming molecules with two (or more) functional groups

WORKSHEET 8D–2 NAMING MOLECULES WITH TWO FUNCTIONAL GROUPS

Table 8D–3 on the following page shows different combinations of butane derivatives with two functional groups. The name of each molecule is shown below its structure.

The worked examples on page 314 demonstrate the process for naming molecules with two different functional groups.

Table 8D–3 Names of butane derivatives with two functional groups

Functional groups	**Chloro**	**Alkene**	**Amino**	**Hydroxyl**	**Carbonyl (ketone)**	**Carbonyl (aldehyde)**	**Carboxylic acid**
Chloro	 1,4-dichlorobutane	 4-chlorobut-1-ene	 4-chlorobutan-1-amine	 4-chlorobutan-1-ol	 4-chlorobutan-2-one	 4-chlorobutanal	 4-chlorobutanoic acid
Alkene		 buta-1,3-diene	 but-3-en-1-amine	 but-3-en-1-ol	 but-3-en-2-one	 but-3-enal	 but-3-enoic acid
Amino			 butane-1,4-diamine	 4-aminobutan-1-ol	 4-aminobutan-2-one	 4-aminobutanal	 4-aminobutanoic acid
Hydroxyl				 butane-1,4-diol	 4-hydroxybutan-2-one	 4-hydroxybutanal	 4-hydroxybutanoic acid
Carbonyl (ketone)					 butane-2,3-dione	 3-oxobutanal	 3-oxobutanoic acid
Carbonyl (aldehyde)						 butanedial	 4-oxobutanoic acid
Carboxylic acid							 butanedioic acid

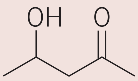
VIDEO 8D–1
NAMING MOLECULES WITH MULTIPLE FUNCTIONAL GROUPS

ISBN 978-1-009-22984-5

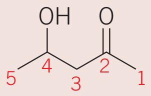
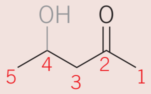
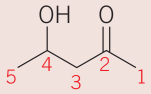
VIDEO
WORKED
EXAMPLE 8D–4

Worked example 8D–4: Naming a molecule with two different functional groups (1)

Write the name of the following molecule.



Solution

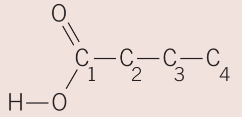
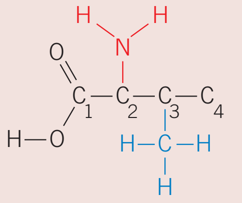
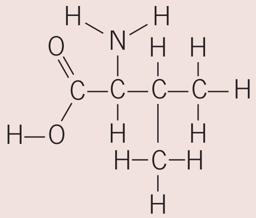
	Logic	Process
Step 1	Identify all functional groups and determine the one which has the highest priority.	Highest priority: carbonyl (ketone) Other functional group: hydroxyl group
Step 2	Number the parent hydrocarbon starting from the end closest to the highest priority functional group.	
Step 3	Write the name of the parent hydrocarbon with the suffix corresponding to the highest priority functional group.	 pentan-2-one
Step 4	Write the alternative name of the remaining functional group and the names of any alkyl groups in alphabetical order as the prefix of the name.	 4-hydroxypentan-2-one

VIDEO
WORKED
EXAMPLE 8D–5

Worked example 8D–5: Naming a molecule with two different functional groups (2)

Draw the structure of 2-amino-3-methylbutanoic acid.

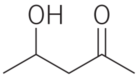
Solution

	Logic	Process
Step 1	Draw the carbons for the parent hydrocarbon. Number the carbons.	$C_1-C_2-C_3-C_4$ 2-amino-3-methyl**butan**oic acid
Step 2	Add the highest priority functional group associated with the suffix of the name.	 2-amino-3-methyl**butanoic acid**
Step 3	Add the structures associated with the prefix of the name.	 2-amino-3-methylbutanoic acid
Step 4	Add the remaining hydrogens.	 2-amino-3-methylbutanoic acid

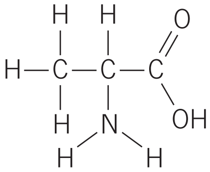
Check-in questions – Set 3

1 Write the names of the following molecules.

a



b



c $CH_3CHClCHCH_2$

2 Represent the following molecules, using their skeletal formula.

a 3-bromopentanoic acid

b hex-5-enal

c 3-aminobutan-1-ol

3 Draw and name a structural isomer of 1-bromopropanone.

VIDEO 8D–2
SKILLS:
ANALYSING
MOLECULE
NAMES

8D SKILLS

Analysing molecule names

Learning to interpret the information embedded in the name of a molecule is an essential skill in this chapter. Each name can be broken up into three parts – a prefix, a parent and a suffix. The prefix describes any alkyl groups, halo groups and other functional groups that are not of the highest priority in the molecule. The parent name describes the longest continuous carbon chain, also known as the parent hydrocarbon. The suffix includes information about the highest priority functional group. The examples below show how names can be separated into prefix, parent and suffix parts. Practise analysing molecule names using this approach to help you become familiar with this system.

Prefix + Parent name + Suffix

2-bromobutane

The structure contains a bromo group attached to the second carbon on the parent hydrocarbon.

The parent hydrocarbon contains four carbons.

The name ends with 'ane' signifying that all C–C bonds are single bonds.

4-methylpentanoic acid

The structure contains a methyl (CH_3) side chain attached to the 4th carbon on the parent hydrocarbon.

The parent hydrocarbon is saturated and contains five carbons.

There is a carboxyl group on the parent hydrocarbon making this molecule a carboxylic acid.

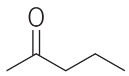
Section 8D questions

1 What elements are in the following functional groups?

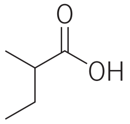
- a carboxyl
- b amide
- c carbonyl
- d ester

2 Write the IUPAC names of the following molecules.

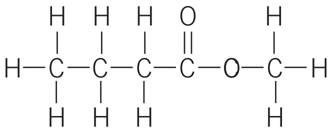
a



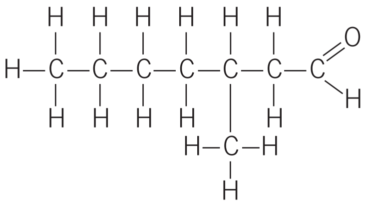
b



c



d



3 Draw the skeletal formulas of the following molecules.

- a 2-ethylbutanal
- b 2,4-dimethylhexanoic acid
- c propyl butanoate

4 Draw the structural formulas of the following molecules.

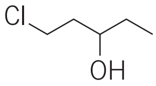
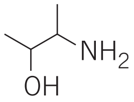
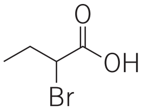
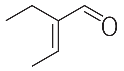
- a heptan-3-one
- b 2-ethylpentanal
- c butanamide

5 Using the semi-structural formula, write and name the following molecules.

- a an aldehyde that is an isomer of butanal
- b a ketone that is an isomer of butanal
- c a carboxylic acid that has a total of five carbon atoms and two methyl groups
- d an ester that has three carbons

6 Draw a diagram showing hydrogen bonding between two propanoic acid molecules.

7 Copy and complete the following table. The first row has been completed as an example.

Structure	Name of functional groups	IUPAC name
	Chloro Hydroxyl	1-chloropentan-3-ol
		
		Pent-4-en-2-one
		
		

8E Physical properties of organic compounds

Study Design:

- Trends in physical properties within homologous series (boiling point and melting point, viscosity), with reference to structure and bonding

Glossary:

Boiling point
Fluid
Kinetic energy
Melting point
n-Alkane
Vapour pressure
Viscosity

ENGAGE

The longest-running experiment

In 1927, an experiment was set up to demonstrate that pitch, the material more commonly known as bitumen used on our roads, is a highly viscous liquid instead of a solid at room temperature. Professor Parnell of The University of Queensland poured a heated sample of pitch into a glass funnel, which was sealed on one end. Three years later in 1930, he cut the stem of the funnel (Figure 8E–1).

Since then, the pitch has very slowly dripped out of the funnel. The process is so slow that it took more than eight years for the first drop to fall. The next five drops took over 40 years to collect. The experiment continues today and is the longest experiment to have ever been conducted. Table 8E–1 below summarises the major events of the experiment. You may notice that the 8th and 9th drops have taken longer than the historical average. This is because air conditioning was installed in the building after the 7th drop, lowering the average temperature of the experiment.

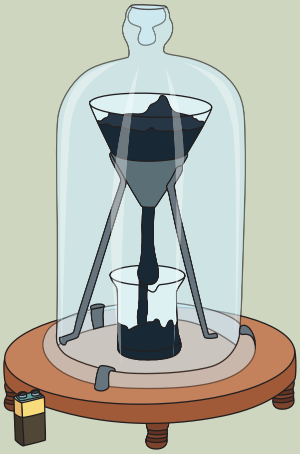


Figure 8E–1 The Pitch drop experiment set up in 1927 is still running today.

Table 8E–1 Timeline of the Pitch drop experiment at the University of Queensland

Date	Event	Duration (years)
1927	Hot pitch poured	
Oct 1930	Stem cut	
Dec 1938	1st drop fell	8.1
Feb 1947	2nd drop fell	8.2
Apr 1954	3rd drop fell	7.2
May 1962	4th drop fell	8.1
Aug 1970	5th drop fell	8.3
Apr 1979	6th drop fell	8.7
Jul 1988	7th drop fell	9.2
Nov 2000	8th drop fell	12.3
Apr 2014	9th drop fell	13.4

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EXPLAIN

Review of intermolecular forces

8B MOLECULES OF CARBON LINK

8C FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS LINK

8D FUNCTIONAL GROUPS: ALDEHYDES, KETONES, CARBOXYLIC ACIDS AND ESTERS LINK

The functional groups we have discussed in previous sections determine the types of intermolecular bonding present between molecules. Functional groups are usually polar, resulting in partially positive and negative regions within a molecule. Polar molecules can interact via electrostatic forces of attraction known as dipole–dipole interactions. In certain cases where a H atom is bonded to a F, N or O atom, hydrogen bonding (a stronger form of dipole–dipole interaction) is possible. In addition, dispersion forces (or London dispersion forces) exist between all molecules regardless of whether they are polar or non-polar. Dispersion forces are the result of instantaneous dipoles caused by the random movement of electrons within an atom or molecule. Table 8E–2 below summarises the types of intermolecular forces present between molecules in each family of organic compounds. You may wish to review how these molecules interact with each other by revisiting the previous sections in this chapter.

Table 8E–2 Types of intermolecular bonding between molecules of different families

Family	Dispersion forces	Dipole–dipole interaction	Hydrogen bonding
Alkane	✓	✗	✗
Alkene	✓	✗	✗
Haloalkane	✓	✓*	✗
Aldehyde	✓	✓	✗
Ketone	✓	✓	✗
Ester	✓	✓	✗
Primary amine	✓	✗	✓
Alcohol	✓	✗	✓
Carboxylic acid	✓	✗	✓

*Not all haloalkanes are polar. For example, tetrachloromethane is a non-polar molecule due to its symmetry. Therefore, dipole–dipole interactions do not exist between its molecules.

A key concept within this section is understanding how the strength of intermolecular forces changes due to structural diversity. Recall that molecules from the same homologous series have the same functional group and therefore possess the same types of intermolecular bonding, as outlined in Table 8E–2. The combination of all different types of intermolecular forces (hydrogen bonding, dipole–dipole interactions and dispersion forces) between two molecules gives the overall strength of intermolecular forces between them. For example, when two alkanols interact, both hydrogen bonding and dispersion forces contribute to the overall strength of intermolecular forces between them (Figure 8E–2).

It may be noted from Figure 8E–2 that the contributions from the hydrogen bonding (red dotted lines) towards the overall intermolecular forces is similar across the three different members of the alkanol homologous series. This is because interactions like hydrogen bonding and dipole–dipole interactions are localised to regions with polar functional groups. In contrast, the number of dispersion forces (blue dotted lines) between the molecules depends on the size of the molecules. Larger members of a homologous series have a greater number of dispersion forces and therefore stronger dispersion forces between molecules. As a result, **larger members of a homologous series also have stronger overall intermolecular forces acting between them than smaller members due to their stronger dispersion forces.**

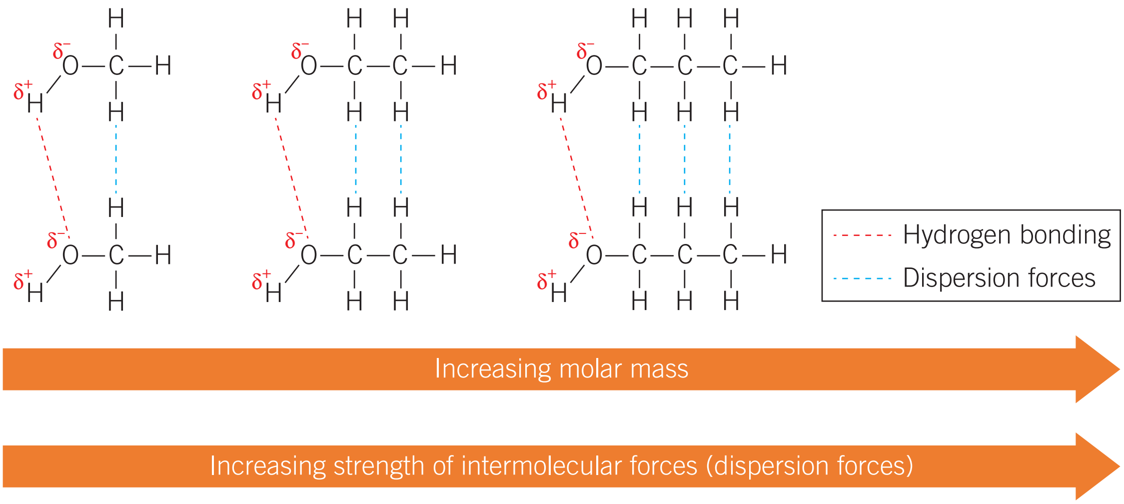
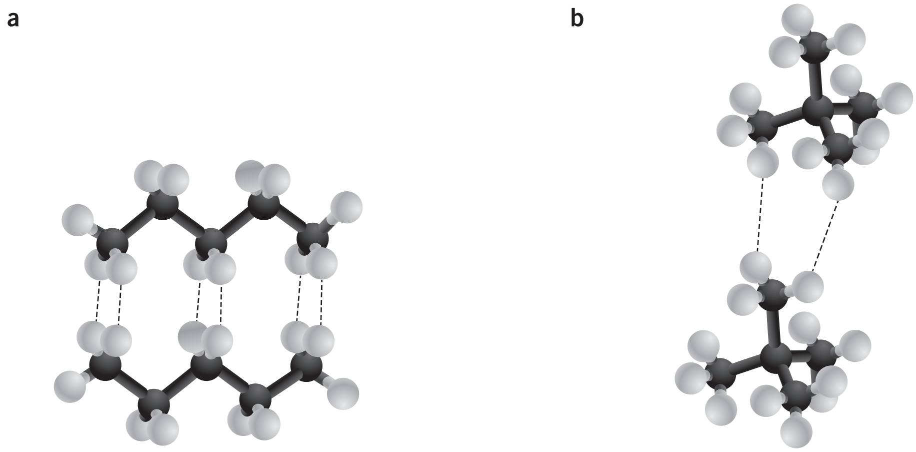


Figure 8E–2 Illustration of the different types of intermolecular forces between members of the alkanol homologous series

The strength of dispersion forces is also dependent on the surface area with which two molecules interact. The greater this surface area, the stronger the dispersion forces holding them together. For example, Figure 8E–3 shows molecules of pentane and 2,2-dimethylpropane interacting. The two molecules are structural isomers with the same molar mass. However, the interaction between the two pentane molecules (straight chain isomers) occurs through greater surface area than the interaction between the two 2,2-dimethylpropane molecules (branched isomers). This is because the straight chain isomer adopts a long and thin rod shape with a high degree of surface area available to interact with other molecules. In contrast, the branched isomer adopts a rounded shape and has reduced surface area for interaction. In general, **the strength of dispersion forces between molecules decreases as the number of alkyl branches in the structure increases.**



- Larger surface area of interaction between molecules
- Stronger dispersion forces
- Stronger overall intermolecular forces

- Smaller surface area of interaction between molecules
- Weaker dispersion foces
- Weaker overall intermolecular forces

Figure 8E–3 Illustration of dispersion forces between: (a) two molecules of pentane and (b) two molecules of 2,2-dimethylpropane. Despite the two pairs of molecules being structural isomers with the same molar mass, the intermolecular force between the straight chain isomers is stronger than the branched isomers due to greater surface area of interaction.

The two concepts discussed on the previous pages are crucial for understanding the trends in physical properties (boiling points, melting points and viscosity) of molecules from the same homologous series. To summarise, molecules from the same homologous series have:

- stronger overall intermolecular forces as the size of the molecule increases.
- weaker overall intermolecular forces as the number of alkyl branches in the structure increases.

Boiling point of organic compounds

Kinetic energy the energy an object or particle has due to its motion

Vapour pressure the pressure exerted by the gas particles of a substance just above its liquid or solid phase

Boiling point the temperature at which a substance begins to boil, which occurs when the vapour pressure of the substance equals the atmospheric pressure

Heating a liquid substance causes its particles to vibrate and move with greater **kinetic energy**. Particles with sufficient kinetic energy can break free of the liquid phase and transition into the gaseous phase. Particles that become gases exert a **vapour pressure** against the surrounding atmosphere. The temperature at which the vapour pressure exerted by these ‘escaped’ gaseous particles equals the atmospheric pressure is the **boiling point** (b.p.) of the substance. The boiling process is usually associated with rapid evaporation, formation of vapours and vigorous bubbling in the liquid phase. Figure 8E–4 shows a simple set-up for determining the boiling point of a substance. A sample of the substance in a test tube is heated to its boiling point (characterised by transition from liquid to gas at constant temperature) using a heat source. A thermometer is suspended above the liquid phase to record the temperature of the gases as the sample evaporates.

Figure 8E–4 Steam and bubbling are observed when water boils at 100°C at sea level (left). An illustration of an apparatus used for determining the boiling point of a sample (right)

At a molecular level, causing an organic substance to boil involves using heat to overcome the intermolecular forces between molecules. Therefore, substances with stronger intermolecular forces have higher boiling points because a greater amount of heat is required to overcome these interactions between molecules. It can be seen from Table 8E–2 that different families of organic compounds possess different types of intermolecular forces with different strengths. When comparing candidates with similar molar mass from each family, compounds capable of strong hydrogen bonding usually have the highest boiling points, followed by those with dipole–dipole interactions and then those with dispersion forces only (Figure 8E–5).

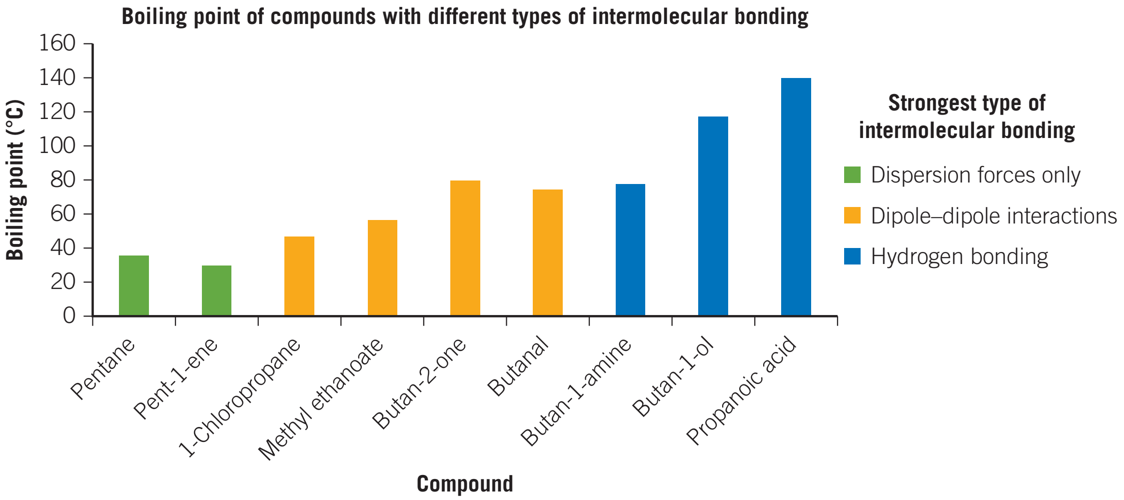


Figure 8E–5 Graph showing the boiling point of compounds with similar molar masses but different types of intermolecular bonding

Since boiling point increases as the overall strength of intermolecular forces increases, we can expect predictable trends for molecules **within the same homologous series**. In particular, the effects of molar mass and alkyl branches and the reasons for these effects are important to note.

Effect of molar mass on boiling point

As molar masses (proportional to the number of carbons) of molecules increase within a homologous series, their boiling points also increase (Figure 8E–6). This is because larger molecules can form a greater number of dispersion forces between molecules. This means that the overall intermolecular forces are stronger in larger members of the same homologous series. More heat is required to overcome these stronger forces and allow the substance to transition from a liquid to a gas state.

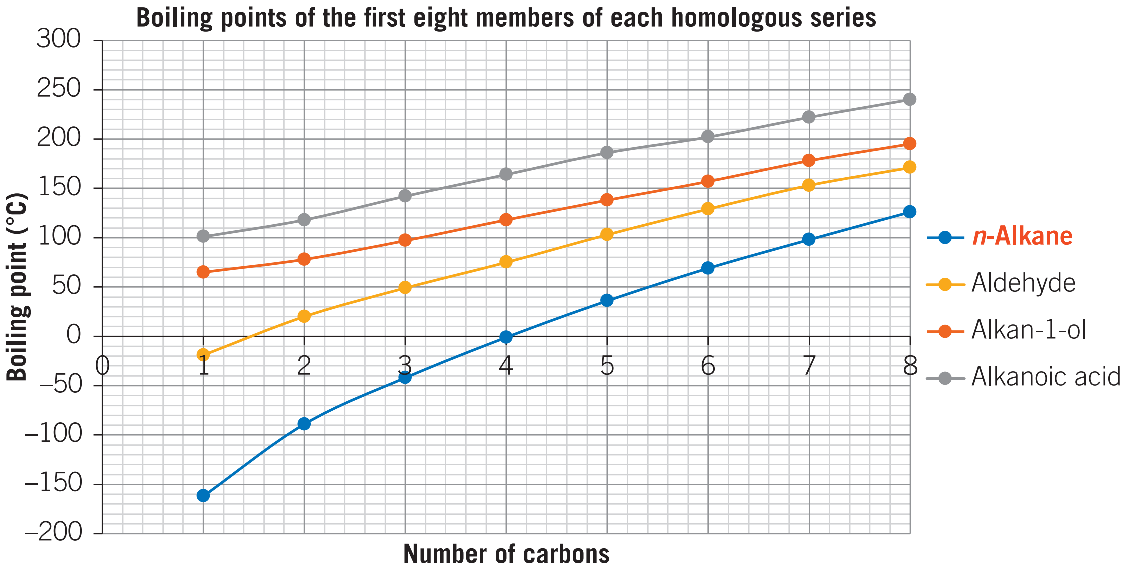


Figure 8E–6 Boiling points increase as molar masses increase within the same homologous series of compounds.

***n*-Alkane** a straight-chain (unbranched) alkane

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Effect of alkyl branches on boiling point

When comparing isomers, the boiling point of compounds decreases as the number or size of alkyl branches increases. This is because molecules with more alkyl branches usually adopt shapes that have less surface area to interact with other molecules. As a result, they generally have weaker dispersion forces and therefore weaker overall intermolecular forces. Less heat is required to overcome the intermolecular forces between more branched isomers, resulting in a lower boiling point. The boiling points of the three C_5H_{12} skeletal isomers shown in Figure 8E–7 demonstrate this trend.

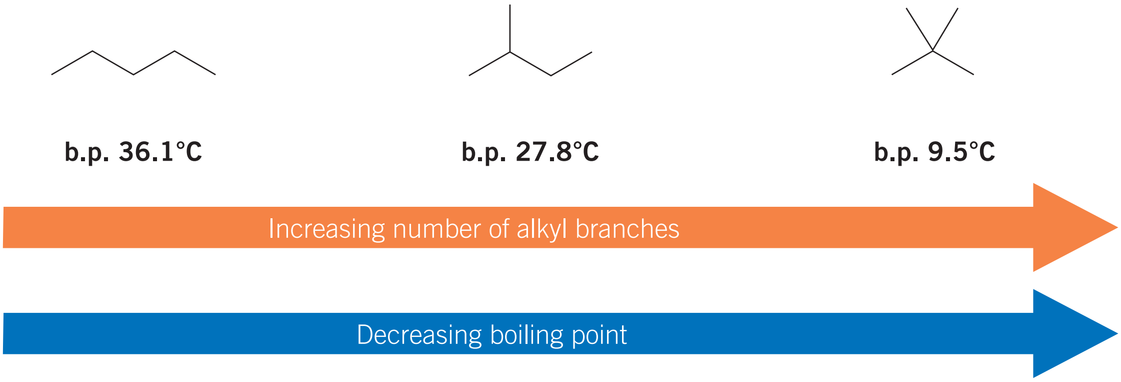

Figure 8E–7 Comparing the boiling point of structural isomers of C_5H_{12}. As the number of alkyl branches increases, the boiling point decreases.

Boiling points of molecules with functional groups are affected in a similar manner by the presence of alkyl branches. Figure 8E–8 shows that alkan-1-ols with increasing number of alkyl branches have decreasing boiling points.

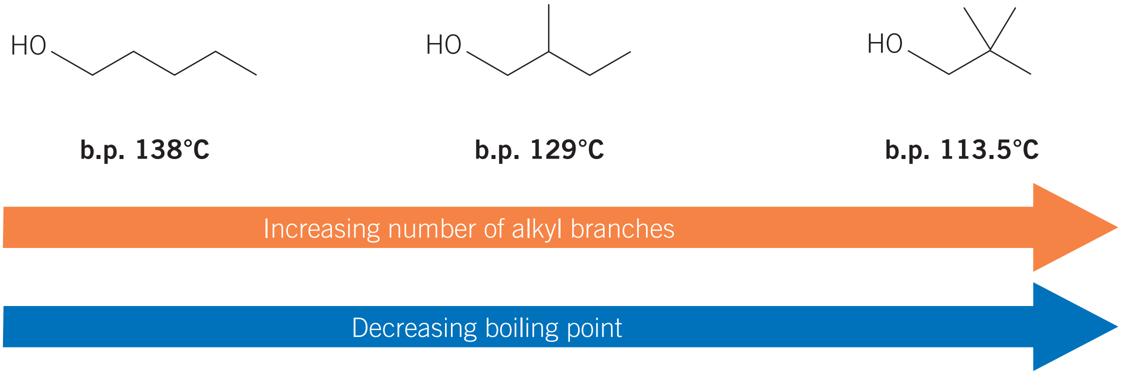

Figure 8E–8 Comparing the boiling point of structural isomers of $C_5H_{12}O$. As the number of alkyl branches increases, the boiling point decreases.

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Melting point of organic compounds

The process of melting involves a substance transitioning from a solid state to a liquid state. Molecules in a solid state are held by their intermolecular forces in fixed positions (Figure 8E–9). Heating a substance would cause its particles to vibrate with increasing kinetic energy. A solid organic substance would melt if the intermolecular forces holding the molecules in their fixed positions are overcome by the kinetic energy of its molecules. The temperature at which a solid substance transitions to a liquid is called its **melting point** (m.p.).

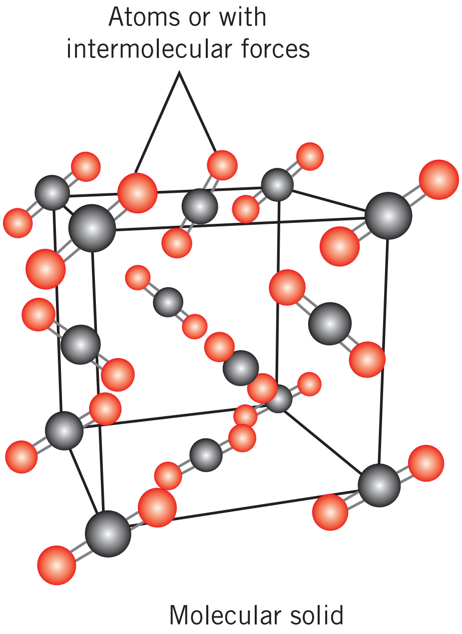

Figure 8E–9 Molecules in the solid state are locked in fixed positions by their intermolecular forces.

Melting point the temperature range from which a solid first starts to transition to a liquid state until this process has finished (i.e. all of the solid has become liquid or completely melted)

The processes of melting and boiling both share the idea of using heat to overcome the interaction between molecules. Therefore, the trends observed in the melting points of substances share similarities with those of the boiling points discussed on pages 320–322. More specifically, larger molecules with stronger intermolecular forces generally have higher melting points (Figure 8E–10). This is because more heat energy is required to overcome stronger intermolecular forces and disrupt the molecules from their fixed positions in the solid state.

Figure 8E–10 General trend of melting points within alkan-1-ol and alkane homologous series

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Check-in questions – Set 1

1 Complete the table below by writing the state (solid, liquid or gas) of the substances at 25°C.

Substance	m.p. (°C)	b.p. (°C)	State at 25°C
A	50	124	
B	–39	16	
C	–60	55	

2 Rank the following molecules in order of increasing boiling point.

- **a** butan-1-ol, ethanol, propan-2-ol, methanol
- **b** pentane, 2,2-dimethylhexane, hexane, 3-methylpentane
- **c** 4-methylpentanoic acid, butanoic acid, 2,3-dimethylbutanoic acid, hexanoic acid

Viscosity of organic compounds

The **viscosity** of a **fluid** is a measure of its resistance to flow due to the intermolecular forces between molecules. We often interact with fluids of varying viscosity in our daily lives. For example, you may notice that more effort is required to pour/squeeze tomato sauce, honey or cooking oil from their containers than it is to pour water out of a bottle. This is because fluids like tomato sauce, honey and oil have a greater resistance to flow or a higher viscosity.

Viscosity
a measure of a fluid's resistance to flow

Fluid
a substance that has no fixed shape and gives way to external pressure. Liquids and gases are considered fluids

Figure 8E–11 Substances like tomato sauce, honey and cooking oil are more viscous than water.

There are numerous methods to compare the viscosity of fluids. One of the simplest ways is to drop a marble down a tube containing the fluid, as shown in Figure 8E–12a. The time it takes the marble to fall a specific distance is recorded. The longer it takes the marble to fall through the fluid, the more viscous the fluid. Another method involves a coiled glass tube, as shown in Figure 8E–12b. The longer it takes the fluid to pass through the coiled tube, the more viscous the fluid.

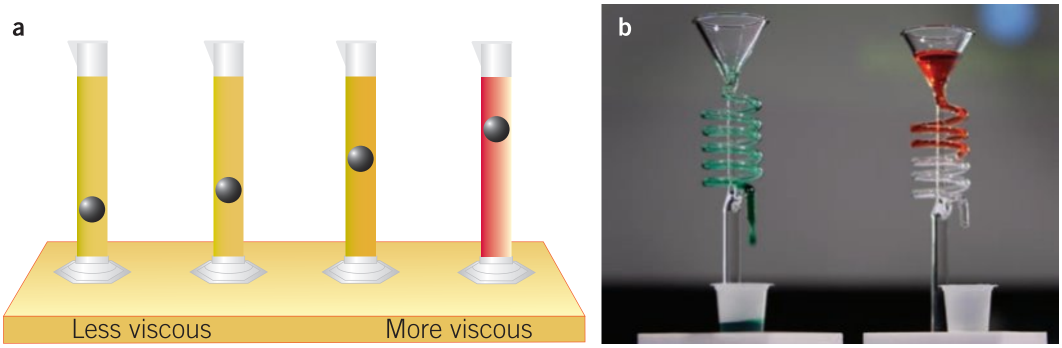


Figure 8E–12 Different ways of comparing viscosity of fluids: (a) dropping a marble through the fluids in tubes and (b) racing the fluids through coiled tubes

At a molecular level, viscosity is another physical property that is linked to the strength of intermolecular bonds. Molecules in a liquid state can flow past each other due to movement caused by their own kinetic energy and due to external forces like being poured out of a container or pushed through a pipe. The intermolecular forces between molecules attempt to hold the molecules together and cause them to resist freely sliding past each other or flowing. The stronger the intermolecular forces between molecules, the higher the viscosity of the substance. When comparing molecules within the same homologous series, **viscosity increases as molar mass increases**. Table 8E–3 shows how the viscosity of *n*-alkanes changes depending on their size.

Another factor that influences viscosity is temperature. As a substance is heated up, the increasing kinetic energy of its molecules gradually overcomes the intermolecular forces between the molecules. This allows the molecules to move past each other more freely. Therefore, **viscosity decreases as temperature increases**. For example, Table 8E–4 shows how the viscosity of ethanol changes as temperature increases.

Table 8E–3 Viscosity of *n*-alkanes at 20°C

n-alkane	Molar mass (g mol^{-1})	Viscosity (mPa s)
Pentane	72	0.224
Hexane	86	0.295
Heptane	100	0.389
Octane	114	0.509

Table 8E–4 Viscosity of ethanol at various temperatures

Temperature (°C)	Viscosity (mPa s)
–25	3.26
0	1.786
25	1.074
50	0.694
75	0.476

VIDEO 8E–1
SKILLS: RESPONDING TO QUESTIONS

8E SKILLS

Responding to questions that ask you to explain your answer

Let's consider the following question:

Butan-1-ol and octan-1-ol are two molecules in the same homologous series. Which molecule has the higher boiling point? Explain your answer.

Questions that require you to compare the properties of two organic molecules in a short-answer response are common but can also be challenging. Demonstrating your understanding in a concise and unambiguous way is critical for obtaining all the marks allocated to that question. Different people may have different styles in how they communicate the necessary information. One way you may wish to structure your response is to use the premise–reasoning–outcome (PRO) strategy:

Premise (P) – the known facts or scientific laws that govern the given scenario
Reasoning (R) – a sequential and logical chain of reasons that link the premise to the outcome
Outcome (O) – the answer or formal response to the scenario

Let's have a look at how the PRO strategy can be applied to formulate a response:

[Boiling point of compounds increases as the strength of their intermolecular forces increases.(P)] [Butan-1-ol and octan-1-ol both take part in hydrogen bonding through their hydroxyl group, and separately through dispersion forces. Octan-1-ol has stronger dispersion forces than butan-1-ol because it's a larger molecule with more electrons. Therefore, more energy is required to overcome the stronger intermolecular forces between octan-1-ol molecules than butan-1-ol molecules.(R)] [As a result, octan-1-ol should have the higher boiling point of the two molecules.(O)]

You may wish to practise using the PRO strategy in some of the Section 8E questions.

Section 8E questions

1 Copy and complete the following table.

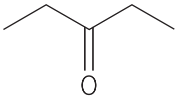
	Intermolecular force(s)	
Compound	**Strongest**	**Other types (if any)**
$CH_3CH_2CHClCH_3$		
$CH_3CH_2CHOHCHO$		
2-aminopropanoic acid		
3-methylpent-1-ene		

2 Draw the structural formula of the following compounds.

- **a** a compound with the molecular formula $C_3H_6O_2$ that has a lower boiling point than propanoic acid
- **b** a compound with the molecular formula C_3H_6O that can form hydrogen bonds between its molecules

3 Define 'viscosity' and describe how it changes with temperature.

4 Arrange the following compounds in order of increasing boiling point and explain your answer.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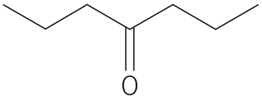
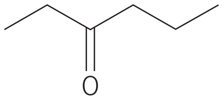
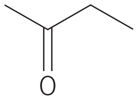

II


III

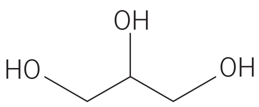

IV

5 Biodiesels are ester molecules produced from plant oils or animal fats. It is desirable for biodiesel to be a low viscosity liquid so that it can be pumped through fuel lines with relative ease. Two esters were produced from natural sources and tested as candidates for biodiesel.

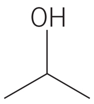
Structure	Source	Name	m.p. (°C)	b.p. (°C)
$C_{11}H_{23}COOCH_3$	Coconut milk	Methyl laurate	4	262
$C_{17}H_{35}COOCH_3$	Fish	Methyl stearate	37	355

- **a** Write the semi-structural formula of both esters.
- **b** Are both esters suitable as biodiesel at room temperature (25°C)? Explain.
- **c** Explain why methyl stearate has a higher melting point than methyl laurate.
- **d** Suggest a way to reduce the viscosity of methyl stearate.

6 Glycerol and propan-2-ol are two compounds containing the hydroxyl functional group. Given their structures below, explain why glycerol is a more viscous liquid than propan-2-ol.



Glycerol



Propan-2-ol

Chapter 8 review

Summary

Create your own set of summary notes for this chapter on paper or in a digital document. A model summary is provided in the Teacher Resources, which can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
8A.1	Recall that carbon prefers to form covalent bonds due to its number of valence electrons	2☐, 4☐
8A.2	Describe the features of covalent bonds, including relative bond strength and bond stability	3☐
8A.3	Recognise that hydrocarbons (including alkanes and alkenes) can form structural isomers	6☐
8A.4	Represent the molecular, structural and semi-structural formulas, as well as the skeletal structures, of organic compounds	11☐, 13☐
8B.1	Determine the systematic IUPAC names of alkanes and alkenes (including branched isomers) from their structures	7☐, 12☐
8B.2	Draw the structural, semi-structural and skeletal formulas of alkanes and alkenes from their IUPAC names	11☐
8B.3	Determine the degree of unsaturation from a compound's molecular formula	5☐
8C.1	Determine the systematic IUPAC names of haloalkanes, amines and alcohols from their structures	1☐, 12☐
8C.2	Draw the structural, semi-structural and skeletal formulas of haloalkanes, amines and alcohols from their IUPAC names	11☐, 13☐
8C.3	Identify and explain the structural features of primary, secondary and tertiary alcohols	8☐
8D.1	Determine the systematic IUPAC name of aldehydes, ketones, carboxylic acids and non-branched esters from their structures	9☐, 10☐, 12☐
8D.2	Draw the structural, semi-structural and skeletal formulas of aldehydes, ketones, carboxylic acids, non-branched esters and primary amides from their IUPAC names	11☐, 13☐
8D.3	Determine the systematic IUPAC names of organic compounds with two functional groups	15☐
8E.1	Recall the key features of different types of intermolecular forces/bonding	14☐, 16☐, 17☐
8E.2	Identify the intermolecular forces/bonds present in different families of organic molecules	14☐, 16☐
8E.3	Discuss the trends in physical properties (boiling point, melting point, viscosity) with reference to structure and bonding of molecules within a homologous series	17☐, 18☐

Multiple-choice questions

1 Which of the following is the correct IUPAC name of $CH_3CH_2CH_2CHClCH_3$?

A 2-chlorohexane

B 1-chloropentane

C 2-chloropentane

D 4-chloropentane

2 Which statement below is incorrect about alkenes?

A Alkenes have a degree of unsaturation greater than or equal to 1.

B The general formula of alkenes is C_nH_{2n}.

C Alkenes can have more than one C=C double bond.

D Alkenes are saturated molecules.

3 Which bond has the highest bond stability?

A C–F

B C–Cl

C C–Br

D C–I

4 Which of the following is **not** a covalent bond?

A C–Br

B C–Li

C C–Si

D C–P

5 The degree of unsaturation of C_4H_6O is

A 0

B 1

C 2

D 3

6 Which of the following is an isomer of 3-ethylpent-2-ene?

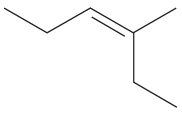
A 3-ethylhex-2-ene

B 3-methylpent-2-ene

C 2,3-dimethylbut-2-ene

D hept-3-ene

7 Which of the following is the correct IUPAC name for the following compound?



A 4-ethylpent-3-ene

B 2-ethylpent-3-ene

C 4-methylhex-3-ene

D 3-methylhex-3-ene

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8 Which of the following is a secondary alcohol?

A 3-methyloctan-2-ol

B 2,2-dimethylhexan-1-ol

C 2-methylbutan-2-ol

D 3-methyloctan-1-ol

9 Which of the following is the correct name for a branched carboxylic acid with the molecular formula $C_5H_{10}O_2$?

A pentanoic acid

B 2-ethylpropanoic acid

C 3-methylbutanoic acid

D methyl butanoate

10 Which functional group is most likely found in a compound with the molecular formula $C_4H_{10}O$?

A carboxyl

B ester

C carbonyl

D hydroxyl

Short-answer questions

11 Draw the structural formulas of the following compounds.

a pentyl propanoate (1 mark)

b 3-ethylpentan-3-amine (1 mark)

c hexan-3-one (1 mark)

d 2-methylbutane (1 mark)

12 **i** Name the homologous series to which each of the following compounds belong.

ii Write the IUPAC name for each compound.

a $CH_3(CH_2)_3CH_2OH$ (2 marks)

b $CH_3CHCHCH_2CH(CH_3)CH_3$ (2 marks)

c $CH_3CH(CH_3)CH_2COCH_3$ (2 marks)

d $CH_3CH_2COOCH_2CH_3$ (2 marks)

13 Draw the skeletal formula of the following compounds.

a 3-methylhexan-2-ol (1 mark)

b 2-chloro-2-methylpentane (1 mark)

c 2-aminobutanoic acid (1 mark)

d butane-2,3-dione (1 mark)

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14 Complete the following table. (4 marks)

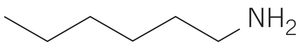
Compound	**Intermolecular force(s)**	
	Strongest	**Other types (if any)**
CH_3COCH_3		
$CH_3CHOHCH_2CH_2Br$		
2-amino-3-methylbutanoic acid		
2-methylhexan-2-ene		

15 The following are incorrect names. Draw the structure they represent, then determine the correct IUPAC name.

- **a** pent-4-ene (2 marks)
- **b** 3-hydroxylbutan-2-amine (2 marks)
- **c** 2-chloro-3-ethylbutane (2 marks)
- **d** 3-bromo-3-propylpropanal (2 marks)

16 Draw a labelled diagram showing all intermolecular forces between two propan-1-ol molecules. (3 marks)

17 The following amines are structural isomers.



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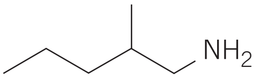

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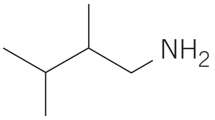

III

- **a** Arrange the molecules in order of increasing viscosity. (1 mark)
- **b** Explain your answer to part **a**. (3 marks)

18 Methane and paraffin wax are both alkanes, but they have very different physical properties as shown in the table below. Explain why the two substances have different boiling and melting points. (3 marks)

Substance	**Molecular formula**	**m.p. (°C)**	**b.p. (°C)**
Methane	CH_4	–182	–162
Paraffin wax	$C_{25}H_{52}$	37	370

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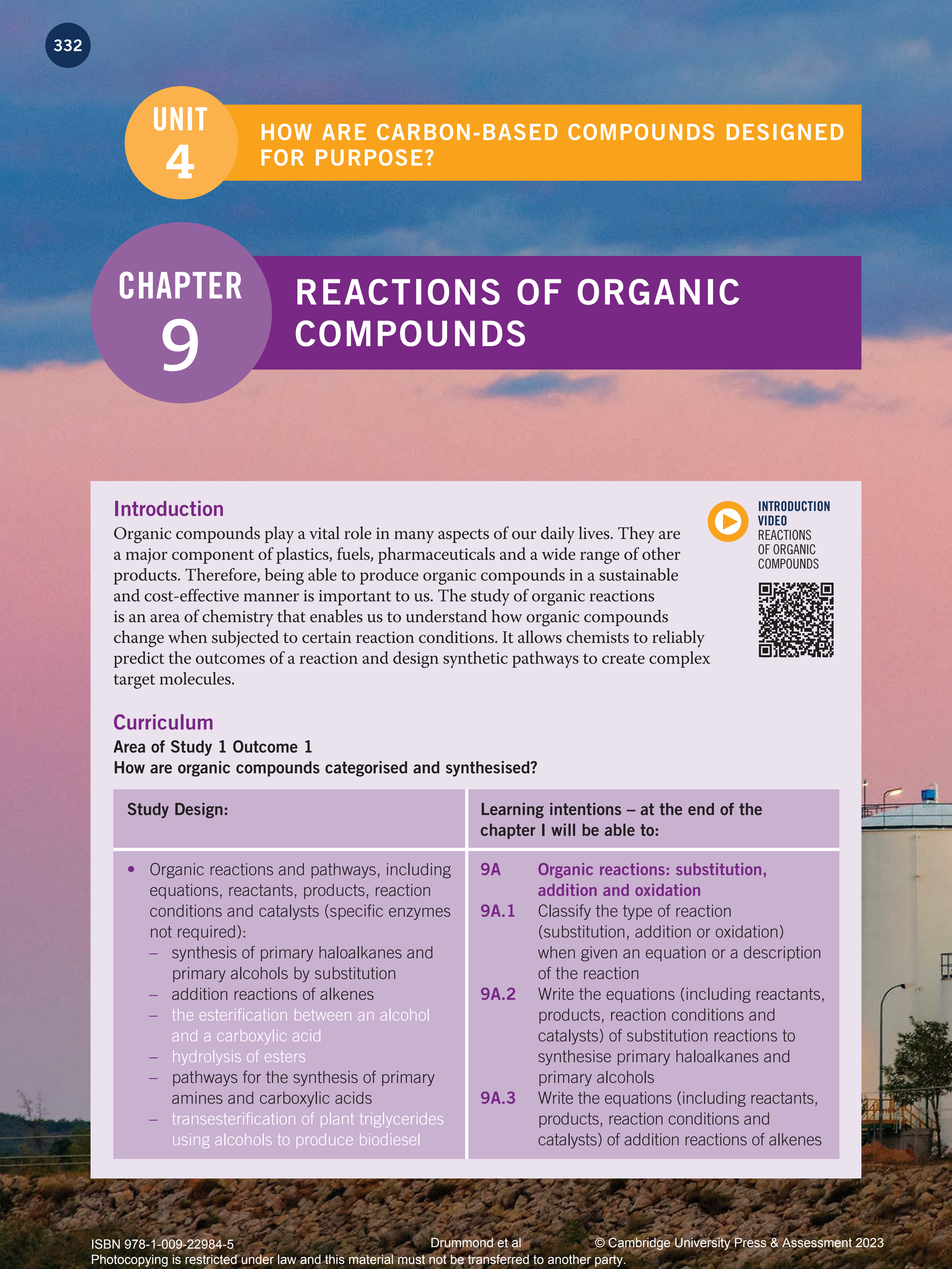

UNIT 4

HOW ARE CARBON-BASED COMPOUNDS DESIGNED FOR PURPOSE?

CHAPTER 9

REACTIONS OF ORGANIC COMPOUNDS

Introduction

INTRODUCTION VIDEO
REACTIONS OF ORGANIC COMPOUNDS

Organic compounds play a vital role in many aspects of our daily lives. They are a major component of plastics, fuels, pharmaceuticals and a wide range of other products. Therefore, being able to produce organic compounds in a sustainable and cost-effective manner is important to us. The study of organic reactions is an area of chemistry that enables us to understand how organic compounds change when subjected to certain reaction conditions. It allows chemists to reliably predict the outcomes of a reaction and design synthetic pathways to create complex target molecules.

Curriculum

Area of Study 1 Outcome 1
How are organic compounds categorised and synthesised?

Study Design:	**Learning intentions – at the end of the chapter I will be able to:**
• Organic reactions and pathways, including equations, reactants, products, reaction conditions and catalysts (specific enzymes not required): – synthesis of primary haloalkanes and primary alcohols by substitution – addition reactions of alkenes – the esterification between an alcohol and a carboxylic acid – hydrolysis of esters – pathways for the synthesis of primary amines and carboxylic acids – transesterification of plant triglycerides using alcohols to produce biodiesel	**9A Organic reactions: substitution, addition and oxidation** **9A.1** Classify the type of reaction (substitution, addition or oxidation) when given an equation or a description of the reaction **9A.2** Write the equations (including reactants, products, reaction conditions and catalysts) of substitution reactions to synthesise primary haloalkanes and primary alcohols **9A.3** Write the equations (including reactants, products, reaction conditions and catalysts) of addition reactions of alkenes

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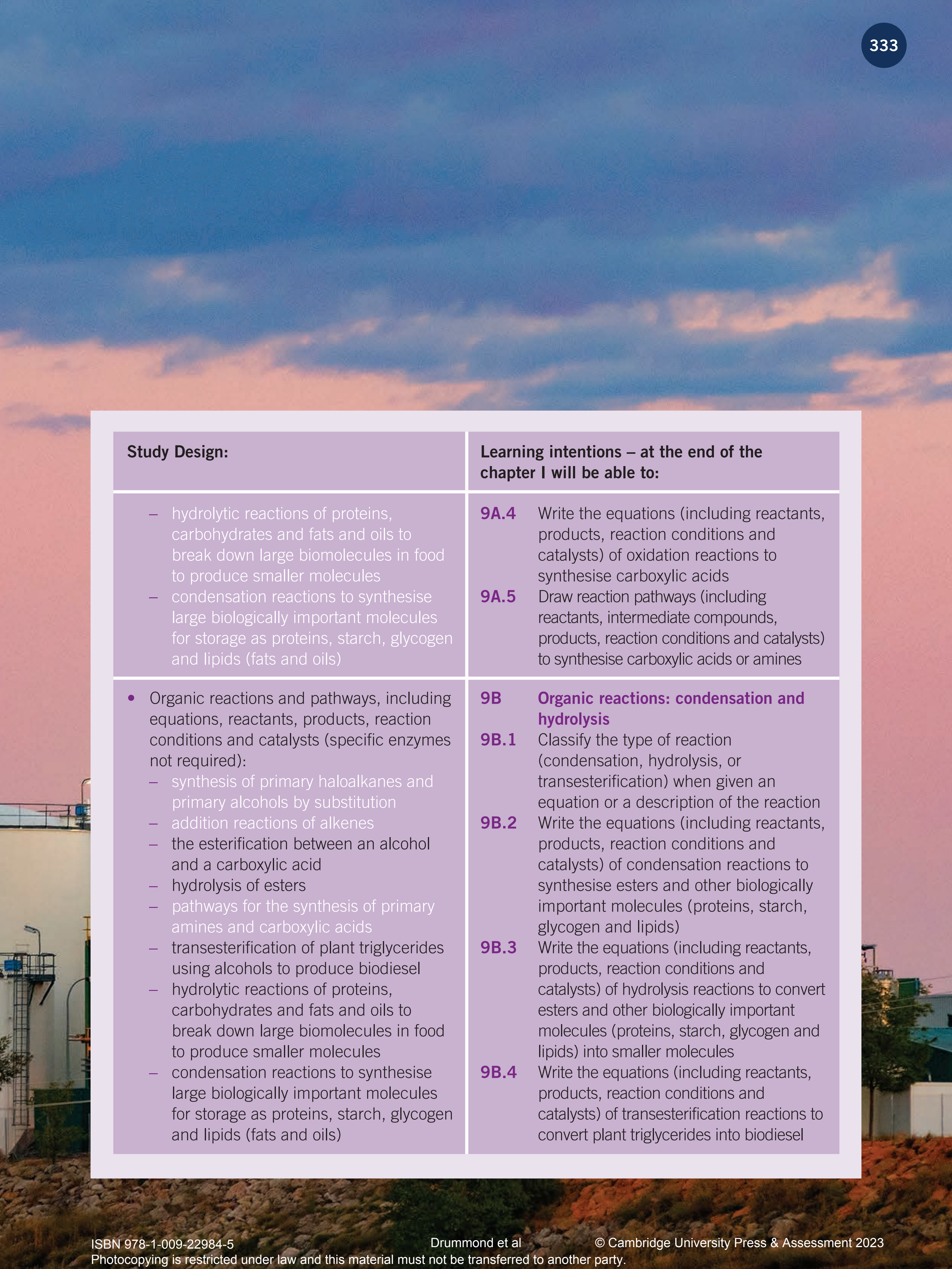
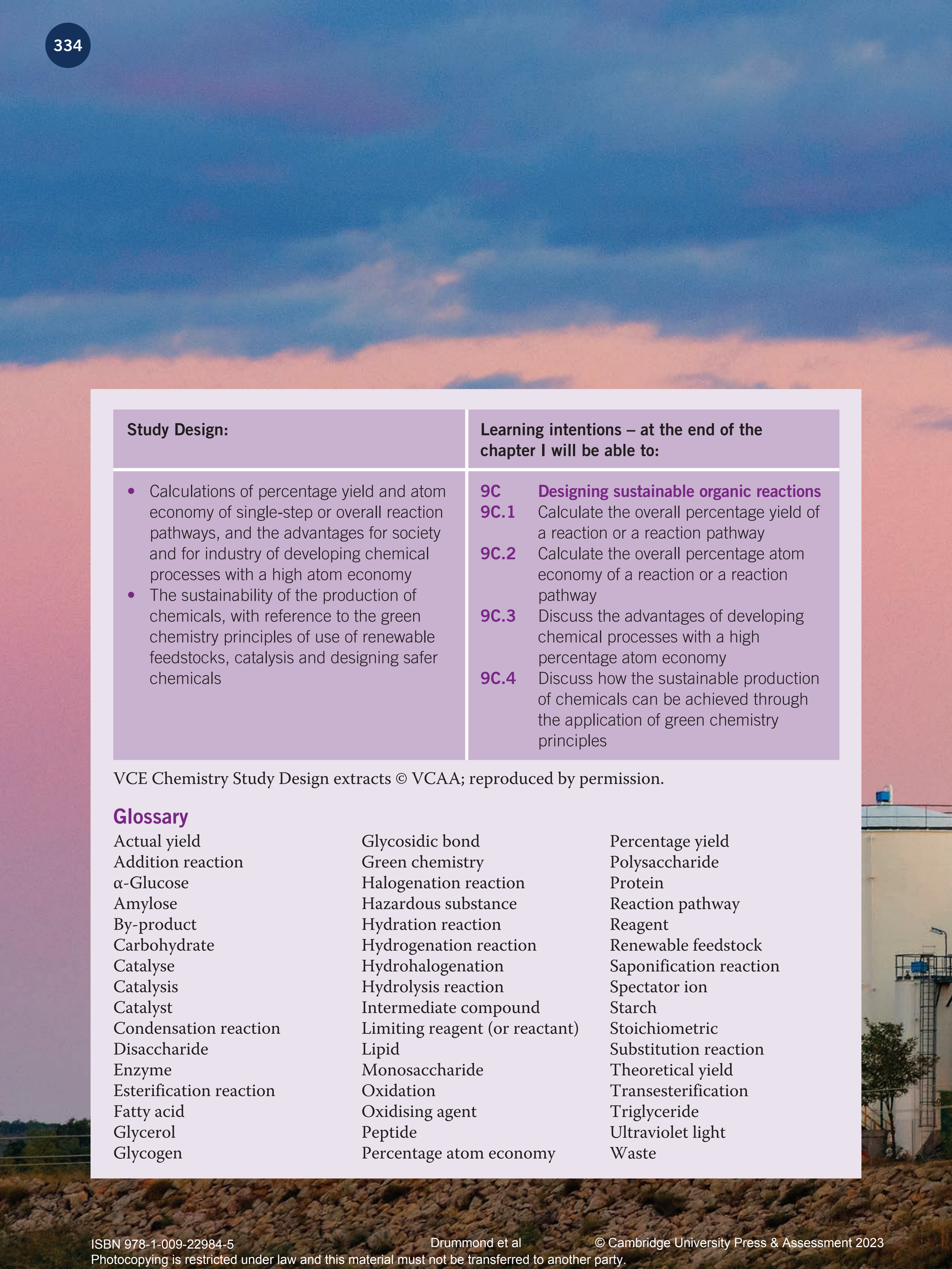


Study Design:	Learning intentions – at the end of the chapter I will be able to:
– hydrolytic reactions of proteins, carbohydrates and fats and oils to break down large biomolecules in food to produce smaller molecules – condensation reactions to synthesise large biologically important molecules for storage as proteins, starch, glycogen and lipids (fats and oils)	**9A.4** Write the equations (including reactants, products, reaction conditions and catalysts) of oxidation reactions to synthesise carboxylic acids **9A.5** Draw reaction pathways (including reactants, intermediate compounds, products, reaction conditions and catalysts) to synthesise carboxylic acids or amines
• Organic reactions and pathways, including equations, reactants, products, reaction conditions and catalysts (specific enzymes not required): – synthesis of primary haloalkanes and primary alcohols by substitution – addition reactions of alkenes – the esterification between an alcohol and a carboxylic acid – hydrolysis of esters – pathways for the synthesis of primary amines and carboxylic acids – transesterification of plant triglycerides using alcohols to produce biodiesel – hydrolytic reactions of proteins, carbohydrates and fats and oils to break down large biomolecules in food to produce smaller molecules – condensation reactions to synthesise large biologically important molecules for storage as proteins, starch, glycogen and lipids (fats and oils)	**9B** **Organic reactions: condensation and hydrolysis** **9B.1** Classify the type of reaction (condensation, hydrolysis, or transesterification) when given an equation or a description of the reaction **9B.2** Write the equations (including reactants, products, reaction conditions and catalysts) of condensation reactions to synthesise esters and other biologically important molecules (proteins, starch, glycogen and lipids) **9B.3** Write the equations (including reactants, products, reaction conditions and catalysts) of hydrolysis reactions to convert esters and other biologically important molecules (proteins, starch, glycogen and lipids) into smaller molecules **9B.4** Write the equations (including reactants, products, reaction conditions and catalysts) of transesterification reactions to convert plant triglycerides into biodiesel



Study Design:	**Learning intentions – at the end of the chapter I will be able to:**
• Calculations of percentage yield and atom economy of single-step or overall reaction pathways, and the advantages for society and for industry of developing chemical processes with a high atom economy • The sustainability of the production of chemicals, with reference to the green chemistry principles of use of renewable feedstocks, catalysis and designing safer chemicals	**9C Designing sustainable organic reactions** **9C.1** Calculate the overall percentage yield of a reaction or a reaction pathway **9C.2** Calculate the overall percentage atom economy of a reaction or a reaction pathway **9C.3** Discuss the advantages of developing chemical processes with a high percentage atom economy **9C.4** Discuss how the sustainable production of chemicals can be achieved through the application of green chemistry principles

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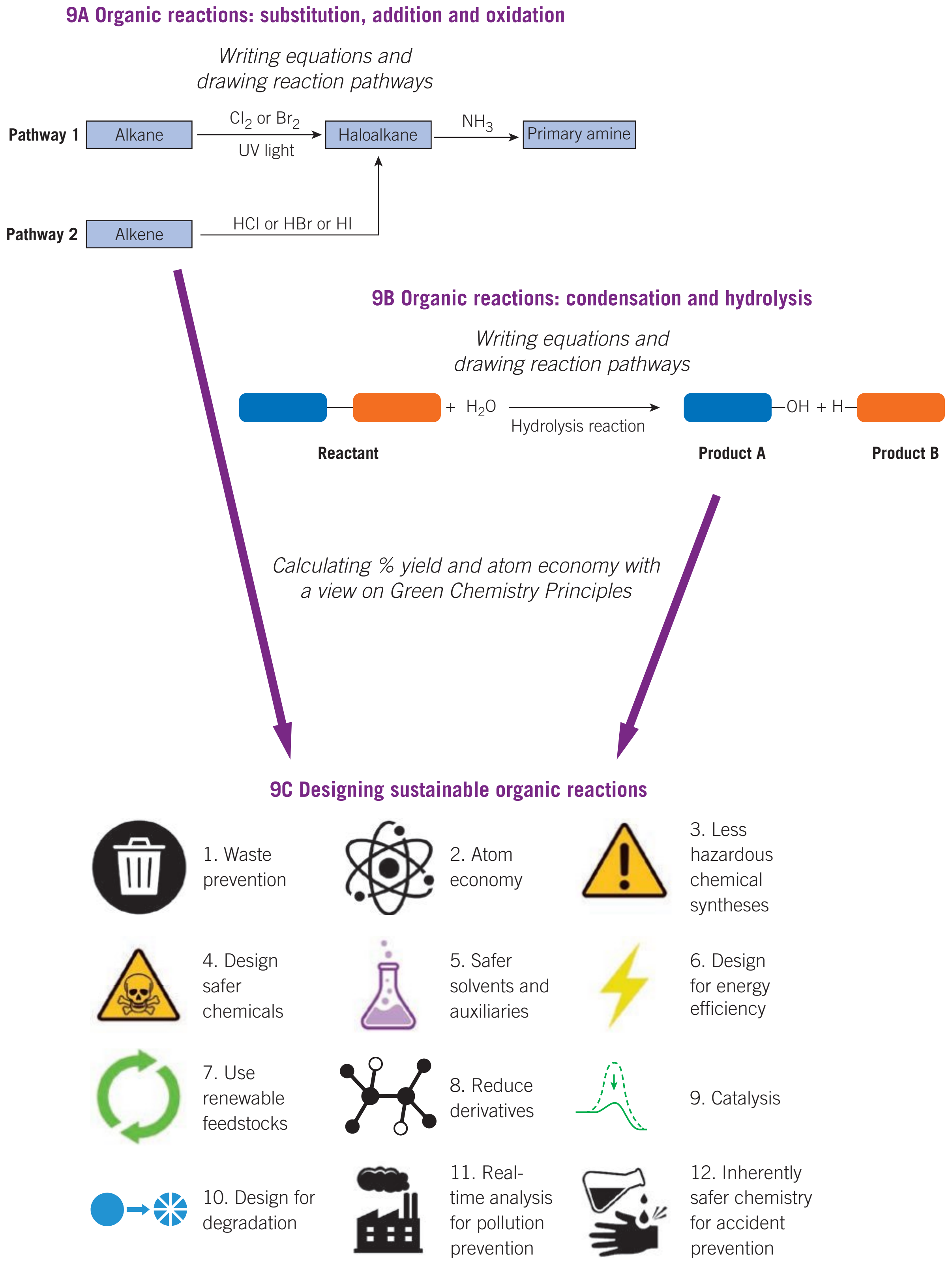
Glossary

Actual yield
Addition reaction
α-Glucose
Amylose
By-product
Carbohydrate
Catalyse
Catalysis
Catalyst
Condensation reaction
Disaccharide
Enzyme
Esterification reaction
Fatty acid
Glycerol
Glycogen
Glycosidic bond
Green chemistry
Halogenation reaction
Hazardous substance
Hydration reaction
Hydrogenation reaction
Hydrohalogenation
Hydrolysis reaction
Intermediate compound
Limiting reagent (or reactant)
Lipid
Monosaccharide
Oxidation
Oxidising agent
Peptide
Percentage atom economy
Percentage yield
Polysaccharide
Protein
Reaction pathway
Reagent
Renewable feedstock
Saponification reaction
Spectator ion
Starch
Stoichiometric
Substitution reaction
Theoretical yield
Transesterification
Triglyceride
Ultraviolet light
Waste

Concept map



9A Organic reactions: substitution, addition and oxidation

Writing equations and drawing reaction pathways

Pathway 1 Alkane $\xrightarrow[\text{UV light}]{Cl_2 \text{ or } Br_2}$ Haloalkane $\xrightarrow{NH_3}$ Primary amine

Pathway 2 Alkene $\xrightarrow{\text{HCl or HBr or HI}}$ Haloalkane

9B Organic reactions: condensation and hydrolysis

Writing equations and drawing reaction pathways

Calculating % yield and atom economy with a view on Green Chemistry Principles

9C Designing sustainable organic reactions

1. Waste prevention
2. Atom economy
3. Less hazardous chemical syntheses
4. Design safer chemicals
5. Safer solvents and auxiliaries
6. Design for energy efficiency
7. Use renewable feedstocks
8. Reduce derivatives
9. Catalysis
10. Design for degradation
11. Real-time analysis for pollution prevention
12. Inherently safer chemistry for accident prevention

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

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9A Organic reactions: substitution, addition and oxidation

Study Design:

- Organic reactions and pathways, including equations, reactants, products, reaction conditions and catalysts (specific enzymes not required):
  - synthesis of primary haloalkanes and primary alcohols by substitution
  - addition reactions of alkenes
  - the esterification between an alcohol and a carboxylic acid
  - hydrolysis of esters
  - pathways for the synthesis of primary amines and carboxylic acids
  - transesterification of plant triglycerides using alcohols to produce biodiesel
  - hydrolytic reactions of proteins, carbohydrates and fats and oils to break down large biomolecules in food to produce smaller molecules
  - condensation reactions to synthesise large biologically important molecules for storage as proteins, starch, glycogen and lipids (fats and oils)

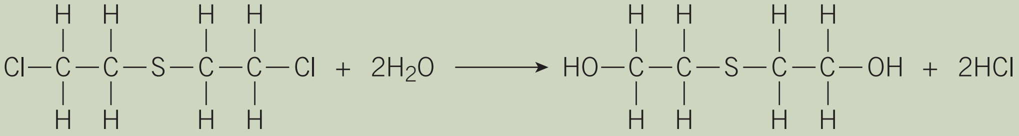
Glossary:

Addition reaction
By-product
Catalyse
Catalyst
Enzyme
Halogenation reaction
Hydration reaction
Hydrogenation reaction
Hydrohalogenation reaction
Intermediate compound
Oxidation
Oxidising agent
Reaction pathway
Reagent
Spectator ion
Substitution reaction
Ultraviolet light

ENGAGE

Mustard gas – a banned chemical warfare agent

The use of chemicals as weapons first occurred in World War I when German forces released chlorine gas (Cl_2) upon the French and British forces in the battle of Ypres. Subsequently, the use of chemical warfare was employed by both sides to cause irreversible and catastrophic damage to the soldiers in trenches. One of the more common chemical agents was mustard gas ($ClCH_2CH_2SCH_2CH_2Cl$). This very reactive substance would produce blisters over the surface of the body upon contact. Mustard gas works by reacting with water on the surface of skin or in lung tissue to produce hydrochloric acid, HCl. The extremely corrosive HCl then causes severe burns to the body. This type of reaction, also known as a substitution reaction, is discussed in detail in this section.



$$ClCH_2CH_2SCH_2CH_2Cl + 2H_2O \longrightarrow HOCH_2CH_2SCH_2CH_2OH + 2HCl$$

Figure 9A–1 Reaction between mustard gas and water to produce HCl

It is estimated from autopsies that about 400 000 soldiers were killed due to mustard gas. The 1925 Geneva Gas Protocol banned the use of any chemical or biological weapons in warfare.

Figure 9A–2 Australian infantry in Ypres, 1917. They are wearing small box respirators, which worked against chlorine gas but could not protect against mustard gas.

EXPLAIN

Reactions of organic compounds

An organic reaction is a chemical reaction that involves organic compounds as reactants. Like all other chemical changes, organic reactions involve breaking of bonds within the reactant molecules followed by formation of new bonds to yield the products. These reactions can be **catalysed** by a variety of substances acting as a **catalyst**, such as acids, bases, **enzymes** and transition metals. They can also be initiated by heat, light or other forms of energy.

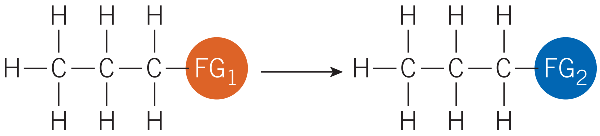
Catalyse
to speed up a reaction

Catalyst
a substance that increases the rate of a chemical reaction by lowering the activation energy by providing an alternative reaction pathway and is itself not consumed as part of the reaction

Enzyme
a protein molecule that acts as a catalyst in a specific biochemical reaction

LINK 9B ORGANIC REACTIONS: CONDENSATION AND HYDROLYSIS

There are many different types of organic reactions, including substitution reactions, addition reactions, oxidation reactions, condensation reactions and hydrolysis reactions. The specific type of reaction that occurs depends on the functional groups present on the reactant molecules and the conditions under which the reaction is carried out. The changes that occur during a reaction usually revolve around modifications to the functional groups in the molecule (Figure 9A–3), which is where your focus should be.



FG_1 and FG_2 represent different functional groups

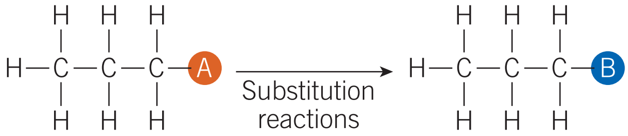
Figure 9A–3 Organic reactions involve a change in the functional group.

Substitution reactions

Substitution reactions involve exchanging an atom (or a group of atoms) in a molecule for another atom (or group of atoms). The general equation for a substitution reaction is shown in Figure 9A–4. In most cases, the atoms of the functional group in the reactant are substituted for new atoms to form the product. Several types of substitution reactions are discussed below.

Substitution reaction
a reaction in which an atom or group of atoms is replaced by another atom or group of atoms

Ultraviolet light
a form of electromagnetic radiation with wavelengths shorter than those of visible light and hence is invisible to most humans



A and B represent different atoms or groups of atoms

Figure 9A–4 General process of substitution reactions

Substitution reactions involving alkanes

8C FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS **LINK**

Alkanes can react with halogens (Cl_2 or Br_2) in the presence of **ultraviolet light** (UV light) to produce haloalkanes in a substitution reaction (Figure 9A–5). In this reaction, a halogen atom from Cl_2 or Br_2 substitutes a hydrogen atom on the alkane. The displaced hydrogen atom bonds with the remaining halogen atom to form hydrogen chloride (HCl) or hydrogen bromide (HBr) as the **by-product** of the reaction. This process is also known as a **halogenation reaction** because it introduces a halogen atom into the organic molecule.

By-product
a product of a chemical reaction or industrial process that is produced as a direct result of the desired reaction, and so appears as part of the fully balanced chemical equation

Halogenation reaction
a chemical reaction that involves the incorporation of one or more halogen atoms into a compound

Reagent
a chemical compound or mixture, typically inorganic, introduced to cause the desired change in an organic substance

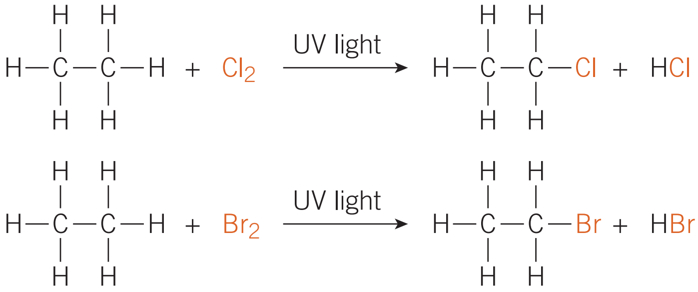


Figure 9A–5 Substitution reactions involving alkanes (ethane in this example) and halogens

A feature of this reaction is that it can be used to introduce more than one halogen atom into the molecule. The substitution reaction can occur more than once on the same molecule if excess Cl_2 or Br_2 **reagent** is added. For example, after methane reacts with Cl_2 to form chloromethane, a second substitution can occur to produce dichloromethane (Figure 9A–6). Further repetition of the same substitution reaction yields trichloromethane and ultimately, tetrachloromethane.

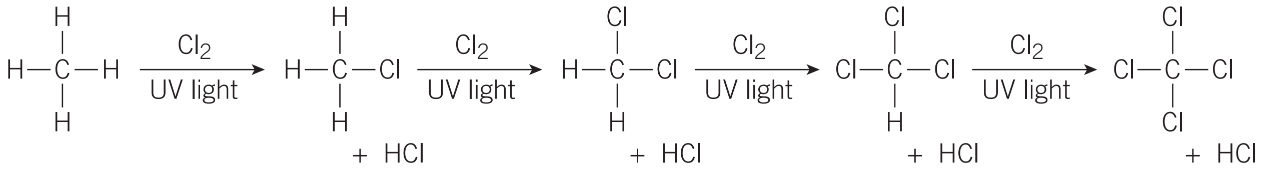


Figure 9A–6 A sequence of substitution reactions between methane and Cl_2 (under UV light) can yield di-, tri- and tetrachloromethane.

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One of the major drawbacks of this reaction is that it is very difficult to exclusively direct the reaction to occur at a specific hydrogen in the molecule. This is not a problem for small alkanes like methane or ethane because the same product is obtained regardless of which hydrogen is substituted. However, in the case of larger alkanes this substitution reaction can lead to more than one haloalkane product. For example, when propane reacts with Cl_2 under UV light, substitution can occur at either the two CH_3 groups at the ends of the molecule or at the CH_2 group in the middle of the molecule. As shown in Figure 9A–7, both scenarios usually occur simultaneously during the reaction, resulting in a mixture of two different products that are positional isomers.

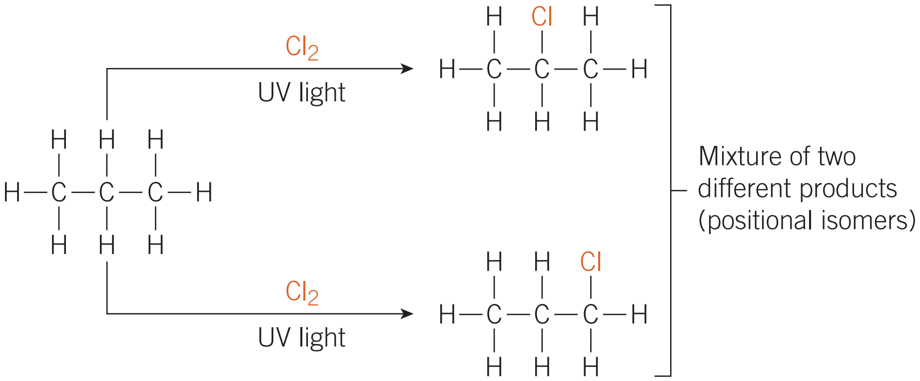


Figure 9A–7 The halogenation reaction between propane and Cl_2 under UV light gives a mixture of two products.

LINK 8C FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS

Substitution reactions involving haloalkanes

Haloalkanes can react with aqueous metal hydroxides (LiOH(aq), NaOH(aq), KOH(aq) etc.) to produce alkanols in a substitution reaction (Figure 9A–8). In this reaction, the hydroxide ion (OH^-) from the metal hydroxide substitutes the halogen atom on the organic molecule. The displaced halide usually couples with the cation from the metal hydroxide to form an ionic by-product. In some cases, the metal cation, which acts as a **spectator ion**, is omitted from the equation.

Spectator ion
a cation or anion that is present on both sides of a chemical equation and remains unchanged during the reaction

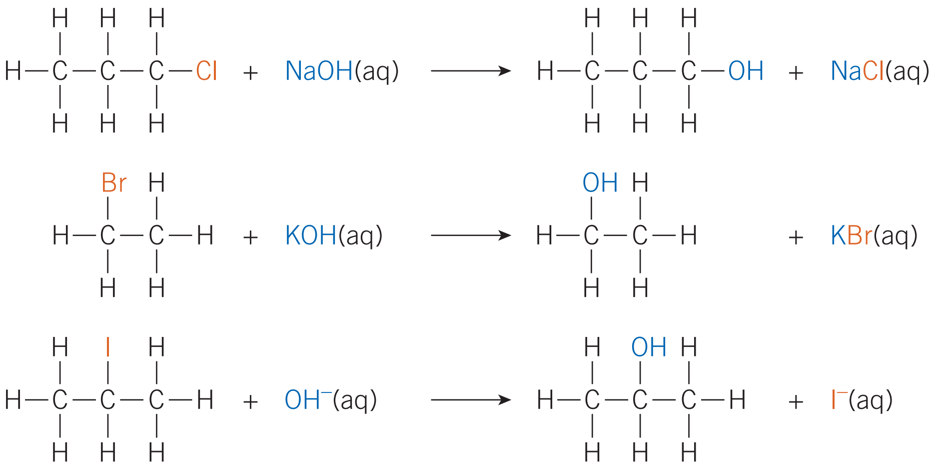


Figure 9A–8 Substitution reactions involving haloalkanes and aqueous metal hydroxides

Haloalkanes can also react with ammonia (NH_3) to form primary amines in a substitution reaction (Figure 9A–9). In this case, the ammonia molecule substitutes the halogen on the organic molecule to install the amino group (NH_2). The by-product of this reaction is a hydrogen halide (HCl, HBr or HI).

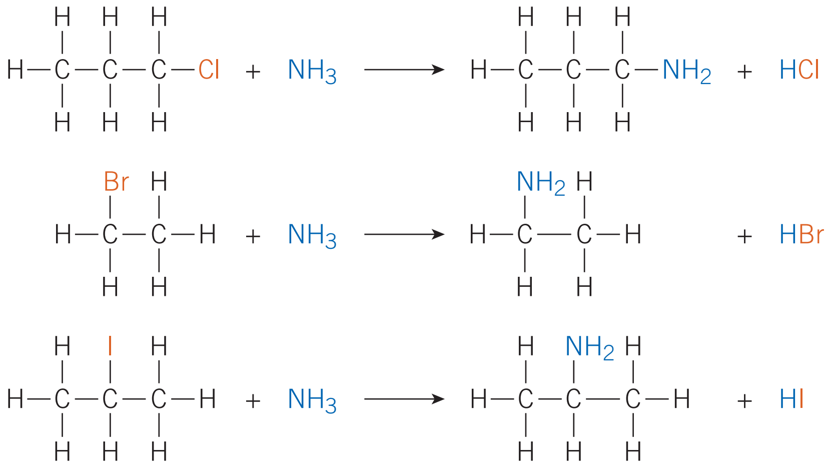
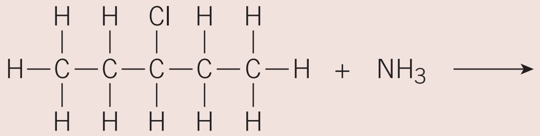


Figure 9A–9 Substitution reactions involving haloalkanes and ammonia

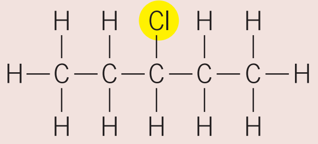
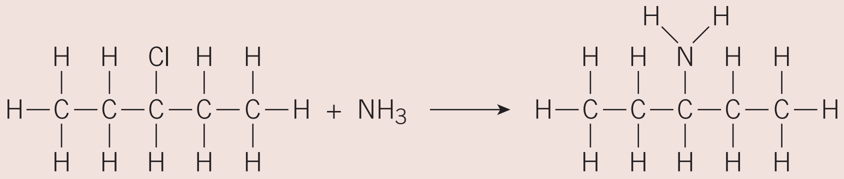
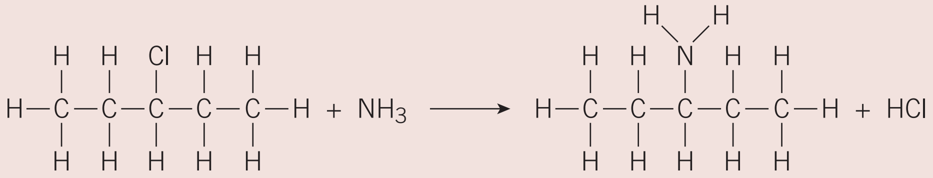
VIDEO
WORKED
EXAMPLE 9A–1

Worked example 9A–1: Substitution reaction of haloalkanes

Complete the following equation by drawing the structural formula of the product and by-products.



Solution

	Logic	Process
Step 1	Identify the functional group of the reactant involved in the reaction.	
Step 2	Recall the type of reaction by analysing the reagents/ reaction conditions.	The reaction is a substitution reaction where an atom or group of atoms in the reactant is replaced by another atom or group of atoms.
Step 3	Draw the product of the reaction in the equation.	
Step 4	Include any by-products and balance the equation.	

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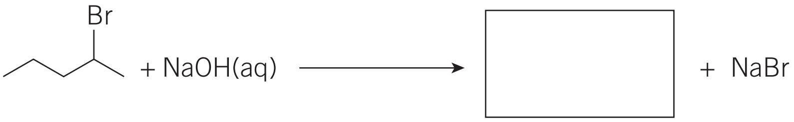
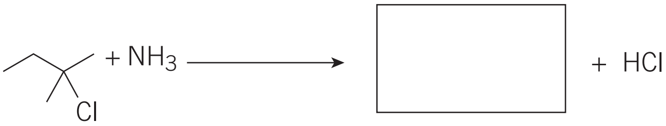
Check-in questions – Set 1

1 Complete the following equations by drawing the missing structure in the box.

a



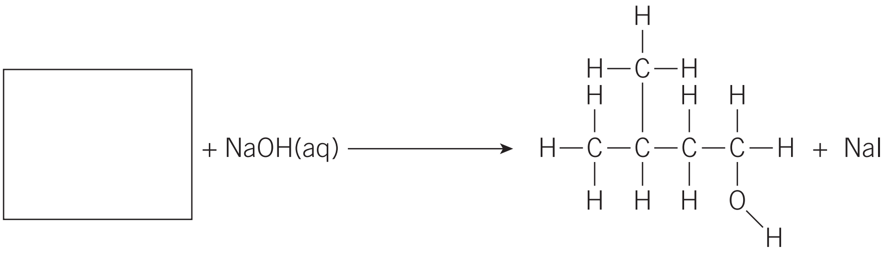
b



c

$\boxed{} + Br_2 \xrightarrow{\text{UV light}} CH_3CH_2CHBrCH_3 + HBr$

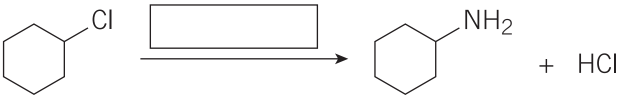
d



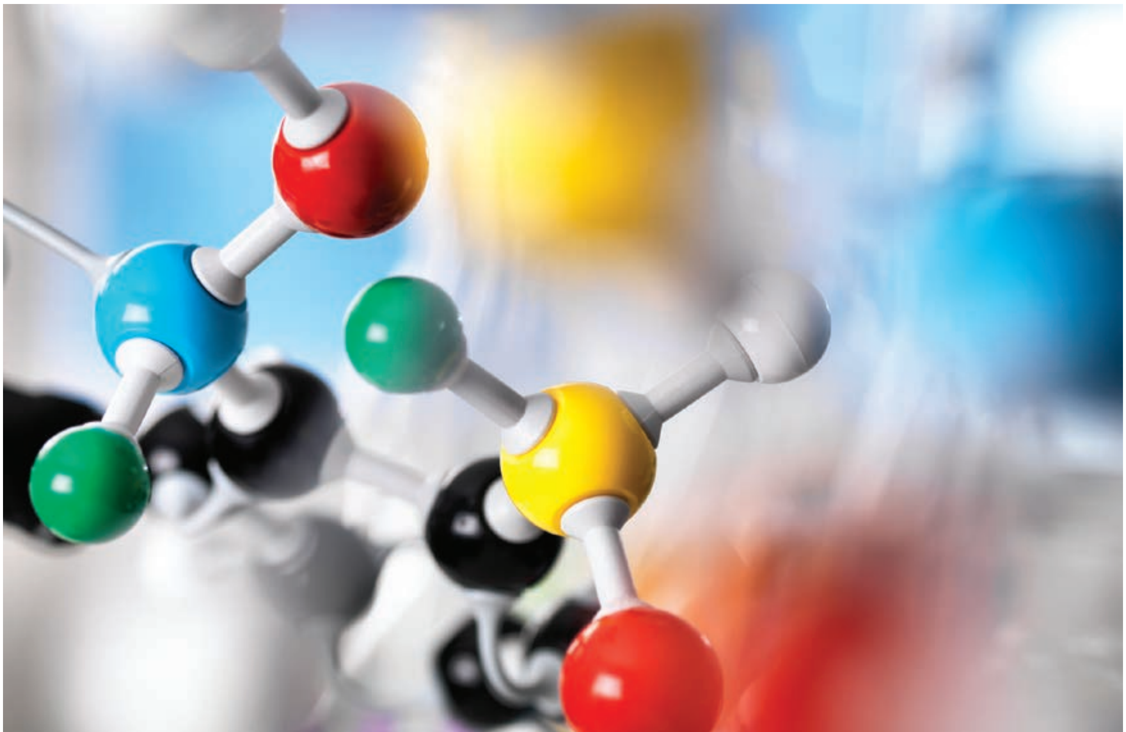
2 Write the missing reagents or reaction conditions in the following equations.

a $C_4H_{10} + \boxed{} \xrightarrow{\boxed{}} C_4H_9Br + HBr$

b



c $C_6H_{13}Cl + \boxed{} \longrightarrow C_6H_{14}O + NaCl$



Addition reactions of alkenes

8B MOLECULES OF CARBON LINK

Addition reaction a reaction in which two or more reactants combine to form a larger product. Addition reactions require an unsaturated reactant

Hydrogenation reaction a reaction in which a hydrogen molecule is added to an unsaturated molecule

Addition reactions of alkenes are chemical reactions in which a molecule is added across the double bond of an alkene. To achieve this, the double bond of the alkene is broken and the two carbon atoms form new single bonds with the added molecule (Figure 9A–10). The resulting molecule is a saturated compound.

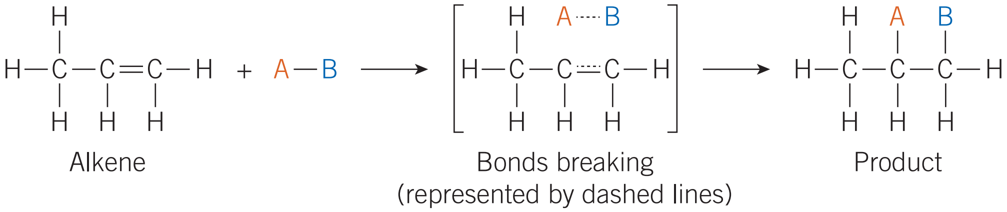


Figure 9A–10 General process of addition reactions of alkenes

As we change the small molecule (A–B in the above figure) in the reaction, we can add different functional groups to the product. This makes alkenes a versatile starting material to synthesise a range of different organic compounds. Different types of addition reactions are given different names depending on the type of molecule (A–B) being added. We will examine a few important types of addition reactions of alkenes in detail. It is worthy to note that while each type of addition reaction has its own name, it is also correct to collectively refer to them all as addition reactions.

Hydrogenation – addition reactions involving hydrogen gas (H_2)

Hydrogenation reactions are a type of addition reaction in which H_2 is added across the C═C double bond of an unsaturated molecule. The C═C double bond is converted to a C–C single bond. This reaction is useful for producing a wide range of food products, including margarine, pharmaceuticals and other industrial materials. Hydrogenation is carried out in the presence of a transition metal catalyst such as nickel (Ni), palladium (Pd) or platinum (Pt) (Figure 9A–12).

Figure 9A–11 Hydrogenation reactions are useful in the creation of margarine and other spreads.

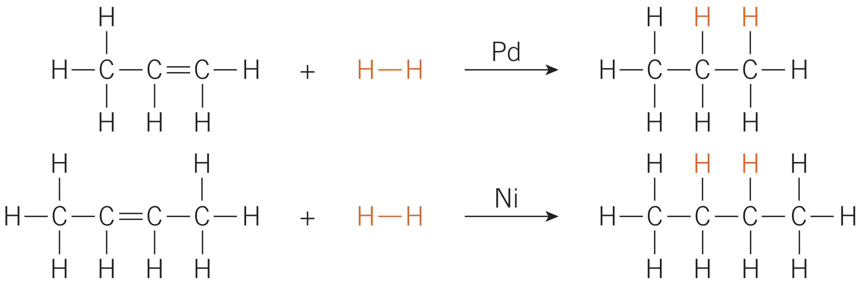


Figure 9A–12 Equations showing the addition of hydrogen (H_2) to an unsaturated alkene producing a saturated alkane

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Halogenation – addition reactions involving a halogen (X_2)

Another type of addition reaction involves the reaction of alkenes with halogens such as Cl_2 and Br_2. The two halogen atoms are added across the C═C double bond to give a molecule with two halo functional groups on neighbouring carbons (Figure 9A–13). As this reaction introduces halogens into the organic molecule, it is called a halogenation reaction.

LINK **8B** MOLECULES OF CARBON

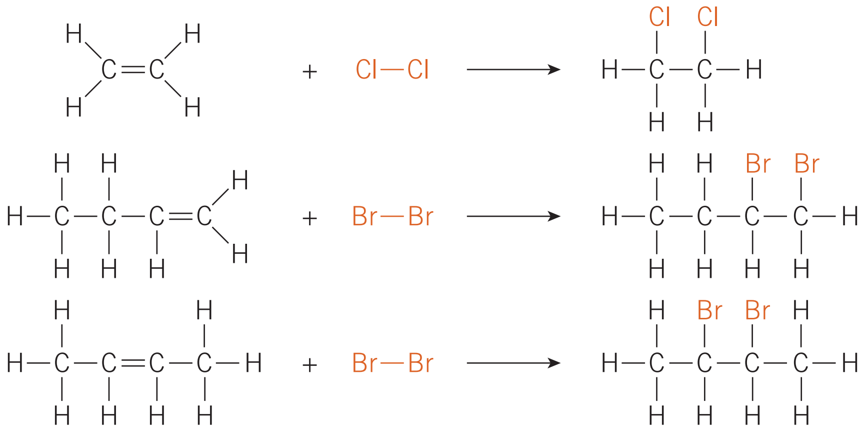

Figure 9A–13 Equations showing the addition of a halogen to an alkene to give a haloalkane

Hydrohalogenation – addition reactions involving a hydrogen halide (HX)

Hydrohalogenation reactions are a type of addition reaction in which a hydrogen halide (HX, where X is a halogen atom) is added across a C═C double bond to form a haloalkane (Figure 9A–14).

LINK **8B** MOLECULES OF CARBON

Hydrohalogenation reaction
a reaction in which a hydrogen halide molecule is added to an unsaturated molecule

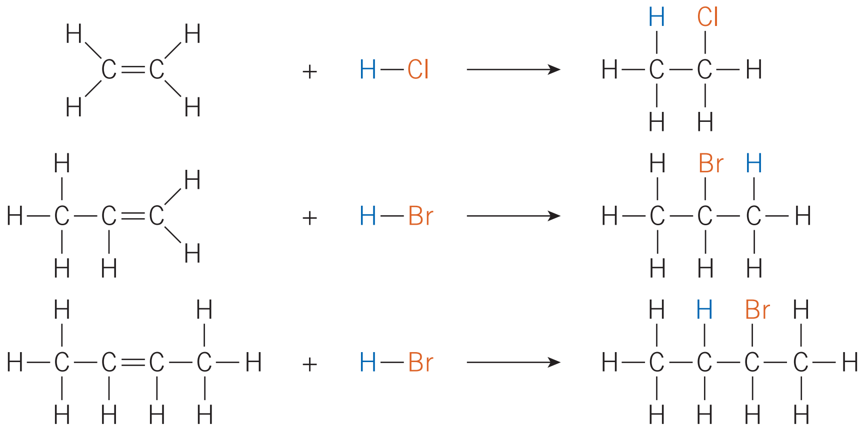

Figure 9A–14 Equations showing the addition of a hydrogen halide (HX) to an alkene producing a haloalkane

It is important to note that two different products may be formed if the alkene starting material is not symmetric. This is because the H–X molecule can orient itself in two different ways during the addition reaction leading to two different structures (Figure 9A–15). For example, when propene reacts with HBr, the Br atom can form a bond with either the first carbon or the second carbon depending on its orientation. As a result, two different positional isomers, 1-bromopropane and 2-bromopropane, are formed as a mixture of products.

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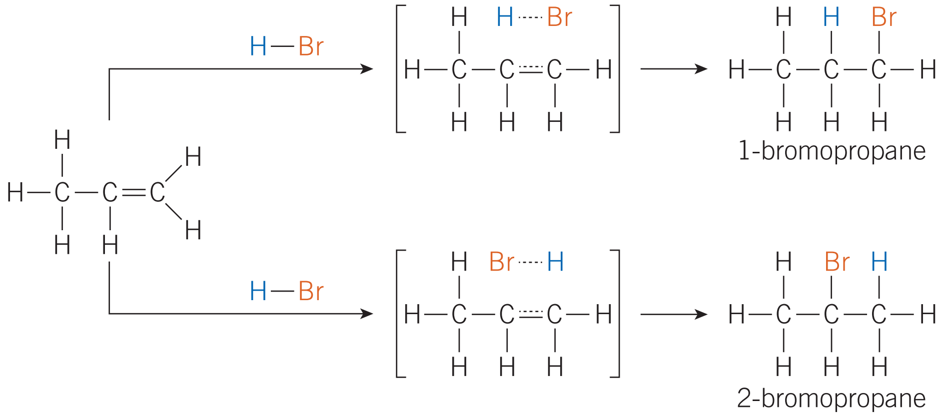

Figure 9A–15 Equation showing the addition of HBr to propene to produce a mixture of 1-bromopropane and 2-bromopropane

Hydration – addition reactions involving water (H_2O)

The addition reaction involving a molecule of water adding across a C═C double bond to give an alcohol is called a **hydration reaction**. The 'hydra' part of the name refers to water being used for the reaction. This reaction is typically performed at high temperature (150–200°C) and uses phosphoric acid (H_3PO_4) or sulfuric acid (H_2SO_4) as a catalyst. For example, the addition of H_2O to but-2-ene in the presence of H_3PO_4 gives the product butan-2-ol. Figure 9A–16 shows examples of hydration reactions of alkenes.

7C COMMERCIAL ELECTROLYTIC CELLS **LINK**

Hydration reaction a reaction in which a water molecule is added to an unsaturated molecule

8C FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS **LINK**

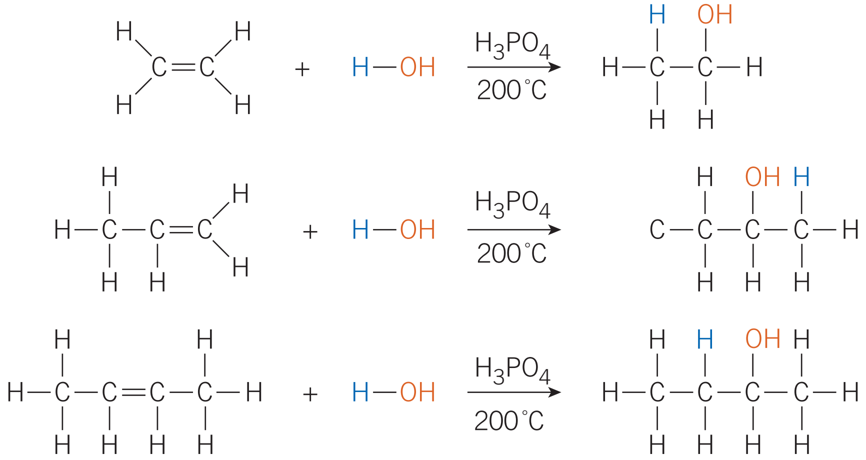

Figure 9A–16 Equations showing the addition reaction of water molecules to alkenes

In a similar fashion to hydrohalogenation, if the alkene is not symmetric, two different products are usually obtained after the reaction. This is because the water molecule can add across the C═C double bond in two different orientations. For example, if pent-2-ene is reacted with H_2O in the presence of H_3PO_4, a mixture of both pentan-2-ol and pentan-3-ol would be formed upon completion of the reaction (Figure 9A–17).

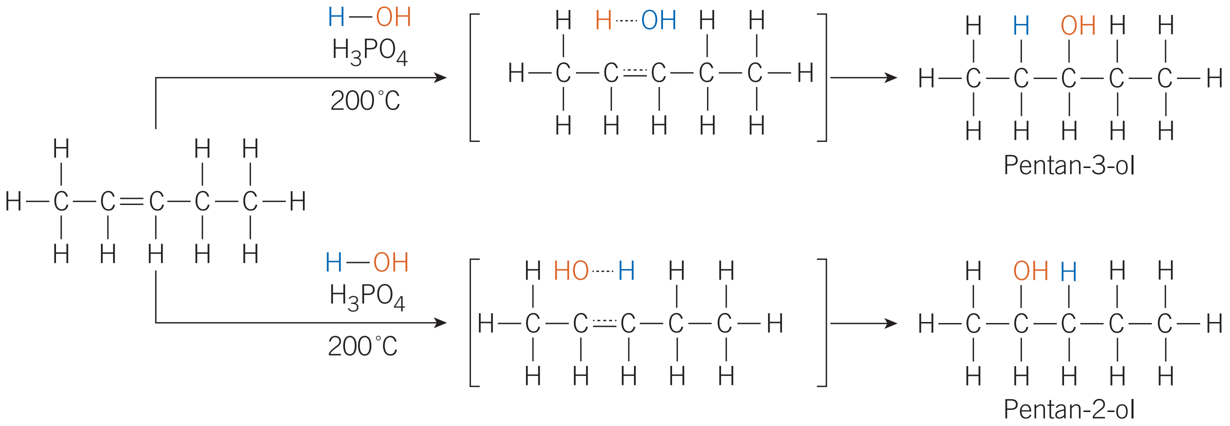

Figure 9A–17 Equations showing the addition of a water molecule (H_2O) to pent-2-ene to produce a mixture of pentan-2-ol and pentan-3-ol

Summary of addition reactions to alkenes

Addition reactions involving alkenes are useful for a variety of applications, including the production of plastics, fuels, pharmaceuticals and other chemicals vital for everyday goods. Some common examples include:

- the addition of hydrogen gas to an alkene to form an alkane, which is commonly used in the production of fuels and margarine
- the addition of halogens (such as Cl_2 or Br_2) to an alkene to form a dihaloalkane, which is used as a solvent, a refrigerant or a starting material for the synthesis of other chemicals
- the addition of water to an alkene to form an alcohol, which is used as a solvent, a fuel or a starting material for the synthesis of other chemicals.

LINK **12A** ORGANIC COMPOUNDS AS MEDICINES

LINK **1A** TYPES OF FUELS

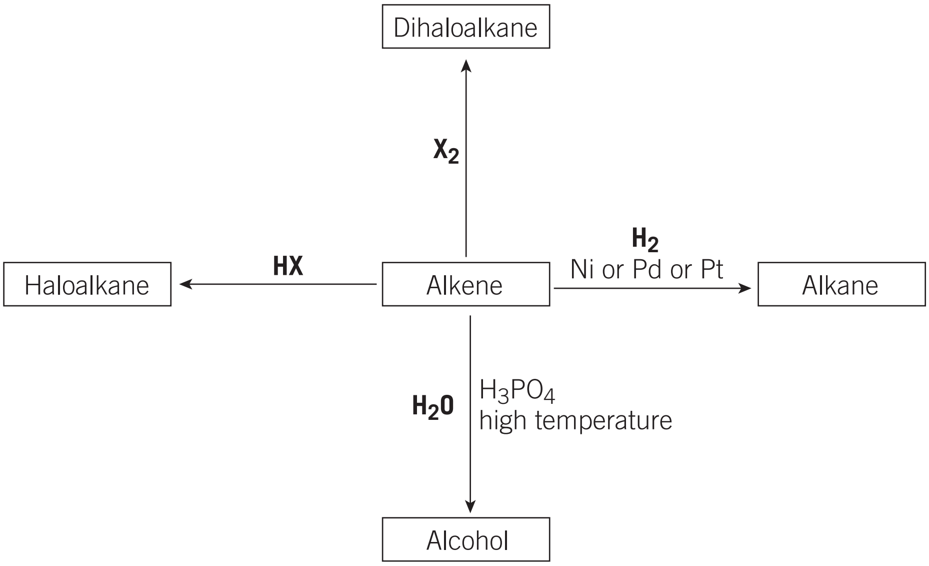

Figure 9A–18 Summary of addition reactions to alkenes, where ‘X’ represents a halogen such as Cl, Br or I

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Figure 9A–19 Halogenation reactions are used in the production of pharmaceuticals such as antibiotics and antidiabetic drugs.

Check-in questions – Set 2

1 Name all products formed during the addition reaction between ethene (CH_2CH_2) and the following small molecules.

a HCl **b** H_2 **c** H_2O **d** Br_2

2 Name and draw the skeletal formula of all products formed during the addition reaction between propene (CH_3CHCH_2) and the following compounds.

a HI **b** H_2 **c** H_2O **d** Cl_2

Oxidation reactions of primary alcohols

3A REDUCTION AND OXIDATION **LINK**

8D FUNCTIONAL GROUPS: ALDEHYDES, KETONES, CARBOXYLIC ACIDS AND ESTERS **LINK**

Oxidation of primary alcohols is a process that converts a primary alcohol into a carboxylic acid or an aldehyde, depending on the specific reaction conditions and the type of **oxidising agent** used. Reacting a primary alcohol with an oxidising agent in the presence of acid (H^+) would give a carboxylic acid. Figure 9A–20 shows common examples of oxidising agents used in this reaction:

- potassium dichromate ($K_2Cr_2O_7$) or dichromate ($Cr_2O_7^{2-}$)
- potassium permanganate ($KMnO_4$) or permanganate (MnO_4^-).

Oxidation a loss of electrons

Oxidising agent the reactant in a redox reaction that causes oxidation. It is itself reduced and therefore will gain electrons – its oxidation number will decrease

Figure 9A–20 Samples of $K_2Cr_2O_7$ (left) and $KMnO_4$ (right) are strong oxidising agents used to oxidise primary alcohols to carboxylic acids.

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Heat can be applied to this reaction to ensure the oxidation proceeds to give a carboxylic acid. An aldehyde can be obtained by performing the reaction at a lower temperature or with a mild oxidising agent. Once the aldehyde is formed, it can be further oxidised to the carboxylic acid by treatment with $KMnO_4$ or $K_2Cr_2O_7$ (Figure 9A–21).

LINK **8D** FUNCTIONAL GROUPS: ALDEHYDES, KETONES, CARBOXYLIC ACIDS AND ESTERS

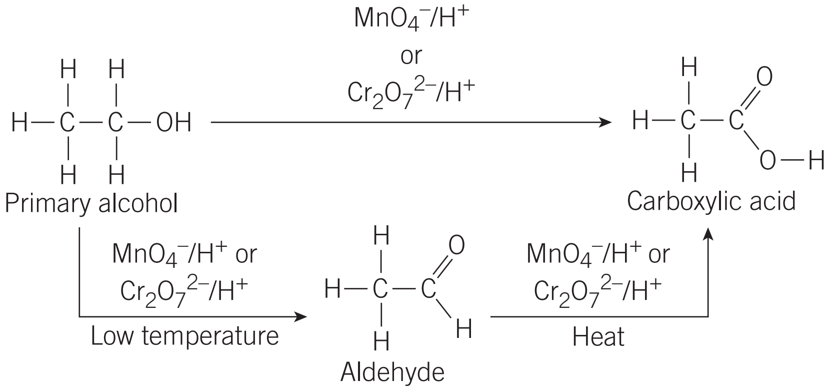


Figure 9A–21 Oxidation of primary alcohols using acidified $KMnO_4$ and $K_2Cr_2O_7$

Organic reaction pathways

Reaction pathways are a sequence of chemical reactions that can convert a relatively cheap and common starting material into a desired product, often with greater molecular complexity. **Intermediate compounds** are formed after each reaction and used in the subsequent reactions until the desired product is eventually formed. Each reaction can also be referred to as a 'step' in the pathway, so the sequence outlined in Figure 9A–22 has a total of three steps.

Reaction pathway a sequence of reactions that convert a simple starting material into a desired product

Intermediate compound a chemical compound that is synthesised from a simpler compound and intended to be used for preparation of more complex molecules

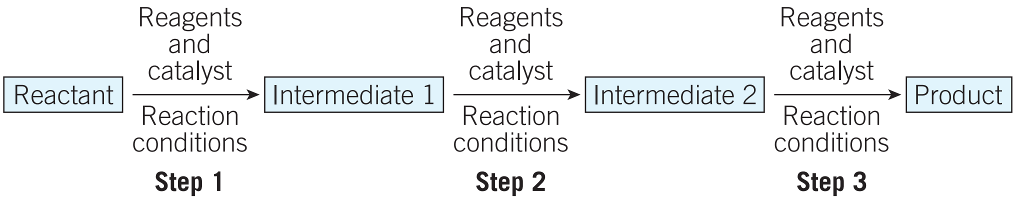


Figure 9A–22 General scheme of a reaction pathway

When drawing a pathway, there is no need to balance the reactants and products of the steps. The focus is on the structure of the reactant, intermediate compounds and the desired product, so all other reagents are written above the arrows. Information about solvent, temperature and time are written below the arrows. States are usually not required for the organic structures but may be important for certain reagents like NaOH(aq).

The design of organic reaction pathways involves selecting and optimising the steps of a chemical synthesis to produce a desired product in an efficient and cost-effective manner. To illustrate this idea, we will use the reactions discussed in this section to construct pathways to synthesise primary amines and carboxylic acids.

Pathways to synthesise primary amines

Figure 9A–23 shows two general pathways for the synthesis of primary amines. Pathway 1 begins with an alkane starting material. A substitution reaction involving the alkane and a halogen under UV light yields a haloalkane intermediate. A second substitution reaction between the haloalkane and ammonia, NH_3, gives the desired primary amine.

Alternatively, Pathway 2 begins with an alkene undergoing an addition reaction with a hydrogen halide to give a haloalkane intermediate. Subsequent reaction with ammonia, NH_3, gives the desired amine product.

10A
ANALYSIS OF
FUNCTIONAL
GROUPS
LINK

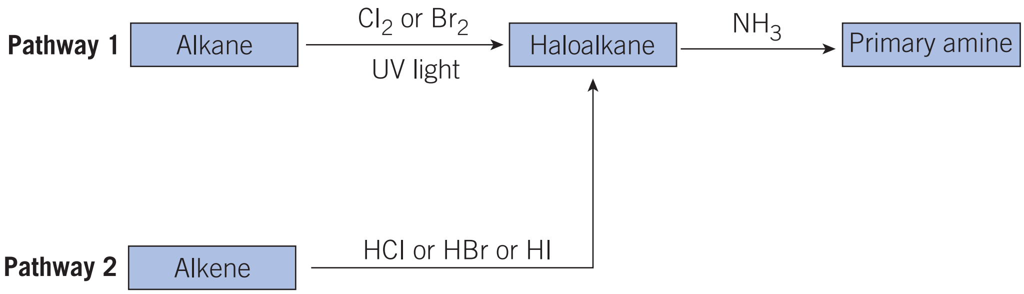


Figure 9A–23 Two general pathways for the synthesis of primary amines from an alkane (Pathway 1) and an alkene (Pathway 2)

Following the general sequence of Pathway 1, Figure 9A–24 shows a two-step sequence for the preparation of ethanamine starting from ethane.

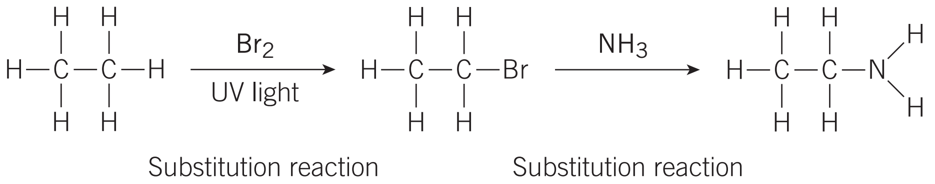


Figure 9A–24 A two-step sequence for the preparation of ethanamine starting from ethane

Following the general sequence of Pathway 2, Figure 9A–25 shows a two-step sequence for the preparation of propan-2-amine starting from propene.

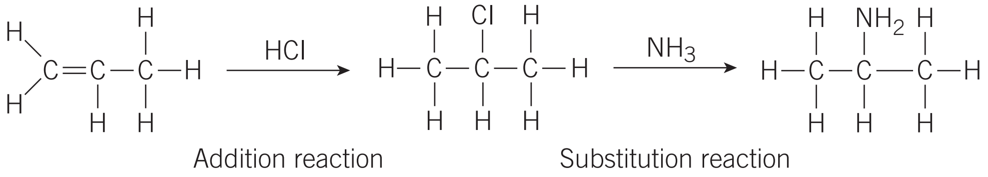


Figure 9A–25 A two-step sequence for the preparation of propan-2-amine starting from propene

Pathways to synthesise carboxylic acids

Carboxylic acids can also be produced from relatively simple starting materials via a sequence of reactions. Figure 9A–26 shows two pathways to produce a carboxylic acid starting from an alkane (Pathway 1) and an alkene (Pathway 2). Pathway 1 begins with a substitution reaction of an alkane to give a haloalkane intermediate. Reacting the haloalkane with aqueous sodium hydroxide in a second substitution reaction produces an alkan-1-ol intermediate. Oxidation of the alcohol with either H^+/MNO_4^- or $H^+/Cr_2O_7^{2-}$ produces the carboxylic acid. Pathway 2 begins with an alkene. After a hydration reaction, the resulting alcohol intermediate intercepts Pathway 1. Oxidation of the alcohol produces the carboxylic acid.

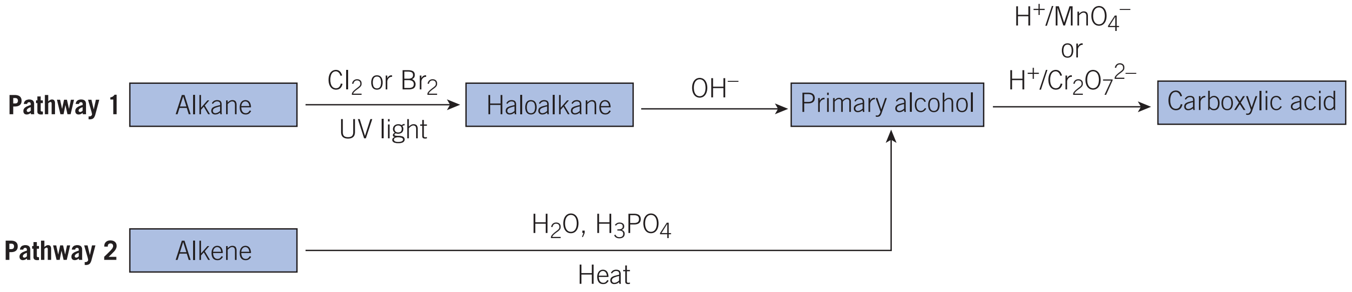


Figure 9A–26 Two general pathways to produce a carboxylic acid starting from an alkane (Pathway 1) and an alkene (Pathway 2)

Using the outline of Pathway 1, Figure 9A–27 below shows a three-step sequence to prepare propanoic acid from propane.

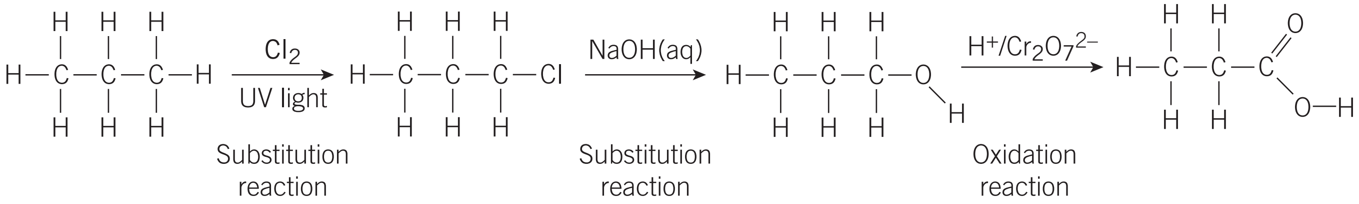


Figure 9A–27 A three-step sequence to prepare propanoic acid from propane

Using the outline of Pathway 2, Figure 9A–28 shows a two-step sequence to prepare ethanoic acid from ethene.

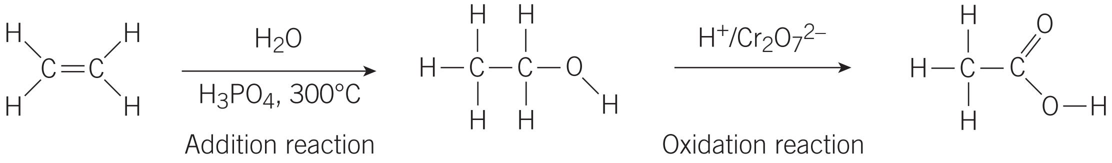


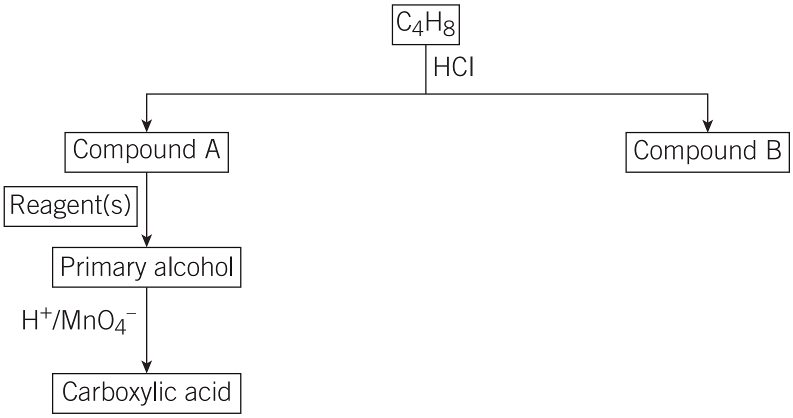
Figure 9A–28 A two-step sequence to prepare ethanoic acid from ethene

Check-in questions – Set 3

1 A reaction pathway to synthesise an amine is shown below.

a Write the semi-structural formula of the saturated hydrocarbon.
b State the reagents and any reaction conditions required to convert the saturated hydrocarbon to the haloalkane (reaction 1).
c State the reagents and any reaction conditions required to convert the haloalkane to the primary amine (reaction 2).

2 The reaction pathway to generate a carboxylic acid is shown below.



WORKSHEET 9A–1 REACTIONS FOR THE SYNTHESIS OF PRIMARY AMINES AND CARBOXYLIC ACIDS

C_4H_8 reacts with HCl to form two unbranched isomers – compound A and compound B. Only compound A can proceed to form a carboxylic acid.

a Identify the type of reaction that converts C_4H_8 into compound A.
b Draw the skeletal structure of compound B.
c State the reagent(s) required to convert compound A into a primary alcohol.
d Draw the structural formula of the carboxylic acid.

Designing a reaction pathway

Designing an efficient, cost-effective and environmentally sustainable reaction pathway requires the consideration of multiple factors. A summary of some of these factors are outlined in Table 9A–1.

Table 9A–1 Factors that influence the design of a reaction pathway

Factor	Attributes
Reagent/starting material	• Cheap • Readily available • Sourced from renewable feedstocks • Low toxicity – safety for the operators/scientists
Intermediate compounds	• Stable – does not degrade after being formed • Easily isolated or purified from the reaction mixture where possible • Low toxicity – safety for the operators/scientists

Factor	Attributes
Product	• Stable – does not degrade after being formed • Easily isolated from the reaction mixture • Can be obtained with a high degree of purity • Low toxicity where possible – safety for the operators/ scientists • Is of commercial value or serves an intended purpose
Waste/by-products	• As few as possible • Toxicity and environmental impact are as low as possible • Have considered opportunities for waste to be used in other chemical processes/manufacturing • Access to responsible waste disposal
Number of steps in the sequence	• As few as possible – fewer number of reactions usually mean less overall waste generated and less energy and reagents required
Overall yield of product	• As high as possible – high yield means that the reactions in the sequence are efficient and there is little starting material left over or by-products being formed.
Reaction conditions	• As mild as possible – extreme reaction conditions such as high temperatures (above 100°C), low temperatures (below 0°C) and high pressures are energy intensive and costly to maintain. Mild conditions such as room temperature and atmospheric pressures are desirable.
Rates of reactions	• Avoid extremely slow reactions as it will hold up (bottleneck) the entire process.

VIDEO 9A–1
REACTION PATHWAYS

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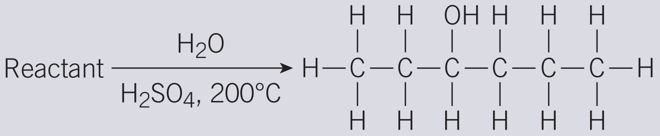
9A SKILLS

Identifying the best reactant for the job

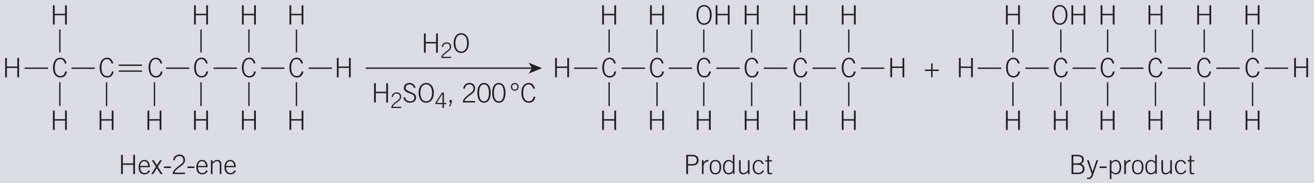
VIDEO 9A–2
SKILLS: IDENTIFYING THE BEST REACTANT

You may encounter situations where you are asked to plan a synthesis of a particular molecule. This is a skill that requires you to consider multiple scenarios to achieve an outcome. For example, consider the equation below and identify the **best** reactant to synthesise hexan-3-ol.

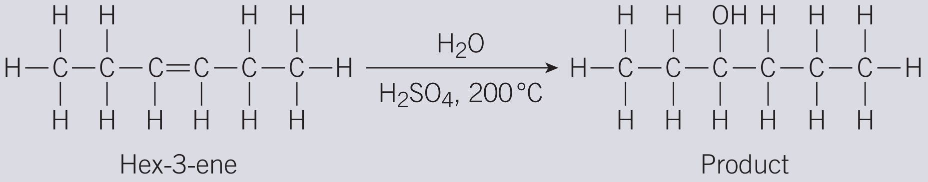


The way to address problems like this is to list all the possible candidates that can be used. The reaction conditions suggest that an addition reaction is being conducted. Therefore, two alkenes fit the requirements: hex-2-ene and hex-3-ene.

Since there is more than one possible answer, how do we decide which is the best reactant? To answer this question, we consider if there are any differences in the outcomes of these two starting materials. Hex-2-ene, a molecule that is not symmetric, would react with H_2O to give two possible products: hexan-3-ol (desired product) and hexan-2-ol (by-product) as shown in the following diagram.



On the other hand, hex-3-ene is symmetric and therefore would react with H_2O to form hexan-3-ol as the only product.



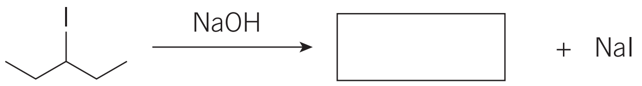
Through selection of more ideal starting materials, we can optimise reactions by reducing the number of by-products formed and maximising the yield.

Section 9A questions

1 Use structural formulas to write equations for the following reactions.
   - a methane reacting with bromine under UV light
   - b 2-chlorobutane reacting with ammonia
   - c 1-bromopropane reacting with aqueous potassium hydroxide

2 Copy these diagrams and complete the following equations by drawing the missing structure in the box.

a



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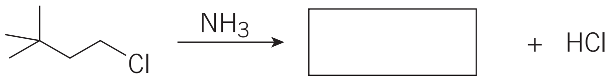

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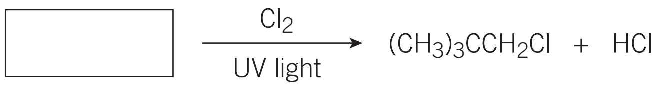

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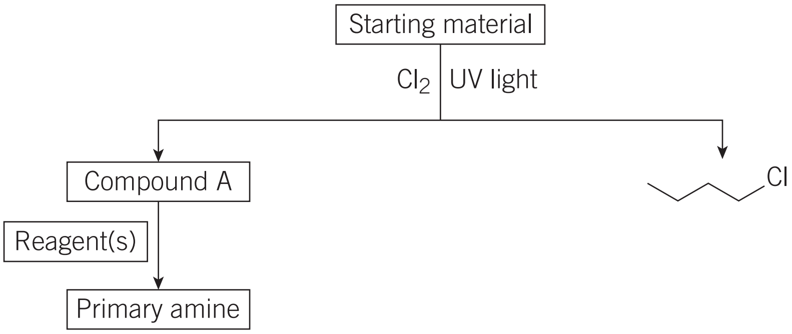
3 Explain the difference between a substitution reaction and an addition reaction in terms of changes made to the reactant.

4 Write the IUPAC name and the semi-structural formula of the product(s) formed when but-2-ene reacts with:

- **a** chlorine.
- **b** water in the presence of phosphoric acid at 250°C.
- **c** hydroiodic acid (HI).
- **d** hydrogen gas in the presence of palladium metal.

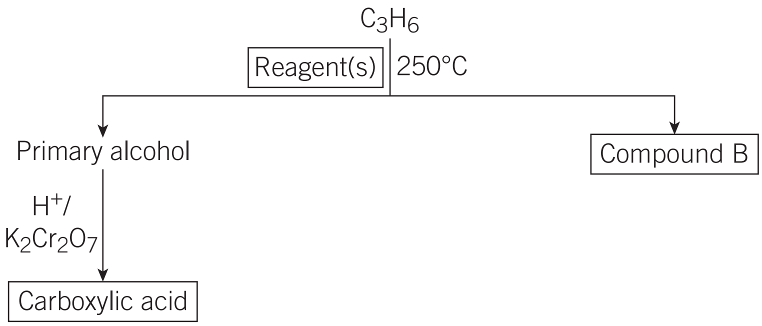
5 Write an equation for the reaction between pent-2-ene and HBr. Use skeletal formula for all organic molecules and show all possible products formed during the reaction.

6 The reaction pathway to synthesise a primary amine is shown below.



- **a** Draw the skeletal formula of the starting material.
- **b** Draw the skeletal formula of compound A.
- **c** State the name of the type of reaction that converts the starting material to compound A.
- **d** State the reagent(s) required to convert the chloroalkane to the primary amine.
- **e** Draw the skeletal structure of the primary amine.

7 The reaction pathway to synthesise a carboxylic acid is shown below.



- **a** Write the reagents required to convert C_3H_6 into a primary alcohol and compound B.
- **b** Write the semi-structural formula of compound B.
- **c** Write the semi-structural formula of the carboxylic acid.

9B Organic reactions: condensation and hydrolysis

Study Design:

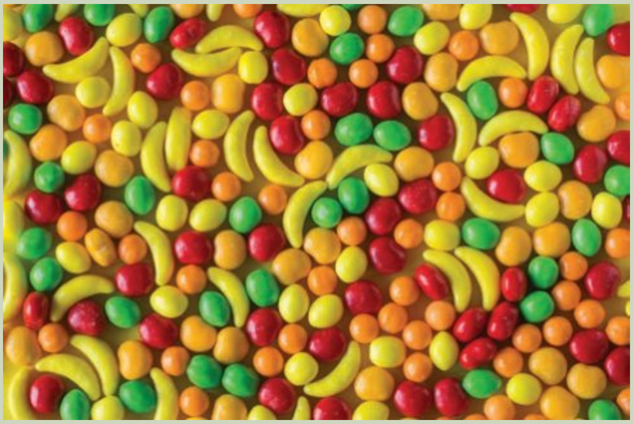
- Organic reactions and pathways, including equations, reactants, products, reaction conditions and catalysts (specific enzymes not required):
  - synthesis of primary haloalkanes and primary alcohols by substitution
  - addition reactions of alkenes
  - the esterification between an alcohol and a carboxylic acid
  - hydrolysis of esters
  - pathways for the synthesis of primary amines and carboxylic acids
  - transesterification of plant triglycerides using alcohols to produce biodiesel
  - hydrolytic reactions of proteins, carbohydrates and fats and oils to break down large biomolecules in food to produce smaller molecules
  - condensation reactions to synthesise large biologically important molecules for storage as proteins, starch, glycogen and lipids (fats and oils)

Glossary:

α-Glucose
Amylose
Carbohydrate
Catalysis
Condensation reaction
Disaccharide
Esterification reaction
Fatty acid
Glycerol
Glycogen
Glycosidic bond
Hydrolysis reaction
Lipid
Monosaccharide
Peptide
Polysaccharide
Protein
Saponification reaction
Starch
Transesterification
Triglyceride

ENGAGE

Are my lollies made from real fruit?



The answer is, generally, no. But, as always, there are certain exceptions. The food industry does not have to use real fruit to make their lollies smell and taste like fruit. The biochemistry of how the receptors in our mouth and nose interact with molecules is extremely complex. For example, pentanoic acid (C_4H_9COOH) has a foul odour that is reminiscent of dirty socks. But if pentanoic acid is heated with ethanol, a pleasant apple-like aroma emerges. The product of this reaction is ethyl pentanoate and, like many other esters, it has a sweet fruity scent that is desirable to our senses. Ethyl pentanoate is added to food items like lollies and chewing gum to give them their distinct flavour and scent. Many other esters are also used as food additives to give the product a desirable smell or taste.

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EXPLAIN

Condensation reactions

Condensation reactions are a type of chemical reaction in which two molecules combine to form a larger molecule, along with the simultaneous release of a small molecule such as water (Figure 9B–1). The small molecule is considered a by-product of the reaction. Condensation reactions are commonly used to form esters, amides, **proteins** and **carbohydrates**. The products of condensation reactions are not only crucial for the normal function of our bodies but also widely used in the materials and pharmaceutical industries.

Condensation reaction
a type of chemical reaction where two molecules combine to form a larger molecule with the release of a small molecule, usually water

Protein
a polymer that consists of amino acids linked by peptide bonds

Carbohydrate
a sugar or a saccharide, ranging from simple sugars (monosaccharides) to complex sugars (polysaccharides)

Figure 9B–1 General process of a condensation reaction

Esterification reactions

A carboxylic acid and an alcohol can undergo a condensation reaction to form an ester and a molecule of water. Heat and an acid catalyst such as H_2SO_4 are commonly used to increase the rate of the reaction. Condensation reactions that form esters are also called **esterification reactions**. An example is shown in Figure 9B–2 in which propanoic acid reacts with ethanol to give ethyl propanoate and water.

LINK **8D** FUNCTIONAL GROUPS: ALDEHYDES, KETONES, CARBOXYLIC ACIDS AND ESTERS

Esterification reaction
a type of condensation reaction that forms an ester from a carboxylic acid and an alcohol

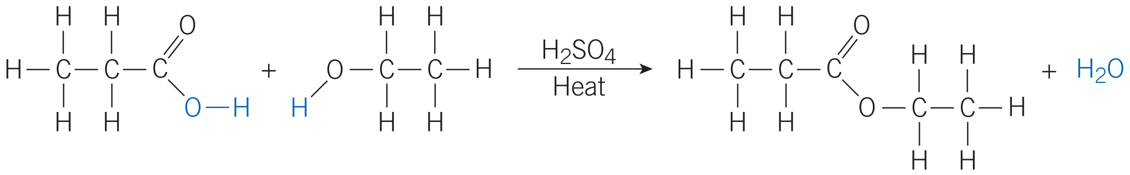


Figure 9B–2 The esterification reaction between propanoic acid and ethanol produces ethyl propanoate and water.

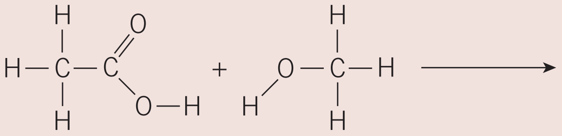
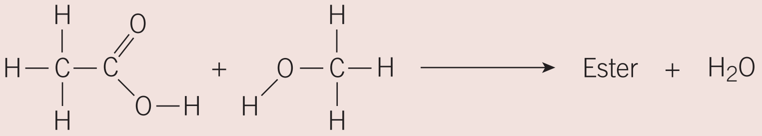
Worked example 9B–1: Drawing an esterification reaction

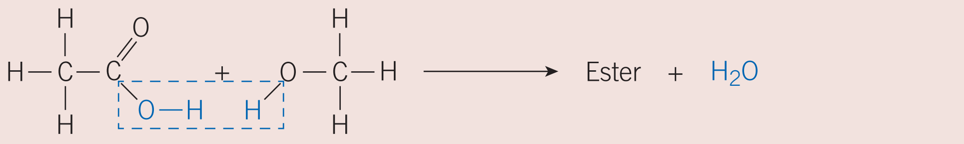
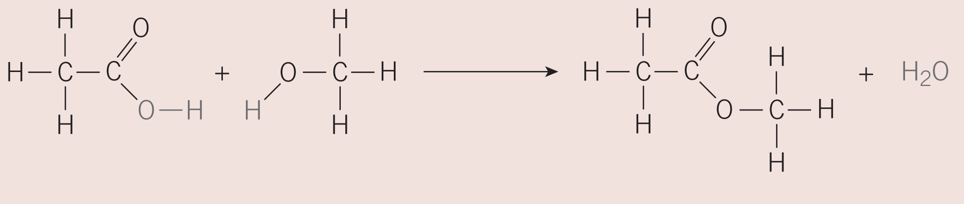
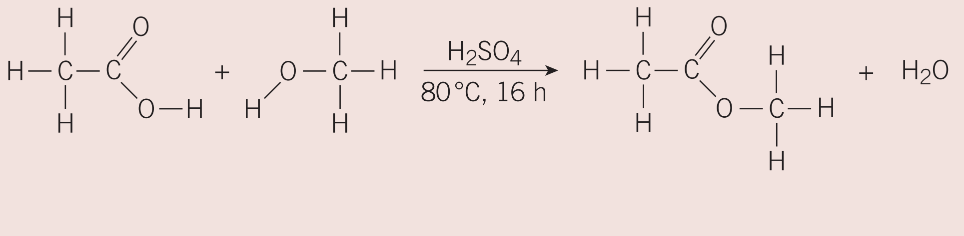
An ester was prepared by reacting ethanoic acid with methanol in the presence of H_2SO_4. The reaction was heated to 80°C for 16 hours.

VIDEO WORKED EXAMPLE 9B–1

Using structural formulas for all organic compounds, draw an equation to describe the reaction above.

Solution

	Logic	Process
Step 1	Draw the structures of the reactants on the left of the arrow.	
Step 2	Recall that a carboxylic acid and an alcohol react in a condensation reaction to form an ester and a molecule of water.	

Step 3	Identify the atoms in the reactants that will form the water molecule.	
Step 4	Draw the structure of the ester using the remaining atoms of the two reactants.	
Step 5	Complete the equation by adding the catalyst and/or any relevant reaction conditions.	

Condensation reactions to form large biologically important molecules

Condensation reactions are important in the synthesis of large biologically important molecules such as **lipids**, proteins and carbohydrates. These molecules are made by living organisms for the long-term storage of energy, structural support, **catalysis** and signalling.

Synthesis of lipids

Lipids are an important class of molecules in our bodies. They make up our cell membranes and are used for fat storage. A particular type of lipids are the **triglycerides**, more commonly known as fats and oils. Fats and oils are part of a healthy diet, and it is essential for our bodies to have a storage of fat as a source of energy. The structure of a triglyceride consists of three ester functional groups and three long hydrocarbon chains derived from fatty acids (Figure 9B–3). The non-polar fatty acid chains make triglycerides insoluble in water.

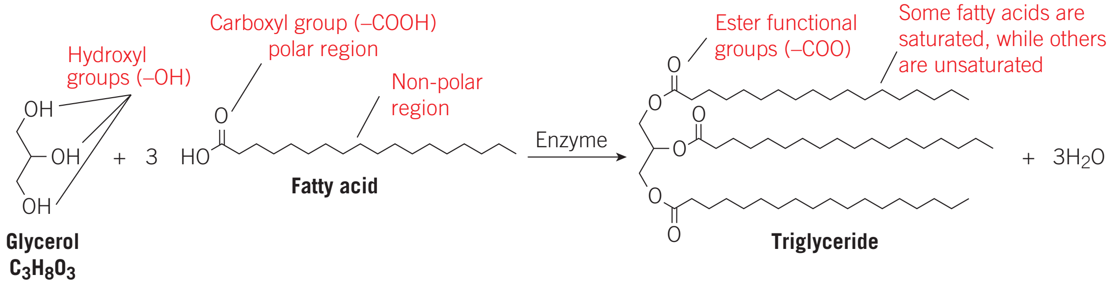


Figure 9B–3 The condensation reaction between glycerol and stearic acid ($C_{17}H_{35}COOH$) gives the corresponding triglyceride and three molecules of water.

Synthesis of triglycerides involves condensation of three **fatty acid** molecules with a **glycerol** molecule. These three fatty acid molecules do not necessarily have to be identical. For each triglyceride, three water molecules are formed as the by-product. In biological systems, enzymes are used to catalyse this reaction.

Lipid
a substance found in living systems that is derived from fatty acids. Common examples include fats and oils

Catalysis
a process in which a catalyst is used to speed up a reaction

Triglyceride
an organic compound in which the three hydroxyl groups of glycerol form esters with three fatty acid molecules

Fatty acid
a compound consisting of a carboxyl group with a long non-polar hydrocarbon chain, which can either be saturated or unsaturated

Glycerol
a compound containing three hydroxyl groups, with the chemical formula $C_3H_8O_3$

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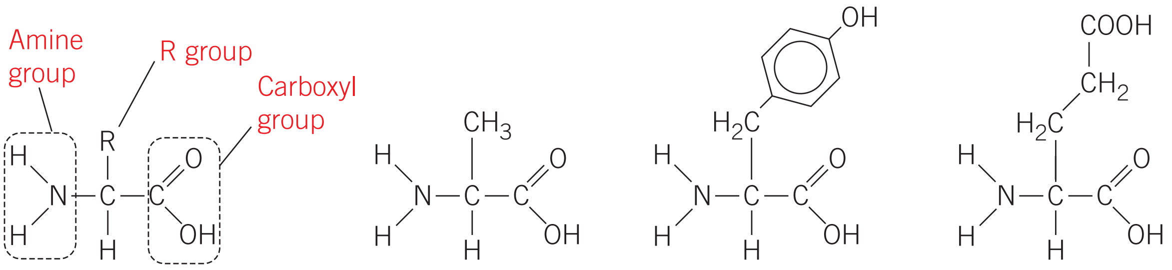
Synthesis of proteins

The basic building blocks for proteins are 2-amino acids (also referred to as α-amino acids). Each 2-amino acid contains a carboxyl functional group and an amino functional group. These two functional groups are part of the backbone of the amino acid. Each 2-amino acid also has a unique R-group that depends on the identity of the amino acid. Our bodies can use any of the twenty 2-amino acids to construct protein molecules. A full list of these 2-amino acids along with their names and three-letter codes is available in the VCE Chemistry Data Book. The general amino acid structure and three examples are shown in Figure 9B–4.

LINK **12B** ENZYMES



General structure of 2-amino acids

Alanine
Ala

Tyrosine
Tyr

Glutamic acid
Glu

Figure 9B–4 Structure, name and three-letter code of selected 2-amino acids. These 2-amino acids are some of the twenty 2-amino acids used by our body to synthesise proteins.

NOTE

The ‘2’ in 2-amino acids refers to the location of the amino functional group in the structure. The $-NH_2$ group is always bonded to the second carbon.
The structures of all 20 2-amino acids are given in your VCE Chemistry Data Book. It is important that you are familiar with how to access this information and the layout of the information.

The condensation reaction to form **peptides** involves the carboxylic acid group of one 2-amino acid reacting with the amino group of another 2-amino acid (Figure 9B–5). As a result, amide bonds, or peptide bonds, are formed between the 2-amino acids. A molecule of water is also generated for each peptide bond that is formed. In a living organism, this reaction occurs at ribosomes.

Peptide
a short sequence of 2-amino acids joined by peptide bonds. Two 2-amino acids joined together by a peptide bond is called a dipeptide; three 2-amino acids make a tripeptide. A longer sequence is called a polypeptide. Proteins are polypeptides containing tens or thousands of 2-amino acids

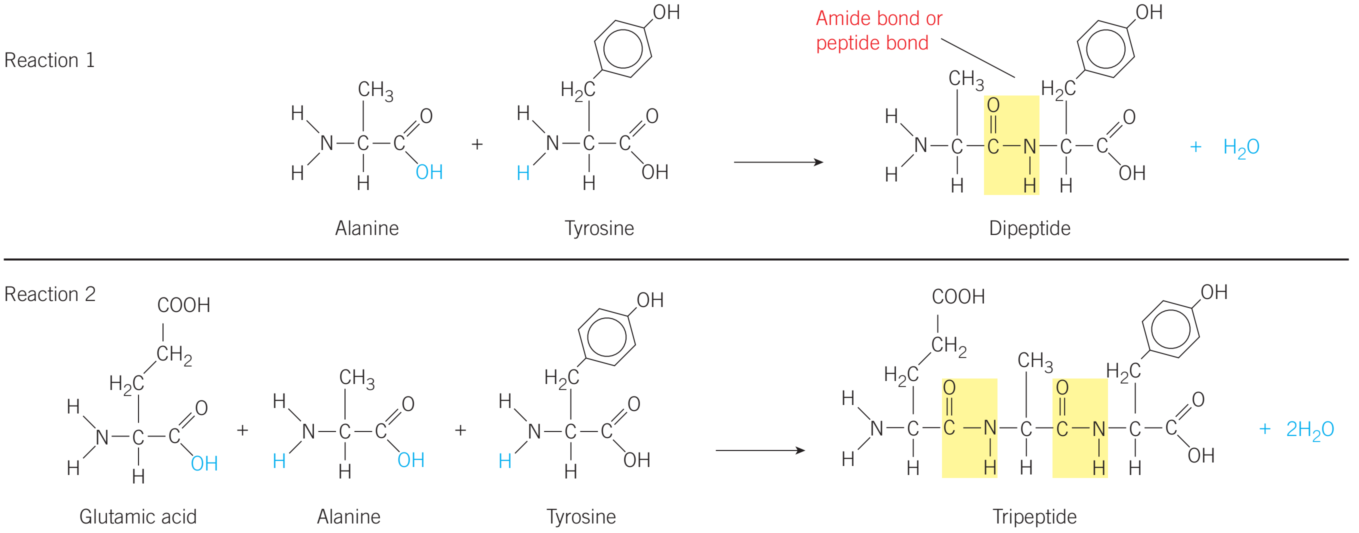


Figure 9B–5 2-Amino acids undergo condensation reactions to form peptides. Reaction 1 shows a possible reaction between alanine and tyrosine to form a dipeptide. Reaction 2 shows a possible reaction between glutamic acid, alanine and tyrosine to form a tripeptide.

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Synthesis of carbohydrates

Carbohydrates refer to a broad class of molecules based on sugar molecules like glucose. The cyclic structure of **α-glucose** consists of a six-membered ring and five hydroxyl groups (Figure 9B–6). A simple sugar molecule like α-glucose is often referred to as a **monosaccharide**. Just like the relationship between 2-amino acids and peptides, molecules of sugar can also condense to form **disaccharides** and **polysaccharides**. Large complex carbohydrates such as **starch** and **glycogen** consist of thousands of glucose units. These polysaccharides are important for short-term storage of energy in living organisms.

α-Glucose a form of glucose in which the hydroxyl group on carbon 1 is on the same side of the six-membered ring as the hydroxyl group on carbon 4

Monosaccharide a single sugar unit

Disaccharide a compound consisting of two sugar units linked by a glycosidic bond

Polysaccharide a compound consisting of many sugar units linked by glycosidic bonds

Starch a polysaccharide of α-glucose joined by glycosidic bonds. Starch is made by plants as a storage of energy

Glycogen a highly branched polysaccharide of α-glucose joined by α-1,4-glycosidic bonds and α-1,6-glycosidic bonds. Glycogen is made by animals as a storage of energy

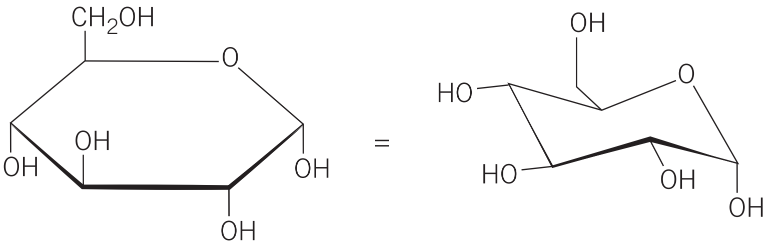

Figure 9B–6 Different ways to represent α-glucose. The structure on the left shows the relative positions of the hydroxyl functional groups on glucose, whereas the structure on the right is a more accurate representation of the molecular shape of glucose.

Disaccharides are formed by the condensation reaction of two monosaccharides. As shown in Figure 9B–7, the reaction between two α-glucose molecules forms a disaccharide and a molecule of water. The new bond formed between the two sugar molecules is called a **glycosidic bond**. Notice that the glycosidic bond is formed between the hydroxyl group on carbon 1 of the first α-glucose molecule and the hydroxyl group on carbon 4 of the second α-glucose molecule. We can be more specific and describe this glycosidic bond as an α-1,4-glycosidic bond. There are other types of glycosidic bonds, as we'll see later.

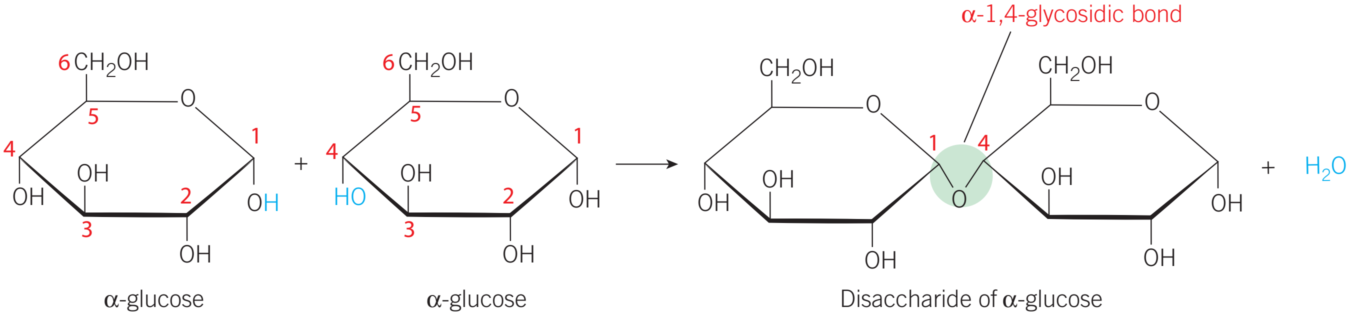

Figure 9B–7 Condensation reaction of two α-glucose molecules to give a disaccharide and water

Condensation can occur between hundreds of α-glucose molecules to form a polysaccharide called **amylose**, a type of starch. Starch molecules are made by plants as a way to store energy. Notice, in Figure 9B–8, that the α-glucose units in amylose combine in a continuous linear structure without any branching. This is because the glycosidic bonds in amylose are predominantly α-1,4-glycosidic bonds.

Glycosidic bond the C–O–C linkage between two monosaccharide units; also called an ether bond

Amylose a type of starch made from α-glucose units bonded to each other through α-1,4-glycosidic bonds

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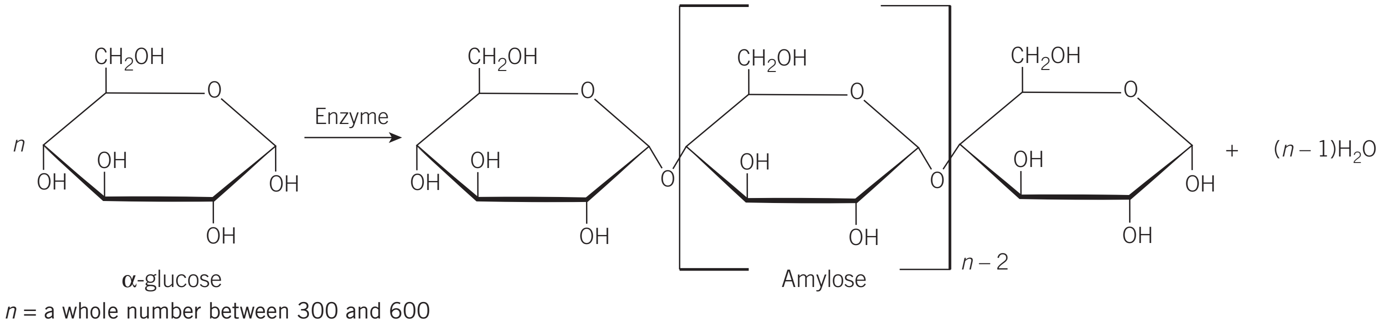

Figure 9B–8 Condensation of α-glucose molecules to give amylose, a linear form of starch

Glycogen is another polysaccharide of glucose. Compared to amylose, the structure of glycogen is highly branched. This is because a mixture of α-1,4-glycosidic bonds and α-1,6-glycosidic bonds exist within glycogen. Notice that glucose units with both α-1,4-glycosidic bonds and α-1,6-glycosidic bonds form the intersection of a branch. Animals synthesise glycogen as a storage of energy. The reason for the extensive branching in the structure will become apparent when we discuss hydrolysis of carbohydrates.

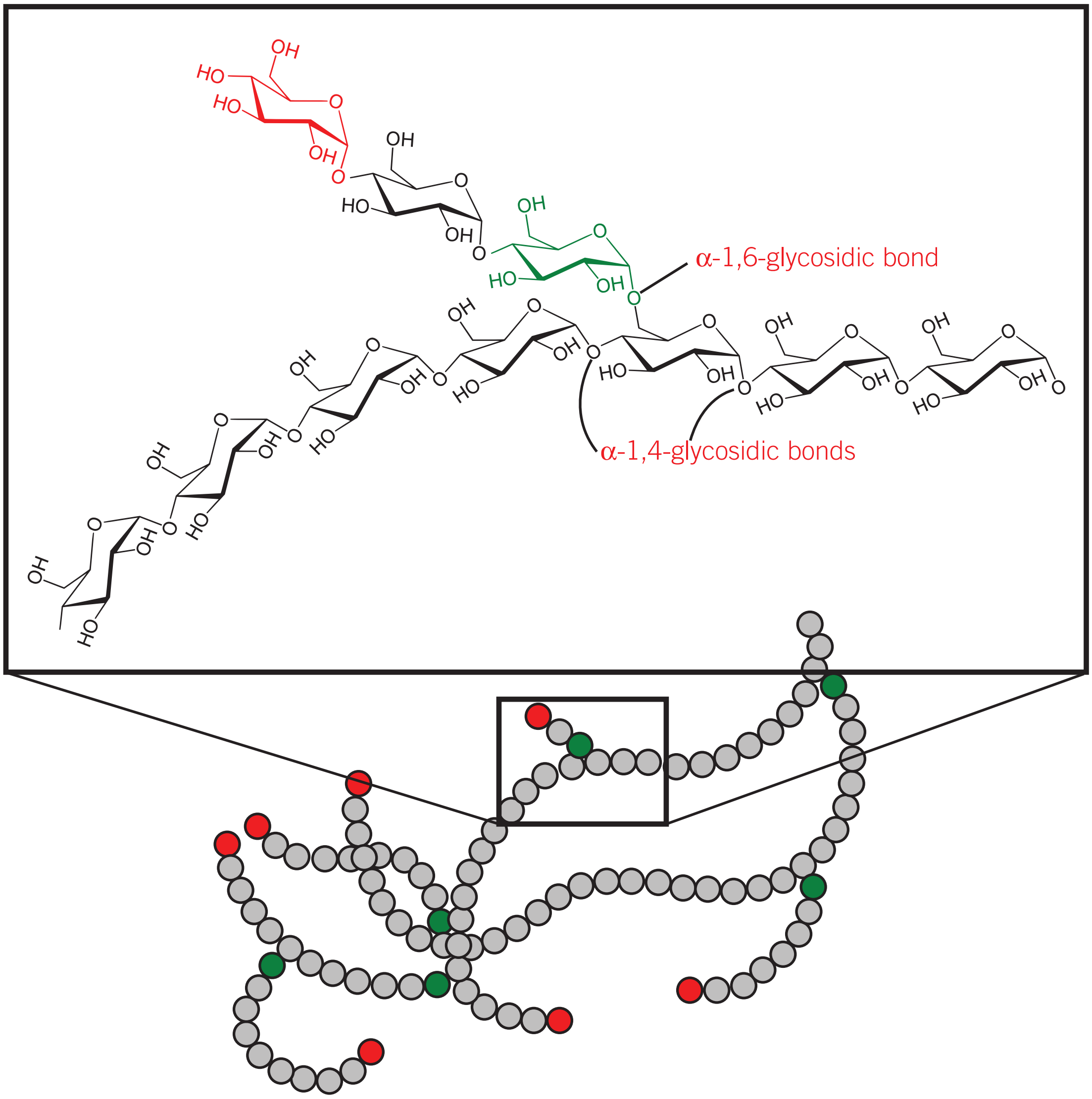

Figure 9B–9 The highly branched structure of glycogen, in which α-glucose units form both α-1,4-glycosidic bonds and α-1,6-glycosidic bonds

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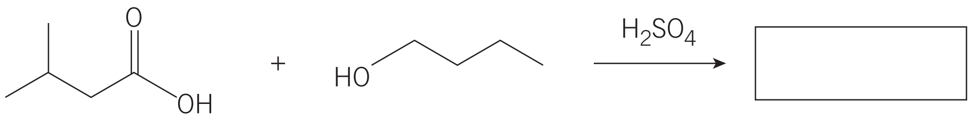
Check-in questions – Set 1

1 Draw all the products formed during the following condensation reactions, in the appropriate format.

a



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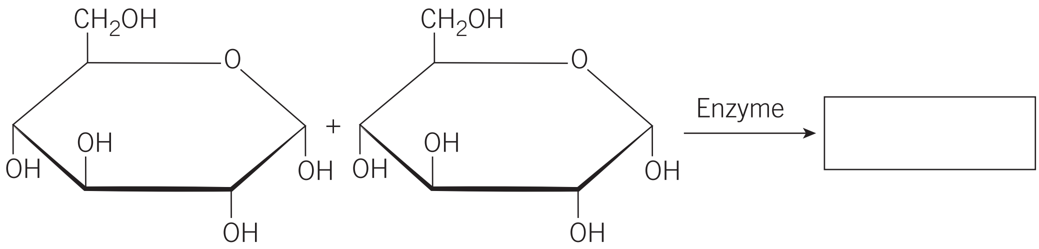

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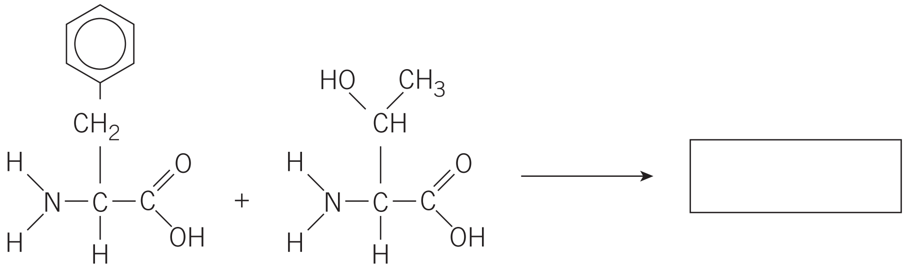

Hydrolysis reaction
a type of chemical reaction involving the addition of water to break a larger molecule into smaller products; *hydro* refers to 'water', *lysis* refers to 'breaking apart'

Hydrolysis reactions

Hydrolysis reactions involve the use of water to break a larger molecule into smaller products. The *hydro* portion of the name refers to 'water' and the *lysis* part refers to 'breaking apart'. Hydrolysis is the reverse process or the backwards reaction of a condensation reaction.

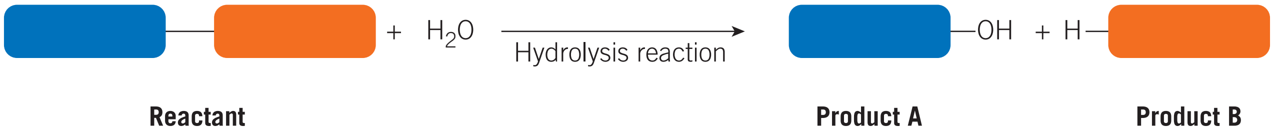

Figure 9B–10 General process for a hydrolysis reaction

Saponification reaction
a reaction that hydrolyses an ester under basic conditions

6A WHAT IS EQUILIBRIUM? LINK

Hydrolysis of esters

Esters can be hydrolysed using water in the presence of a NaOH or KOH catalyst. This reaction is also called a **saponification reaction**. The products are a carboxylic acid and an alcohol. As an example, Figure 9B–11 shows the hydrolysis reaction of propyl butanoate to produce butanoic acid and propan-1-ol. Excess water is typically used in hydrolysis reactions to push the reaction to completion.

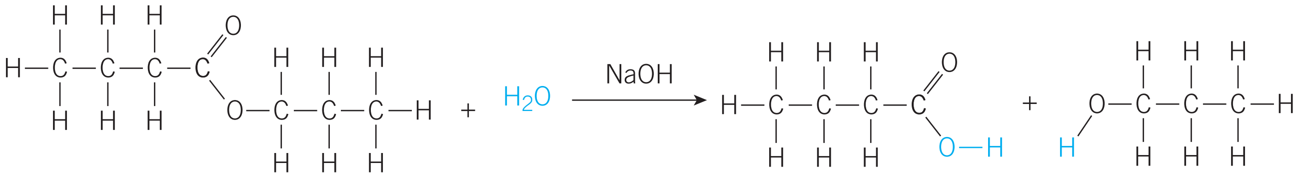

Figure 9B–11 Base hydrolysis of propyl butanoate catalysed by NaOH to produce butanoic acid and propan-1-ol

Hydrolysis of food molecules

The food we consume is broken down by our bodies via a series of chemical reactions. Hydrolysis is one of the first transformations to affect chemical compounds in our food. Our bodies produce a variety of enzymes to speed up the hydrolysis process.

Hydrolysis of fats and oils (lipids)

The triglyceride molecules we consume are hydrolysed in our bodies into glycerol and fatty acids (Figure 9B–12). Special enzymes in the digestive system, such as lipase, help speed up this process. Subsequently, the glycerol and fatty acid molecules can supply our bodies with energy. Outside of our bodies, triglycerides can also be saponified using the same reaction conditions that would normally hydrolyse an ester.

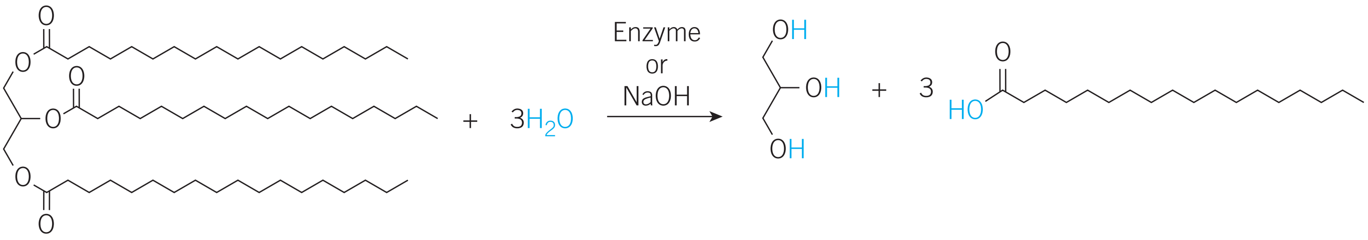

Figure 9B–12 Equation showing the hydrolysis of triglyceride molecules to give glycerol and fatty acids. This reaction can be catalysed by enzymes or by using NaOH.

Hydrolysis of proteins

A variety of food items, including eggs, fish, meat, legumes and dairy, provide us with a rich source of proteins. Once these foods are consumed, the body begins to hydrolyse the polypeptide molecules into smaller peptides and 2-amino acids via hydrolysis reactions. Again, enzymes in the body, such as trypsin and pepsin, have been specifically designed to carry out this reaction. The 2-amino acids from the hydrolysis reaction can be used for energy or building blocks for the body's own proteins. Peptides can also be hydrolysed by boiling in a strong aqueous acid, such as HCl.

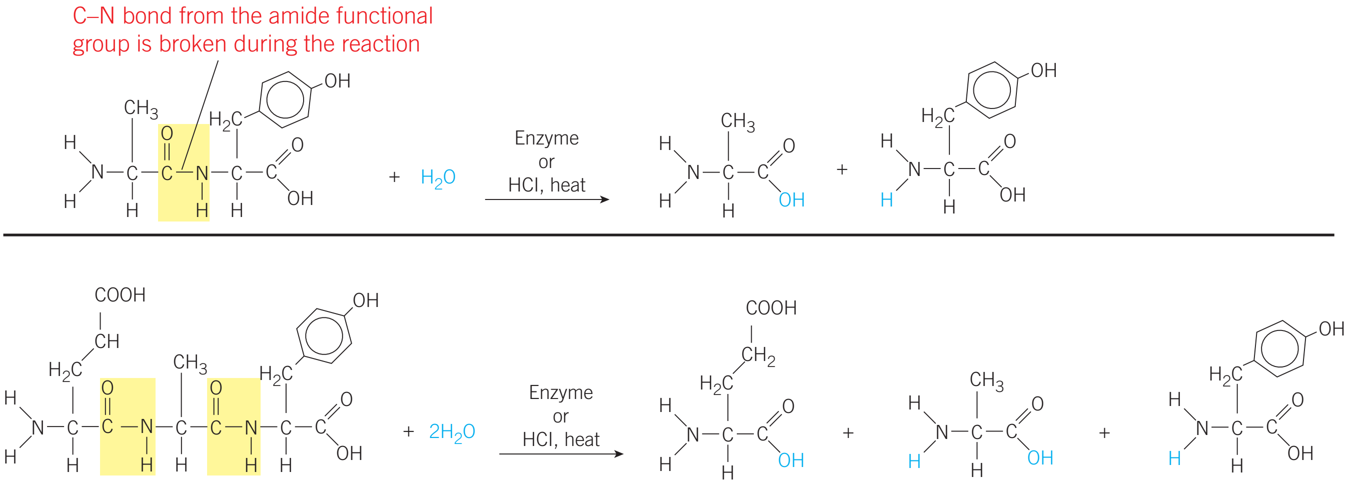
C–N bond from the amide functional group is broken during the reaction

Figure 9B–13 Equations showing the hydrolysis of peptide molecules to give amino acids. This reaction can be catalysed by enzymes or by using HCl(aq) with heat.

WORKSHEET 9B–1 CONDENSATION AND HYDROLYSIS REACTIONS

1B PRODUCTION OF CHEMICAL ENERGY IN NATURE

LINK

Hydrolysis of carbohydrates

Hydrolysis of stored starch or glycogen produces glucose molecules, which living organisms use for energy (ATP) production in cellular respiration. Again, specific enzymes are responsible for speeding up the hydrolysis reaction in biological systems.

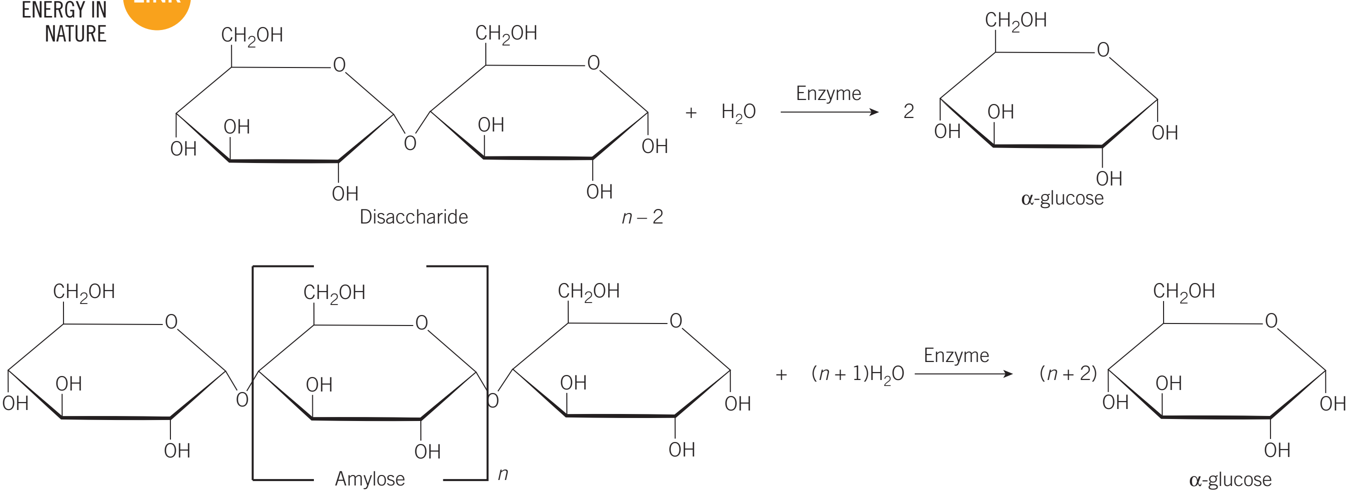

Figure 9B–14 Equations showing the hydrolysis of a disaccharide (top) and polysaccharide (bottom) to give monosaccharides

These enzymes work by hydrolysing the glucose unit at the termini (plural of *terminus*) of the polysaccharide structure. Glycogen, which has a branched structure, has significantly more termini than the linear structure of amylose. Consequently, the structure of glycogen allows a greater number of hydrolysis reactions to occur simultaneously, releasing glucose at a faster rate than amylose. This is an important distinction because animals have the need to perform energy-intensive tasks, such as running, swimming or comprehending a chemistry textbook.

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Transesterification reactions

Synthesising biodiesel from plant-based triglycerides utilises a reaction called **transesterification**. Transesterification involves reacting an ester with an alcohol in the presence of a base to form a new ester. The alcohol becomes the new alkyl group on the ester product. In the case of producing biodiesel, a triglyceride molecule (usually sourced from oils and fats from plants and animals) reacts with a small alcohol, such as methanol or ethanol, to give an ester of a fatty acid (biodiesel) and glycerol. If methanol is used, a fatty acid methyl ester is produced and if ethanol is used, a fatty acid ethyl ester is produced. A typical reaction to synthesise biodiesel involves adding the plant oil to a solution of NaOH in methanol. The NaOH acts as a catalyst in the reaction.

LINK **1A** TYPES OF FUELS

Transesterification a reaction involving an ester and an alcohol to form a new ester. The alcohol involved becomes the new alkyl group of the ester product

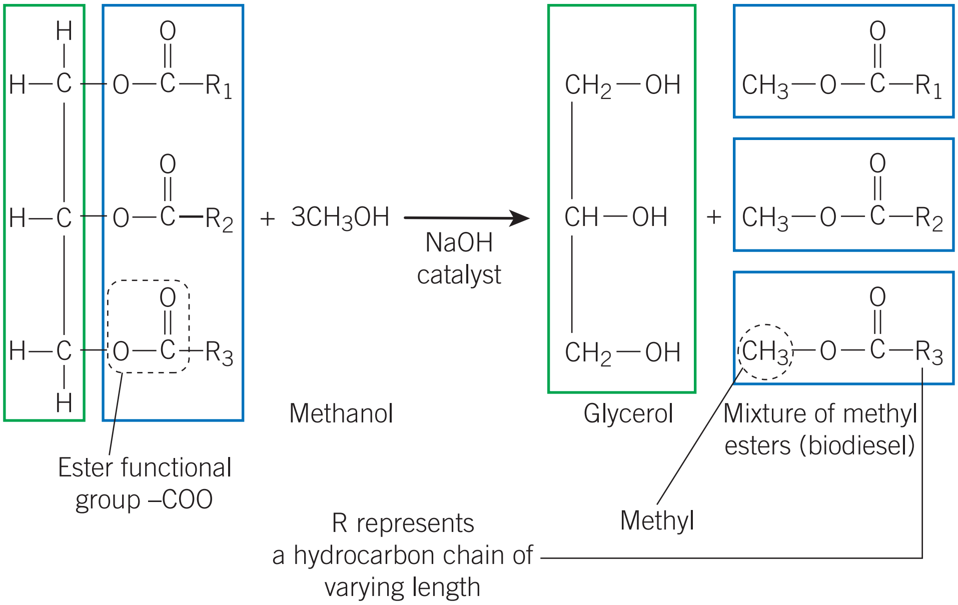
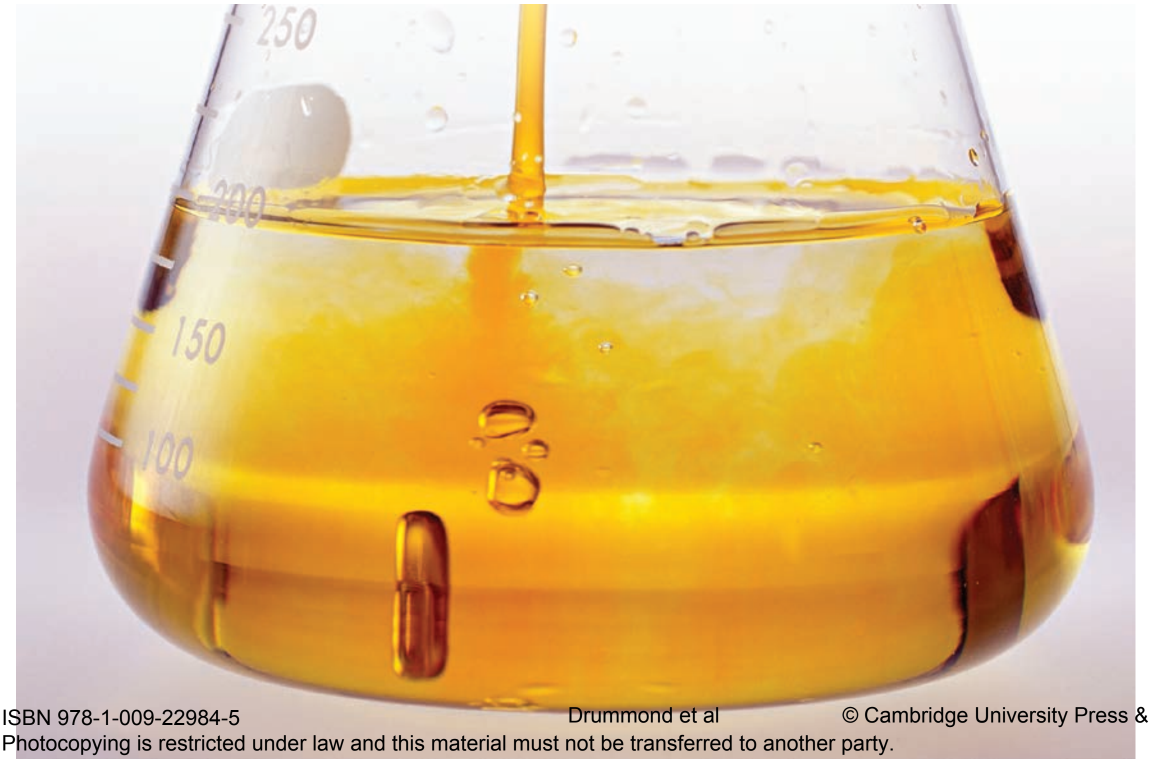


Figure 9B–15 Transesterification reaction between a triglyceride and methanol, producing a mixture of esters, or biodiesel

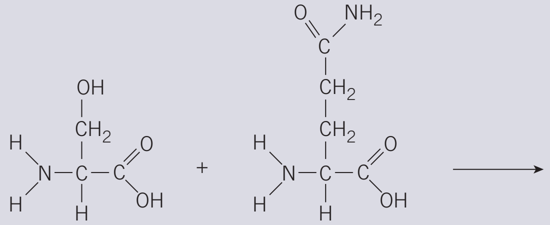


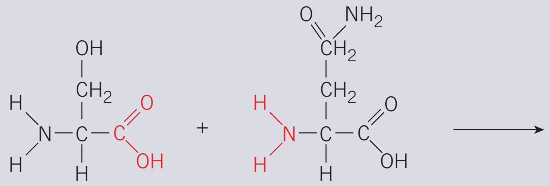
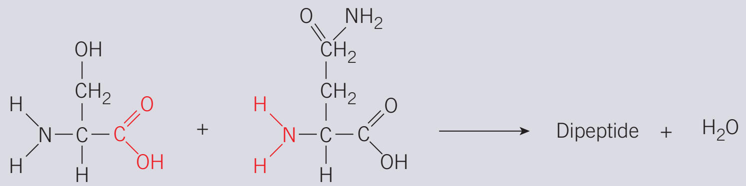
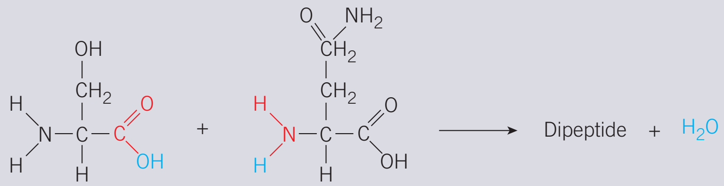
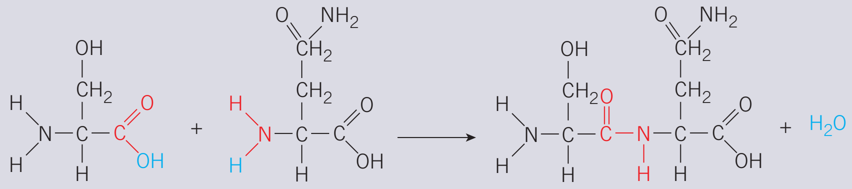
9B SKILLS

Focus on the functional groups and simplifying the problem

VIDEO 9B–1
SKILLS: FOCUS ON THE FUNCTIONAL GROUPS

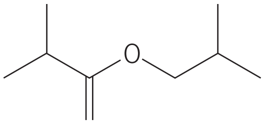
Drawing the product of a condensation reaction can be challenging if complex starting materials are involved. An example of this is drawing a dipeptide product from two amino acids. The way to address this is to focus on the relevant functional groups (carboxyl and amino) and ignore the extra complexities in the amino acids. Below is an approach to tackle such a question.



Step 1	Identify the carboxyl and amino groups that will react.	
Step 2	Recall that a carboxylic acid and an amine react in a condensation reaction to form a dipeptide and a molecule of water.	
Step 3	Identify the atoms in the reactants that will form the water molecule and write H_2O on the product side of the equation.	
Step 4	Draw the structure of the dipeptide using the remaining atoms of the two reactants. Recall that only the functional groups involved in the reaction (red) will change. The majority of the structure (black) can be copied directly from the starting amino acids.	

Section 9B questions

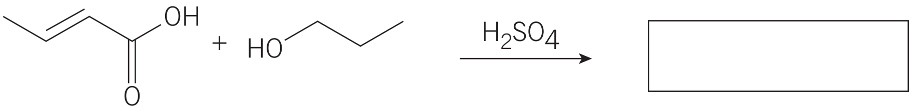
1 Esters can be used to add flavour to a food. The structure of an ester that has a fruity scent is shown below.



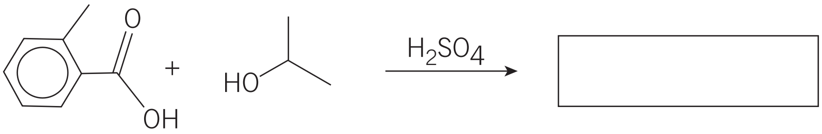
Give the name and draw the structures of the two organic compounds used to produce this ester.

2 Draw all products of the following reactions.

a

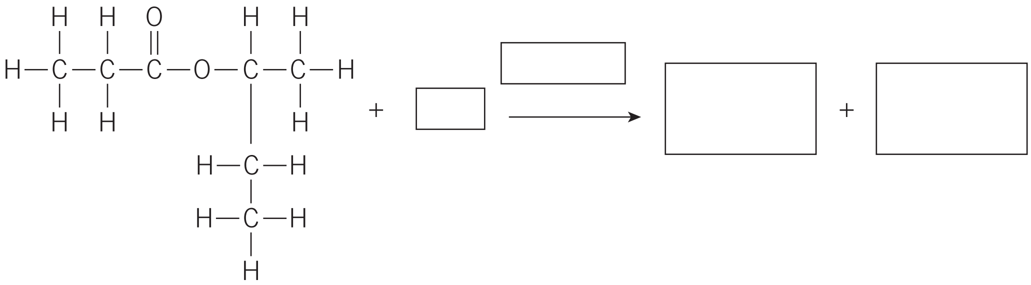


b

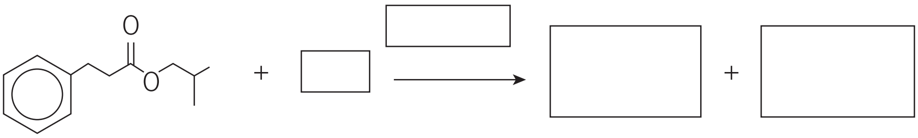


3 Complete the equations of the following hydrolysis reactions.

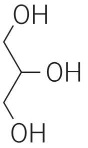
a



b

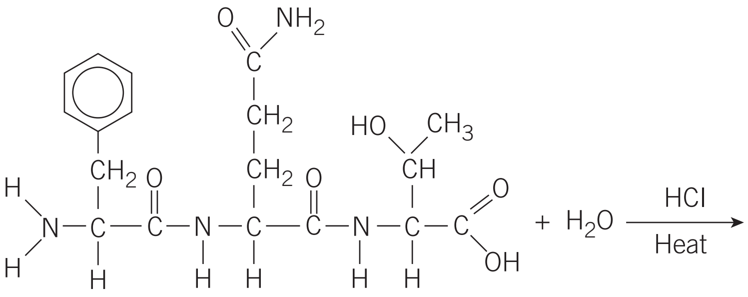


4 Draw the structure of the **two** different triglycerides that can be formed from the following condensation reaction.



$+ \quad 2\ CH_3(CH_2)_{10}COOH \quad + \quad CH_3(CH_2)_7CH{=}CH(CH_2)_7COOH \longrightarrow$

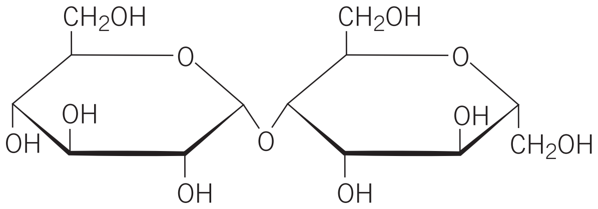
5 Draw the structural formula of the products in the following reaction.



6 A sample of a protein isolated from egg white needs to be hydrolysed to analyse its amino acid composition. In a high school laboratory, the specific enzymes required to hydrolyse the peptide are not available.

- **a** Describe an experiment you could conduct to hydrolyse the protein.
- **b** Determine the number of amino acids in the protein if 0.0134 mol of the protein reacted with 0.2412 mol of water during the hydrolysis.

7 Table sugar, or sucrose, is a disaccharide with the structure shown below.



- **a** Circle the glycosidic bond in sucrose.
- **b** Draw the products of the hydrolysis reaction of sucrose.

8 During the synthesis of biodiesel, it is important to make sure that the reagents are not contaminated with water. This is because a by-product would form if water was introduced to the reaction.

- **a** What is the functional group found in the by-product?
- **b** What type of reaction caused the by-product to form?

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9C Sustainable production of organic compounds

Study Design:

- Calculations of percentage yield and atom economy of single-step or overall reaction pathways, and the advantages for society and for industry of developing chemical processes with a high atom economy
- The sustainability of the production of chemicals, with reference to the green chemistry principles of use of renewable feedstocks, catalysis and designing safer chemicals

Glossary:

Actual yield
Green chemistry
Hazardous substance
Limiting reagent (or reactant)
Percentage atom economy
Percentage yield
Renewable feedstock
Stoichiometric
Theoretical yield
Waste

ENGAGE

Valuable natural products

Many organic compounds that are used in everyday products, such as plastics and pharmaceuticals, can be produced using sustainable methods. Identifying and using renewable feedstocks, such as plant biomass and waste materials, is a key driver of sustainability. Curcumin, sourced from the spice turmeric, is an example of an organic compound with medicinal properties that can be sourced from a renewable feedstock. There is some evidence to indicate that it has a variety of potential health benefits, including anti-inflammatory and anticancer effects, but research is ongoing. It could be used as a natural remedy for a range of conditions, such as inflammation and arthritis. Alternatively, it can also be synthesised using green chemistry techniques to reduce the use of hazardous chemicals and waste generation. As a result, curcumin is an example of a potentially valuable medicinal compound that can be sustainably produced from a renewable source.

Figure 9C–1 Powder from the spice turmeric contains the medicinal compound curcumin.

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EXPLAIN

Evaluating the efficiency of reactions and pathways

Evaluating the outcome of a reaction is an important part of performing any reaction. After all, it would be pointless and even wasteful to start a reaction without assessing its results. At times, this assessment may simply involve making observations to gain an experience. Other times, specific measurements and data are collected in a scientifically rigorous manner to evaluate the efficiency of a reaction. **Percentage yield** and **percentage atom economy** are two separate measurements that contribute to determining whether a reaction is efficient at producing the intended product in a cost-effective and sustainable manner.

Percentage yield a measure of the amount of product obtained as a percentage of the theoretical maximum amount of product that could be obtained from a reaction

Percentage atom economy the measure of the percentage of the atoms in the reactants that are incorporated into the desired product

Percentage yield

Recall that reactions do not always proceed until all reactants are converted to products. In fact, most reactions reach a dynamic equilibrium where the reaction vessel contains a mixture of reactants and products. A method to evaluate whether the reaction is efficient at producing the desired product is to determine its percentage yield. The percentage yield of a chemical reaction is a measure of the amount of the **actual yield** as a percentage of the **theoretical yield**. This is summarised in the formula below.

6C LE CHÂTELIER'S PRINCIPLE LINK

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

Actual yield the actual quantity of product obtained from a reaction

The actual yield is the quantity of product that is obtained from the reaction. This is quoted as either the mass, usually in grams, or amount, in mol, of product. The theoretical yield is the maximum quantity of product that can be obtained if all the **limiting reagent** (or **reactant**) is converted to the product. The theoretical yield is calculated using the stoichiometry of the reaction.

The following worked examples demonstrate how to determine and apply percentage yield of reactions in different scenarios.

VIDEO WORKED EXAMPLE 9C–1

Worked example 9C–1: Calculating the percentage yield when the mass of reactant is known

A 45 g sample of ethanol was oxidised to ethanoic acid using acidified $KMnO_4$. The product was purified by distillation and had a mass of 38 g. Calculate the percentage yield of this oxidation reaction.

Solution

	Logic	Process
Step 1	Write an equation for the reaction.	$CH_3CH_2OH \xrightarrow{H^+/KMnO_4} CH_3COOH$ Note that it is not always necessary to fully balance the equation. In this case, it is sufficient to just balance the carbon atoms on both sides of the equation. The equation shows a 1:1 ratio of reactant to product.
Step 2	Determine the amount, in mol, of the reactant.	$n(CH_3CH_2OH) = \frac{m}{M}$ $= \frac{45\ g}{46\ g\ mol^{-1}}$ $= 0.98\ mol$

Theoretical yield the theoretical maximum quantity of product that could be obtained from a reaction if all the limiting reagent is converted to the product

Limiting reagent (or **reactant**) the reagent that is completely used up in a reaction and therefore limits the amount of product that can be formed

Step 3	Use the mole ratio to determine the amount, in mol, of product that could be obtained if all the reactant is converted to product.	$n(CH_3COOH) = \frac{1}{1} \times n(CH_3CH_2OH)$ $= 0.98$ mol
Step 4	Determine the mass of the product in Step 3. **This is the theoretical yield.**	$m(CH_3COOH) = n \times M$ $= 0.98 \text{ mol} \times 60 \text{ g mol}^{-1}$ $= 58.7$ g
Step 5	Calculate the percentage yield.	$\text{Percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100$ $= \frac{38 \text{ g}}{58.7 \text{ g}} \times 100$ $= 65\%$

Worked example 9C–2: Calculating the mass of product when the percentage yield is known

VIDEO
WORKED EXAMPLE 9C–2

The addition reaction between but-2-ene and Br_2 has a 93.0% yield. If 35.0 g of but-2-ene was added to excess Br_2, calculate the mass of the product obtained.

Solution

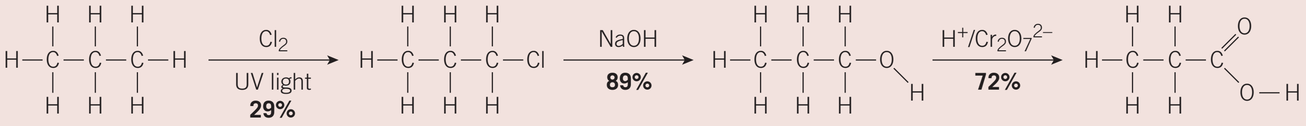
	Logic	Process
Step 1	Write an equation for the reaction.	$CH_3CHCHCH_3 + Br_2 \rightarrow CH_3CHBrCHBrCH_3$
Step 2	Determine the amount, in mol, of the reactant.	$n(CH_3CHCHCH_3) = \frac{m}{M}$ $= \frac{35.0 \text{ g}}{56.0 \text{ g mol}^{-1}}$ $= 0.625$ mol
Step 3	Use the mole ratio to determine the amount, in mol, of product that could be obtained if all the reactant is converted to product.	$n(CH_3CHBrCHBrCH_3)$ $= \frac{1}{1} \times n(CH_3CHCHCH_3)$ $= 0.625$ mol
Step 4	Determine the mass of the product in Step 3. **This is the theoretical yield.**	$m(CH_3CHBrCHBrCH_3) = n \times M$ $= 0.625 \text{ mol} \times 215.8 \text{ g mol}^{-1}$ $= 135$ g
Step 5	Calculate the actual yield.	$\text{Actual yield} = \frac{\text{Percentage yield}}{100} \times \text{theoretical yield}$ $\text{Actual yield} = \frac{93.0\%}{100\%} \times 135 \text{ g}$ $= 125$ g $m(CH_3CHBrCHBrCH_3)_{actual} = 125$ g

The percentage yield can also be determined for a multi-step reaction pathway. In this case, the percentage yields of each individual step are multiplied to give the overall percentage yield of the entire pathway. This means that the yield of every step influences the overall percentage yield. A single low-yielding reaction in a sequence can drastically affect the amount of product that is formed at the end. Furthermore, given that actual yields are always less than 100%, long sequences usually suffer from poor overall percentage yield of product.

VIDEO
WORKED
EXAMPLE 9C–3

Worked example 9C–3: Calculating the overall percentage yield

A reaction pathway for the synthesis of propanoic acid is shown below. Given the percentage yields of each individual step stated below the arrows, calculate the overall percentage yield of the sequence.



Solution

	Logic	Process
Step 1	Recall that the individual percentage yields of each step are multiplied together to obtain the overall percentage yield of the pathway.	Overall percentage yield $= \frac{29}{100} \times \frac{89}{100} \times \frac{72}{100} \times 100$ $= 19\%$

Percentage atom economy

Waste
unwanted substances that have no further value in production

Designing reactions that produce less **waste** or no waste is an essential goal of green chemistry. By-products formed during a reaction contribute to the waste that may need to be processed and disposed of at the end of a reaction. Atom economy is one way of evaluating the amount of potential by-products that could form during a reaction. Percentage atom economy is the measure of the percentage of the atoms in the reactants that are incorporated into the desired product. One of the aims of designing a green process is to maximise atom economy so that the product accounts for as much of the material added to the reaction as possible. A reaction with high atom economy would generate fewer by-products and, by extension, less waste. The illustration in Figure 9C–2 compares reactions with high versus low atom economy.

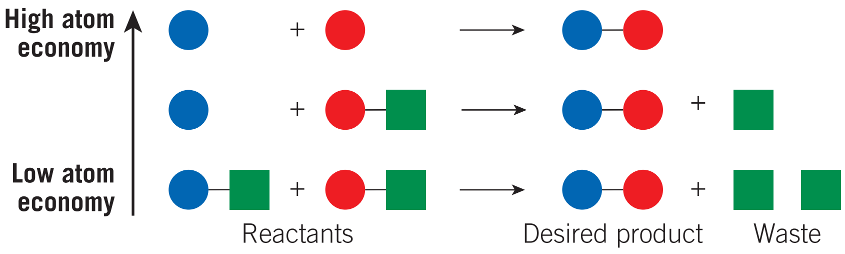


Figure 9C–2 Illustration of reactions with high and low atom economy

NOTE

Waste may include by-products from a reaction, contaminated solvents after a reaction, unreacted starting materials that are uneconomical to reclaim or excess products that are not needed further down the production line.

Atom economy can be calculated by dividing the total molar mass of the desired product by the molar mass of all reactants, then expressed as a percentage. The equation below summarises this process.

$$\text{Percentage atom economy} = \frac{\text{molar mass of desired product}}{\text{molar mass of all reactants}} \times 100$$

Given that mass is conserved in all reactions, we can assume that the mass of all products equals the mass of all reactants. Therefore, the alternative equation for atom economy is:

$$\text{Percentage atom economy} = \frac{\text{molar mass of desired product}}{\text{molar mass of all products}} \times 100$$

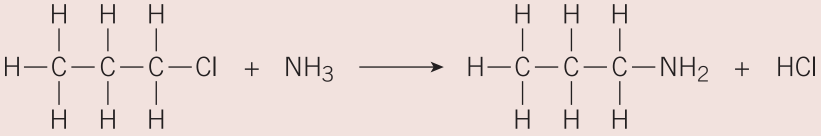
It is worthwhile noting that reagents that remain chemically unchanged at the end of a reaction are not included in the calculation of atom economy. This includes substances like solvents and catalysts.

Worked example 9C–4 demonstrates a calculation of percentage atom economy of a given reaction.

Worked example 9C–4: Calculating percentage atom economy

VIDEO
WORKED
EXAMPLE 9C–4

The following reaction is used to synthesise propan-1-amine from 1-chloropropane. Calculate the percentage atom economy of the reaction.



Solution

	Logic	Process
Step 1	Calculate the total molar mass of all products.	$M(CH_3CH_2CH_2NH_2) + M(HCl) = 59.0 + 36.5$ $= 95.5\ g\ mol^{-1}$
Step 2	Calculate the molar mass of the desired product.	$M(CH_3CH_2CH_2NH_2) = 59.0\ g\ mol^{-1}$
Step 3	Calculate percentage atom economy.	$\text{Percentage atom economy} = \frac{59\ g\ mol^{-1}}{95.5\ g\ mol^{-1}} \times 100$ $= 61.8\%$

A similar procedure can be used to calculate the atom economy of a reaction pathway. In this case, the reactants added at each step need to be clearly identified. It is important to only account for the reactants **added** after the first step so that the main organic compound is not double-counted at each subsequent step.

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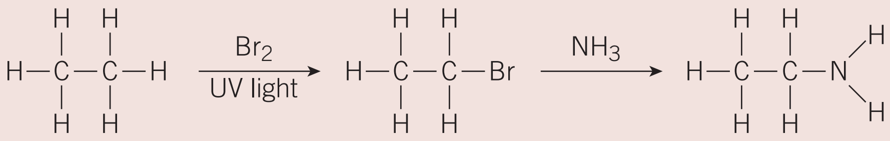
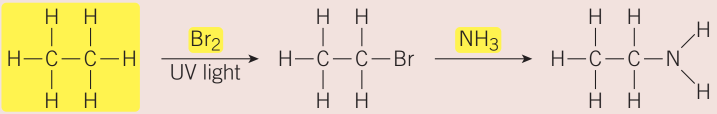
VIDEO
WORKED
EXAMPLE 9C–5

Worked example 9C–5: Calculating the percentage atom economy of a reaction pathway

Calculate the percentage atom economy of the reaction pathway shown below.

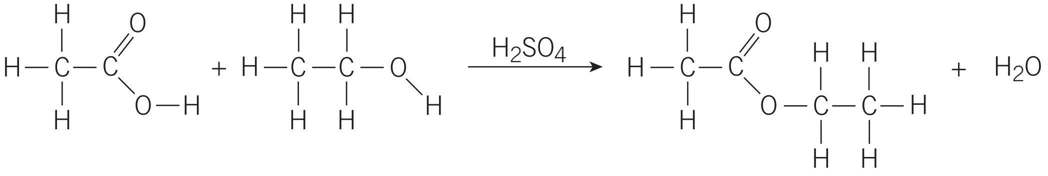


Solution

	Logic	Process
Step 1	Identify all added reactants in the sequence.	
Step 2	Calculate the total molar mass of all added reactants.	$M(CH_3CH_3) + M(Br_2) + M(NH_3) = 30 + 159.8 + 17$ $= 206.8\ g\ mol^{-1}$
Step 2	Calculate the molar mass of the desired product.	$M(CH_3CH_2NH_2) = 45.0\ g\ mol^{-1}$
Step 3	Calculate percentage atom economy.	Percentage atom economy $= \frac{45.0\ g\ mol^{-1}}{206.8\ g\ mol^{-1}} \times 10$ $= 21.8\%$

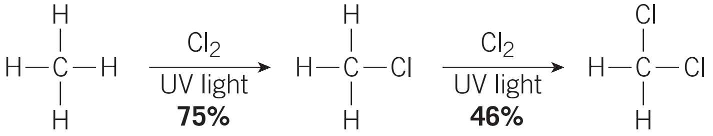
Check-in questions – Set 1

1 A 56 g sample of ethanoic acid reacted with excess ethanol in the presence of H_2SO_4 catalyst according to the reaction shown below. The reaction produced 42 g of ethyl ethanoate.



- **a** Calculate the percentage yield of the reaction.
- **b** Calculate the percentage atom economy of the reaction.

2 The reaction pathway to synthesise dichloromethane is shown below.



WORKSHEET
9C–1
CALCULATING
PERCENTAGE
YIELD AND
PERCENTAGE
ATOM ECONOMY

- **a** Calculate the overall percentage yield of the reaction pathway.
- **b** Calculate the overall percentage atom economy for the reaction pathway.

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Applying green chemistry principles to sustainable chemical production

A sustainable chemical process is one that minimises environmental impact and consumption of non-renewable resources while maintaining or improving the economic and social benefits associated with the product. Towards this end, Paul Anastas and John Warner published the 12 principles of **green chemistry** in 1998. The main concept behind these green chemistry principles is to use our knowledge, skills and creativity in the field of chemistry to reduce or eliminate the use and production of **hazardous substances**. In turn, continuous improvement in manufacturing processes would minimise threats to our health and reduce the impact on the environment and other living organisms.

Green chemistry the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances

Hazardous substance a substance that can cause harm to your health or the environment

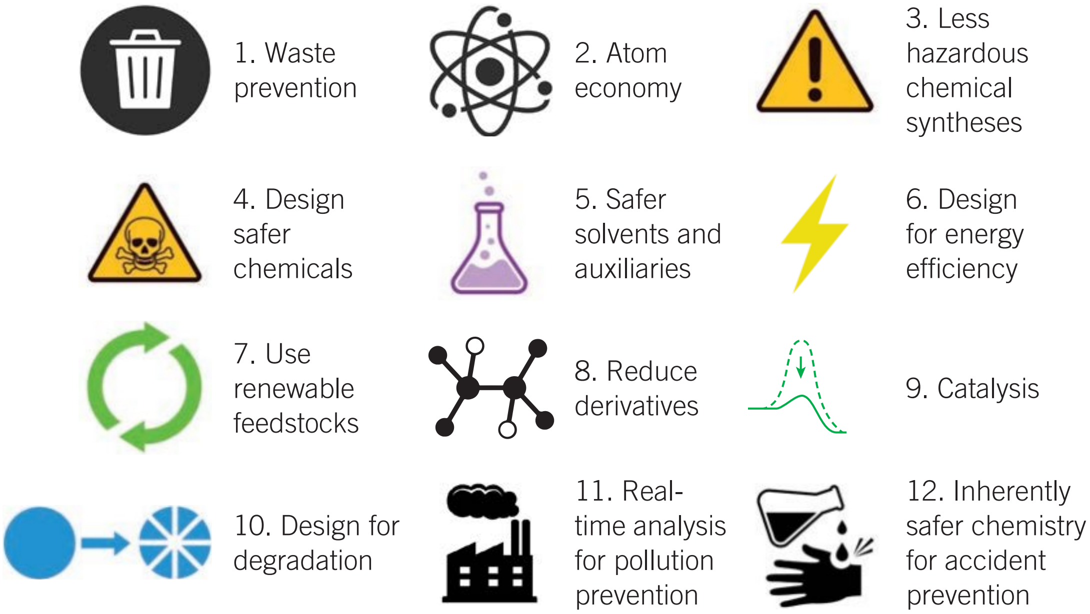

Figure 9C–3 The 12 principles of green chemistry proposed by Anastas and Warner

When applying green chemistry to achieve sustainability in organic synthesis, we strive to:

- use **renewable feedstocks** where possible.
- use catalysis to reduce or eliminate by-products and decrease the energy demands of the reaction.
- design safer chemicals that have low toxicity to humans and other living organisms and low impact on the environment.

LINK **1A** TYPES OF FUELS

Renewable feedstock raw material that is used to supply an industrial process and can be readily replenished

LINK **4A** FUEL CELLS

Use of renewable feedstocks

As discussed in Chapter 4, renewable feedstocks are resources that can be replenished at a faster rate than they are consumed. Using renewable feedstocks, such as biomass derived from plant, animal or waste materials, in chemical production can provide several advantages over traditional petrochemical feedstocks. These include:

- reducing dependence on finite, non-renewable resources.
- reducing the amount of waste produced since many renewable feedstocks are by-products of other industries.
- creating economic growth opportunities in rural areas where the agricultural feedstocks are grown and processed.

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UNIT 1 LINK

7A FEATURES OF ELECTROLYTIC CELLS LINK

9B ORGANIC REACTIONS: CONDENSATION AND HYDROLYSIS LINK

1A TYPES OF FUELS LINK

However, it is important to note that there are also challenges associated with using renewable feedstocks, such as scalability, consistency, cost-competitiveness and agriculture's impact on the environment. Additionally, the sustainability benefits of renewable feedstocks depend on the specific feedstock and how it is produced, processed and transported.

An example of using renewable feedstocks in the production of organic compounds is the conversion of triglycerides, which are sourced from animal fat or plant oil, to give biodiesel. The specific transesterification reaction involved in this process was discussed in Section 9B. Another example is the synthesis of bioethanol from corn or sugar cane feedstocks. Agricultural production of sugar cane takes less than one year from seed. Upon harvesting, the glucose from the feedstock can be converted to bioethanol, which is a versatile chemical with applications as a fuel, solvent, cleaning agent, antiseptic and other industrial uses.

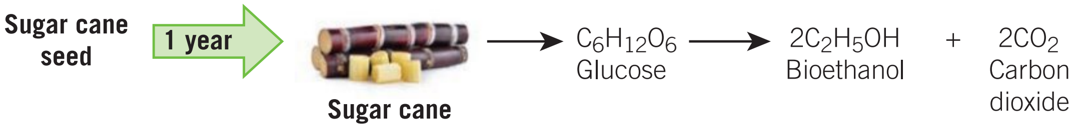

Figure 9C–4 Production of bioethanol from sugar cane, a renewable feedstock

Catalysis

5B FACTORS AFFECTING REACTION RATE LINK

Stoichiometric the quantity of reagents, as a molar ratio, as prescribed by the balanced equation of a reaction

As discussed in Chapter 5, catalysis is the process of using a catalyst to increase the rate of a chemical reaction. In most catalytic reactions, only a small amount of catalyst is required to speed up the transformation because the catalyst is not consumed during the reaction. In contrast, reactions that are not catalysed require **stoichiometric** reagents to affect the chemical change and/or require higher temperature and pressure to drive the reaction forwards. In summary, catalysis is an important part of sustainable production of organic compounds because it has the potential to:

- reduce the energy demand of conducting a reaction.
- reduce the time required to obtain products.
- reduce the amount of waste generated upon completion of a reaction.

Furthermore, the development of new catalysts enables new reaction pathways that may have been too slow or ineffective in the past to become commercially viable. Such an advancement allows us to build complex molecular structures with fewer reaction steps, achieve higher atom economy and use less energy or hazardous substances compared to existing technologies. An example of this is the synthesis of ibuprofen, an anti-inflammatory medicine. The industrial production of ibuprofen in 1961 by the Boots Pure Drug Company required six steps using stoichiometric reagents (Figure 9C–5). The sequence suffers from low atom economy and uses various hazardous substances like aluminium trichloride ($AlCl_3$) to effect the chemical transformations.

Advancements in catalysis enabled a more efficient sequence to be developed in 1992 by the Hoechst Company. Beginning with the same starting material, the newer sequence takes advantage of two catalytic reactions to build the same ibuprofen product in just three steps. In comparison with the earlier process, the Hoechst Company process has higher atom economy, generates less waste and recycles the hydrogen fluoride (HF) used in the first step for use in subsequent batches. Examples like this demonstrate how catalysis can make our chemical manufacturing greener and more sustainable.

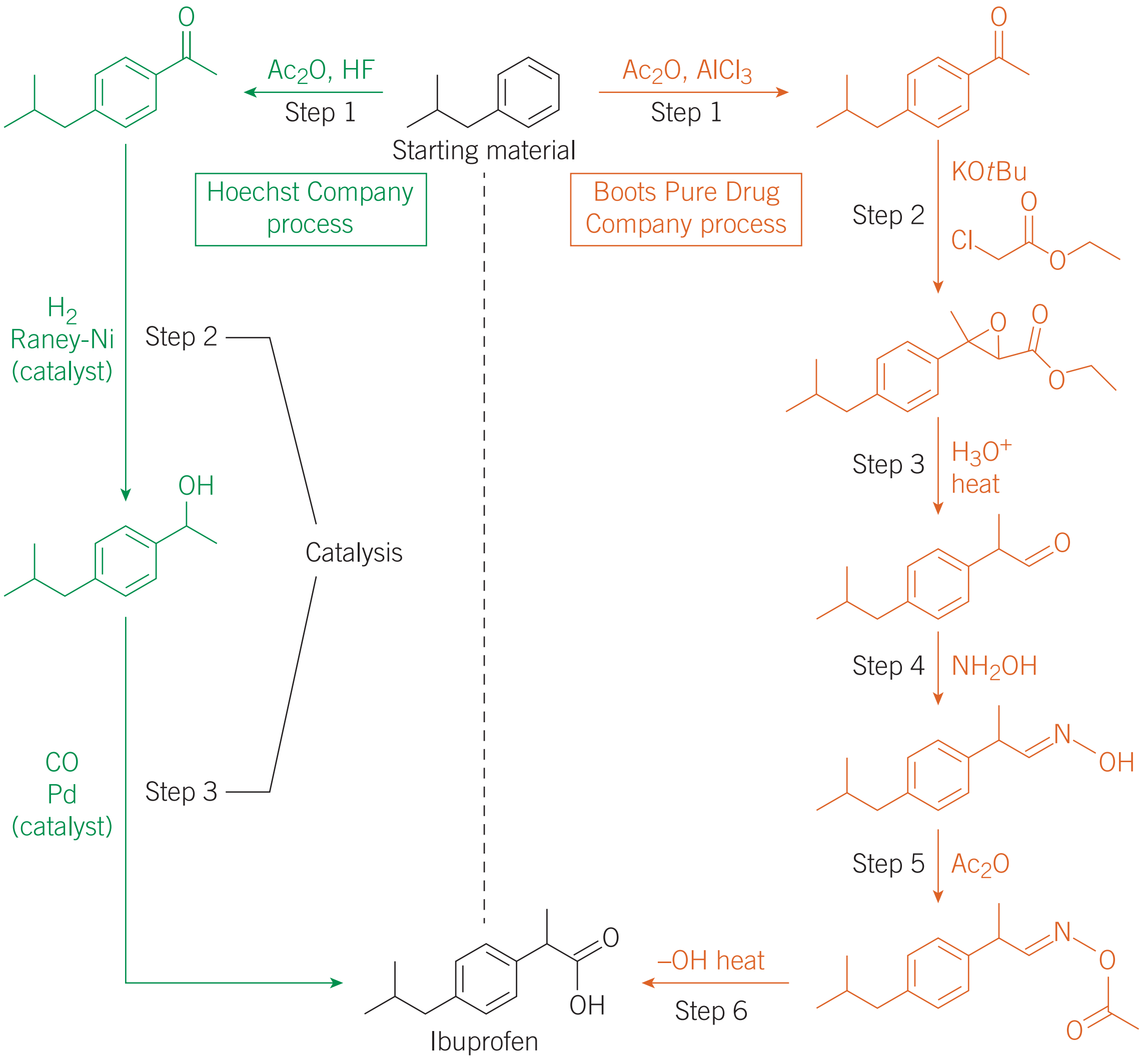

Figure 9C–5 Two alternative synthetic pathways to synthesise ibuprofen. The green pathway by Hoechst Company features two catalytic steps to produce the desired product in a total of three steps. In contrast, the orange pathway by Boots Pure Drug Company involves six steps using stoichiometric reagents.

Designing safer chemicals

Designing safer chemicals is one of the 12 principles of green chemistry and an important aspect of achieving sustainable chemical manufacturing. Certain chemicals are safe to handle, while others are more toxic to humans and animals or have a greater impact on the environment. Towards this end, reactions and processes should be designed to reduce or eliminate the use and production of hazardous chemicals. Some of the strategies to achieve this include:

- use less toxic or non-toxic starting materials and reagents
- develop reactions that produce less by-products (high atom economy) or non-toxic by-products
- design chemicals that break down into non-toxic or less toxic substances to reduce their impact on the environment
- explore structurally similar compounds that can serve the same purpose with less toxicity.

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An example of using a structurally related substance as a replacement for a toxic compound is toluene. The structure and reactivity of a compound are the main determinants of its toxicity. Certain structures can interact with enzymes, receptors or molecules in our body leading to adverse effects. Traditionally, benzene was used as a common solvent in many organic reactions. However, the frequency of its use has diminished when it was discovered that benzene oxidised in the liver to form a carcinogen that led to leukaemia, a cancer of the blood cells (Figure 9C–6). We can avoid benzene's toxic effects by using toluene, a viable replacement in most cases. Compared to benzene, toluene has an extra methyl group. The added methyl group in toluene means that its oxidation in the liver produces benzoic acid, a non-toxic compound.

Through understanding how reactions work, the by-products that are formed and how molecules interact with living organisms, we can design safer reactions and produce safer chemicals. This would not only benefit our lives but also the lives of all other living organisms and the environment that we all inhabit.

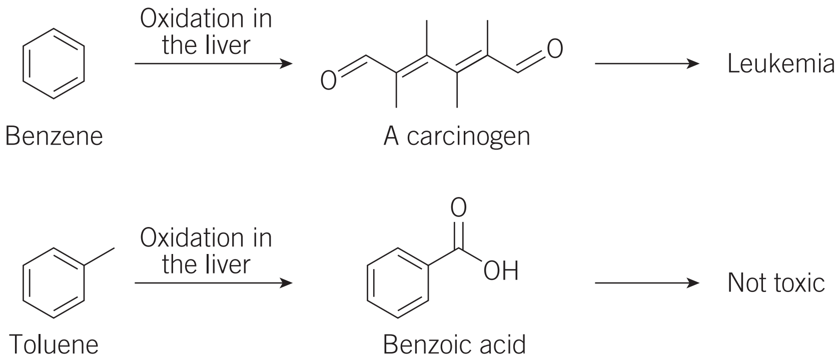

Figure 9C–6 Comparison of toxic effects of benzene and toluene in our body

VIDEO 9C–1
SKILLS: A DEEPER DIVE INTO ATOM ECONOMY

9C SKILLS

A deeper dive into atom economy

A part of the current Study Design requires you to address 'the advantages for society and for industry of developing chemical processes with a high atom economy'. This necessitates you having the skill to link the concept of atom economy to broader contexts from society and industry. While processes with high atom economy generate fewer by-products, you may need to incorporate more depth in your responses should the question demand it.

For example, consider the question:

Explain why chemical processes with higher atom economy are beneficial to the environment.

A simple response such as 'Processes with high atom economy generate fewer by-products' would unlikely afford you full marks.

To access all available marks, you may need to consider **why** generating fewer by-products during manufacturing of organic compounds is a beneficial trait.

For example:

Reactions that have high atom economy produce fewer by-products. This means that less waste is generated and disposed of into the environment, reducing the environmental impact of running the reaction.

Some other advantages of high atom economy are summarised in the table below. You and your peers may be able to collaboratively think of more. Applying them in a suitable context is a skill you should continue to practise.

Table 9C–1 Advantages of reactions with high percentage atom economy

Advantage	Explanation
Less environmental impact	Reactions that have high percentage atom economy produce fewer by-products. This means that less waste is generated and disposed of into the environment, reducing the environmental impact of running the reaction.
Better safety	By-products formed during a reaction may potentially be toxic to humans. Handling the waste after a reaction and transporting it to a waste facility are also potential hazards. Therefore, reactions that produce fewer by-products are likely to be safer to conduct.
Reduced cost	Using reactions with high percentage atom economy is one of the ways to save on the costs associated with an industrial process. This is because reactions with high atom economy generate less waste, which in an industrial process is associated with the need for frequent equipment cleaning, maintenance and disposal of waste. Therefore, high atom economy may reduce the overall cost of producing the desired product.
Better quality of product	Reactions with high percentage atom economy form fewer by-products, which may potentially lead to products of higher quality. The product formed during the reaction needs to be separated from any by-products that are also formed. Forming fewer by-products leads to a simpler separation process, resulting in a higher purity of the desired product.

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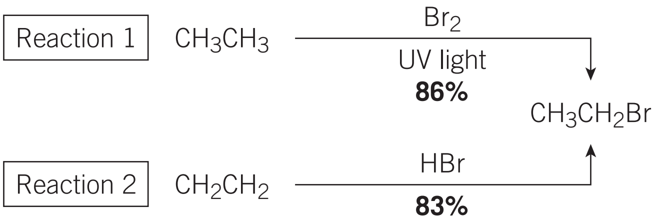
Section 9C questions

1 During a hydrolysis reaction, 93 g of butyl ethanoate reacted to give 22 g of ethanoic acid. Calculate the percentage yield of the reaction.

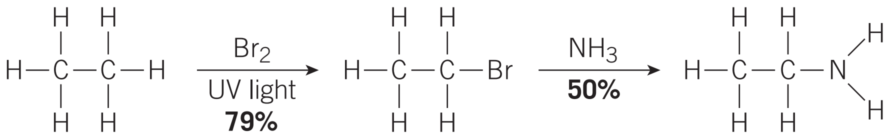
2 Chloromethane and bromomethane are two molecules that can be produced from methane via a substitution reaction.
   - a In each case, calculate the percentage atom economy of the reaction.
   - b Why is there a difference seen between the percentage atom economy of the two processes?

3 Bromoethane can be synthesised from two different reactions, as shown below.



   - a Calculate the percentage atom economy of each reaction.
   - b If a percentage yield of 86.0% can be achieved for Reaction 1, calculate the mass of product if 100 g of CH_3CH_3 was reacted.
   - c From a sustainability perspective, which reaction is preferred when synthesising bromoethane? Explain your choice.

4 The reaction pathway to synthesise ethanamine is shown below.



   - a Calculate the overall percentage yield of the reaction pathway.
   - b Determine the percentage atom economy of the reaction sequence.

5 Define 'percentage atom economy' and explain why manufacturing processes with high percentage atom economy are potentially safer for the workers at a chemical plant.

6 Renewable feedstock, such as sugar cane, can be converted to ethanol, a valuable industrial chemical. Research two other renewable feedstocks and the product(s) derived from them.

7 How does catalysis contribute to sustainable chemical manufacturing?

8 How can improving the catalyst used for a reaction lead to a more sustainable manufacturing process?

Chapter 9 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
9A.1	Classify the type of reaction (substitution, addition or oxidation) when given an equation or a description of the reaction	2☐, 6☐
9A.2	Write the equations (including reactants, products, reaction conditions and catalysts) of substitution reactions to synthesise primary haloalkanes and primary alcohols	6☐, 11☐
9A.3	Write the equations (including reactants, products, reaction conditions and catalysts) of addition reactions of alkenes	1☐, 2☐, 7☐, 11☐
9A.4	Write the equations (including reactants, products, reaction conditions and catalysts) of oxidation reactions to synthesise carboxylic acids	3☐, 10☐
9A.5	Draw reaction pathways (including reactants, intermediate compounds, products, reaction conditions and catalysts) to synthesise carboxylic acids or amines	10☐, 16☐
9B.1	Classify the type of reaction (condensation, hydrolysis or transesterification) when given an equation or a description of the reaction	12☐, 15☐
9B.2	Write the equations (including reactants, products, reaction conditions and catalysts) of condensation reactions to synthesise esters and other biologically important molecules (proteins, starch, glycogen and lipids)	5☐, 11☐, 12☐
9B.3	Write the equations (including reactants, products, reaction conditions and catalysts) of hydrolysis reactions to convert esters and other biologically important molecules (proteins, starch, glycogen and lipids) into smaller molecules	4☐, 11☐, 13☐
9B.4	Write the equations (including reactants, products, reaction conditions and catalysts) of transesterification reactions to convert plant triglycerides into biodiesel	15☐
9C.1	Calculate the overall percentage yield of a reaction or a reaction pathway	9☐, 16☐
9C.2	Calculate the overall percentage atom economy of a reaction or a reaction pathway	8☐, 14☐
9C.3	Discuss the advantages of developing chemical processes with a high percentage atom economy	14☐, 16☐
9C.4	Discuss how the sustainable production of chemicals can be achieved through the application of green chemistry principles	14☐, 15☐

Multiple-choice questions

1 Which of the following can convert an alkene to an alkane?

A H_2O
B HCl
C $KMnO_4$
D H_2

2 Consider the following equation:

$$CH_2CH_2 + H_2O \rightarrow CH_3CH_2OH$$

This reaction is an example of

A a condensation reaction.
B a substitution reaction.
C an addition reaction.
D a hydrolysis reaction.

3 Which of the following is converted to hexanoic acid by acidified potassium dichromate?

A hexan-1-ol
B hexan-1-amine
C 1-chlorohexane
D methyl hexanoate

4 Which of the following is converted to hexanoic acid by treatment with aqueous sodium hydroxide?

A hexan-1-ol
B hexan-1-amine
C 1-chlorohexane
D methyl hexanoate

5 An ester with the formula $CH_3CH_2COOCH_2CH_3$ is made from

A propanol and propanoic acid.
B propanol and ethanoic acid.
C ethanol and propanoic acid.
D ethanol and ethanoic acid.

6 Which of the following is a substitution reaction?

A $C_3H_7Cl \rightarrow C_3H_6$
B $C_3H_7Cl \rightarrow C_3H_6Cl_2$
C $C_3H_6 \rightarrow C_3H_8O$
D $C_3H_6 \rightarrow C_3H_8$

7 An alkene with the molecular formula C_5H_{10} was reacted with H_2 in the presence of a Ni catalyst. The product was 2-methylbutane. Which one of the following could **not** be the alkene?

A $CH_2C(CH_3)CH_2CH_3$
B $CH_3CH_2C(CH_3)CH_2$
C $(CH_3)_2CCHCH_3$
D $CH_3CHCHCH_2CH_3$

8 Methane and chlorine react to produce trichloromethane according to the following equation.

$$CH_4 + 3Cl_2 \rightarrow CHCl_3 + 3HCl$$

The percentage atom economy of the reaction is

A 7%
B 52%
C 77%
D 87%

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9 Excess acidified potassium permanganate was used to oxidise 1.50 g of propan-1-ol. After the reaction mixture was purified, 0.78 g of propanoic acid was obtained. The percentage yield of the reaction is

A 42%
B 44%
C 52%
D 64%

10 The following reaction pathway is used to make a carboxylic acid.

$$\text{Ethene} \xrightarrow{X} \text{Ethanol} \xrightarrow{Y} \text{Ethanoic acid}$$

The reagents X and Y, respectively, are

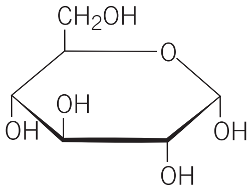
A acidified $KMnO_4$ and water/catalyst.
B NaOH and acidified $KMnO_4$.
C water/catalyst and acidified $KMnO_4$.
D HCl and water/catalyst.

Short-answer questions

11 Write a balanced equation for the reaction of the following substances. Show any relevant reaction conditions and/or catalysts required for the reaction.

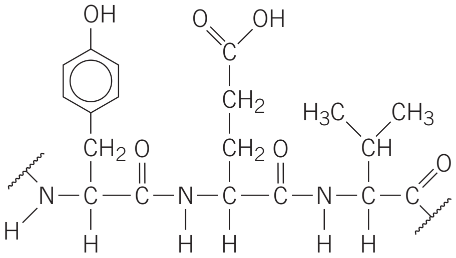
a	but-1-ene + Cl_2	(1 mark)
b	propane + Br_2	(1 mark)
c	ethene + H_2	(1 mark)
d	1-iodobutane + NH_3	(1 mark)
e	methanol + 2-methylpropanoic acid	(1 mark)
f	butyl ethanoate + H_2O (base hydrolysis)	(1 mark)

12 Glycogen is a highly branched polysaccharide of α-glucose. The structure of α-glucose is shown below.



a	Draw the structure of a disaccharide of α-glucose with an α-1,4-glycosidic bond.	(1 mark)
b	Draw the structure of a disaccharide of α-glucose with an α-1,6-glycosidic bond.	(1 mark)
c	What type of reaction converts α-glucose into a disaccharide?	(1 mark)

13 A section of a protein is shown below.



a	How many amino acid units are shown in the section of the protein?	(1 mark)
b	Circle all peptide bonds shown in the section of the protein.	(1 mark)
c	Give the names of the amino acids in the section of the protein.	(1 mark)
d	If the protein consisted of 81 amino acid units, calculate the mass of water required to fully hydrolyse 0.0035 mol of the protein.	(2 marks)

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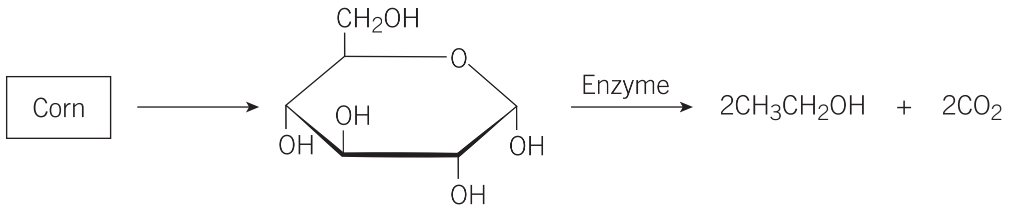
14 Plant-based biomass, such as corn, can be converted to bioethanol, a valuable fuel source and industrial solvent. A summary of the process is given below.



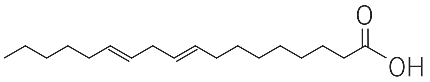
a Select a specific part of the process and explain how it relates to a green chemistry principle and sustainable production of chemicals. (3 marks)

b Discuss a potential disadvantage of using corn as a feedstock. (2 marks)

c Calculate the percentage atom economy of the reaction that converts glucose into bioethanol. (2 marks)

d Explain why manufacturing processes with higher percentage atom economy are potentially more environmentally friendly. (2 marks)

15 Linolelaidic acid is a molecule found in processed vegetable oil. Its structure is shown below.



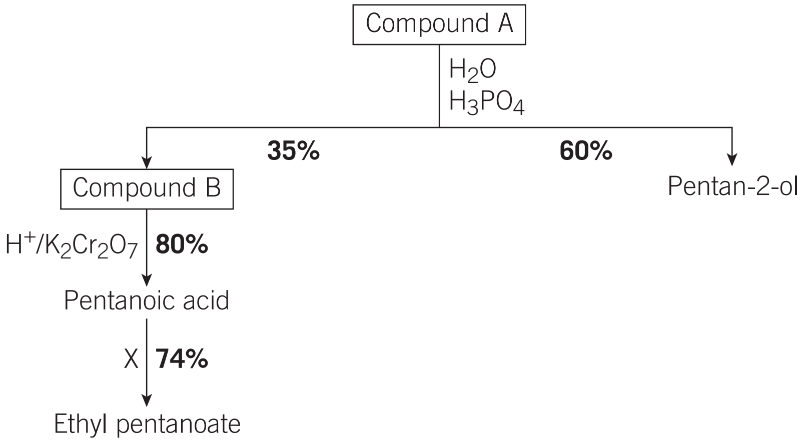
a Draw the structure of the triglyceride formed from linolelaidic acid. (1 mark)

b Draw an equation showing the conversion of the triglyceride in part **a** to a biodiesel using methanol. (2 marks)

c What type of reaction is outlined in part **b**? (1 mark)

d An alternative to biodiesel is petrodiesel, a resource obtained from fossil fuels. From a sustainability perspective, describe the advantages of using biodiesel over petrodiesel. (2 marks)

16 The reaction pathway shown below was used to synthesise ethyl pentanoate.



a Give the semi-structural formula of compound A. (1 mark)

b Draw the structural formula of compound B. (1 mark)

c Name the type of reaction that converts pentanoic acid to ethyl pentanoate (marked by X). (1 mark)

d Give the reagents required to convert pentanoic acid to ethyl pentanoate (marked by X). (1 mark)

e Calculate the overall percentage yield of converting compound A to ethyl pentanoate. (2 marks)

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UNIT 4 HOW ARE CARBON-BASED COMPOUNDS DESIGNED FOR PURPOSE?

CHAPTER 10 LABORATORY ANALYSIS OF ORGANIC COMPOUNDS

Introduction

In Area of Study 1 for Unit 4, you learned about organic compounds, the different types of organic compounds and the different types of reactions to synthesise organic compounds. In this chapter, you will explore how to analyse the products of these reactions using various experimental techniques. You will start by investigating qualitative techniques that are used to test for the presence of various functional groups. This will be followed by examining procedures that determine the purity of these organic compounds. To conclude, you will revisit the topic of volumetric analysis with a focus on redox titrations for the calculation of unknown concentrations.

INTRODUCTION VIDEO
LABORATORY ANALYSIS OF ORGANIC COMPOUNDS

Curriculum

Area of Study 2 Outcome 2
How are organic compounds analysed and used?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Qualitative tests for the presence of carbon–carbon double bonds, hydroxyl and carboxyl functional groups • Measurement of the degree of unsaturation of compounds using iodine	**10A Analysis of functional groups** **10A.1** Explain how qualitative tests can be used to determine the presence of carbon–carbon double bonds **10A.2** Explain how qualitative tests can be used to determine the presence of hydroxyl functional groups **10A.3** Explain how qualitative tests can be used to determine the presence of carboxyl functional groups **10A.4** Design experimental methods to test for carbon–carbon double bonds, and hydroxyl and/or carboxyl functional groups **10A.5** Determine the presence of carbon–carbon double bonds, and hydroxyl and/or carboxyl functional groups through analysing experimental data **10A.6** Describe how a redox titration with iodine can be used to determine the number of carbon–carbon double bonds in a molecule **10A.7** Calculate the number of carbon–carbon double bonds in an unsaturated hydrocarbon

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Applications and principles of laboratory analysis techniques in verifying components and purity of consumer products, including melting point determination and distillation (simple and fractional) • Volumetric analysis, including calculations of excess and limiting reactants using redox titrations (excluding back titrations)	**10B** **Analysis of purity and concentration** **10B.1** Define 'purity' **10B.2** Describe how the melting point of a consumer product can help determine the identity and purity of a consumer product **10B.3** Compare simple and fractional distillation **10B.4** Draw a diagram of the experimental setup for simple and fractional distillation **10B.5** Explain how simple distillation can be used to verify the components and purity of a consumer product **10B.6** Explain how fractional distillation can be used to verify the components and purity of a consumer product **10B.7** Define 'end point' and 'equivalence point' **10B.8** Describe the use of an indicator in an redox titration **10B.9** Define 'standard solution' **10B.10** State the key characteristics of a primary standard solution **10B.11** List the steps involved in a redox titration, including glassware involved **10B.12** Calculate the concentration of an unknown solution from given experimental data

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Glossary

Analyte
Baeyer's test
Concordant
End point
Equivalence point
Free radical
Melting point
Monounsaturated
Polyunsaturated
Purity
Qualitative
Quantitative
Standard solution
Titrant

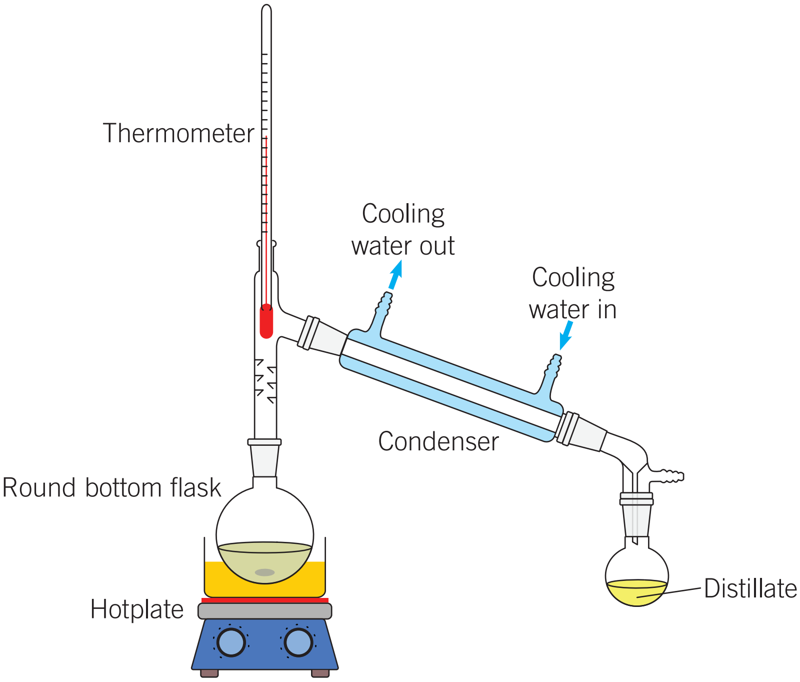
Concept map

10A Analysis of functional groups

Qualitative tests to determine the presence of carbon-carbon double bonds and hydroxyl and carboxyl functional groups

10B Analysis of purity and concentration

Experimental techniques, including distillation, melting point determination and volumetric analysis, to determine purity and concentration



See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

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10A Analysis of functional groups

Study Design:
- Qualitative tests for the presence of carbon–carbon double bonds, hydroxyl and carboxyl functional groups
- Measurement of the degree of unsaturation of compounds using iodine

Glossary:
Baeyer's test
Free radical
Monounsaturated
Polyunsaturated
Qualitative
Quantitative

ENGAGE

Functional groups all around us

Ant bites. Vinegar. Aspirin. Lemon juice. Vitamin C. What do they all have in common? Interestingly, they all contain different compounds that are all linked by being carboxylic acids. In this section, we will focus on the carboxyl functional group that forms carboxylic acids, as well as two other functional groups – the carbon–carbon double bond and the hydroxyl group – and the qualitative tests that can be used to identify them.

Figure 10A–1 Compounds containing the carboxyl functional group are found in many situations, such as formic acid in ant bites (left), 2-acetoxybenzoic acid in aspirin (centre), citric acid and ascorbic acid in oranges and lemons (right).

EXPLAIN

Qualitative versus quantitative

No doubt you've heard the terms **qualitative** and **quantitative** in previous years of science when analysing various forms of data. In this section, the tests presented to check for the presence of carbon–carbon double bonds, hydroxyl and carboxyl functional groups are all qualitative. This means data that are discrete or categorical and are a description of the results observed. In Section 10B, you will look at volumetric analysis of organic compounds, which results in numerical values being obtained. This is an example of quantitative data.

Qualitative the non-numerical characterisation of a substance or sample based on its observable properties

LINK **10B** ANALYSIS OF PURITY AND CONCENTRATION

Quantitative the numerical determination of the quantity or concentration of a substance or component in a sample

NOTE

A way to remember the difference between qualitative and quantitative is to think of the 'l' in qualitative as meaning 'language' and the 'n' in quantitative as meaning 'numerical'. Alternatively, quantitative is derived from the word 'quantity' so is therefore finding a measurable quantity.

8B MOLECULES OF CARBON LINK

Qualitative tests for carbon–carbon double bonds

In Section 8B, you learned about the difference between alkanes and alkenes. As a reminder, the main difference is that alkanes are saturated, whereas alkenes are unsaturated. In terms of alkenes, this means that the family is characterised by the presence of one or more carbon–carbon double bonds. We can see this difference illustrated by the structural formulas of ethane and ethene in Figure 10A–2.

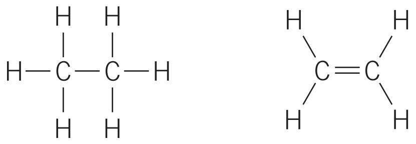

Figure 10A–2 Structural formulas of ethane (left) and ethene (right) show that ethene is characterised by the presence of a carbon–carbon double bond.

9A ORGANIC REACTIONS: SUBSTITUTION, ADDITION AND OXIDATION LINK

There are a number of instances where it may be important to test a sample to identify whether it contains an alkane or an alkene. In particular, this can be useful when analysing whether a hydrogenation reaction converting an alkene to an alkane has gone to completion. One laboratory technique to achieve this is known as the bromine test.

9A ORGANIC REACTIONS: SUBSTITUTION, ADDITION AND OXIDATION LINK

Bromine test

The bromine test works on the principle that alkanes and alkenes react differently in the presence of halogens. Let's focus on how ethane and ethene would react with bromine.

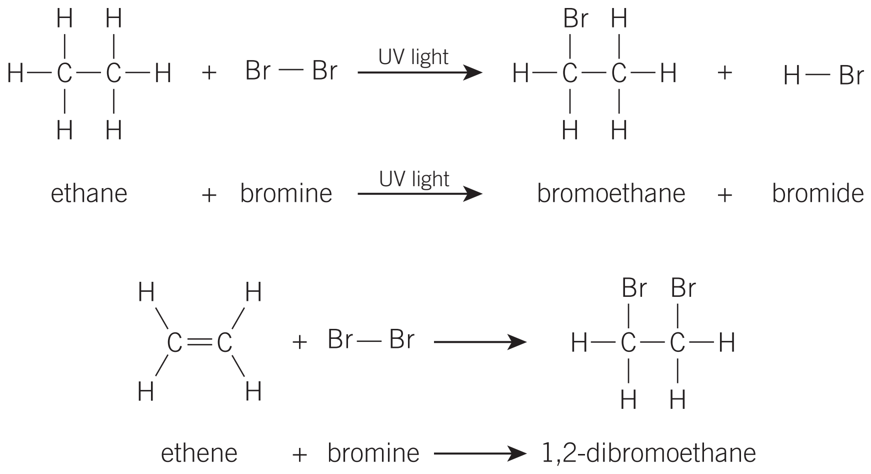

Figure 10A–3 The reactions of ethane (top) and ethene (bottom) with bromine

9A ORGANIC REACTIONS: SUBSTITUTION, ADDITION AND OXIDATION LINK

Free radical a short-lived uncharged molecule with an unpaired valence electron

It can be seen from the equations that the biggest difference in the reactions is the conditions required for the reaction to occur. Due to the presence of the reactive carbon–carbon double bond, ethene is able to react easily with bromine in an addition reaction. However, the alkane is less reactive and so the reaction can only take place in the presence of UV light. The UV light forms reactive bromine **free radicals**, which can then replace a hydrogen atom on the ethane via a substitution reaction.

Let's now investigate how the bromine test takes advantage of this difference to allow us to detect the presence of carbon–carbon double bonds.

Figure 10A–4 When a reaction takes place, the bromine solution changes from a yellow-orange colour (left) to colourless (right). This forms the basis of the bromine test.

At room temperature, bromine is often used dissolved in water. This is due to the very toxic, corrosive and environmentally hazardous nature of pure bromine liquid. Bromine water is a yellow-orange colour. However, when bromine water reacts with either an alkane or an alkene, the yellow-orange colour disappears and the solution becomes colourless (Figure 10A–4). This allows for a qualitative way to determine whether or not a reaction has occurred.

So how does this help us determine whether or not the substance is an alkane or an alkene, or to put it another way, whether there is a carbon–carbon double bond present? We can answer this by looking at a flow chart of possible results (Figure 10A–5). Here it can be seen that the bromine solution will only change from yellow-orange to colourless in the dark if a carbon–carbon double bond is present. If the solution remains yellow-orange in the dark, it can be moved into the light, where it should then become colourless. This acts as a control to indicate that an alkane is present and not that the reaction has failed.

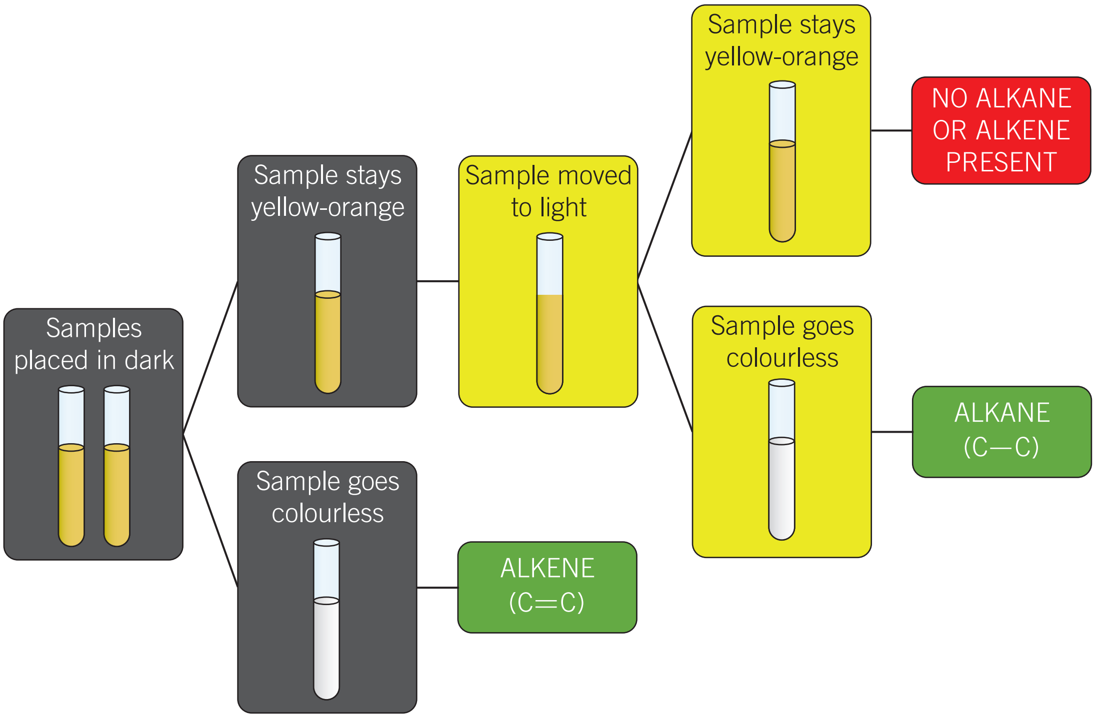

Figure 10A–5 The possible results of the outcome of the bromine test for the presence of a carbon–carbon double bond

Baeyer's test

Baeyer's test a test for an unsaturated carbon–carbon bond, such as an alkene

Another qualitative test that can be performed to detect the presence of a carbon–carbon double bond, in order to distinguish between alkanes and alkenes, is known as **Baeyer's test**. Similar to the bromine test, Baeyer's test is based on observing a colour change that occurs if a chemical reaction occurs. In this instance, the reaction involves mixing the alkane or alkene with potassium permanganate, which is purple in colour. When a reaction takes place, manganese(IV) oxide is formed, which appears black (or brown) in colour. However, not only is there a discolouration (from purple to colourless), but the manganese(IV) oxide forms a solid precipitate. The combination of observing the precipitate and the discolouration indicates that a reaction has occurred.

NOTE

Baeyer's test will detect any species that oxidises in solution, including both hydroxyl and carbonyl functional groups, which are discussed later in the section. Therefore, this test is of limited value unless it is known that the species being tested are hydrocarbons.

Let's look at the reactions that would occur in the Baeyer's test, using the same examples of ethane and ethene (Figure 10A–6).

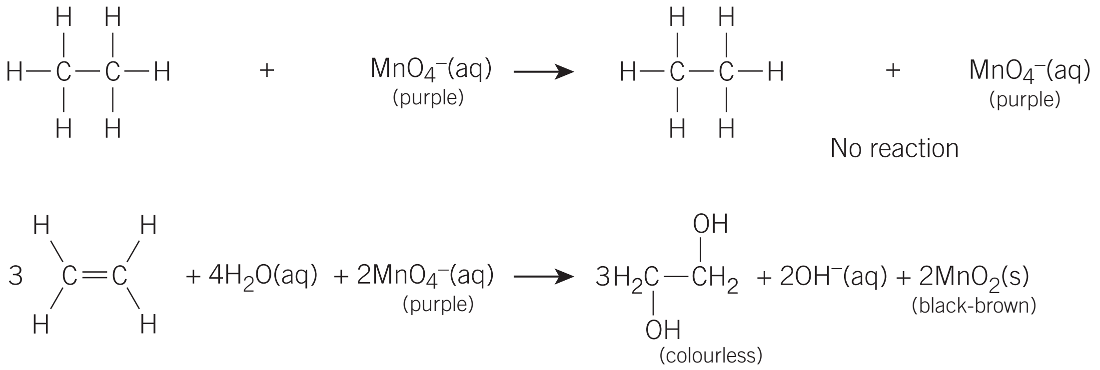

Figure 10A–6 The reactions of ethane (top) and ethene (bottom) that would occur in the Baeyer's test. Ethane doesn't react and the tube stays purple, whereas ethene will oxidise to ethane-1,2-diol, which is colourless, and manganese dioxide, which is black (or brown).

We can summarise the results of this test by generating another flow chart, as shown in Figure 10A–7.

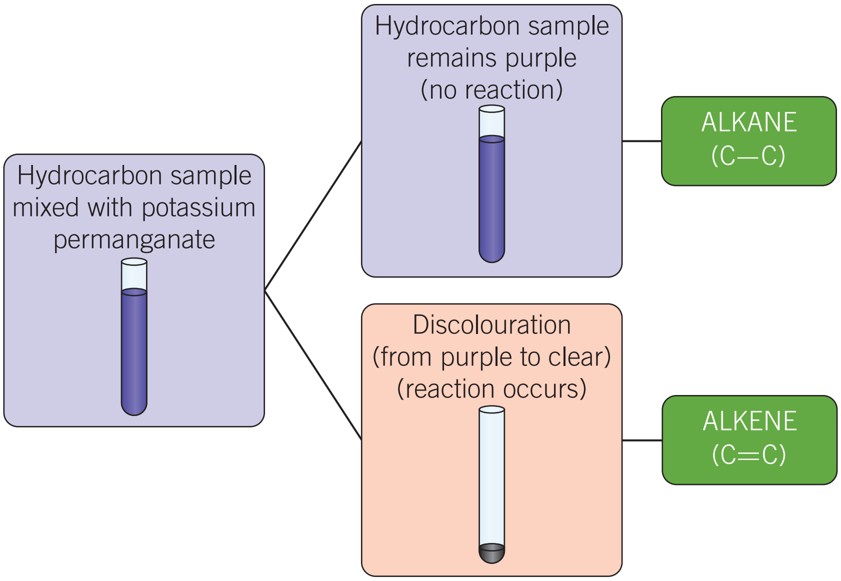

Figure 10A–7 The possible results of the outcome of the Baeyer's test for the presence of a carbon–carbon double bond

Quantitative analysis of carbon–carbon double bonds

If you've paid attention to commercials discussing fats in food products, you have probably heard the terms **monounsaturated** and **polyunsaturated**. These terms refer to how many carbon–carbon double bonds are present in the fat: monounsaturated fats have a single carbon–carbon double bond, whereas polyunsaturated fats have multiple carbon–carbon double bonds.

It is possible to determine the number of carbon–carbon double bonds in a molecule by performing an addition reaction with iodine. This reaction occurs similarly to the one that was described in the bromine test, however, iodine (I_2) is used in place of bromine. An example reaction with ethene is shown in Figure 10A–8.

Monounsaturated an organic compound that contains one carbon–carbon double bond

Polyunsaturated an organic compound that has two or more C═C double bonds or C≡C triple bonds

LINK **9A** ORGANIC REACTIONS: SUBSTITUTION, ADDITION AND OXIDATION

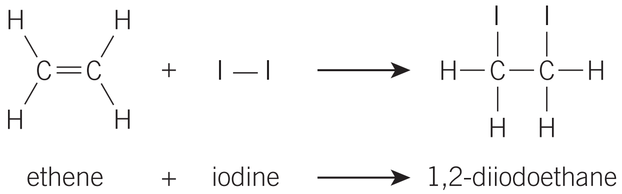

Figure 10A–8 An addition reaction between ethene and iodine to produce 1,2-diiodoethane

From Figure 10A–8, we can observe that the addition reaction occurs in a mole ratio of 1 : 1 between carbon–carbon double bonds and iodine. This means that we can use the mole ratio of any given reaction to tell us how many carbon–carbon double bonds exist. As an example, if hydrocarbon X contained two carbon–carbon double bonds, we would need twice as many moles of iodine to react completely with it (that is, our carbon–carbon double bond to iodine ratio would be 1 : 2).

Before we go through a worked example of one of these calculations, we must first understand how to determine when this reaction has gone to completion. The principle behind this is similar to the bromine test in that a colour change is observed. Iodine, which in schools is typically dissolved in acetic acid (also known as Hanus solution) is an orange-red colour. However, when it reacts with the hydrocarbon, the iodide ion (I^-) is colourless. To determine the amount of iodine required, the reaction is conducted by repeatedly adding small amounts of Hanus solution to the hydrocarbon until the orange-red colour completely disappears. This is an example of a redox titration, which you will learn more about in Section 10B.

LINK **10B** ANALYSIS OF PURITY AND CONCENTRATION

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VIDEO WORKED EXAMPLE 10A–1

Worked example 10A–1: Using the mole ratio to determine the number of carbon–carbon double bonds in an unknown hydrocarbon

A 6.90 g sample of an unknown hydrocarbon (M = 138 g mol^{-1}) reacts completely with 25.38 g of iodine (I_2). How many carbon–carbon double bonds are present in the hydrocarbon?

Solution

	Logic	Process
Step 1	Calculate the amount, in mol, of each reactant.	$n(\text{hydrocarbon}) = \frac{m}{M}$ $= \frac{6.90\text{ g}}{138\text{ g mol}^{-1}}$ $n(\text{hydrocarbon}) = 0.0500\text{ mol}$ $n(I_2) = \frac{m}{M}$ $= \frac{28.38\text{ g}}{253.8\text{ g mol}^{-1}}$ $n(I_2) = 0.1000\text{ mol}$
Step 2	Determine the mole ratio of the reactants.	$n(\text{hydrocarbon}) : n(I_2)$ $= 0.0500\text{ mol} : 0.1000\text{ mol}$ $n(\text{hydrocarbon}) : n(I_2)$ $= 1:2$
Step 3	State the number of carbon–carbon double bonds present.	As two moles of iodine are required to react completely with one mole of the hydrocarbon, there must be two carbon–carbon double bonds present in the unknown hydrocarbon.

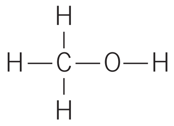
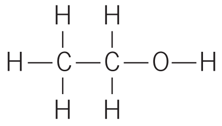
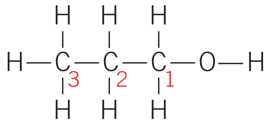
Qualitative tests for hydroxyl functional groups

What are hydroxyl functional groups?

8C FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS LINK

Recall from Section 8C that a hydroxyl functional group is –OH bonded to a hydrocarbon chain. This family of organic compounds is referred to as alcohols, examples of which are shown in Table 10A–1.

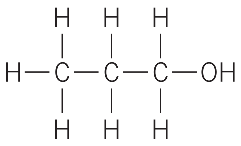
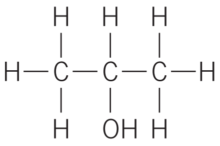
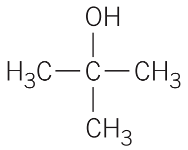
Table 10A–1 Structures of three alcohols

Name	Molecular formula	Structural formula	Semi-structural formula
Methanol	CH_4O		CH_3OH
Ethanol	C_2H_6O		CH_3CH_2OH
Propan-1-ol	C_3H_8O		$CH_3CH_2CH_2OH$

You should also recall here the rules for naming alcohols larger than ethanol and that the position of the hydroxyl group on the parent hydrocarbon chain must be included in the name. You should also recall the difference between primary, secondary and tertiary alcohols from Section 8C. Examples with a description of each are outlined in Table 10A–2.

LINK **8C** FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS

Table 10A–2 Examples of, and the distinction between, primary, secondary and tertiary alcohols

	Alcohol type		
	Primary	**Secondary**	**Tertiary**
Structural formula	 $\mathrm{H-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-OH}$	 $\mathrm{H-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{OH}{C}}-\overset{H}{\underset{H}{C}}-H}$	 $\mathrm{H_3C-\overset{OH}{\underset{CH_3}{C}}-CH_3}$
Name	Propan-1-ol	Propan-2-ol	2-methylpropan-2-ol
Distinction	The carbon atom that the –OH functional group is bonded to is only bonded to one other carbon atom.	The carbon atom that the –OH functional group is bonded to is bonded to two other carbon atoms.	The carbon atom that the –OH functional group is bonded to is bonded to three other carbon atoms.

Esterification

LINK **9B** ORGANIC REACTIONS: CONDENSATION AND HYDROLYSIS

Esterification reactions, which you learned about in Section 9B, can be used to confirm the presence of primary, secondary and tertiary alcohols – that is, the hydroxyl functional group. Simply, these reactions are performed by mixing an alcohol with a carboxylic acid to produce an ester. An example of the procedure is shown in Figure 10A–9.

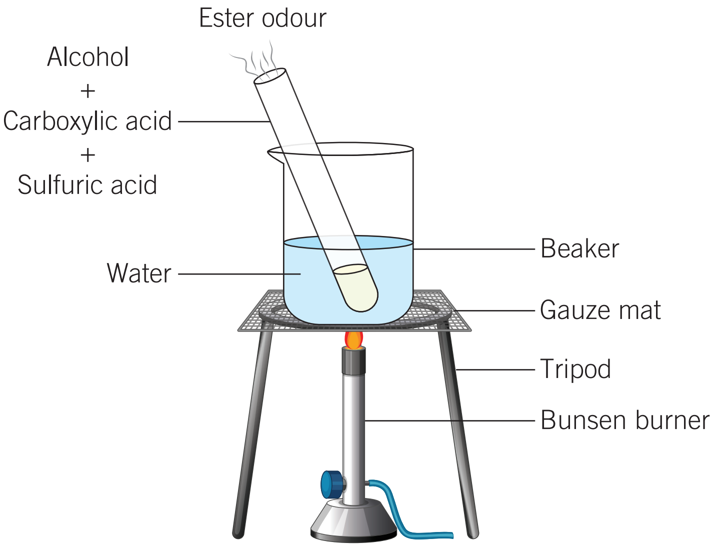


Figure 10A–9 Experimental set-up of an esterification reaction

Concentrated sulfuric acid, the catalyst, is added to the test tube, and the contents of the test tube are heated. Both the sulfuric acid catalyst and the heat speed up the rate of reaction to produce the ester. If an ester is produced, it is detected by its odour. An example reaction is shown below.

$$\text{ethanol} + \text{ethanoic acid} \xrightarrow{\text{sulfuric acid}} \text{ethyl ethanoate} + \text{water}$$

$$CH_3CH_2OH(aq) + CH_3COOH(aq) \xrightarrow{H_2SO_4} CH_3COOCH_2CH_3(aq) + H_2O(l)$$

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If an organic compound containing a hydroxyl group is not present, then no ester odour is produced and it is not an esterification reaction. This is summarised in Figure 10A–10.

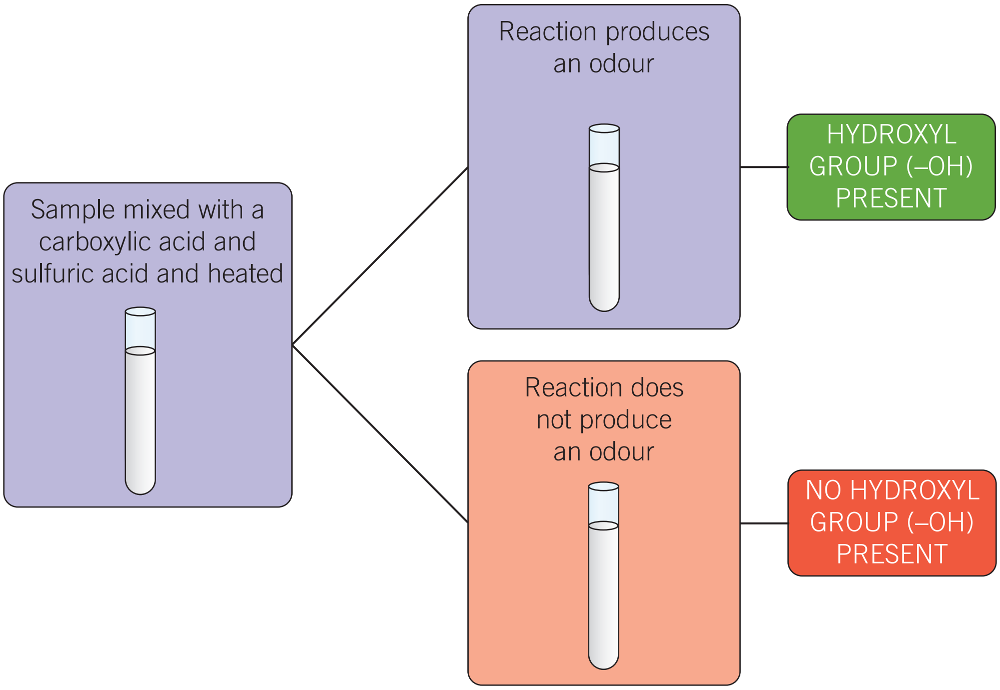
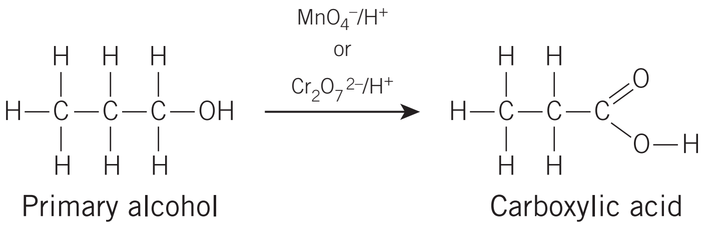


Figure 10A–10 The possible results of the outcome of an esterification test for the presence of a hydroxyl functional group

Oxidation

If you want to distinguish between primary and secondary alcohols compared to tertiary alcohols, a redox reaction can be performed. Primary and secondary alcohols can both be oxidised, however, tertiary alcohols cannot.

An example of a chemical equation for this oxidation reaction is given below.



In this reaction, a small amount of an oxidising agent, such as acidified potassium dichromate, $K_2Cr_2O_7$, can be added to the alcohol in a test tube. The contents are mixed before being placed in a heated water bath for a few minutes. Originally, this solution will be orange; however, if a primary or secondary alcohol is present, the solution will change colour from orange to green, as represented in Figure 10A–11.

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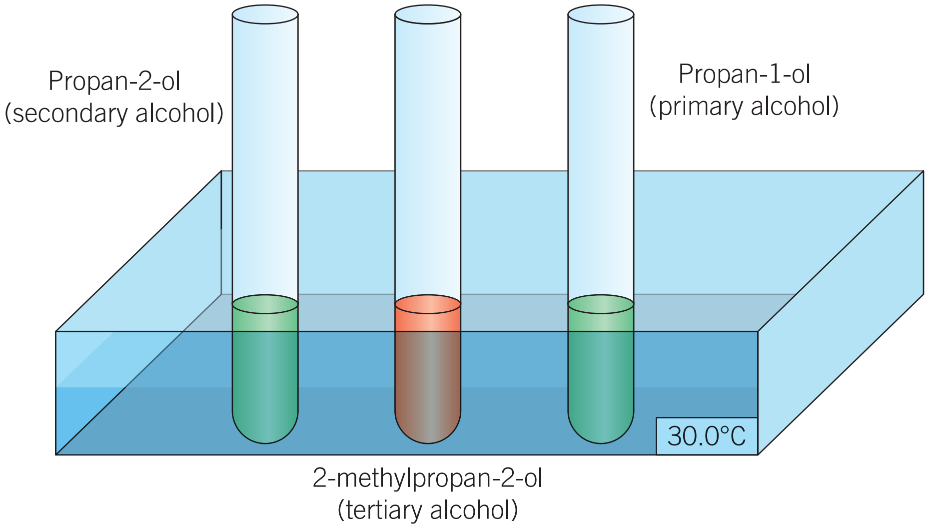


Figure 10A–11 Oxidation reaction for primary, secondary and tertiary alcohols. If a colour change occurs, then either a primary or secondary alcohol is present. If no colour change occurs, a tertiary alcohol is present.

The potential outcomes of this test are summarised in Figure 10A–12.

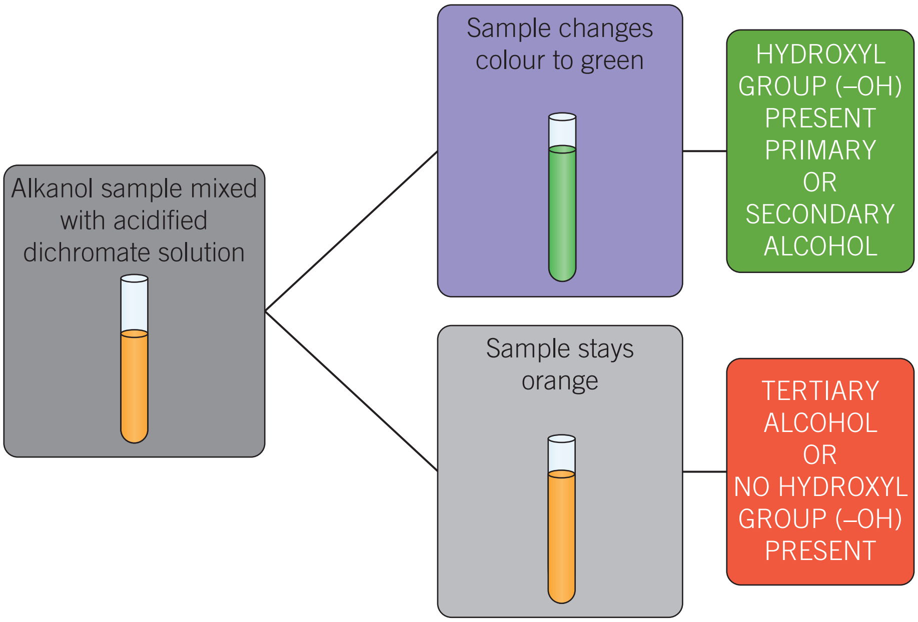


Figure 10A–12 The possible results of an oxidation test for the presence of a hydroxyl functional group

Check-in questions – Set 1

1 What reacts more readily with a halogen – an alkane or an alkene?
2 If you conducted a bromine test only in the light, would you be able to differentiate between an alkane and an alkene? Explain why or why not.
3 If you want to test for the presence of a hydroxyl functional group, you can mix the sample with a carboxylic acid to see if an ester forms. What two other steps must be performed?

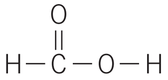
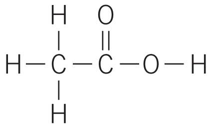
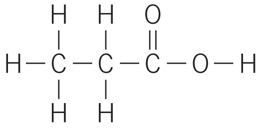
8D FUNCTIONAL GROUPS: ALDEHYDES, KETONES, CARBOXYLIC ACIDS AND ESTERS **LINK**

Qualitative tests for carboxyl functional groups

What are carboxyl functional groups?

Recall from Section 8D that a carboxyl functional group is –COOH bonded to a hydrocarbon chain. This family of organic compounds is referred to as carboxylic acids, examples of which are shown in Table 10A–3.

Table 10A–3 Structures of the first three carboxylic acids

Name	Common name	Structural formula	Semi-structural formula
Methanoic acid	Formic acid	 $H-\overset{\overset{O}{\|}}{C}-O-H$	$HCOOH$
Ethanoic acid	Acetic acid	 $H-\overset{\overset{H}{\mid}}{\underset{\underset{H}{\mid}}{C}}-\overset{\overset{O}{\|}}{C}-O-H$	CH_3COOH
Propanoic acid	Propionic acid	 $H-\overset{\overset{H}{\mid}}{\underset{\underset{H}{\mid}}{C}}-\overset{\overset{H}{\mid}}{\underset{\underset{H}{\mid}}{C}}-\overset{\overset{O}{\|}}{C}-O-H$	CH_3CH_2COOH

9B ORGANIC REACTIONS: CONDENSATION AND HYDROLYSIS **LINK**

Esterification

As you learned in Section 9B and earlier in this chapter, when testing for hydroxyl groups, esterification reactions can be used to confirm the presence of carboxyl groups as well. Simply, these reactions are performed by mixing an alcohol with a carboxylic acid to produce an ester, as was shown in Figure 10A–9 on page 393.

If an ester is produced, it is detected by its ester odour. An example reaction can be found earlier in this chapter on page 393. If an organic compound containing a carboxyl group is not present, then no ester odour will be produced and it is not an esterification reaction.

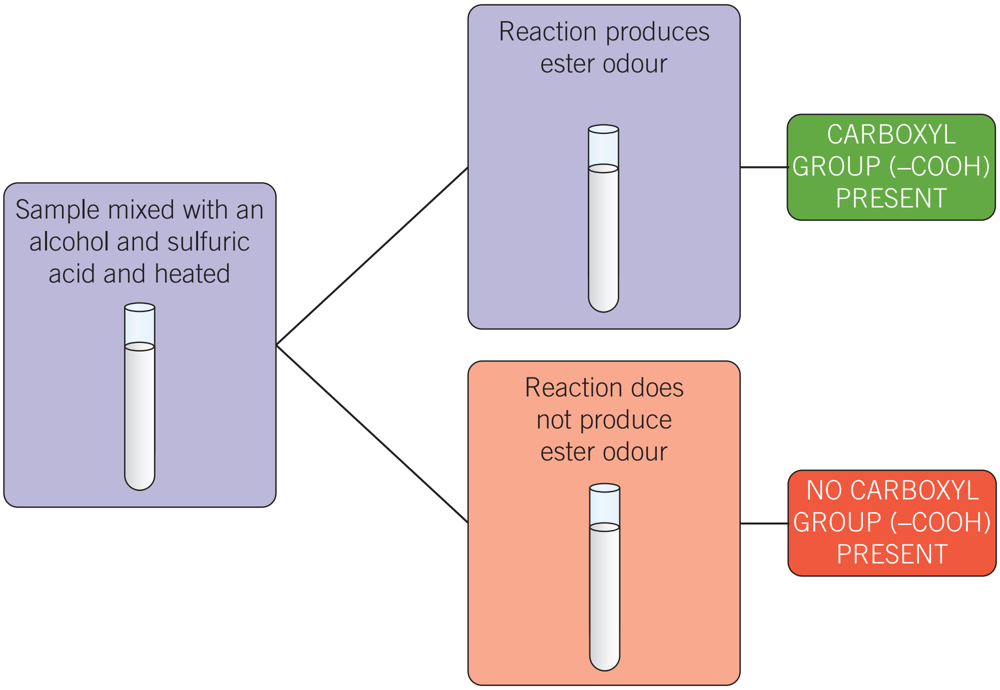


Figure 10A–13 The possible results of an esterification test for the presence of a carboxyl functional group

Litmus test

You might recall from Unit 2 that litmus is a water-soluble substance extracted from lichens. Litmus can be used either as a solution or absorbed onto filter paper. Litmus turns red under acidic conditions and blue under basic conditions.

LINK UNIT 2

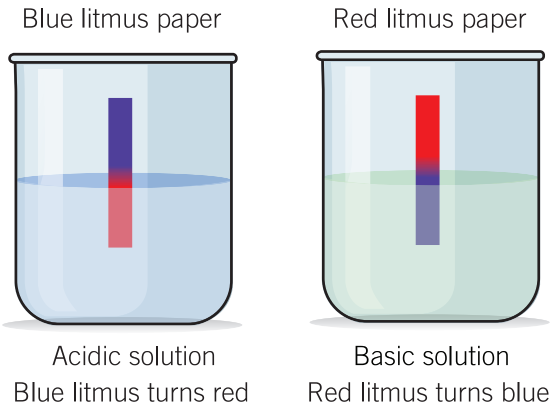


Figure 10A–14 Change in colour of litmus paper under both acidic (left) and basic (right) conditions

If litmus paper is placed into an aqueous solution of a carboxylic acid, the appearance of a red colour confirms the presence of a carboxyl functional group, or carboxylic acid.

An example of the dissociation of ethanoic acid when reacted with water is shown below.

ethanoic acid	+	water acid	→	ethanoate acid	+	hydronium acid
$CH_3COOH(aq)$	+	$H_2O(l)$	→	$CH_3COO^-(aq)$	+	$H_3O^+(aq)$

Reacting with sodium carbonate

You will recall from Unit 2 that reacting acids with metal carbonates results in the production of a salt, water and carbon dioxide, as shown in the example equation below.

LINK UNIT 2

Acid + Metal carbonate → **Salt + Water + Carbon dioxide**

$$C_4H_6O_6(aq) + Na_2CO_3(s) \rightarrow Na_2C_4H_4O_6(aq) + H_2O(l) + CO_2(g)$$

Confirmation of the presence of a carboxyl group can be seen through the bubbling of the solution, indicating that a gas is produced. To confirm that this gas is indeed carbon dioxide, a delivery tube can be passed from the reaction mixture into a solution of limewater. If the limewater changes from clear to cloudy, then carbon dioxide is produced. This is shown in Figure 10A–15.

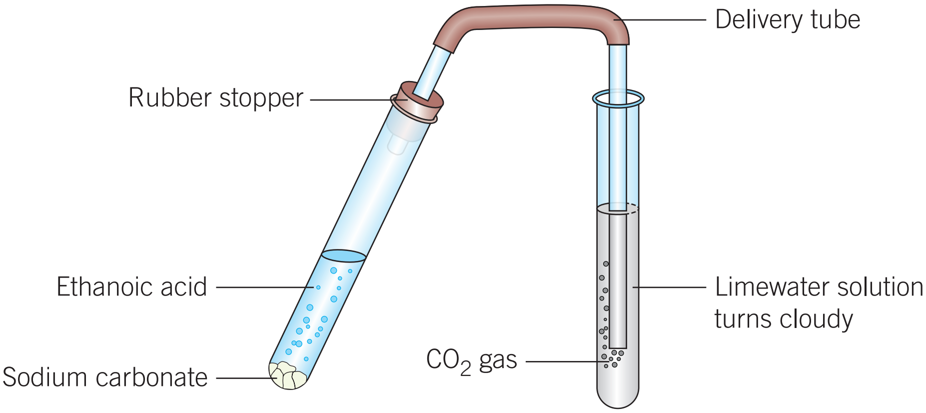


Figure 10A–15 In an acid and metal carbonate reaction, the presence of carbon dioxide is indicated by bubbling the gas produced through limewater and determining if the limewater turns cloudy.

Summarising qualitative tests

WORKSHEET 10A–1
ANALYSING QUALITATIVE TESTS TO DETERMINE THE PRESENCE OF FUNCTIONAL GROUPS

So far in this chapter, you've learned about a number of different tests checking for the presence of carbon–carbon double bonds, hydroxyl and carboxyl functional groups.

Table 10A–4 shows a summary of the different tests associated with each functional group, as well as what result confirms a positive result.

Table 10A–4 Summary of tests for different functional groups

Functional group	Chemical test	Positive result
Carbon–carbon double bond (C=C)	Bromine	Solution changes from yellow-orange to colourless
	Baeyer's	Solution changes from black (or brown) to colourless
Hydroxyl (–OH)	Esterification	Ester odour
	Oxidation	Solution changes from orange to green
Carboxyl (–COOH)	Esterification	Ester odour
	Litmus	Blue litmus turns red
	Metal carbonate	Carbon dioxide gas bubbled through limewater changes it from clear to cloudy.

VIDEO 10A–1
SKILLS: IDENTIFYING AN UNKNOWN SUBSTANCE

10A SKILLS

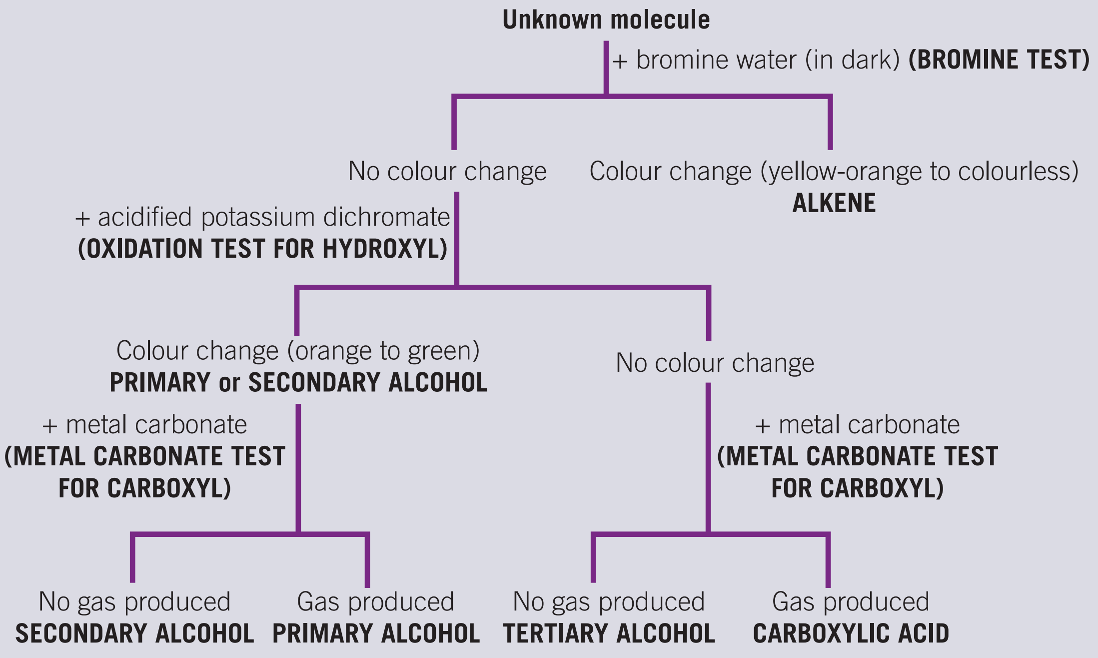
Identifying an unknown substance

Refer back to the Study Design dot point for Section 10A, shown below:

- *qualitative tests for the presence of carbon–carbon double bonds, hydroxyl and carboxyl functional groups*

The authors feel that the intent of this Study Design dot point is for students to use a flow chart idea to help identify an unknown substance from an alkane, alkene, alcohol or carboxylic acid.

An example of what a flow chart for this could look like, given the tests presented in this chapter, is shown below.



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Being able to use your knowledge of organic molecules learned in Chapter 8 with your knowledge of organic reactions learned in Chapter 9, and combining this with your knowledge of the different tests and results learned in this section will be important in helping you determine the identity of an unknown organic molecule.

You could use this flow chart as a basis for adding detail, such as:

- colour coding to represent the specific colour change observed in certain tests.
- examples of structural formulas of the resulting organic molecules that are determined from each pathway.
- examples of chemical equations to show the reactions taking place.

Flow charts such as these are useful ways to condense your understanding into smaller and more easily memorisable visual pieces of information.

Section 10A questions

1 A sample is known to contain either propane or propene.

  a To determine what the compound is, a scientist first performs a bromine test. When the test is conducted in the dark, the sample remains a yellow-orange colour. When the test is conducted in the presence of a UV light source, the same result is obtained. Is it possible to conclude if the sample is propane or propene from these results? Why or why not?

  b Describe another test that the scientist could perform to determine if the sample is propane or propene.

2 An esterification test can be used to detect the presence of both a carboxyl and a hydroxyl functional group.

  a Explain why it is possible to use this test to detect both functional groups.

  b Describe the positive result that is obtained from this test.

  c Is this result qualitative or quantitative? Why?

3 For each of the following types of data, state whether they are quantitative or qualitative.

  a red litmus paper turning blue

  b a sample changing colour from orange to green

  c a sample giving a pH reading of 3.0

  d the absorbance of a solution increasing as the colour of the sample gets darker

  e observing the production of bubbles during a chemical reaction

4 You receive two samples from a laboratory. You know that one contains a primary alcohol and the other contains a tertiary alcohol. However, the labelling got smudged in transport and you can no longer read it.

  a Use a flow chart to demonstrate the steps you would undertake to determine which sample is the primary alcohol and which is the tertiary alcohol.

  b Describe another test, not included in your flow chart from part **a**, that could be performed to help you better distinguish between the two unknown samples.

5 A 2.76 g sample of an unknown hydrocarbon ($M = 138\ \text{g mol}^{-1}$) reacts completely with 15.23 g of iodine (I_2). How many carbon–carbon double bonds are present in the hydrocarbon?

10B Analysis of purity and concentration

Study Design:

- Applications and principles of laboratory analysis techniques in verifying components and purity of consumer products, including melting point determination and distillation (simple and fractional)
- Volumetric analysis, including calculations of excess and limiting reactants using redox titrations (excluding back titrations)

Glossary:

Analyte
Concordant
End point
Equivalence point
Melting point
Purity
Standard solution
Titrant

ENGAGE

Organic versus inorganic disinfectants

Nature's oldest organic disinfectant, known as hypochlorous acid (HOCl), is actually produced by white blood cells in the human body. This means it is used to fight off pathogenic infections. This is the primary reason why hypochlorous acid is present in many hand sanitisers, as it targets bacterial pathogens on the skin without causing any irritation. Advantages for medical institutes and businesses of using this organic disinfectant, not to mention the human body, is that it is not harmful to humans (or animals and plants), releases non-harmful chemicals, fumes or residues and is biodegradable. Other examples of organic disinfectants include vinegar (acetic acid) and hydrogen peroxide.

Organic disinfectants are preferred over inorganic disinfectants, like chloramines used to chlorinate drinking water, for the same anti-pathogenic purpose. If high amounts of chloramines are ingested it can lead to stomach aches, vomiting and diarrhoea, or even death. It can also cause pipe corrosion, which subsequently allows metals such as iron, copper and lead to be present in our drinking water.

Redox titrations are very useful in helping to quantitively determine the level of substances in water supplies, while maintaining the levels of these substance within desired concentrations. In this section, you will learn about laboratory techniques that are used to test the purity and composition of consumer products. Volumetric analysis using redox titrations, such as the one described to test water purity, is one such technique that will be covered along with melting point determination and distillation.

Figure 10B–1 Collecting a water sample to analyse the water purity

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EXPLAIN

As well as qualitative tests to identity the presence of different functional groups to assess the success of a chemical reaction, quantitative tests to determine the **purity** of a product are also critically important. Depending on the type of consumer product in question, impurities can have a range of unwanted effects, from health issues to inaccurate research results. While the following tests can also give an indication about the identity of the components within a sample, we will look at this aspect more closely when we discuss instrumental techniques in Chapter 11.

Purity the degree to which a substance or compound is free from contaminants or other unwanted materials

LINK **11A** MASS SPECTROMETRY

Analysing purity

To analyse purity, common laboratory techniques take advantage of a couple of properties of samples. If the sample in question is a solid, we can use the melting point of the substance to determine whether it is pure. If the sample in question is a liquid, we can use the boiling point of that substance to determine whether it is pure. While the properties measured are slightly different in these situations, the basis for how they assess purity is the same. In these experiments, there are two main outcomes:

- The sample has a fixed, sharp value for the boiling or melting point. This indicates that the sample is pure.
- The sample has a melting or boiling point that occurs across a range, rather than a single discrete value. This indicates that the sample is impure.

Let's now look specifically at three different techniques that apply these principles to determine the purity of products.

Melting point determination

Melting point determination is a common laboratory technique from which the purity of a solid can be established. The **melting point** is defined as the temperature range from which a solid first starts to transition to a liquid state until this process has finished (that is, all of the solid has become liquid or completely melted).

Melting point the temperature range from which a solid first starts to transition to a liquid state until this process has finished (i.e. all of the solid has become liquid or completely melted)

For a pure solid, the melting point is contained within a very narrow (or sharp) range. Usually, this will be within 1–2°C. The melting point of a pure substance is also characteristic for that compound. This means that the melting point can be used to give an indication of the identity of the compound in a sample. For example, pure citric acid, an acidity regulator used in cooking, has a melting point of 153°C. If we had a sample of unknown colourless, translucent crystalline material, performed a melting point analysis of it and found that the melting point was 153°C, this would suggest that the sample may be citric acid.

When a solid contains impurities, the melting point is altered in two ways. Firstly, it begins to melt at a lower temperature. Secondly, it melts across a larger range of temperatures. To understand this, we need to picture what a pure and an impure solid would look like at a molecular level (Figure 10B–2).

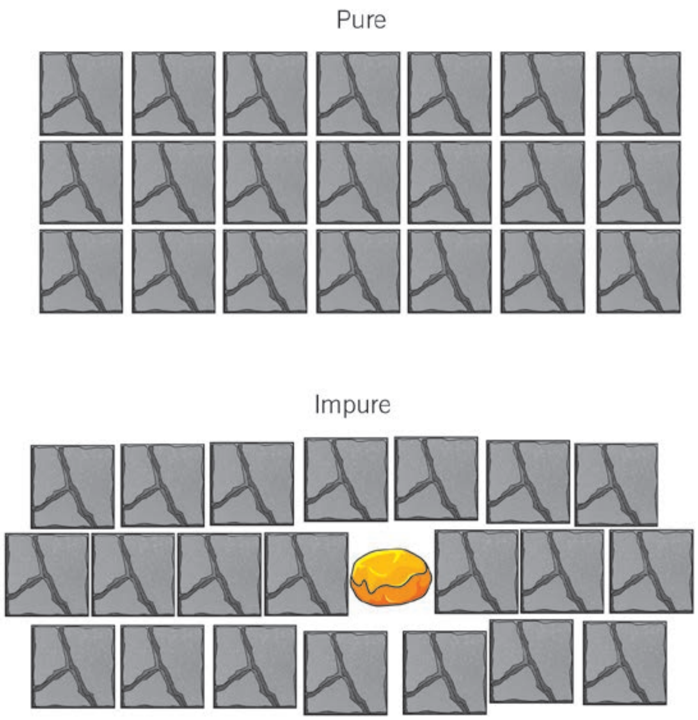

Figure 10B–2 The crystals in a pure substance are arranged in a more ordered fashion (top) compared to when there is an impurity present (bottom).

It can be seen that in a pure substance, the crystals can be arranged in an ordered fashion. This means that they are able to pack more closely together, which allows for stronger intermolecular forces. However, this is not the case when there is a contaminant or impurity present in the substance (that is, the substance is impure). In these cases, the impurity disrupts the ordered structure and causes the crystals to have a greater level of disorder, weakening the intermolecular forces between them. For this reason, a pure substance will have a higher melting point than the same substance that contains impurities.

A good example of this can be seen by looking at the melting point of pure ice compared to ice formed in the ocean (ice containing salt and other impurities). As you would probably know, the melting point of pure ice is 0°C at 101.3 kPa. However, the melting point of ice formed in sea water is lower than this; it would start melting at around −2°C at 101.3 kPa.

So how is this measured in a laboratory to test the purity of consumer products? The technique involves the use of a melting point apparatus, as shown in Figure 10B–3.

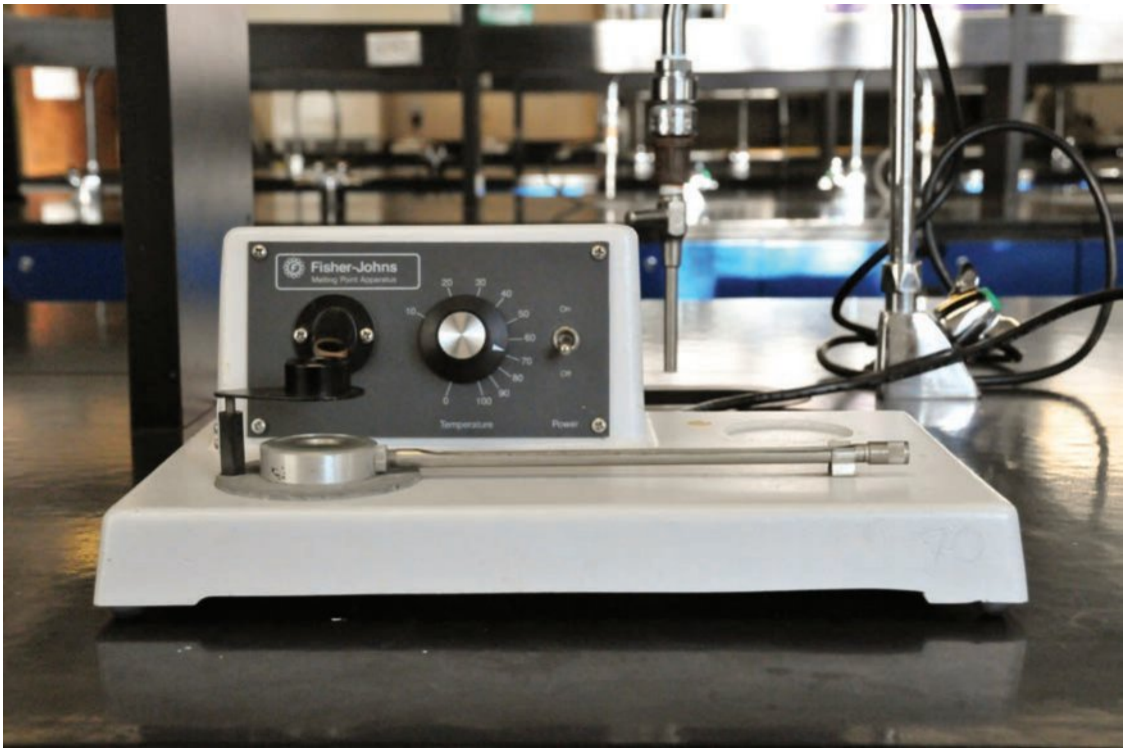

Figure 10B–3 A melting point apparatus can be used to measure the melting point of a sample so that its purity can be analysed.

While there are a number of variations of this machine, they all function with the same basic characteristics.

- They have a port where a sample can be inserted, usually inside a thin tube (known as a capillary tube).
- They have a way of raising the temperature applied to the sample until it melts.
- They have a way of observing a magnified image of the sample, so it can be monitored for when it begins to melt and when it has melted completely.

The process that is observed is represented in Figure 10B–4.

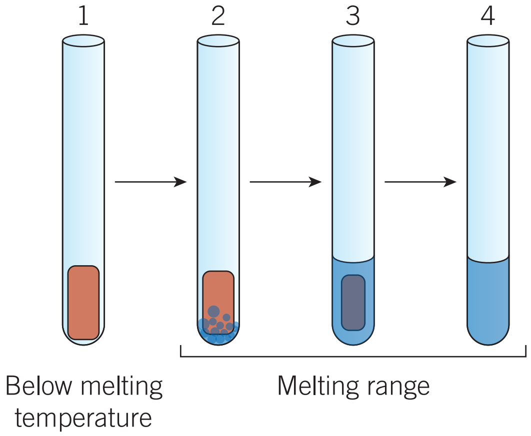

Figure 10B–4 The steps that a solid sample goes through during melting point determination allow the melting range and purity to be determined.

As a reminder, the higher the purity of a sample, the smaller the temperature range for the sample to go from beginning to melt to completely melted (tubes 2–4). However, if a sample has lower purity, it will begin to melt (tube 2) at a lower temperature and the temperature range between the initial and final melting point (tubes 2–4) will be greater.

Melting point determination allows us to assess the purity and components of a solid sample. However, what if our sample is a liquid? For this, we use a technique known as distillation. Depending on the nature of the liquid sample, we can either use simple distillation or fractional distillation.

Simple distillation

Simple distillation is a method used to both separate and purify liquids. It is based on the fact that different liquids have different boiling points. The process of simple distillation is often used in a laboratory setting to separate and purify different chemicals, or to separate a mixture of liquids into its individual components.

However, there is also a long history of using distillation techniques in Australia outside of the laboratory. Prior to colonisation, many First Nations peoples utilised steam distillation: by placing wet plant matter over a controlled fire, a person could be placed over the fire in the manner of a ‘steam bath’ and be exposed to the medicinal vapours. *Eucalyptus dives* (the broad-leaved peppermint from New South Wales and Victoria) was used in such a manner for the treatment of fevers. These benefits of eucalyptus oils were soon noticed by early colonists, and in late 1788, colonists began distilling *Eucalyptus piperita* for medicinal purposes. You will look at the medicinal aspects of chemistry in further detail in Section 12A.

LINK **12A** ORGANIC COMPOUNDS AS MEDICINES

In the laboratory setting, the process of simple distillation involves heating a mixture of liquids in a flask and collecting the vapour that is produced. The vapour is then cooled and condensed back into a liquid form, which is collected in a separate container. The liquid that is collected is called the distillate. This is illustrated in Figure 10B–5.

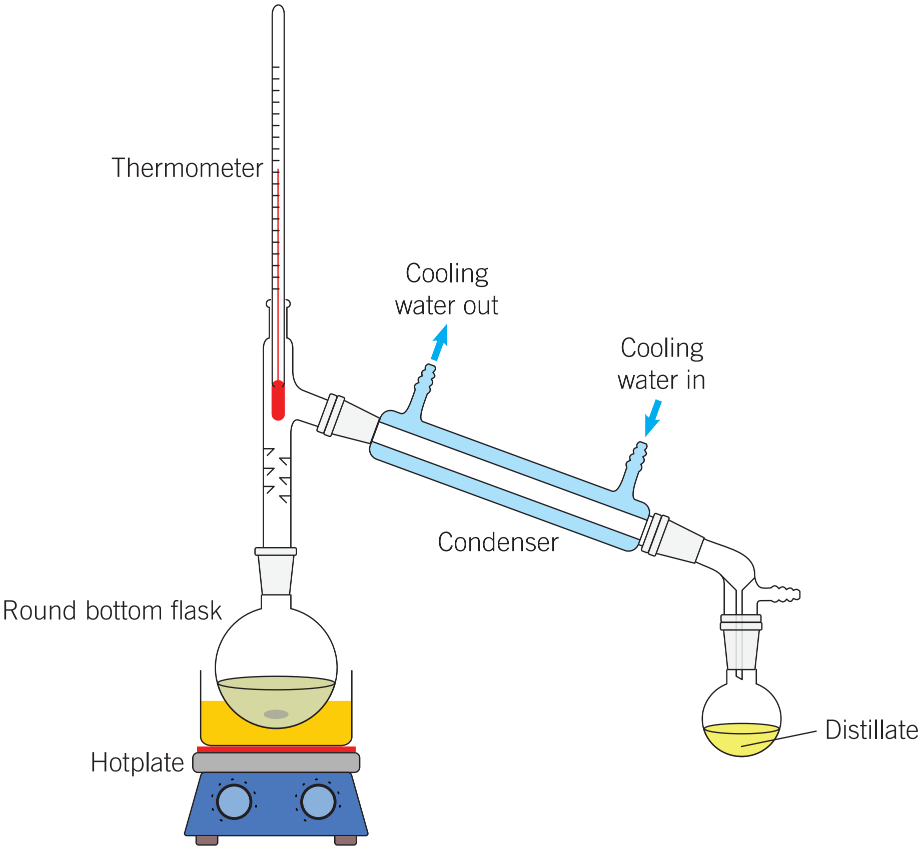

Figure 10B–5 The general setup of a simple distillation experiment

VIDEO 10B–1
SIMPLE DISTILLATION OF ETHANOL AND WATER

To understand how this can be used to verify the components and purity of a compound in a consumer product, let's focus on an example: propyl ethanoate ($C_5H_{10}O_2$), which is an ester found in plant extracts and has the flavour and odour of pear. It is miscible in alcohols, such as ethanol.

Propyl ethanoate has a boiling point of 102°C. Ethanol, on the other hand, has a boiling point of 78.5°C at 101.3 kPa. As the boiling points of these two liquids are quite different, simple distillation can be used for the analysis of mixtures containing these two components. If our plant contained nothing other than propyl ethanoate and ethanol, we would expect our experiment to proceed as follows.

The process of simple distillation starts by heating the mixture of propyl ethanoate and ethanol. As the temperature increases to 78.5°C, the ethanol will begin to boil. The gas will then travel up the cylinder and through the condenser, where it will cool down and turn back into a liquid state. This liquid is then collected in a separate container as the distillate.

The first distillate, containing pure ethanol, could then be removed and a clean round bottom flask attached to the end of the condenser. The experiment could then be allowed to continue with the mixture being heated until it reaches 102°C at 101.3 kPa, at which point we would see the remaining liquid turn into vapour. This would again travel up the tube and into the condenser, where it would cool down and turn back into liquid propyl ethanoate to be collected as a second distillate. In this way, we could finish the experiment with one flask containing pure ethanol and one flask containing pure propyl ethanoate. If these results were obtained, this would allow us to have a high level of confidence that the plant extract that we purchased does indeed contain a mixture of propyl ethanoate and ethanol.

While these are the ideal results for separating a mixture that contains only these components, let's now look at some other findings that could be obtained in this simple distillation and discuss what they would mean for the analysis of our plant extract (Table 10B–1).

Table 10B–1 Analysis of results from the simple distillation of a plant extract that is thought to contain only ethanol and propyl ethanoate

Observation	Analysis
A distillate is collected at a temperature lower than the boiling point of ethanol.	The mixture contains a component other than ethanol and propyl ethanoate. This may suggest that impurities are present.
No distillate is collected around the boiling point of ethanol.	It is likely that the mixture does not contain any ethanol. This suggests that the plant extract has not been prepared correctly.
A distillate is collected at a temperature greater than the boiling point of propyl ethanoate.	The mixture contains a component other than ethanol and propyl ethanoate. This may suggest that impurities are present.

This example highlights the fact that simple distillation can be used to provide some indication about both the purity of a consumer product and the identity of the components within it. Simple distillation is a relatively simple and inexpensive process, but it is not always effective for separating liquids with similar boiling points. In such cases, a technique called fractional distillation may be used. Fractional distillation is similar to simple distillation, but it involves a more complex set-up that allows for a more accurate separation of liquids with similar boiling points.

Fractional distillation

As briefly discussed in Section 1A, fractional distillation is a method used to separate different components in a mixture. It is based on the principle that different components in a mixture have different boiling points.

LINK **1A** TYPES OF FUELS

During fractional distillation, a mixture is heated until it vapourises and the vapour then passes through a fractionating column. The column is filled with packing materials, such as glass beads or metal mesh, that help to slow down the vapour. There is a temperature gradient across the fractionating column – the highest temperature occurs at the bottom (as it is closest to the heat source) and the lowest temperature occurs at the top of the column. This gradient allows for different vapour components to condense at different temperatures. If they condense before reaching the top of the fractionating column, they will run back down the column towards the round bottom flask.

From this point, the process proceeds in a similar fashion to simple distillation. The first distillate that is collected will contain the component of the mixture that has the lowest boiling point, as this will remain as a vapour until it reaches the top of the fractionating column and then passes into the condenser, where it cools further until it condenses back to a liquid and is captured in the conical flask. This flask is then removed and replaced with a fresh flask. As the mixture continues to be heated, the component with the second lowest boiling point will reach the top of the fractionating column and go through the same process. This continues to be repeated until all of the different distillates, or fractions, are collected.

Each fraction contains a different component of the mixture, depending on its boiling point. This experimental setup is illustrated in Figure 10B–6.

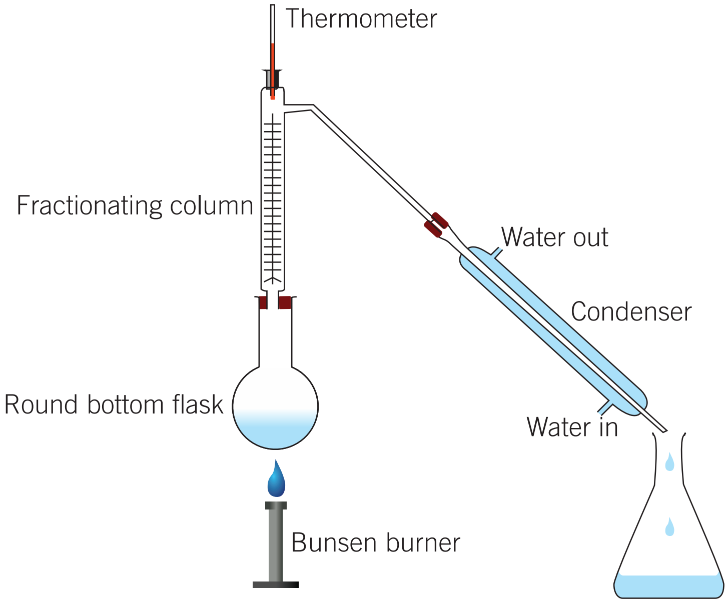

Figure 10B–6 The setup of a fractional distillation experiment

Fractional distillation is commonly used in the chemical and oil industries to identify the components of a substance (not purity, as these fractions contain a mixture of hydrocarbons). For example, it can be used to separate crude oil into different fractions, such as petrol, diesel and jet fuel. An example of how crude oil is separated by fractional distillation at an industrial level is shown in Figure 10B–7. It can be seen that each distillate is collected simultaneously by having condensers branching off from each level of the fractionating column. This helps make the process more efficient.

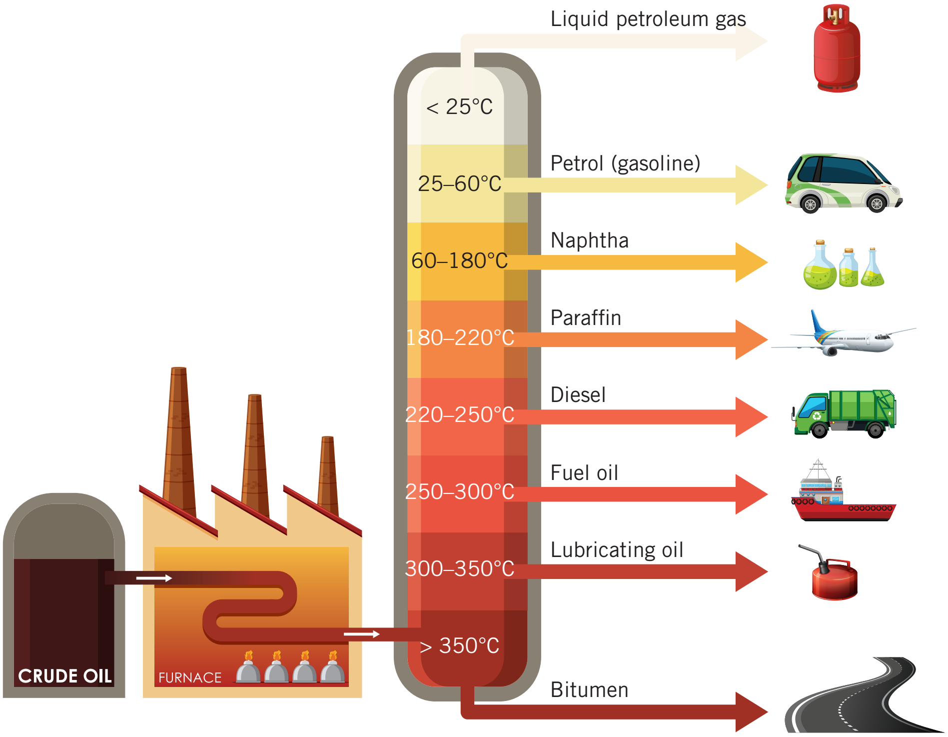

Figure 10B–7 The process for fractional distillation of crude oil at an industrial level

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Fractional distillation can also be used in the laboratory setting to separate and purify different chemicals. By analysing the fractions collected during fractional distillation, scientists can determine the composition and purity of the original mixture, in a similar way to the procedure described for simple distillation. As an example, under reduced pressure, fractional distillation is used to isolate essential oils like citronella or limonene. Distillation can be used to extract and purify the natural organic compounds in plants, such as extracting limonene from orange peel, which typically makes up more than 95% of the peel. Limonene ($C_{10}H_{16}$) is also an unsaturated hydrocarbon, which means that it can be put through a bromine water test, as outlined in Section 10A.

LINK **10A** ANALYSIS OF FUNCTIONAL GROUPS

Volumetric analysis

Volumetric analysis allows for the accurate determination of an unknown concentration for a solution. The concept of volumetric analysis was discussed in Unit 2 through the application of acid–base titrations. However, in Unit 4, we will be focusing purely on redox titrations. As with other types of volumetric analysis, redox titrations are a type of chemical analysis used to determine the concentration of a substance in a solution. However, in this instance, they are based on the principle of oxidation–reduction reactions, where electrons are transferred from one molecule to another. In a redox titration, a solution of known concentration, called the **titrant**, is slowly added to a solution of unknown concentration, called the **analyte**, until the reaction between the two is complete.

LINK **UNIT 2**

Titrant
a solution of known concentration that is added in titration

Analyte
a solution of unknown concentration in titration that is the subject of analysis

Redox titration is a precise and reliable method for measuring the concentration of a wide variety of chemicals, making it an important tool for many different fields.

In the food industry, redox titration is used to determine the purity or concentration of a compound. For example, it can be used to measure the concentration of ascorbic acid (vitamin C) in a vitamin C tablet or in different brands of orange juice, by titrating with an iodine solution. Redox titration is a powerful tool that can be used in a wide range of applications. In addition to the food industry, it is also commonly used in the pharmaceutical and water industries, as well as in environmental monitoring.

A redox titration is performed similarly to other forms of volumetric analysis. The required equipment and its arrangement is illustrated in Figure 10B–8.

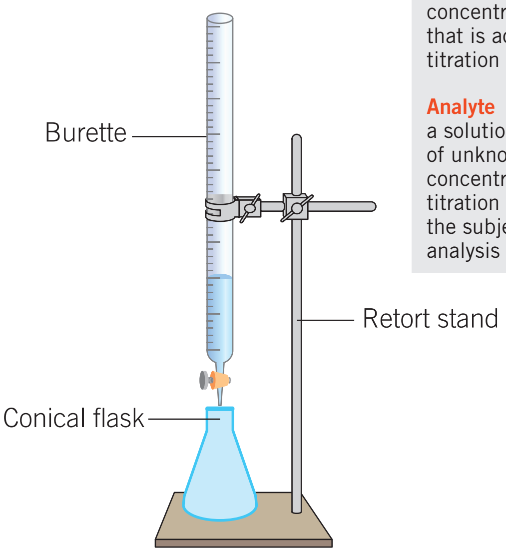


Figure 10B–8 The experimental set-up for a redox titration

Preparation of standard solutions

A critical part of any titration experiment is the preparation of the **standard solution**. To accurately calculate the concentration of the unknown oxidising agent or reducing agent, the standard solution needs to be made up correctly. For a compound to be considered suitable to be used as a primary standard, it needs to fulfil the following criteria:

- have a high molar mass to allow for accurate weight measurement on a balance with minimal error
- have a high stability/low level of reactivity
- be available with a high level of purity
- inexpensive
- be soluble in water or other common solvents.

Standard solution
a solution that contains a precisely known concentration; often used in volumetric analysis

To prepare a primary standard for a titration, an accurate and precise mass of the compound needs to be weighed out on an electronic balance and made up to an accurate volume in a volumetric flask. Primary standards can be used to standardise other solutions. These other solutions are often referred to as secondary standards and can also be used in titrations.

Common primary standards for redox titrations include potassium dichromate ($K_2Cr_2O_7$) and potassium iodate (KIO_3).

VIDEO WORKED EXAMPLE 10B–1

Worked example 10B–1: Calculating an accurate mass to use for preparing a primary standard

You require 100.0 mL of a 0.250 mol L^{-1} solution of potassium dichromate ($K_2Cr_2O_7$) to use as a primary standard. Calculate the mass of potassium dichromate that must be weighed out.

Solution

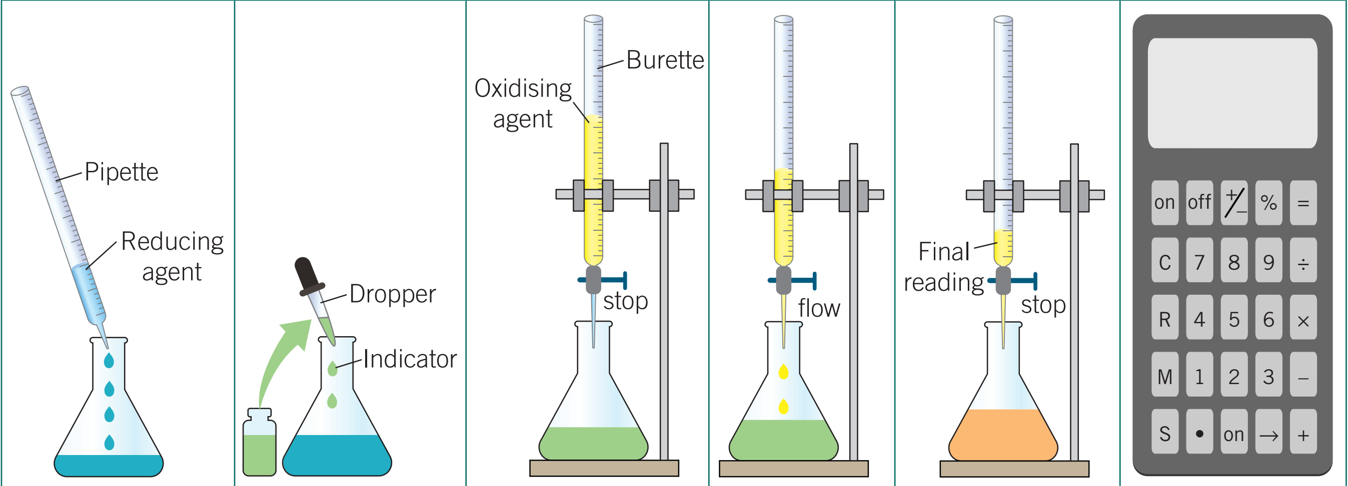
	Logic	Process
Step 1	Use $n = c \times V$ to calculate the amount, in mol, of potassium dichromate required.	$n(K_2Cr_2O_7) = c \times V$ $= 0.1000\ L \times 0.250\ mol\ L^{-1}$ $= 0.250\ mol$
Step 2	Use the periodic table to calculate the molar mass of potassium dichromate.	$M(K_2Cr_2O_7) = 294.2\ g\ mol^{-1}$
Step 3	Use $m = n \times M$ to calculate the mass of potassium dichromate required.	$m(K_2Cr_2O_7) = n \times M$ $= 0.250\ mol \times 294.2\ g\ mol^{-1}$ $= 7.36\ g$

Performing a titration

As mentioned previously, the purpose of performing a redox titration is to determine the unknown concentration of an oxidising agent or a reducing agent. To do this, that solution undergoes a redox reaction with a solution of known concentration, the titrant. Let's go through the steps involved in conducting this experiment.

For this scenario, we are going to have a reducing agent with an unknown concentration in the conical flask and an oxidising agent as our primary standard in the burette. It is important to note that you could perform this experiment with the solutions in either location.

The main steps in performing a titration are shown in Figure 10B–9. Each of these steps is explained in detail.



Step 1	Step 2	Step 3	Step 4	Step 5	Step 6
The reducing agent, with unknown concentration, is added to the conical flask using a pipette.	An indicator is added to the solution. It is important to note that depending on the redox reaction being performed, an indicator may not be required. Some redox reactions involve a colour change that can be monitored without the need for an indicator.	The oxidising agent, with known concentration, is added to the burette. The initial volume reading is recorded.	The tap of the burette is turned to the flow position and the oxidising agent is added in a dropwise fashion into the conical flask.	Once the indicator (or oxidising agent/ reducing agent) changes colour, the tap is moved back to the stop position. The final volume reading on the burette is recorded. The total volume added to the conical flask is recorded. Process is repeated until three **concordant** results are obtained.	The total volume of solution required for the redox reaction to go to completion is used to calculate the unknown concentration.

Figure 10B–9 The main steps in performing a redox titration

In step 5, the importance of obtaining concordant results was described. In the following table, five example titre volumes have been recorded for an experiment. You can see that volumes 2, 3 and 4 are concordant, and so, only the average of these three values should be used for performing any subsequent calculations.

Concordant in titration, the volume of two or more titres that are within 0.10 mL of each other

Table 10B–2 Determining concordant titration results

Titre volumes (mL)				
1	2	3	4	5
24.10	24.65	24.60	24.70	24.85

NOTE

For accurate redox titrations, the rinsing of each piece of glassware with the correct solutions is important.

An easy way to remember this is that instruments with the term 'flask' in them, such as conical flask and volumetric flask, are rinsed with de-ionised water.

The other instruments, such as the pipette and burette, are rinsed with the solutions that go into them prior to using them to deliver specific volumes as outlined in the steps above.

Indicators

A titration reaction is performed until the amount, in moles, of reducing agent and oxidising agent are in the correct stoichiometric ratio for the redox reaction to have gone to completion. This is known as the **equivalence point**. However, it is not always something that can be visualised when performing the experiment. Therefore, we use a way to observe this occurring. When acid–base titrations were studied in Unit 2, the concept of indicators was discussed. Acid–base indicators change colour in response to changes in the pH of the solution, and the time at which the indicator changes colour is known as the **end point**. It is important to realise that the equivalence point and the end point are not identical.

UNIT 2 LINK

Equivalence point the point in a titration when the amount, in moles, of reactants is present in the stoichiometric ratio that achieves neutralisation

End point the point in titration when the indicator changes colour

The concept is exactly the same in redox titrations, however, it is often not necessary for an additional indicator to be added. This is because some of the compounds used as primary or secondary standards in redox titrations will undergo a colour change of their own when the reaction occurs. Two common processes that are utilised during redox titrations, and their associated colour changes, are listed below.

- Potassium permanganate is a strong oxidising agent that is commonly used as a standard solution in redox titrations. As it is reduced, it goes through a number of colour changes (Figure 10B–10). This property allows for the end point to be visualised without the addition of an indicator.

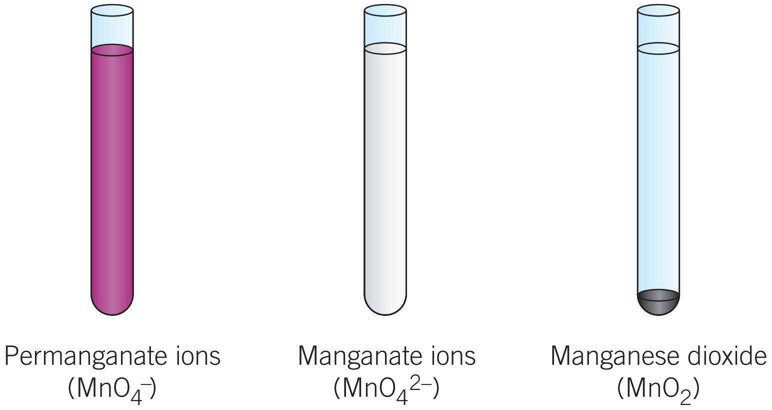
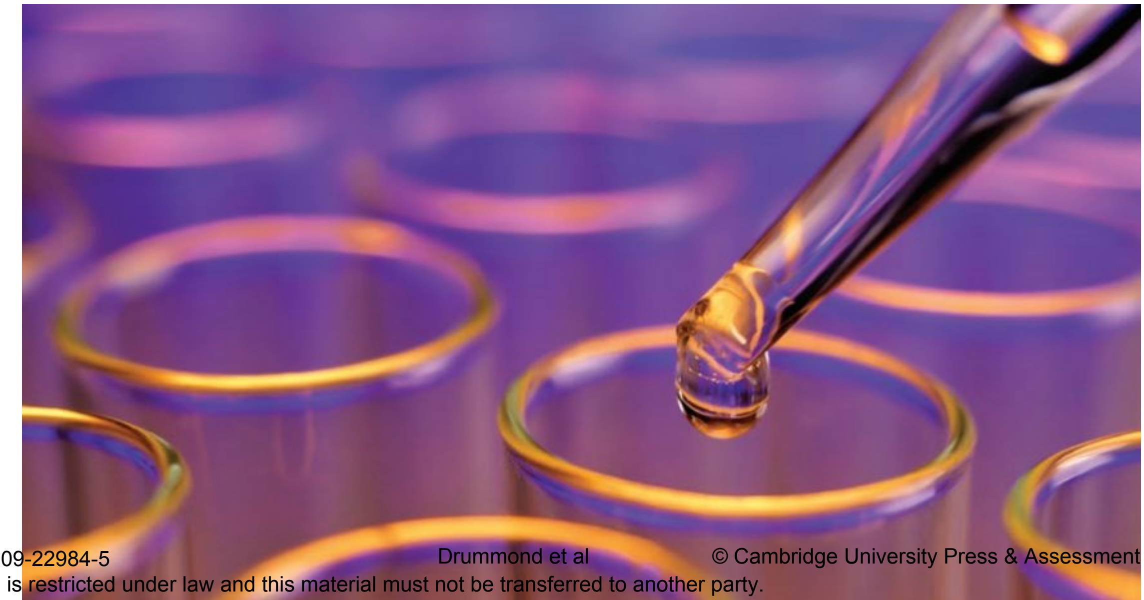


Figure 10B–10 Potassium permanganate undergoes a number of colour changes as it is reduced during a redox titration.

- Iodine is another common oxidising agent that can be used in redox titrations. When iodine is used as the titrant, it is common to utilise starch as an indicator. Unlike in the example above, starch isn't participating in the redox titration. However, during the redox titration, iodine is being reduced to iodide ions (I^-). These iodide ions are able to participate in a separate reaction with the starch, which forms a characteristic dark blue-purple colour. A colour change in the analyte from colourless to purple is used to visualise the end point in these titrations.



Titration calculations

The process to calculate the unknown concentration of a solution in any redox titration uses the same series of steps as those used in an acid–base titration. These steps are illustrated in the flow chart in Figure 10B–11.

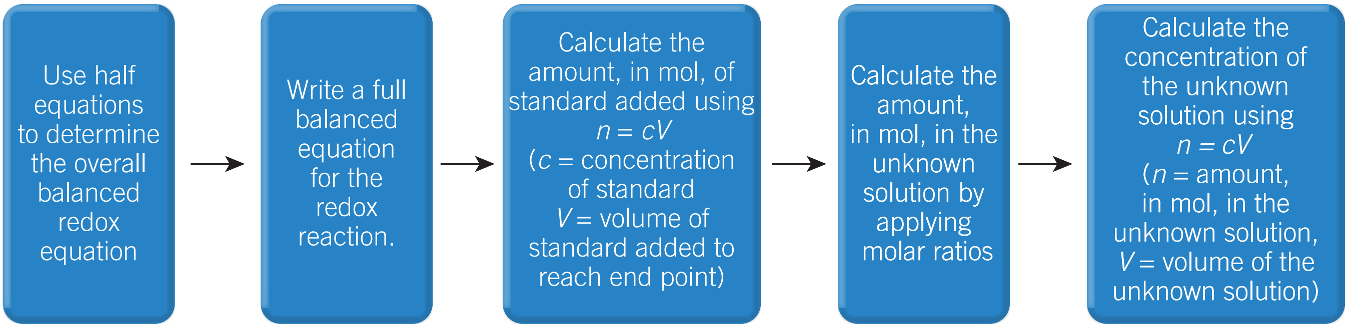


Figure 10B–11 Calculating the unknown concentration of any solution in a redox titration

Worked example 10B–2: Redox titration calculations

VIDEO
WORKED EXAMPLE 10B–2

WORKSHEET 10B–1
CALCULATIONS FOR REDOX TITRATIONS

A student performed a redox titration to determine the concentration of a solution of iron(II) ions (Fe^{2+}) using acidified potassium permanganate ($KMnO_4$) as the oxidising agent. The student used 25.00 mL of 0.100 M $KMnO_4$ to titrate a 50.00 mL sample of the Fe^{2+} solution. The half-equations occurring are:

$$Fe^{2+}(aq) \rightarrow Fe^{3+}(aq) + e^-$$

$$MnO_4^-(aq) + 8H^+(aq) + 5e^- \rightarrow Mn^{2+}(aq) + 4H_2O(l)$$

Determine the concentration of the Fe^{2+} solution.

Solution

	Logic	Process
Step 1	Write a balanced equation for the overall redox reaction.	$MnO_4^-(aq) + 5Fe^{2+}(aq) + 8H^+(aq) \rightarrow Mn^{2+}(aq) + 5Fe^{3+}(aq) + 4H_2O(l)$
Step 2	Extract the relevant information from the question.	$V(MnO_4^-) = 0.0250$ L $c(MnO_4^-) = 0.100$ M $V(Fe^{2+}) = 0.0500$ L
Step 3	Calculate the amount, in mol, of potassium permanganate using $n = cV$.	$n(MnO_4^-) = c \times V$ $= 0.100 \text{ M} \times 0.0250 \text{ L}$ $= 0.00250$ mol
Step 4	Calculate the amount, in mol, of iron(II) ions using molar ratios.	$n(Fe^{2+}) = n(MnO_4^-) \times 5$ $= 0.00250 \text{ mol} \times 5$ $= 0.0125$ mol
Step 5	Calculate the concentration of iron(II) ions using $n = cV$.	$c(Fe^{2+}) = \frac{n}{V}$ $= \frac{0.0125 \text{ mol}}{0.0500 \text{ L}}$ $= 0.250$ M

10B SKILLS

Calculation process for redox titrations

VIDEO 10B–2
SKILLS: CALCULATION PROCESS FOR REDOX TITRATIONS

In this section, you learned about performing calculations in a volumetric analysis for redox titrations. As you saw with these calculations, the unknown concentration of one reactant needs to be determined from information known about the other reactant. As such, questions for volumetric analysis include many numerical values. It is therefore important when writing symbols for given equations to assign more information to the chemical species to which the value refers. Here, this is termed 'notations'. It is also important to follow key steps in a process where the reactants and numerical values change in a problem but the key steps of the process do not. These steps are outlined using the example question below.

Question:

Aliquots of 20.00 mL of a brand of orange juice with an unknown concentration of ascorbic acid ($C_6H_8O_6$) are reacted with a 0.00500 M iodine solution, placed in the burette. A starch indicator is added to the conical flask with the orange juice. During this reaction the iodine will react (be reduced) with the ascorbic acid to form iodide. When the ascorbic acid has been used up, the remaining iodine will react with the starch indicator and change from a blue-black colour to a very pale blue-grey colour. This is the end point of the titration. The mean titre volume delivered is 30.45 mL. The reaction occurs according to the following equation:

$$C_6H_8O_6(aq) + I_2(aq) \rightarrow 2I^-(aq) + 2H^+(aq) + C_6H_6O_6(aq).$$

Determine the concentration of the ascorbic acid in the orange juice.

Solution:

	Logic	Process
Step 1	Write the respective half-equations for the reduction and oxidation reactions.	Oxidation half-equation: $C_6H_8O_6(aq) \rightarrow 2H^+(aq) + C_6H_6O_6(aq) + 2e^-$ Reduction half-equation: $I_2(aq) + 2e^- \rightarrow 2I^-(aq)$
Step 2	Write a balanced redox equation by combining the two half-equations from Step 1.	$C_6H_8O_6(aq) + I_2(aq) \rightarrow 2I^-(aq) + 2H^+(aq) + C_6H_6O_6(aq)$
Step 3	Use the information in the stem of the question to write down what is known and unknown. Clearly include notation about which species each value refers to, as opposed to just *c* or *V*.	$c(C_6H_8O_6) = ?$ $V(C_6H_8O_6) = 20.00\text{ mL} = 0.02000\text{ L}$ $c(I_2) = 0.00500\text{ mol L}^{-1}$ $V(I_2) = 30.45\text{ mL} = 0.03045\text{ L}$
Step 4	Determine the amount, in mol, of iodine. Again, use specific notation, $n(I_2)$, as opposed to just *n*. *Remember to keep the full number in the calculator for this step in the calculations.	$n(I_2) = c(I_2) \times V(I_2)$ $= 0.00500\text{ mol L}^{-1} \times 0.03045\text{ L}$ $= 1.52 \times 10^{-4}\text{ mol}$

	Logic	Process
Step 5	Use the mole ratio in the balanced equation from Step 2 to determine the amount, in mol, of ascorbic acid. Again, use specific notation, $n(C_6H_8O_6)$, as opposed to just '*n*'. *Remember to keep the full number in the calculator again for this step in the calculations.	$n(C_6H_8O_6) = n(I_2)$ $= 1.52 \times 10^{-4}$ mol
Step 6	Calculate the unknown concentration of ascorbic acid, using correct notation.	$c(C_6H_8O_6) = \frac{n(C_6H_8O_6)}{V(C_6H_8O_6)}$ $= \frac{1.52 \times 10^{-4} \text{ mol}}{0.02000 \text{ L}}$ $= 0.00761 \text{ mol L}^{-1}$

Remember, in these types of questions, obviously you are attempting to calculate the unknown concentration of a reactant, but it is equally important for your teacher or examiner to follow each step in your process of working. If by chance you were to enter a number incorrectly into your scientific calculator, at least the person assessing your work will be able to identify whether you have followed the correct process and written down the correct values for each step in this process.

Section 10B questions

1 Melting point determination can be used to determine the purity and identity of a consumer product.
   - a What is the melting point of a substance?
   - b Compare the results that you would expect to observe in a melting point determination experiment for a pure substance and an impure sample of the same substance.
   - c How can melting point determination be used to give an indication of the identity of the sample?

2 Simple distillation is a process that can be used to purify and check the purity of consumer products.
   - a What property of a substance is exploited in simple distillation?
   - b An 80% v/v solution of ethanol in water in a conical flask is processed through simple distillation. The first distillate is collected at 80°C, just above the boiling point of ethanol. Will this distillate have a higher or lower concentration of ethanol than the starting solution?
   - c What might be one explanation for why the observed result would be different to the expected result for part **b**?

3 In a redox titration, 25.00 mL of an unknown solution of MnO_4^- was titrated with a solution of Fe^{2+} with a concentration of 0.0100 M. The balanced half-equations for the reaction are:

$$MnO_4^- + 8H^+ + 5e^- \rightarrow Mn^{2+} + 4H_2O$$
$$Fe^{2+} \rightarrow Fe^{3+} + e^-$$

The end point was reached after the addition of 20.00 mL of the Fe^{2+} solution.
   - a What is the balanced equation for the overall titration reaction?
   - b What is the amount, in moles, of Fe^{2+} added?
   - c What is the amount, in moles, of MnO_4^- in the unknown solution?
   - d What is the concentration of the unknown MnO_4^- solution?

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Chapter 10 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
10A.1	Explain how qualitative tests can be used to determine the presence of carbon–carbon double bonds	3☐, 13☐
10A.2	Explain how qualitative tests can be used to determine the presence of hydroxyl functional groups	9☐, 13☐
10A.3	Explain how qualitative tests can be used to determine the presence of carboxyl functional groups	13☐
10A.4	Design experimental methods to test for carbon–carbon double bonds, and hydroxyl and/or carboxyl functional groups	13☐
10A.5	Determine the presence of carbon–carbon double bonds, and hydroxyl and/or carboxyl functional groups through analysing experimental data	7☐
10A.6	Describe how a redox titration with iodine can be used to determine the number of carbon–carbon double bonds in a molecule	4☐
10A.7	Calculate the number of carbon–carbon double bonds in an unsaturated hydrocarbon	13☐
10B.1	Define ‘purity’	1☐
10B.2	Describe how the melting point of a consumer product can help determine the identity and purity of a consumer product	12☐
10B.3	Compare simple and fractional distillation	6☐, 12☐
10B.4	Draw a diagram of the experimental set-up for simple and fractional distillation	12☐
10B.5	Explain how simple distillation can be used to verify the components and purity of a consumer product	10☐
10B.6	Explain how fractional distillation can be used to verify the components and purity of a consumer product	12☐
10B.7	Define ‘end point’ and ‘equivalence point’	2☐
10B.8	Describe the use of an indicator in a redox titration	5☐
10B.9	Define ‘standard solution’	11☐
10B.10	State the key characteristics of a primary standard solution	8☐
10B.11	List the steps involved in a redox titration, including glassware involved	11☐
10B.12	Calculate the concentration of an unknown solution from given experimental data	11☐

Multiple-choice questions

1 The degree to which a substance is free from contaminants or unwanted materials is known as its
- **A** purity.
- **B** composition.
- **C** boiling point.
- **D** melting point.

2 The instant at which a permanent colour change is observed in a redox titration is called the
- **A** indicator.
- **B** end point.
- **C** concordant result.
- **D** equivalence point.

3 Qualitative tests to determine the presence of a carbon–carbon double bond involve
- **A** measuring the boiling point of the hydrocarbon.
- **B** measuring the melting point of the hydrocarbon.
- **C** observing the colour change associated with an addition reaction.
- **D** separating the components of the hydrocarbon through fractional distillation.

4 Which of the following is a correctly balanced equation for the reaction between iodine and a hydrocarbon containing one carbon–carbon double bond?
- **A** $C_6H_{14} + I_2 \rightarrow C_6H_{12}I_2$
- **B** $C_6H_{14} + I_2 \rightarrow C_6H_{12}I_2 + H_2I_2$
- **C** $C_6H_{12} + I_2 \rightarrow C_6H_{12}I_2 + H_2$
- **D** $C_6H_{12} + I_2 \rightarrow C_6H_{12}I_2$

5 What is the main reason why an indicator isn't always used in a redox titration?
- **A** They are expensive and not readily available.
- **B** They only work for acid–base titrations.
- **C** They don't accurately measure the end point in redox reactions.
- **D** They aren't necessary if a permanent colour change is observed directly in the redox reaction.

6 Which of the following is an advantage of fractional distillation over simple distillation?
- **A** It can produce more than one distillate.
- **B** It can separate components that have similar boiling points.
- **C** It can be done more cost effectively and with less equipment.
- **D** It can be performed at much lower temperatures and so is more environmentally friendly.

7 If a carboxyl functional group was present in a hydrocarbon, it would
- **A** turn red litmus paper blue.
- **B** change colour when reacted with bromine.
- **C** have an ester odour after reacting with an alcohol.
- **D** have a melting point lower than expected for its pure compound.

8 Which of the following is **not** a key characteristic of a primary standard solution used in a redox titration?

A It reacts readily with the air.

B It is soluble in water and other common solvents.

C It has a high molar mass to allow for accurate weighing.

D It is inexpensive, non-toxic and readily available for purchasing.

9 The colour change that occurs when a primary alcohol is reacted with potassium dichromate is

A green to orange.

B orange to green.

C green to colourless.

D orange to colourless.

10 A sample, which could be pure or a mixture of substances, is distilled. Which row of the table correctly matches an observation with a valid conclusion about the purity of the sample?

	Observed result	Conclusion about purity
A	A single distillate is obtained at the expected boiling point.	The sample contains impurities.
B	Two distillates are obtained.	The sample is pure.
C	A single distillate is obtained at the expected boiling point.	Only one of the expected components is present in the sample.
D	Two distillates are obtained.	Both of the expected components are present in the sample.

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Short-answer questions

11 Oxalic acid ($C_2H_2O_4$) can be used in pottery to create light-coloured ceramics. The working concentration range for oxalic acid for this purpose is between 0.05 mol L^{-1} and 0.15 mol L^{-1}. A new product has gone on the market for this purpose, called PotOx, but customers have claimed that the results they are obtaining aren't suitable. There is a suggestion that this is because the oxalic acid in the product is at a higher concentration than the recommended value. Your lab has been asked to test this hypothesis by performing a redox titration.

a Potassium dichromate ($K_2Cr_2O_7$) is to be used as the standard solution for this titration. Define the term 'standard solution'. (1 mark)

b You are required to prepare 100.0 mL of a 0.200 mol L^{-1} standard solution. What mass of potassium dichromate should be weighed out? (2 marks)

c With the standard solution prepared, you are now ready to perform your redox titration. For the titration, 1.25 g of PotOx was weighed and dissolved in de-ionised water (as per the manufacturer's instructions) made up to the 200 mL mark of a volumetric flask. Describe the next steps involved in conducting this experiment, including the glassware required. (5 marks)

d The oxidation and reduction half-equations occurring during this titration are provided below. What is the overall reaction?

Reduction: $Cr_2O_7^{2-}(aq) + 14H^+(aq) + 6e^- \rightarrow 2Cr^{3+}(aq) + 7H_2O(l)$

Oxidation: $C_2O_4^{2-}(aq) \rightarrow 2CO_2(g) + 2e^-$ (1 mark)

e Having completed three titrations, you determine the average titre to be 15.00 mL. What is the amount, in mol, of potassium dichromate needed to reach the end point? (1 mark)

f What is the concentration of oxalic acid, in mol L^{-1}, in the sample? (1 mark)

g Is the customer hypothesis about PotOx correct? (1 mark)

12 A scientist has received two samples of new products to store in their laboratory. One of the samples is a bullion bar created from pure silver (melting point = 961.8°C). The other is a cleaning product that is a high-quality vinegar, composed of acetic acid (boiling point = 118°C) in water (boiling point = 100°C).

a Explain why melting point determination is a more suitable technique than distillation to assess the purity of the bullion bar. (2 marks)

b Three different batches of bullion bar were received from different suppliers. The results from the melting point determination are presented below.

	Batch 1	Batch 2	Batch 3
Melting point (°C)	961.6–962.0	958.2–960.5	961.7–961.9

Which of the three batches is impure? What features of the data indicate this? (2 marks)

c Draw a diagram of the experimental set-up that you would use to test the purity and components of the cleaning product. (2 marks)

d Describe the results that you would expect from the experiment described in part **c** if the mixture did not contain any other contaminants. (2 marks)

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13 A range of samples has been produced from conducting organic reactions. These samples have been labelled 1–5. The scientist that created the samples has passed them to you to analyse. To ensure that the testing is unbiased, they have not told you what the expected compound is in each sample. They have asked you to conduct a number of qualitative tests and report back your findings on what functional groups the potential samples contain. The results of your analyses are found in the table below.

	Qualitative test performed				
Sample number	**Bromine water test**	**Reaction with potassium dichromate**	**Litmus test**	**Reaction with alcohol**	**Baeyer's test**
1	Becomes colourless in dark	Sample is orange	Blue litmus paper stays blue	No smell produced	Red precipitate forms
2	Becomes colourless in light	Sample is orange	Blue litmus paper turns red	Ester odour	Sample is purple
3	Becomes colourless in light	Sample is orange	Blue litmus paper stays blue	No smell produced	Sample is purple
4	Becomes colourless in light	Sample is green	Blue litmus paper stays blue	No smell produced	Sample is purple
5	Inconclusive	Sample is green	Blue litmus paper stays blue	Ester odour	Red precipitate forms

a Which two samples have conflicting results? Explain your choices. (3 marks)

b Assuming all of the results are correct for sample 3, what can you conclude about this compound? (2 marks)

c Which sample contains more than one functional group and what functional groups does it contain? (2 marks)

d Since you have done such a good job with the initial samples, the scientist sends through a sixth sample, which they need identified. They know that this sample is either an alkane or an alkene, but aren't sure which. Design an experiment that you could use to determine what the sixth sample is. Make sure that you include a description of the results that may be observed and what you could conclude from them. (5 marks)

e The results show that the sixth sample does in fact contain a carbon–carbon double bond. However, the scientist would like more information and asks you to determine the number of carbon–carbon double bonds that are present. You are given the following information:

$m(\text{sample 6}) = 12.2\text{ g}$

$M(\text{sample 6}) = 304.5\text{ g mol}^{-1}$

You find that this reacts completely with a 200.0 mL 0.802 mol L^{-1} iodine solution. How many carbon–carbon double bonds are present in the molecule in sample 6? (3 marks)

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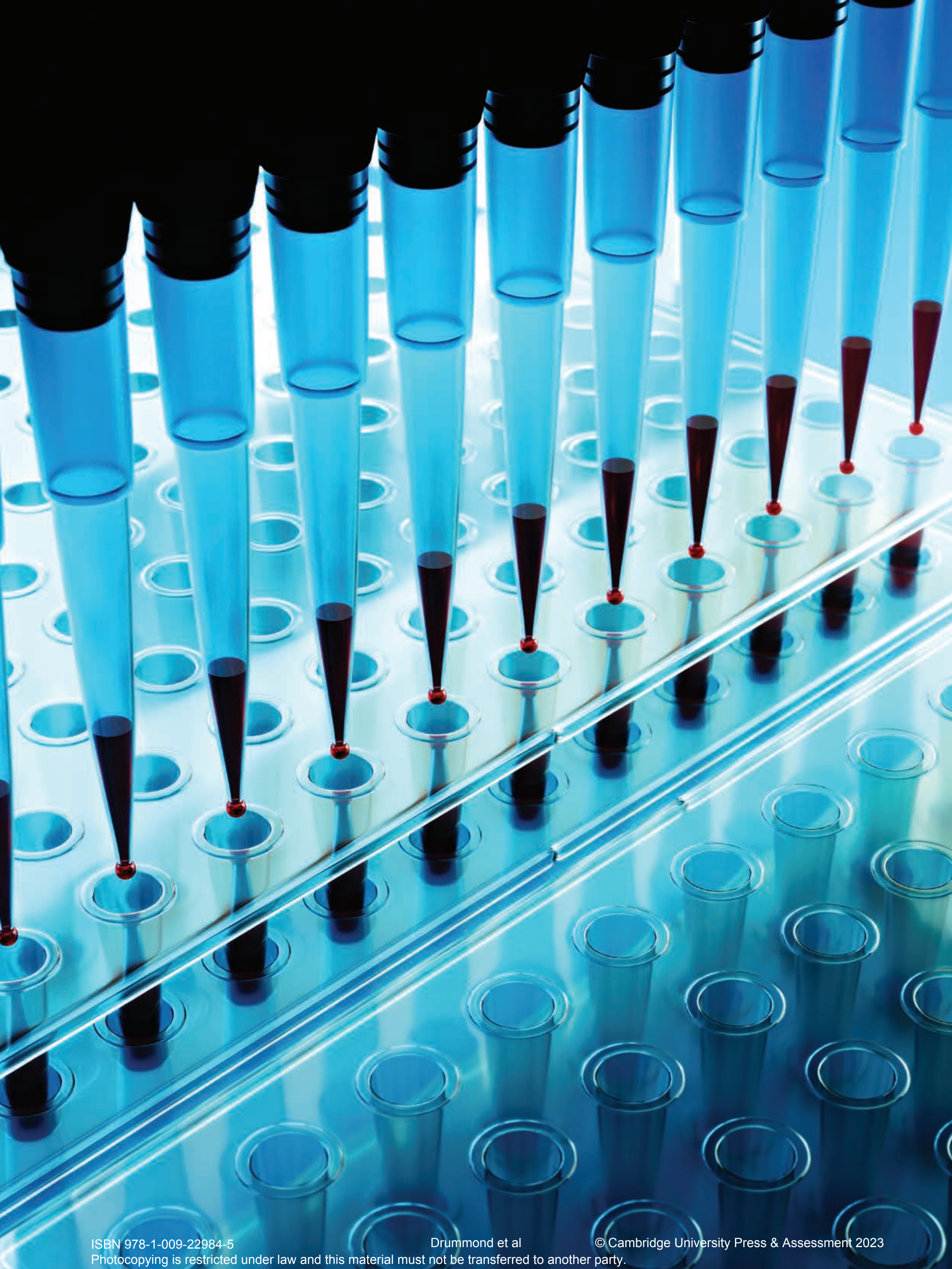

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UNIT 4 HOW ARE CARBON-BASED COMPOUNDS DESIGNED FOR PURPOSE?

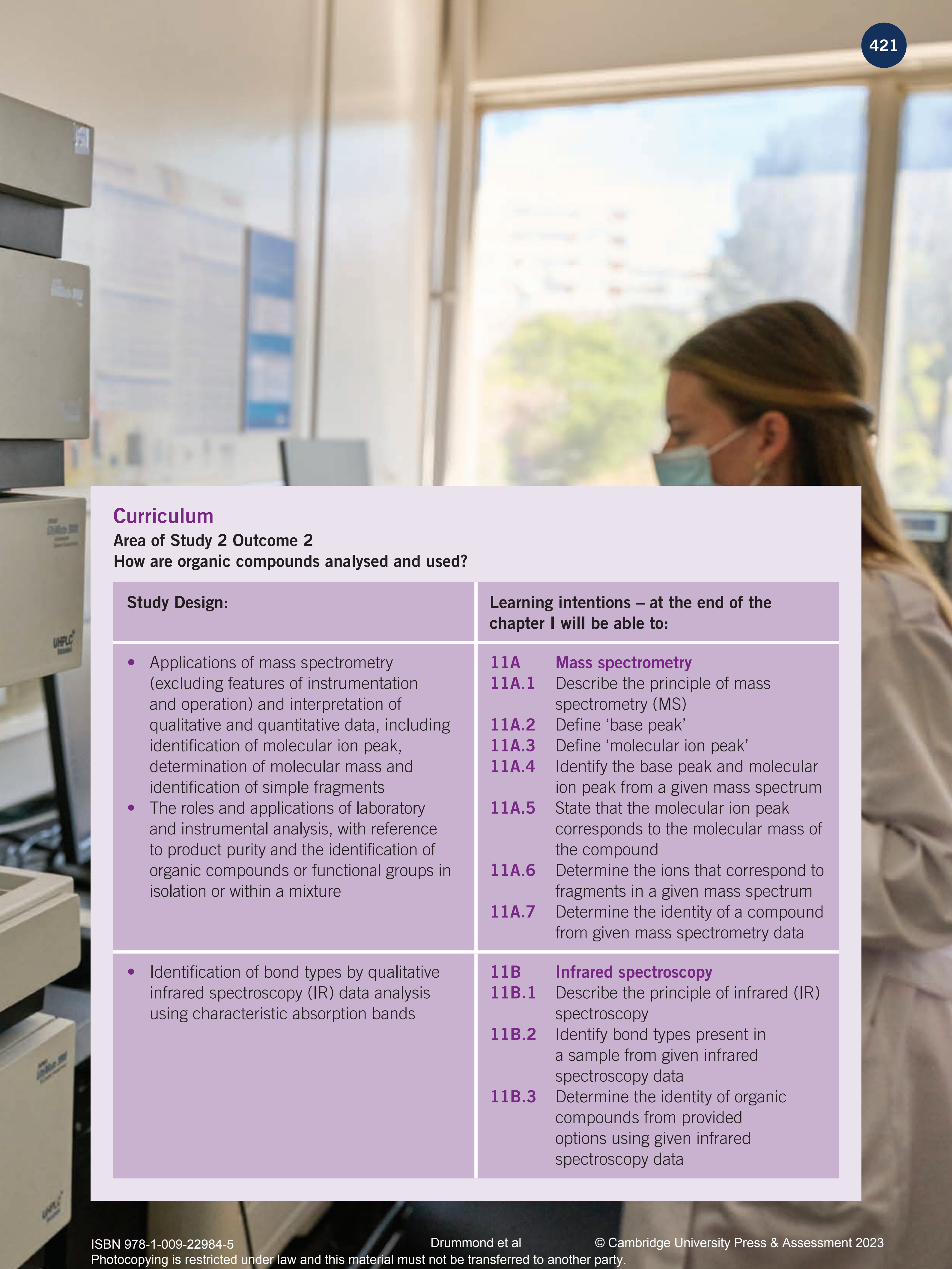
CHAPTER 11 INSTRUMENTAL ANALYSIS OF ORGANIC COMPOUNDS

Introduction

INTRODUCTION VIDEO
INSTRUMENTAL ANALYSIS OF ORGANIC COMPOUNDS

Technological advancements are happening all around us – electric vehicles, artificial intelligence, mRNA vaccines – and the world of chemistry is no different! The advancement of highly sophisticated instruments has brought a whole new dimension to the field and the use of these is often referred to as instrumental analysis. It's a fascinating area of chemistry that combines our theoretical knowledge with state-of-the-art technology to help us delve into the intricate details of chemical compounds. It's like Sherlock Holmes meeting James Bond in the realm of science – using advanced gadgets and profound knowledge to solve mysteries at the molecular level.

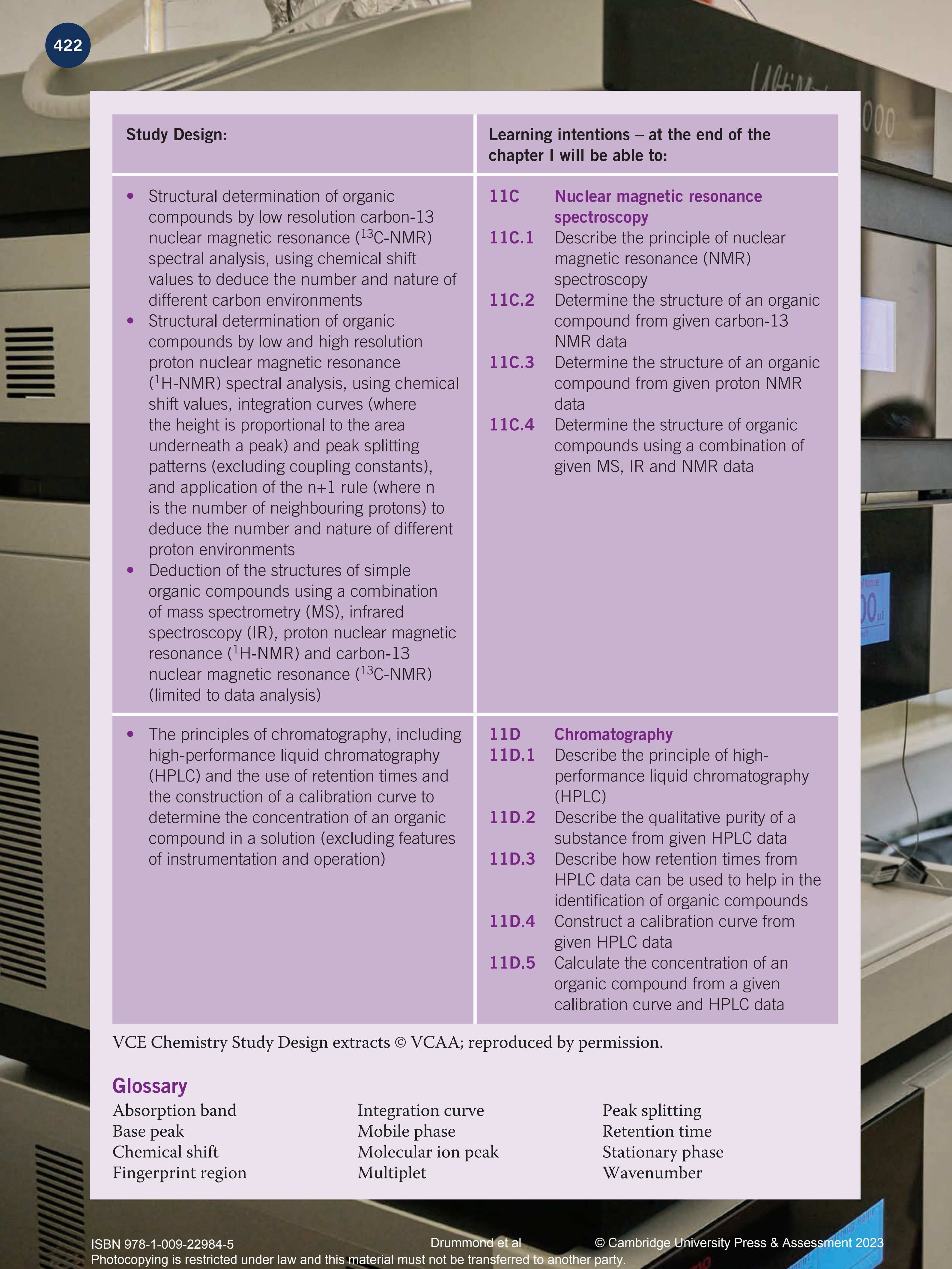
These instruments are not just useful in a laboratory setting, they also have real-life applications. Have you ever wondered how forensic scientists can identify the minutest trace of a substance at a crime scene? Or how pharmaceutical companies ensure that the medicine you take is safe and effective? Instrumental techniques, such as mass spectrometry (MS), infrared spectroscopy (IR) and nuclear magnetic resonance (NMR) spectroscopy, are the unsung heroes behind the scenes. Mass spectrometry allows us to analyse the composition of a sample down to its individual atoms. Infrared spectroscopy can identify specific functional groups in molecules, aiding in the identification of substances. And NMR spectroscopy? It provides information about the structure of a molecule, helping us understand how it's put together. From ensuring the purity of drinking water and developing new medicines, to exploring the vastness of space, instrumental analysis plays a critical role in many facets of modern life. In this chapter, you will learn about the principles behind these techniques and how the data they generate can be analysed.



Curriculum

Area of Study 2 Outcome 2
How are organic compounds analysed and used?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
- Applications of mass spectrometry (excluding features of instrumentation and operation) and interpretation of qualitative and quantitative data, including identification of molecular ion peak, determination of molecular mass and identification of simple fragments - The roles and applications of laboratory and instrumental analysis, with reference to product purity and the identification of organic compounds or functional groups in isolation or within a mixture	**11A Mass spectrometry** **11A.1** Describe the principle of mass spectrometry (MS) **11A.2** Define 'base peak' **11A.3** Define 'molecular ion peak' **11A.4** Identify the base peak and molecular ion peak from a given mass spectrum **11A.5** State that the molecular ion peak corresponds to the molecular mass of the compound **11A.6** Determine the ions that correspond to fragments in a given mass spectrum **11A.7** Determine the identity of a compound from given mass spectrometry data
- Identification of bond types by qualitative infrared spectroscopy (IR) data analysis using characteristic absorption bands	**11B Infrared spectroscopy** **11B.1** Describe the principle of infrared (IR) spectroscopy **11B.2** Identify bond types present in a sample from given infrared spectroscopy data **11B.3** Determine the identity of organic compounds from provided options using given infrared spectroscopy data



Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Structural determination of organic compounds by low resolution carbon-13 nuclear magnetic resonance (^{13}C-NMR) spectral analysis, using chemical shift values to deduce the number and nature of different carbon environments • Structural determination of organic compounds by low and high resolution proton nuclear magnetic resonance (^{1}H-NMR) spectral analysis, using chemical shift values, integration curves (where the height is proportional to the area underneath a peak) and peak splitting patterns (excluding coupling constants), and application of the n+1 rule (where n is the number of neighbouring protons) to deduce the number and nature of different proton environments • Deduction of the structures of simple organic compounds using a combination of mass spectrometry (MS), infrared spectroscopy (IR), proton nuclear magnetic resonance (^{1}H-NMR) and carbon-13 nuclear magnetic resonance (^{13}C-NMR) (limited to data analysis)	**11C Nuclear magnetic resonance spectroscopy** **11C.1** Describe the principle of nuclear magnetic resonance (NMR) spectroscopy **11C.2** Determine the structure of an organic compound from given carbon-13 NMR data **11C.3** Determine the structure of an organic compound from given proton NMR data **11C.4** Determine the structure of organic compounds using a combination of given MS, IR and NMR data
• The principles of chromatography, including high-performance liquid chromatography (HPLC) and the use of retention times and the construction of a calibration curve to determine the concentration of an organic compound in a solution (excluding features of instrumentation and operation)	**11D Chromatography** **11D.1** Describe the principle of high-performance liquid chromatography (HPLC) **11D.2** Describe the qualitative purity of a substance from given HPLC data **11D.3** Describe how retention times from HPLC data can be used to help in the identification of organic compounds **11D.4** Construct a calibration curve from given HPLC data **11D.5** Calculate the concentration of an organic compound from a given calibration curve and HPLC data

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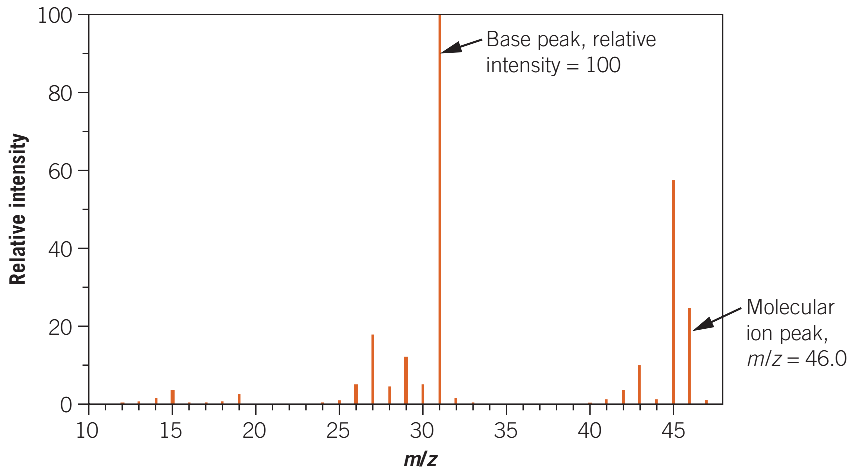
Glossary

Absorption band
Base peak
Chemical shift
Fingerprint region
Integration curve
Mobile phase
Molecular ion peak
Multiplet
Peak splitting
Retention time
Stationary phase
Wavenumber

Concept map

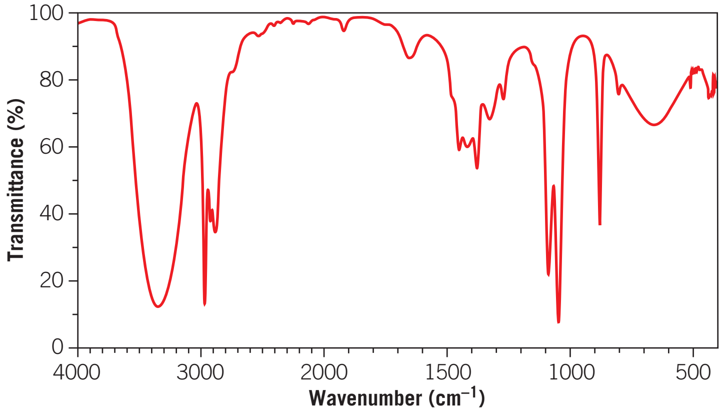
11A Mass spectrometry

Technique for determining the mass and identity of organic compounds



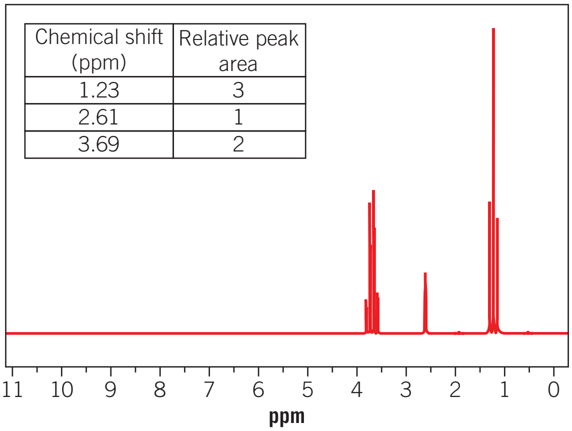
11B Infrared spectroscopy

Technique for identifying functional groups in organic compounds



11C Nuclear magnetic resonance spectroscopy

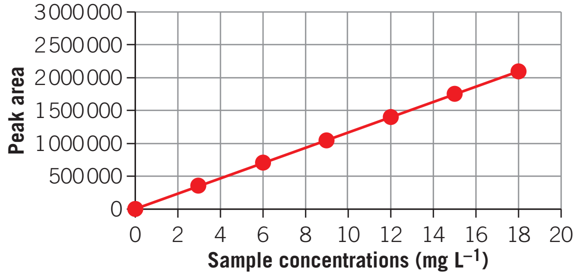
Technique for determining the identity and structure of organic compounds



Chemical shift (ppm)	Relative peak area
1.23	3
2.61	1
3.69	2

11D Chromatography

Technique for separating organic compounds in mixtures, analysing purity and determining concentration



See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

11A Mass spectrometry

Study Design:

- Applications of mass spectrometry (excluding features of instrumentation and operation) and interpretation of qualitative and quantitative data, including identification of molecular ion peak, determination of molecular mass and identification of simple fragments
- The roles and applications of laboratory and instrumental analysis, with reference to product purity and the identification of organic compounds or functional groups in isolation or within a mixture

Glossary:
Base peak
Molecular ion peak

ENGAGE

Chemistry that's out of this world!

Figure 11A–1 The Mars *Curiosity* rover

Have you ever been travelling somewhere by plane and, as you were passing through the security checkpoints, been taken aside to have an extra test that involved swabbing your carry-on luggage, your clothes and your shoes? This screening measure is used to detect traces of explosives and uses an extremely sensitive and accurate device called a mass spectrometer. Incredibly, mass spectrometry hasn't only proved to be a useful technique on this planet. The Mars *Curiosity* rover, which landed on Mars in 2012, has now been collecting data about our planetary neighbour for over a decade. Part of the information that is being analysed by *Curiosity* is the detection of key elements and organic compounds that may make Mars suitable for habitation. This is done through an in-built mass spectrometer within the rover itself. In this section, you will learn about mass spectrometry and how to interpret the data that it generates to gain qualitative and quantitative information about organic compounds.

EXPLAIN

What is mass spectrometry (MS)?

Mass spectrometry is a powerful analytical technique used to determine the masses and abundances of atoms and molecules in a sample. It is used in many areas of chemistry, including drug discovery, environmental analysis and forensic science. The principle of mass spectrometry is based on the fact that ions, which are atoms or molecules that have gained or lost one or more electrons, can be separated based on their mass-to-charge ratio (m/z). The process involves three main steps: ionisation, separation and detection.

In the first step, the sample is ionised to produce positively charged ions. It works by vaporising the sample and passing it through a stream of high-energy electrons. These electrons collide with the sample molecules or atoms, knocking one or more electrons off and creating positive ions.

For an example molecule, M, the equation for this process could be written as:

$$M \rightarrow M^+ + e^-$$

Ions in the mass spectrometer are unstable and can fragment further. For example, a bond in the M^+ ion may break, producing two smaller fragments, X and Y. One of X or Y will have a positive charge and the other will be uncharged. For example, the fragmentation of M^+ may proceed as:

$$M^+ \rightarrow X^+ + Y$$

or

$$M^+ \rightarrow X + Y^+$$

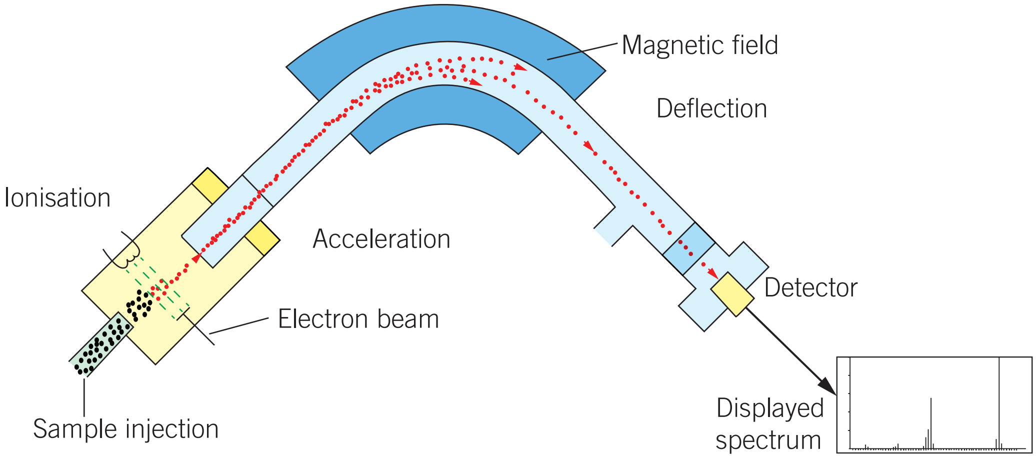


Figure 11A–2 A diagrammatic representation of a mass spectrometer, highlighting the different stages of the process, from ionisation of the sample through to detection at the end

Once ionised, the ions are accelerated through an electric field and separated based on their *m*/*z* ratio by a magnetic field. The separated ions are then detected, typically by a detector that measures the ion current as a function of *m*/*z*. This process is illustrated in Figure 11A–2, although it is important to realise that you aren't required to understand the principles of the instrument.

Analysing mass spectrometry data

Mass spectrometry is a powerful analytical technique used to determine the molecular weight and structural information of organic compounds. To analyse mass spectrometry data of organic compounds, it is important to first understand the terms 'base peak' and 'molecular ion'. The **base peak** refers to the highest intensity peak in a mass spectrum, while the **molecular ion peak** represents the molecular weight of the compound. It is important to note that occasionally more than one molecular ion peak can be present. This occurs in instances where the analysed compound contains elements with multiple stable isotopes. A common example involves organic compounds containing a chlorine atom, which would have two molecular ion peaks – one corresponding to the compound containing chlorine-35 and the other to the compound containing chlorine-37.

Base peak
the highest intensity peak in a mass spectrum

Molecular ion peak
the ion peak that represents the molecular weight of the compound

Mass spectrometry data is typically displayed as a graph of relative intensity versus mass-to-charge ratio (*m/z*), where the mass-to-charge ratio represents the mass of the ion divided by its charge. The mass-to-charge ratio is represented on the *x*-axis, while the relative intensity is represented on the *y*-axis. The peaks in the mass spectrum correspond to the various ions produced by the compound during the ionisation process.

The mass-to-charge ratio is an important parameter in mass spectrometry because it provides information about the mass of the ion, as well as its charge. The relative intensity of each peak in the mass spectrum provides information about the abundance of each ion produced during the ionisation process. The most abundant peak in the spectrum is the base peak, which is assigned a relative intensity of 100%. Other peaks are assigned a relative intensity based on their abundance relative to the base peak.

In addition to the base peak and molecular ion, there are other important features in a mass spectrum, such as fragmentation peaks and isotopic peaks, which can provide valuable information about the compound. Fragmentation peaks arise from the fragmentation of the molecular ion during the ionisation process, while isotopic peaks are caused by the presence of isotopes in the sample. The analysis of these peaks, along with the base peak and molecular ion, can provide important structural information about the compound, allowing for its identification.

VIDEO 11A–1
IMPORTANT FEATURES OF A MASS SPECTRUM

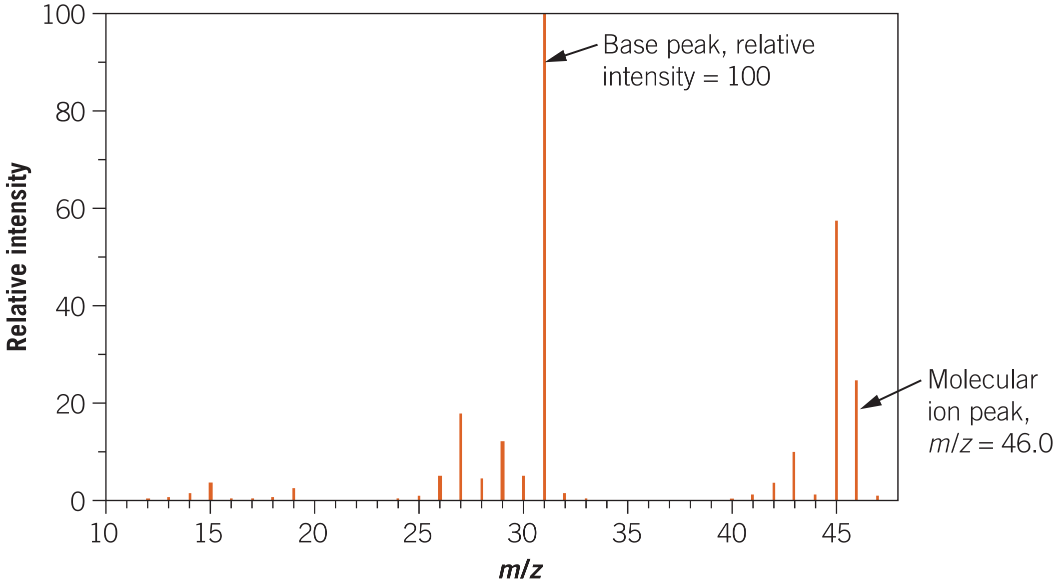


Figure 11A–3 Mass spectrum for ethanol (C_2H_5OH)

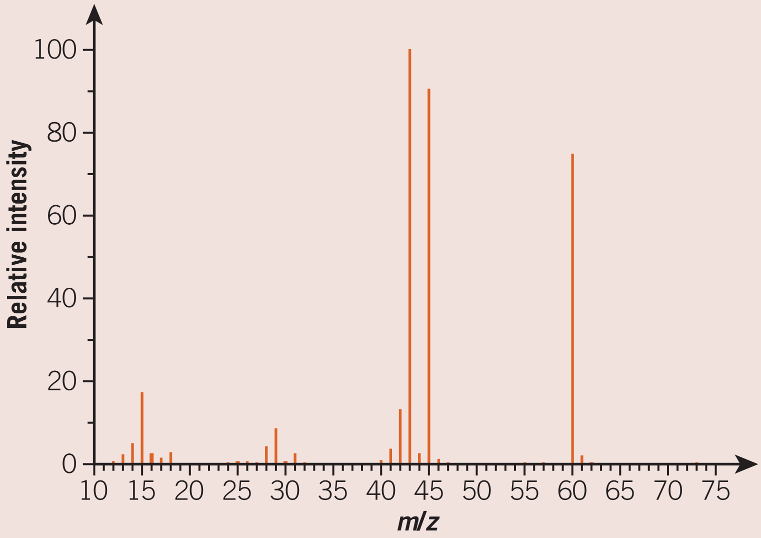
WORKSHEET 11A–1
ANALYSING MASS SPECTROMETRY DATA

Figure 11A–3 shows the mass spectrum that would be produced for a sample of ethanol. There are a number of key features that we can observe in this spectrum. Firstly, the molecular ion is the peak with the highest *m*/*z* (that is, the one furthest to the right). This tells us that ethanol has a molecular weight of 46.0 g mol^{-1}. It is also possible to observe the base peak, which is seen at an *m*/*z* of 31.0. This is the most abundant peak in the spectrum and so is given the relative intensity of 100. As this peak has an *m*/*z* of 15 less than the molecular ion, it could be suggested that this is ethanol having lost a methyl ($-CH_3$) group. Determining the fragments that correspond to given peaks in a mass spectrum will be covered in Worked examples 11A–1 and 11A–2.

Worked example 11A–1: Using the molecular ion to differentiate between compounds

VIDEO WORKED EXAMPLE 11A–1

Mass spectrometry data have been generated from an organic compound. By analysing the spectrum below, determine whether the compound is ethanol or ethanoic acid.



Solution

	Logic	Process
Step 1	Determine the molecular masses of ethanol and ethanoic acid.	M(ethanol) = 46 M(ethanoic acid) = 60
Step 2	Identify the mass of the molecular ion.	Molecular ion mass = 60
Step 3	Determine which compound is present.	As the molecular ion mass corresponds to the molecular mass of ethanoic acid, this must be the compound present in the sample.

Worked example 11A–2: Determining fragments from a given compound

VIDEO WORKED EXAMPLE 11A–2

Determine the ions that produce fragments occurring at an m/z of 15, 43 and 86 in a mass spectrum of hexane.

Solution

	Logic	Process
Step 1	Write the semi-structural formula of hexane.	Hexane = $CH_3CH_2CH_2CH_2CH_2CH_3$
Step 2	Determine the molecular mass of hexane.	M(hexane) = 86
Step 3	Determine the masses produced by fragmenting hexane at each carbon-carbon bond.	$CH_3 = 15$ $CH_3CH_2 = 29$ $CH_3CH_2CH_2 = 43$ $CH_3CH_2CH_2CH_2 = 57$ $CH_3CH_2CH_2CH_2CH_2 = 71$
Step 4	Identify and write the fragments corresponding to the masses in the question.	m/z of 15 = $[CH_3]^+$ m/z of 43 = $[CH_3CH_2CH_2]^+$ m/z of 86 = molecular ion = $[CH_3CH_2CH_2CH_2CH_2CH_3]^+$

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Check-in questions – Set 1

1 The x-axis of a mass spectrum is often labelled m/z. What do 'm' and 'z' represent in this instance?

2 Explain why ethane and propane both produce fragments in mass spectrometry with an m/z of 29, but methane does not.

3 Would you expect to see the same molecular ion for butane and methylpropane? Explain why or why not.

Mass spectrometry for identification of compounds

Due to its sensitivity and nature of analysis, mass spectrometry can be an incredibly powerful technique for the identification of compounds in mixtures. As described earlier, compounds will produce characteristic fragmentation patterns when they are ionised within a mass spectrometer. In a sample containing a single compound, the analysis can be performed relatively easily to determine the identity of the compound. However, in a mixture, this process can become far more complicated. Indeed, many samples that are analysed by mass spectrometry do involve complex mixtures, such as blood samples that are used for drug testing of athletes. Fortunately, in these instances, the large numbers of fragmentation patterns that are detected can be analysed using specialised computer software to search through large databases. This allows for quite definitive conclusions to be drawn about the identity of organic components within these complex mixtures.

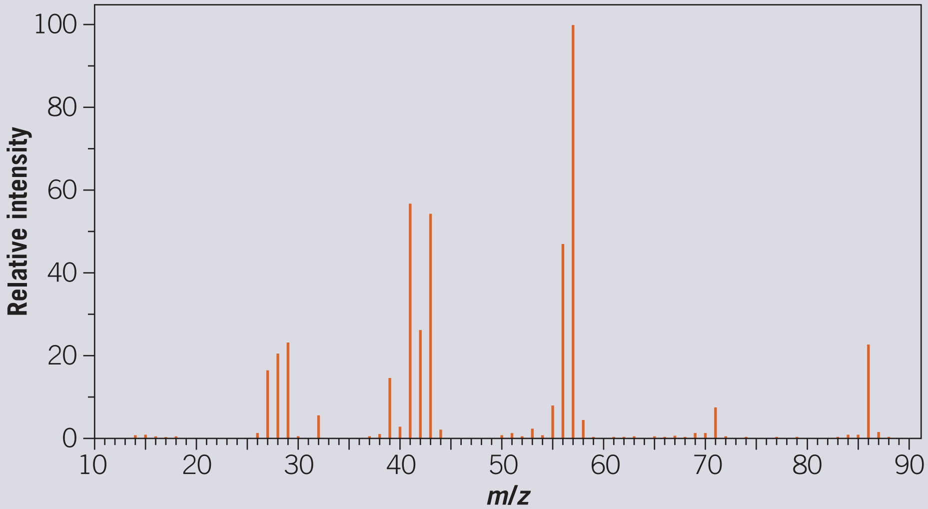
VIDEO 11A–2
SKILLS: MASS SPECTROMETRY SKILLS

11A SKILLS

Mass spectrometry skills

In Worked example 11A–2, we looked at a question that involved determining the fragments that corresponded to given m/z values from mass spectrometry data. In this instance, the steps shown involved determining the masses of all the different fragments that could be produced by breaking hexane at each carbon–carbon bond. The masses of these were then calculated by adding together the masses of all the elements in the fragment.

However, you may get questions that involve a slightly more complicated molecule or more complex spectra that you are trying to figure out. In these instances, it can be useful to flip the way that you attempt to solve these problems and start with the molecular ion and work out what has been subtracted from that. To illustrate this, let's look at the mass spectrum for hexane.



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As in Worked example 11A–2, we can see the molecular ion peak at an *m/z* of 86. However, what if we were asked to identify the fragment that created the peak at an *m/z* of 71? As in the worked example, we could try to identify what fragments add up to 71. A quicker method, however, would be to realise that an *m/z* of 71 is equivalent to the molecular ion (*m/z* = 86) with a loss of 15. A common fragment in mass spectrometry is $-CH_3^+$, which has an *m/z* of 15. Knowing this, we can quickly identify that the *m/z* peak at 71 is the molecular ion having lost a methyl group. This highlights that it can sometimes be more efficient to think about what might have been lost from the molecular ion, rather than trying to add up fragments to get the correct *m/z*.

Section 11A questions

1 What does the base peak represent in a mass spectrum?

2 What is the molecular ion in a mass spectrum, and why is it important?

3 What is the mass-to-charge ratio in mass spectrometry, and how is it used to analyse data?

4 You have a sample that contains an unknown compound. You know that it's either pentane (C_5H_{12}) or 2-methylbutane (C_4H_{10}). You run a mass spectrometry test and find a molecular ion peak at an *m/z* of 72. Based on this data, which compound is likely to be in your sample? Explain your answer.

5 Propane (C_3H_8) exhibits a molecular ion peak at *m/z* = 44 in its mass spectrum. What might be a fragment responsible for a peak observed at *m/z* = 29?

6 A sample of butanol (C_4H_9OH) is subjected to mass spectrometry.
  a Identify the *m/z* value that would correspond to the molecular ion.
  b If a prominent peak is observed at *m/z* = 31, what fragment might this represent?
  c Propose another possible fragment for butanol and the corresponding *m/z* value you would expect to see for it.

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11B Infrared spectroscopy

Study Design:

- Identification of bond types by qualitative infrared spectroscopy (IR) data analysis using characteristic absorption bands

Glossary:
Absorption band
Fingerprint region
Wavenumber

ENGAGE

The laws of science or the science of the laws?

In Australia, as with most other countries in the world, there are laws regarding the level of blood alcohol that a person can legally drive with. For drivers with a full license, the legal limit is 0.05 grams of alcohol per 100 millilitres of blood. For probationary drivers here, the concentration needs to be 0.00 grams of alcohol per 100 millilitres of blood. Due to the dangers of drink driving, police regularly perform random checks of drivers using breathalysers. A breathalyser is able to measure alcohol in a person's breath and then use this to calculate the alcohol concentration in the blood. If a driver fails this test, they often undergo a second, more sensitive, test. The technology used in the second test involves a form of spectroscopy called infrared (IR) spectroscopy. In this section, you will learn about the principles of IR spectroscopy and how the data generated from it can be used to determine the presence of functional groups within organic compounds.

Figure 11B–1 In a breathalyser (or breath analyser), breath is blown into the sample chamber and analysed by a beam of infrared radiation to detect the concentration of alcohol in your blood.

EXPLAIN

What is infrared (IR) spectroscopy?

Infrared spectroscopy is a powerful tool for identifying functional groups in organic compounds. This is because different bond types absorb infrared radiation at characteristic frequencies, which are referred to as **absorption bands**. The position of these absorption bands provides valuable information about the bond types present in the molecule, which can be used to identify the functional groups.

Absorption band a range of wavelengths in the IR spectrum where absorption of infrared light occurs

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Analysing IR spectroscopy data

The **fingerprint region** in an infrared spectrum for organic compounds refers to the range of **wavenumbers**, typically between 500 cm^{-1} and 1500 cm^{-1}, where a complex pattern of absorption bands occurs due to the combination and deformation vibrations of all the atoms in the molecule. This region is often referred to as the fingerprint region because the unique pattern of absorption bands serves as a unique 'fingerprint' for the compound, enabling it to be identified.

The fingerprint region is useful because it provides a wealth of information about the overall structure and composition of the molecule. In this region, each compound has its own unique absorption spectrum, which can be used to identify the compound by comparison with known spectra in a library. The pattern of peaks in the fingerprint region is due to the molecular vibrations that involve multiple bonds, which are specific to the individual molecule. Since the fingerprint region is unique for each molecule, it is a useful region for identifying unknown compounds. The fingerprint region is often the last region analysed because it is the most complex, and the pattern of absorption bands is unique to each molecule. Therefore, it is used as a confirmatory test to verify the identification of a compound after functional group analysis has been performed.

Besides the fingerprint region, IR spectroscopy provides information about the different bond types present in a compound. This is possible because different bond types have characteristic wavenumber ranges where they absorb (Table 11B–1). For example, the carbonyl group (C=O) has a characteristic absorption band in the range of 1630–1820 cm^{-1}, while the hydroxyl group (–OH) has a broad absorption band in the range of 3200–3600 cm^{-1}. Similarly, the amino group (–NH_2) has a characteristic absorption band in the range of 3300–3500 cm^{-1}. By analysing the positions and intensities of these absorption bands, the functional groups present in the molecule can be determined and this information is then used to identify the compound. In addition, the absence of certain absorption bands can also be used to rule out the presence of particular functional groups.

Fingerprint region
the part of an infrared spectrum that is found between 500 cm^{-1} and 1500 cm^{-1}, which, like a fingerprint, is unique and characteristic of a compound

Wavenumber
a measure of frequency denoting the number of wavelengths per unit distance, usually in reciprocal centimetres (cm^{-1}), with higher values corresponding to higher energy transitions in a molecule

Table 11B–1 Characteristic ranges for infrared absorption

Bond	Wavenumber (cm^{-1})
C–Cl (chloroalkanes)	600–800
C–O (alcohols, esters, ethers)	1050–1410
C=C (alkenes)	1620–1680
C=O (amides)	1630–1680
C=O (aldehydes)	1660–1745
C=O (acids)	1680–1740
C=O (ketones)	1680–1850
C=O (esters)	1720–1840
C–H (alkanes, alkenes, arenes)	2850–3090
O–H (acid)	2500–3500
O–H (alcohols)	3200–3600
N–H (amines and amides)	3300–3500

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Let's look at an example using the infrared spectrum for ethanol (Figure 11B–2). From this, we can see that in the fingerprint region there is a complicated series of absorption bands. It is likely that the signal from the C–O bond is in this region (1050–1410 cm^{-1}), but it is hard to definitively locate it and so it isn't usually a focus of the analysis. A prominent feature of the spectrum is the absorption band between 3200 and 3600 cm^{-1}, which is the signal for the O–H bond. Also, we can see an absorption band between 2850 and 3090 cm^{-1}, which corresponds to the signal from the C–H bonds.

Lastly, although we are talking about absorption bands, you may notice that the *y*-axis of the spectrum in Figure 11B–2 is labelled as 'Transmittance (%)'. Absorbance is a measure of the amount of radiation absorbed by the sample, whereas transmittance is a measure of the amount not absorbed and therefore transmitted through the sample. A high absorbance will be seen as a transmittance trough on the spectrum.

VIDEO 11B–1 IMPORTANT FEATURES IN INFRARED SPECTROSCOPY DATA

WORKSHEET 11B–1 ANALYSING INFRARED SPECTROSCOPY DATA

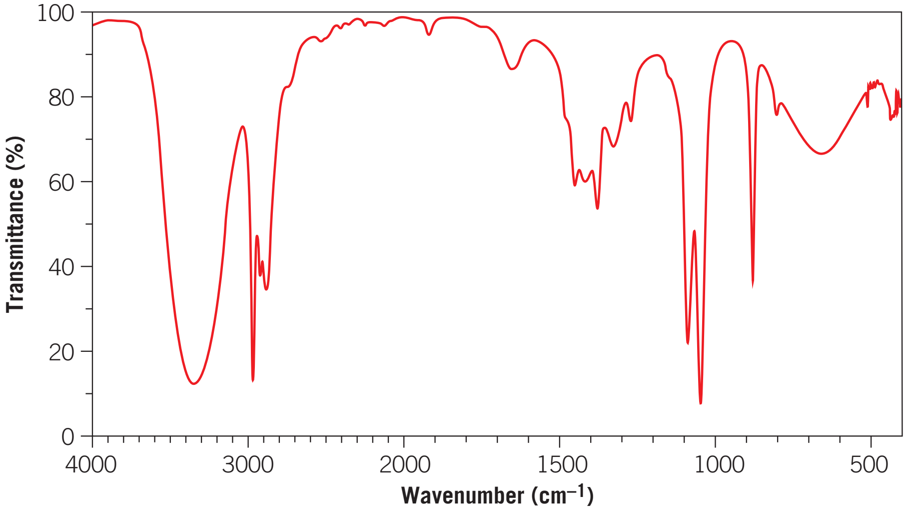
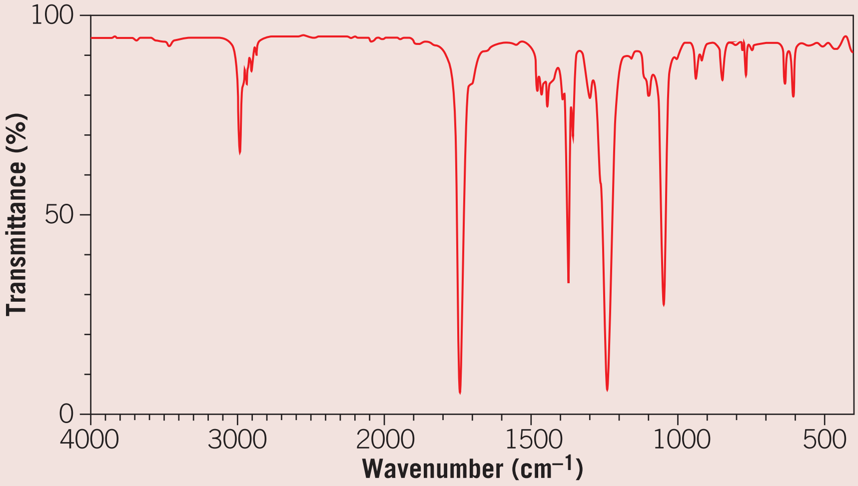


Figure 11B–2 Infrared spectrum for ethanol (C_2H_5OH)

VIDEO WORKED EXAMPLE 11B–1

Worked example 11B–1: Analysing the IR spectrum of a compound

A sample with the molecular formula $C_4H_8O_2$ is analysed by infrared spectroscopy and the spectrum produced is shown below. By analysing this spectrum, explain why the sample must contain an ester and not a carboxylic acid.



Solution

	Logic	Process
Step 1	Determine the absorption bands that you would expect to see for an ester.	1720–1840 cm^{-1} for C=O (ester)
Step 2	Determine the absorption bands that you would expect to see for a carboxylic acid.	1680–1740 cm^{-1} for C=O (acid) 2500–3500 cm^{-1} for O–H (acid)
Step 3	Determine the absorption bands present in the spectrum.	1730–1760 cm^{-1} 2950–3050 cm^{-1}
Step 4	Use the information from Steps 1–3 to explain why the sample is an ester and not a carboxylic acid.	The presence of an absorption band at 1730–1760 cm^{-1} indicates the presence of a C=O bond, but could be from an ester or a carboxylic acid. The presence of an absorption band at 2950–3050 cm^{-1} indicates the presence of a C–H bond, but could be from an ester or a carboxylic acid. The absence of a broad peak at 2500–3500 cm^{-1} suggests it cannot be a carboxylic acid and so it must be an ester.

Check-in questions – Set 1

1 In the context of infrared spectroscopy, what is meant by the term ‘fingerprint region’?

2 What information can infrared spectroscopy data tell you about organic compounds?

3 What bond type does an absorption band at the following wavenumber ranges represent?
  - a 1620 cm^{-1} to 1680 cm^{-1}
  - b 2500 cm^{-1} to 3500 cm^{-1}
  - c 3300 cm^{-1} to 3500 cm^{-1}

11B SKILLS

VIDEO 11B–2
SKILLS: IR SPECTROSCOPY QUESTIONS

IR spectroscopy questions

Having explored the analysis of IR spectroscopy data in this section, you may think that the best approach is simply to look at the spectrum and compare the absorption bands seen with a table of wavenumber ranges corresponding to bond types. While this strategy will definitely be a good starting point, there are instances when it may not be enough to give you a definitive answer or there is an alternative method that may provide a quicker path to the solution.

Let’s think about this using the example question below.

Question:

You are provided with an infrared spectrum of an unknown compound. You are told that the compound has the molecular formula C_2H_6O. Using the spectrum, determine the bond types present and suggest what the compound may be.

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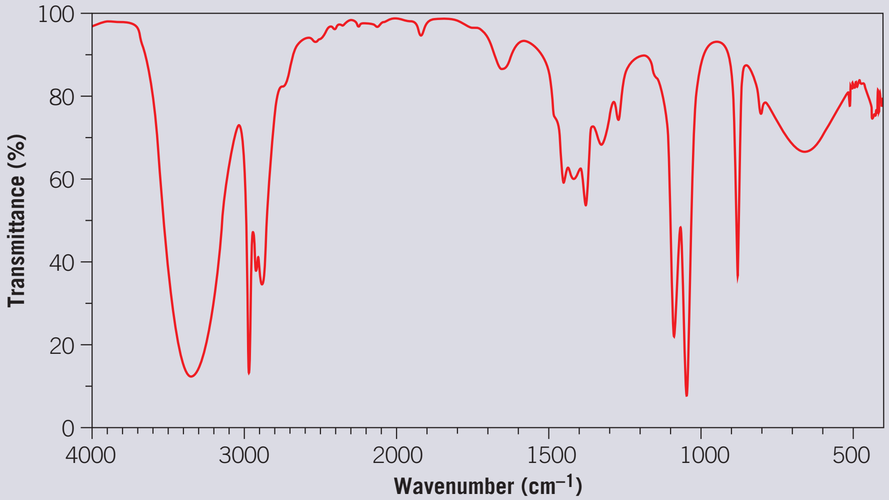


Answer:

If we focus on the left-hand side of the spectrum, we can see an absorption band within the range of 3200–3500 cm^{-1}. Using Table 11B–1, we would be able to determine that this could correspond to an O–H or an N–H bond type. However, using the additional information provided in the question in the form of the molecular formula, we can automatically disregard the N–H bond option, as there are no nitrogen atoms present. As this must be an O–H bond type for alcohols, and there is an additional absorption band corresponding to a C–H bond type, we can combine this with the molecular formula provided to suggest the unknown compound is ethanol.

For a question like this, it could be a beneficial first step to cross out options in the table that are not possible based on the formula information provided. This will ensure that you don't make mistakes during your analysis and make the process quicker.

Section 11B questions

1 What is the principle of infrared spectroscopy, and how does it work?

2 What is the fingerprint region in an infrared spectrum, and why is it important?

3 What is the process for analysing infrared spectroscopy data, and what information can be obtained?

4 In an infrared spectrum, you notice a broad, strong absorption peak between 3200–3600 cm^{-1}.

  a What functional group is most likely present in the compound?

  b What other evidence in the spectrum might you look for to support this?

5 A scientist in an organic chemistry lab has performed a reaction to produce ethanol from chloroethane. To test whether the reaction has been successful, the scientist performs infrared spectroscopy on a sample of the unused reactant and a sample of the reaction material.

  a Using Table 11B–1, identify the absorption bands that you might expect to see for each sample.

  b From your answer to part **a**, would any absorption bands be difficult to observe in an IR spectra? Explain.

  c Describe what information from the obtained IR spectrum would help you determine if the reaction the scientist had conducted had been successful.

  d What other technique might provide useful additional data to help determine whether the reaction had been successful?

11C Nuclear magnetic resonance spectroscopy

Study Design:

- Structural determination of organic compounds by low resolution carbon-13 nuclear magnetic resonance (^{13}C-NMR) spectral analysis, using chemical shift values to deduce the number and nature of different carbon environments
- Structural determination of organic compounds by low and high resolution proton nuclear magnetic resonance (^{1}H-NMR) spectral analysis, using chemical shift values, integration curves (where the height is proportional to the area underneath a peak) and peak splitting patterns (excluding coupling constants), and application of the n+1 rule (where n is the number of neighbouring protons) to deduce the number and nature of different proton environments
- Deduction of the structures of simple organic compounds using a combination of mass spectrometry (MS), infrared spectroscopy (IR), proton nuclear magnetic resonance (^{1}H-NMR) and carbon-13 nuclear magnetic resonance (^{13}C-NMR) (limited to data analysis)

Glossary:

Chemical shift
Integration curve
Multiplet
Peak splitting

ENGAGE

The brains behind MRI

One of the greatest advances in modern medicine has been the development of magnetic resonance imaging or MRI. MRI has provided doctors with a relatively quick and non-invasive way to obtain high-resolution images of the skeletal system, organs, tissues and central nervous system. It has become an invaluable tool for the diagnosis of neurological conditions like multiple sclerosis and stroke, as well as structural issues or blockages in the heart. MRI is also extensively used for the screening and diagnosis of cancer in multiple organs, such as the liver, pancreas and ovaries. For their contribution to the discovery of MRI technology and its subsequent contribution to the medical field, Sir Peter Mansfield from the University of Nottingham and Paul Lauterbur from Stony Brook University were awarded the 2003 Nobel Prize in Physiology or Medicine. In this section, you will be learning about nuclear magnetic resonance (NMR), the principles of which MRI machines are based on.

As well as understanding two different types of NMR, you will also gain an understanding of how they can be used to produce data that allows for the structure of organic compounds to be determined.

Figure 11C–1 A patient being positioned for an MRI scan (left). An MRI scan of the brain (right)

ISBN 978-1-009-22984-5

EXPLAIN

What is nuclear magnetic resonance (NMR)?

Nuclear magnetic resonance (NMR) is a technique used to study the structure of molecules. It works based on the fact that certain atomic nuclei, such as those of hydrogen or carbon, have an intrinsic magnetic moment or spin. When a sample containing these nuclei is placed in a strong magnetic field, the spins of the nuclei align either parallel or antiparallel to the magnetic field.

When a magnetic field is applied to the nuclei, they can absorb and emit electromagnetic radiation at certain frequencies, just like tuning to a radio station. This is because the spins of the nuclei can flip between the two energy levels, and the energy difference between these levels determines the frequency of electromagnetic radiation that can be absorbed or emitted. By measuring these frequencies, NMR can provide information about the structure and dynamics of molecules, including their composition, arrangement, and interactions with other molecules. This makes NMR an essential tool in many fields, including chemistry, biochemistry and medicine.

Carbon-13 NMR

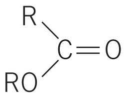
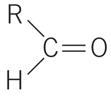
Carbon-13 is one of two naturally occurring stable isotopes of carbon, the other being carbon-12. Carbon-13 NMR (also referred to as ^{13}C NMR), works by measuring the magnetic properties of the carbon-13 nuclei in a molecule. The principle behind carbon-13 NMR is based on the fact that carbon-13 nuclei possess a magnetic moment, which is a property of some atomic nuclei that makes them behave like tiny bar magnets. When placed in a strong magnetic field, the carbon-13 nuclei align themselves either with or against the field, depending on their energy levels. By applying a radiofrequency pulse, the nuclei can be made to absorb energy and 'flip' their alignment. As the nuclei relax back to their original state, they emit energy in the form of electromagnetic radiation. The frequency of this radiation is unique to each carbon atom, and it is detected by a receiver coil to generate a carbon-13 NMR spectrum.

Chemical shift the position of a signal in the nuclear magnetic resonance (NMR) spectrum relative to the signal produced by a reference compound, usually tetramethylsilane (TMS); measured in parts per million, ppm

Analysing carbon-13 NMR data

NMR spectra show the signals produced by the nuclei of the atoms in the molecule being studied, and the position of these signals is referred to as the **chemical shift**. The chemical shift values give important information about the environment of the atoms in the molecule, which can help identify the molecule's structure (Table 11C–1).

Table 11C–1 Typical chemical shift values for carbon-13 NMR data relative to TMS = 0

Type of carbon	Chemical shift (ppm)
$R–CH_3$	8–25
$R–CH_2–R$	20–45
$R_3–CH$	40–60
$R_4–C$	36–45
$R–CH_2–X$	15–80
$R_3C–NH_2$, $R_3C–NR$	35–70
$R–CH_2–OH$	50–90
$RC≡CR$	75–95
$R_2C{=}CR_2$	110–150
RCOOH	160–185
	165–175
	190–200
$R_2C{=}O$	205–220

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The chemical shift is measured in parts per million (ppm) and is relative to a reference compound. The reference compound typically used is tetramethylsilane (TMS), which is given a chemical shift of 0 ppm. The chemical shift is influenced by the magnetic field experienced by the nucleus, which is in turn affected by the environment of the atom. Atoms with different electron environments will produce signals at different chemical shift values. For example, atoms that are in a more electron-rich environment will have signals at lower chemical shift values, while atoms in a more electron-poor environment will have signals at higher chemical shift values.

The number of peaks in a carbon-13 NMR spectrum corresponds to the number of carbon environments. By analysing the chemical shift values and comparing to tables of reference data, scientists can identify the nature of the different carbon environments and get information about the overall structure of the molecule.

Figure 11C–2 shows the carbon-13 NMR spectrum for ethanol. It can be observed that there are two peaks, which correspond to the two carbon environments in ethanol. These peaks occur at a chemical shift of 20 ppm (the carbon in the $–CH_3$ environment) and 58 ppm (the carbon in the $–CH_2–OH$ environment).

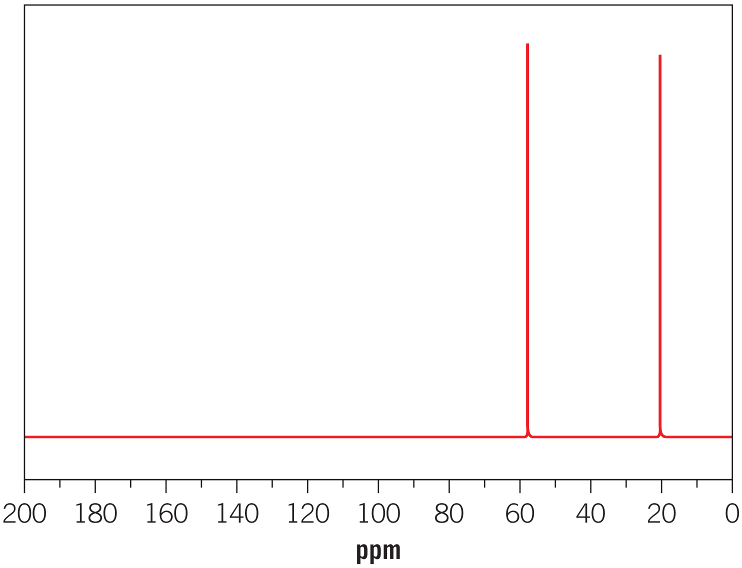

Figure 11C–2 Carbon-13 NMR spectrum for ethanol

Hydrogen-1 NMR

Hydrogen NMR (also referred to as proton NMR or ^{1}H NMR) is a type of nuclear magnetic resonance (NMR) spectroscopy that is used to study the properties of hydrogen-containing molecules. Hydrogen is abundant in nature and has a magnetic moment or spin, making it an ideal target for NMR spectroscopy. By exploiting the magnetic properties of hydrogen nuclei, important information about the chemical structure and dynamics of molecules can be obtained.

Hydrogen NMR works in the same way as carbon-13 NMR by placing a sample containing hydrogen atoms in a strong magnetic field, causing the hydrogen atoms to align either parallel or anti-parallel to the field. By applying an oscillating electromagnetic field at a specific frequency, the hydrogen atoms can be excited and emit a signal that can be detected. The frequency of the signal depends on the chemical environment of the hydrogen atom, such as the type of atoms attached to it and their spatial arrangement. By analysing the hydrogen NMR spectrum, information about the chemical structure and dynamics of the molecule can be obtained, including the number of hydrogen atoms, the types of functional groups present and the connectivity of the atoms within the molecule. Hydrogen NMR is widely used in many fields, including chemistry, biochemistry and medicine, to study the properties of molecules and to develop new drugs and materials. There are two types of hydrogen NMR that you need to be aware of: low-resolution and high-resolution. Low-resolution proton NMR provides basic information about the number of different types of protons (hydrogen environments) present in a molecule based on the number of peaks in the spectrum and their relative numbers based on peak areas. High-resolution proton NMR, on the other hand, provides more detailed information by displaying the splitting of peaks due to neighbouring protons, giving insights into the structural arrangement of the molecule. We will explore how to analyse all of these aspects of NMR data.

Analysing hydrogen-1 NMR data

When analysing data from a hydrogen-1 NMR spectrum, there are three main features that you need to look out for.

Chemical shift values

Similar to carbon-13 NMR, the number of peaks in a proton NMR spectrum corresponds to the number of hydrogen environments (Table 11C–2). By analysing the chemical shift values and comparing to tables of reference data, scientists can identify the nature of the different hydrogen environments and get information about the overall structure of the molecule.

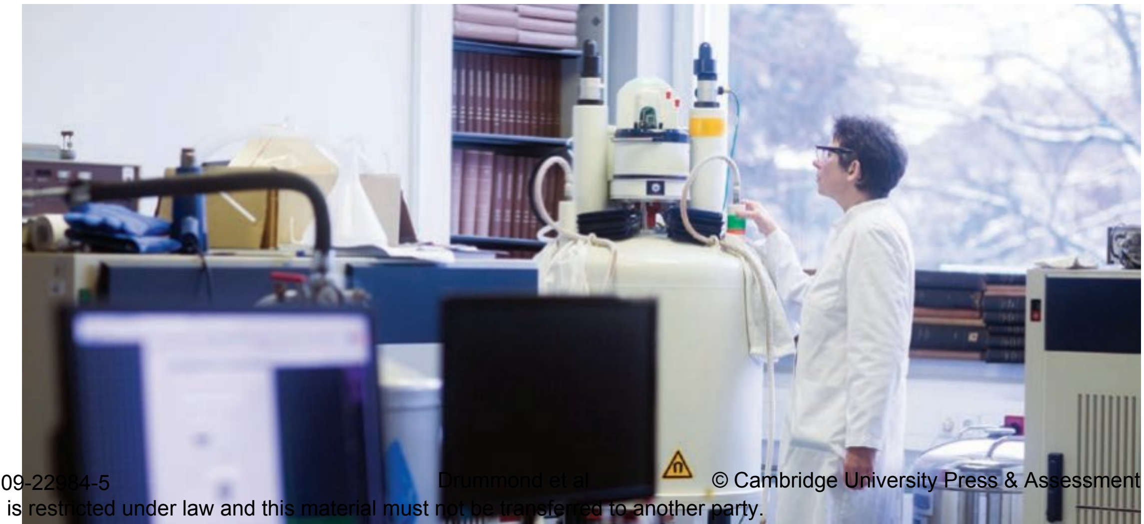

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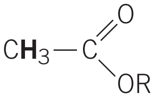
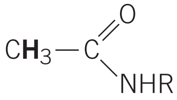
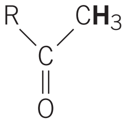
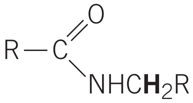
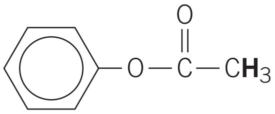
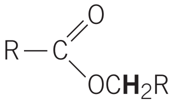
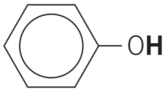
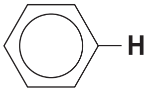
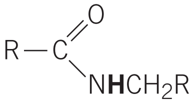
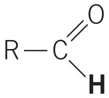
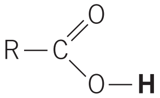
Table 11C–2 Typical chemical shift values for hydrogen-1 NMR data relative to TMS = 0

Type of proton	Chemical shift (ppm)
R–C**H**$_3$	0.9–1.0
R–C**H**$_2$–R	1.3–1.4
RCH=CH–C**H**$_3$	1.6–1.9
R$_3$–C**H**	1.5
 or 	2.0
	2.1–2.7
R–C**H**$_2$–X (X = F, Cl, Br or I)	3.0–4.5
R–C**H**$_2$–OH, R$_2$–C**H**–OH	3.3–4.5
	3.2
R—O—C**H**$_3$ or R—O—C**H**$_2$R	3.3–3.7
	2.3
	3.7–4.8
R–O–**H**	1–6 (varies considerably under different conditions)
R–N**H**$_2$	1–5
RHC=C**H**R	4.5–7.0
	4.0–12.0
	6.9–9.0
	8.1
	9.4–10.0
	9.0–13.0

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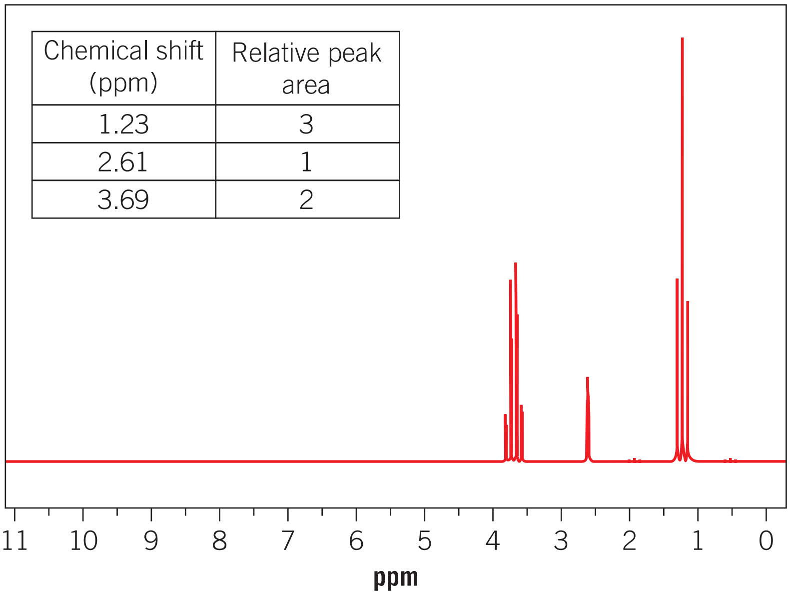
We can see from the spectrum in Figure 11C–3 that we have three different environments with chemical shift values at around 1.2, 2.6 and 3.6 ppm. From this, we can determine that there are three unique hydrogen environments present in our unknown compound.



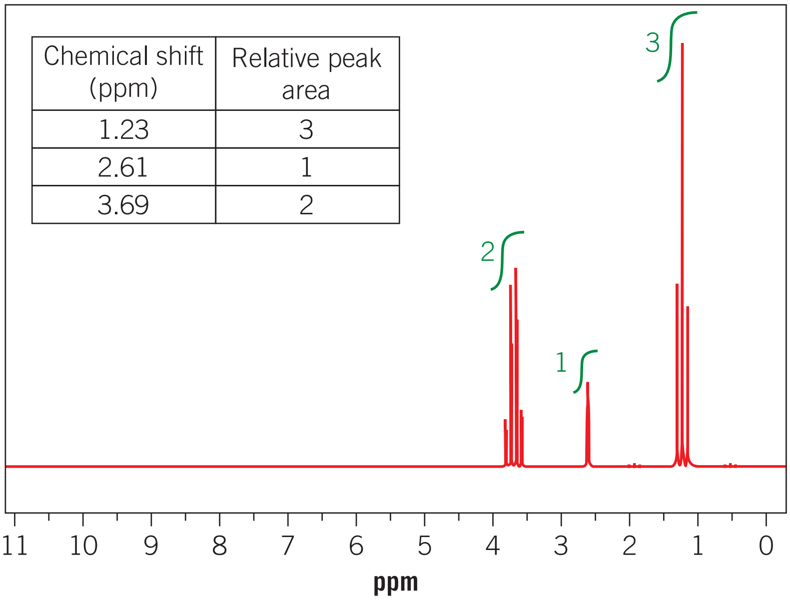
Chemical shift (ppm)	Relative peak area
1.23	3
2.61	1
3.69	2

Figure 11C–3 Proton NMR of a compound with the molecular formula C_2H_6O, with chemical shift values of 1.23, 2.61 and 3.69

Integration curves

Integration curve the area under a peak that directly correlates to the number of protons producing that particular signal in the spectrum

The **integration curve** is a plot of the intensity of the NMR signal as a function of the chemical shift. The integration curve provides information about the relative number of hydrogen atoms that produce each signal in the NMR spectrum. The area under the integration curve, measured in arbitrary units, is proportional to the number of hydrogen atoms that produce each signal, and this information can be used to determine the relative number of each type of hydrogen atom in the molecule. For example, if a peak has an integration value of 2, it means that it contains twice as many hydrogen atoms as a peak with an integration value of 1. By analysing the integration curve in conjunction with the chemical shift values, scientists can identify the types of atoms present in the molecule and determine its overall structure.



Chemical shift (ppm)	Relative peak area
1.23	3
2.61	1
3.69	2

Figure 11C–4 Proton NMR of a compound with the molecular formula C_2H_6O, displaying integration curves

We can see from the information provided in Figure 11C–4 that our relative peak areas are 3 : 1 : 2 for the environments at 1.23 ppm, 2.61 ppm and 3.69 ppm, respectively. From this, we can determine that there are three times more hydrogen atoms in the environment at 1.23 than the one at 2.61. Similarly, there are twice as many hydrogen atoms in the environment at 3.69 than the one at 2.61. With this information and that gained from the chemical shift data, we now know the number of hydrogen environments and the number of hydrogen atoms in these environments. To be able to determine how they are arranged though, we need to analyse the peak splitting.

Peak splitting

Proton NMR can produce either low or high resolution data. In high resolution proton NMR, what might have appeared as a single peak on a low resolution spectrum is split into a cluster of peaks. **Peak splitting** occurs when the signals from a set of equivalent hydrogen atoms are split into multiple peaks due to the influence of neighbouring hydrogen atoms. The resulting peaks in the NMR spectrum are called **multiplets** and can provide important information about the molecular structure. The number of peaks in a multiplet is determined by the number of hydrogen atoms on neighbouring carbon atoms and follows the rule $n + 1$, where n is equal to the number of neighbouring hydrogen atoms. For example, the signal from a proton that has three hydrogen atoms on the neighbouring carbon atom ($n = 3$) will be split into a quartet ($3 + 1 = 4$). If there are two neighbouring carbon atoms, n is equal to the total number of hydrogen atoms bonded to them. The signal from hydrogen atoms not bonded to carbon atoms will not undergo peak splitting (that is, will always be a singlet). For example, the signal from the hydrogen in a hydroxyl group (–OH) will always be a singlet. The multiplets can provide important information about the connectivity of the atoms in the molecule and can be used to help determine the molecular structure.

Peak splitting the division of a signal into several smaller peaks due to interactions with adjacent nuclei

Multiplet the resulting peaks when peak splitting occurs in an NMR spectrum, which can provide important information about molecular structure

VIDEO 11C–1 UNDERSTANDING FEATURES IN NMR DATA

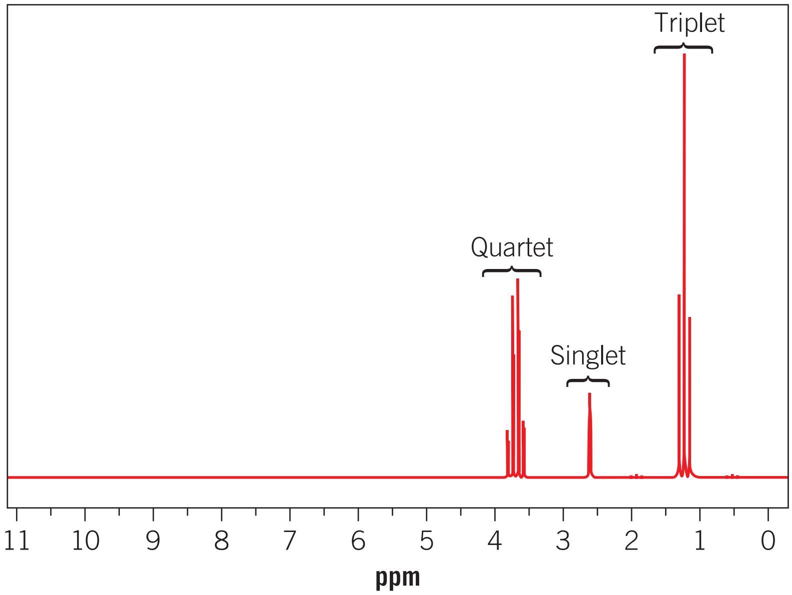


Figure 11C–5 High-resolution proton NMR of a compound with the molecular formula C_2H_6O

From this, we can see that we have a triplet, a singlet and a quartet present at 1.23 ppm, 2.61 ppm and 3.69 ppm respectively. This tells us about the number of hydrogen atoms in the neighbouring environment.

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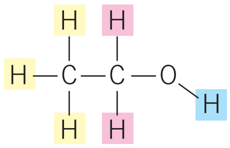


All of this information, combined with the provided molecular formula, C_2H_6O, is consistent with the unknown compound being ethanol.

If we focus on the environment at 1.23 ppm, we now know the following information.

- It has three hydrogen atoms in its environment (highlighted in yellow).
- The triplet tells us the neighbouring environment has two hydrogen atoms.
- The relative peak area indicates the neighbouring environment is the one at 3.69 ppm.

Moving onto the environment at 2.61 ppm, we now know the following information.

- It has one hydrogen atom in its environment (highlighted in blue).
- The singlet tells us there are no neighbouring hydrogen atoms.

Moving onto the environment at 3.69 ppm, we now know the following information.

- It has two hydrogen atoms in its environment (highlighted in pink).
- The quartet tells us the neighbouring environment has three hydrogen atoms.
- The relative peak area indicates the neighbouring environment is the one at 1.23 ppm.

Check-in questions – Set 1

WORKSHEET 11C–1 ANALYSING NMR DATA

1 Given a hydrogen NMR spectrum with a peak that splits into a triplet, what can be inferred about the hydrogen causing this signal?

2 What does the area under a peak or integration curve represent in hydrogen NMR?

3 If a carbon-13 NMR spectrum for a compound shows three distinct peaks and a hydrogen-1 NMR spectrum for the same compound shows six distinct peaks, how many unique carbon and hydrogen environments does this compound have?

NMR for identification of compounds

NMR spectroscopy can be used to give an indication on the identification of samples. As seen throughout this section, NMR can provide an array of data on organic compounds. This includes chemical shifts indicating the number of carbon or hydrogen environments, integration curves illustrating the numbers of carbon or hydrogen atoms in these environments and peak splitting providing evidence for the number of hydrogen atoms on neighbouring carbon atoms. Using all of this information, often in combination with a known molecular formula, can aid in the determination of the structure of the analysed compound. In this way, NMR can help provide the identity of compounds in samples.

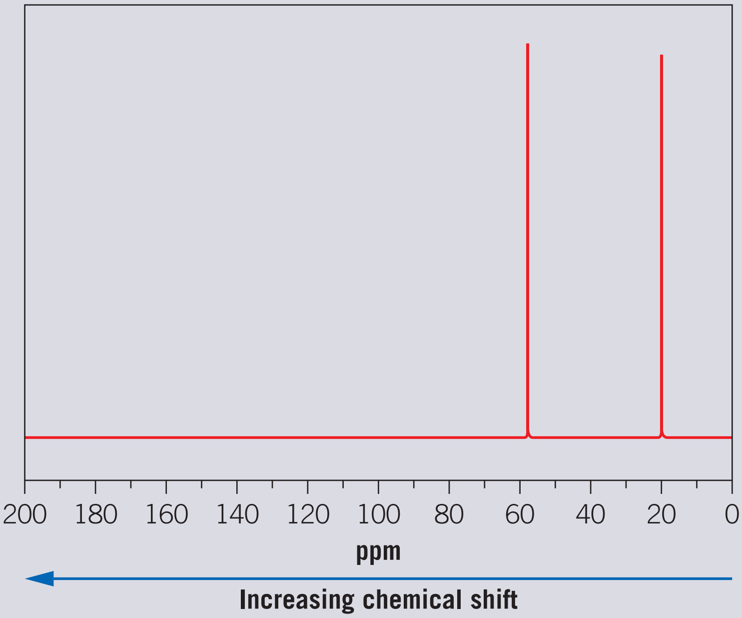
Analysing data from multiple sources

WORKSHEET 11C–2 DATA ANALYSIS USING MULTIPLE INSTRUMENTAL ANALYSIS TECHNIQUES

Across the first three sections of this chapter, it has become clear that instrumental analysis can provide valuable information about organic compounds. While each individual technique gives useful insights into the samples they are analysing, often the most value is gained when data from the different instruments are combined. In fact, it is a common exam question to be provided with spectra from MS, IR and NMR and asked to determine the structure and identity of the unknown compound.

11C SKILLS

Analysing NMR spectra
When analysing NMR spectra, care needs to be taken with chemical shift values on the *x*-axis. The scale on the *x*-axis goes the opposite way to what you might expect, with the smallest chemical shift values found on the right-hand side and the largest chemical shift values found on the left-hand side. This is true for both ^{13}C and ^{1}H NMR spectra.



Section 11C questions

1 Compare the following techniques:
   a carbon-13 NMR and low-resolution proton NMR
   b low-resolution proton NMR and high resolution proton NMR.

2 When analysing NMR data, one of the things that you might look at is the integration curve information.
   a What information does the integration curve in a proton NMR spectrum provide?
   b In a compound with the formula C_3H_8O, if the integration curve shows a ratio of 6 : 1 : 1, what could be the possible structure of this compound?
   c Another compound that has the molecular formula C_3H_8O is an ether with the semi-structural formula of $CH_3CH_2OCH_3$. What would be the integration curve for this compound?

3 Another feature that can be analysed in NMR data is peak splitting.
   a Is peak splitting associated with low resolution or high resolution proton NMR?
   b What information does peak splitting provide about the structure of a molecule?
   c Draw the structure for butan-1-ol, $CH_3CH_2CH_2OH$, and label each different hydrogen environment and indicate what the peak splitting would be for that environment.

4 You have a sample that contains an unknown compound. You know that it's either acetone (CH_3COCH_3) or ethanol (CH_3CH_2OH). You run a carbon-13 NMR test and find two distinct peaks: one at around 20 ppm and another at around 170 ppm. Based on these data and the information in Table 11C–1, which compound is likely in your sample? Justify your answer.

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11D Chromatography

Study Design:

- the principles of chromatography, including high-performance liquid chromatography (HPLC) and the use of retention times and the construction of a calibration curve to determine the concentration of an organic compound in a solution (excluding features of instrumentation and operation)

Glossary:

Mobile phase
Retention time
Stationary phase

ENGAGE

Blood tests – studying won't help, but chromatography will

One of the most common tests that a doctor may order when a patient has symptoms of an illness is a blood test. Performing a blood test allows the doctor to get results that indicate whether there is something abnormal present in the patient's blood or whether some of the levels of normal compounds are not in their usual range. However, while blood may be relatively simple to obtain as a sample, it is quite complex in its composition. In fact, a study that looked at all of the proteins present in the blood identified around 3700 different proteins! Therefore, in order to analyse a blood sample, the pathologists need a way of first simplifying and separating this complex mixture. They do this using a technique known as chromatography. In this section, you will learn about the principles of chromatography, including a specific form called high-performance liquid chromatography or HPLC, and then proceed to learn about how chromatography data can be analysed.

EXPLAIN

What is chromatography?

LINK UNIT 1

In Unit 1, you started to learn about chromatography. In particular, the technique of thin-layer chromatography (TLC) was discussed. As a reminder, chromatography is a general term that is used to describe a number of different techniques that are responsible for separating compounds in a mixture. Chromatography can be helpful for assessing both the purity and identification of organic compounds. Chromatography is widely used in many fields, including pharmaceuticals, food science and environmental science to analyse complex mixtures and determine the composition and purity of individual components. In this section, we will specifically discuss high-performance liquid chromatography or HPLC.

High-performance liquid chromatography (HPLC)

High-performance liquid chromatography (HPLC) is a powerful analytical technique used to separate, identify and quantify the components of complex mixtures. The basic principle of HPLC is that the separation of different components of a sample is based on their interactions with a stationary phase and a mobile phase. The **stationary phase** is typically a solid material or a liquid immobilised on a solid support, while the **mobile phase** is a liquid that flows through the stationary phase. The interaction between the components of the sample and the stationary phase is controlled by the chemical and physical properties of both the sample and the stationary phase, as well as the conditions of the mobile phase.

In HPLC, the sample is injected into a column containing the stationary phase. As the mobile phase flows through the column, the different components of the sample interact with the stationary phase to varying degrees, causing them to separate from each other. The more strongly a component interacts with the stationary phase, the longer it takes to elute from the column. The time at which a component elutes from the column is known as the **retention time**, R_t. As the components elute from the column, they are detected by a detector, such as an ultraviolet–visible (UV–visible) spectrophotometer, which produces a signal that is proportional to the concentration of the component.

Stationary phase a solid, liquid or gel that remains static during a chromatography experiment

Mobile phase the liquid or gas that flows during a chromatography experiment, which transports the compounds to be separated at different rates over the stationary phase

Retention time the time taken from when the sample is added to the column to when it is eluted; symbol R_t

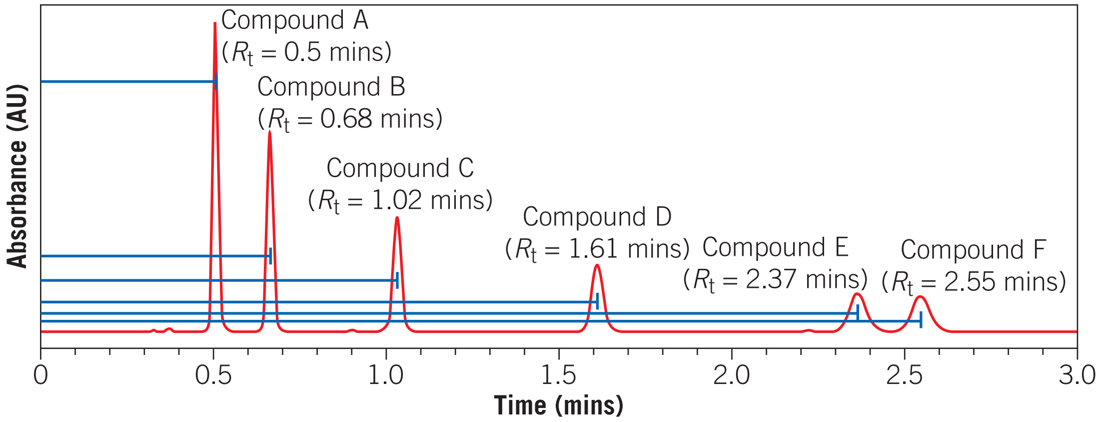

Figure 11D–1 This chromatogram shows peaks representing compounds that are detected when they elute from the HPLC. The time taken to elute from the column is called the retention time (R_t).

VIDEO 11D–1 UNDERSTANDING HPLC CHROMATOGRAMS

We can explore this further by imagining an HPLC column that contains a polar stationary phase and a non-polar mobile phase. When a polar stationary phase (for example, silica) and a non-polar mobile phase (for example, hexane) are used in HPLC, the separation of components in a sample is based on their relative polarities. Polar compounds will have a stronger interaction with the polar stationary phase and therefore will elute more slowly from the column compared to non-polar compounds, which will interact more with the

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non-polar mobile phase and elute faster. At the beginning of the separation, the non-polar compounds in the sample will be carried quickly by the non-polar mobile phase, while the polar compounds will be more strongly retained by the polar stationary phase, causing them to elute more slowly. As the separation proceeds, the non-polar compounds will be eluted first, followed by the less polar compounds, and finally the more polar compounds. As mentioned earlier, the detection of the separated compounds would then be achieved by the use of UV–visible spectroscopy. The resulting chromatogram will show a series of peaks representing the different components of the sample, with the retention time of each peak indicating its relative polarity. We can apply this analysis to the chromatogram represented in Figure 11D–1 (on the previous page). Assuming that this sample was run on the same column as just described, we can make the following conclusions:

WORKSHEET 11D–1 ANALYSING HPLC DATA

- Compound A has the shortest retention time and so is the most non-polar or least polar compound. It will have interacted the least with the stationary phase.
- Compound F has the longest retention time and so is the most polar or least non-polar compound. It will have interacted the most with the stationary phase.

VIDEO WORKED EXAMPLE 11D–1

Worked example 11D–1: Determining relative polarity from HPLC data

An HPLC column containing a polar silica matrix is used to separate a mixture containing three compounds, designated compounds A, B and C. Hexane is used as the non-polar mobile phase. The retention times for the compounds are 3.25 minutes (Compound B), 4.15 minutes (Compound A) and 9.79 minutes (Compound C). Determine the relative polarities of the three compounds.

Solution

	Logic	Process
Step 1	Extract the information about the properties of the stationary phase and mobile phase from the question.	Stationary phase = polar Mobile phase = non-polar
Step 2	Determine the order that the compounds eluted in the HPLC.	The compound with the shortest retention time will have eluted first, whereas the longest retention time will have eluted last. 1st = Compound B (3.25 mins) 2nd = Compound A (4.15 mins) 3rd = Compound C (9.79 mins)
Step 3	Use the information in Steps 1 and 2 to determine the relative polarities of the compounds.	The most polar compound will interact with the stationary phase the most and so take the longest to elute. The most non-polar compound will interact with the mobile phase the most and be eluted first. Order in increasing polarity: B < A < C

Check-in questions – Set 1

1. What is the basic principle behind high-performance liquid chromatography (HPLC)?
2. What does the term ‘retention time’ mean in HPLC?
3. If two compounds, A and B, are separated by HPLC with a polar stationary phase and compound A has a longer retention time than compound B, what can be inferred about the properties of these two compounds?

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Calibration curves and calculating unknown concentrations

To accurately quantify a specific compound, it is essential to construct a calibration curve that relates the concentration of the compound to the measured response of the instrument, such as absorbance. A calibration curve is a plot of the instrument response against the concentration of a series of known standards, which allows for the determination of the unknown concentration of the compound in the sample.

To construct a calibration curve using HPLC, a series of solutions with known concentrations of the compound of interest are prepared. These solutions are typically prepared by diluting a stock solution of the compound. The concentration range of the standards should cover the expected range of the unknown samples.

The prepared standards are then injected into the HPLC instrument, and the peak area or height of the compound of interest is measured. This is then plotted against the known concentration of the standards to construct a calibration curve.

After the calibration curve has been constructed, it can be used to determine the concentration of an unknown sample. To do this, you would first conduct the same measurement for the unknown sample as was done for the known standards, which is typically the peak area or height.

To calculate the concentration of the unknown sample, you would first plot the instrument response on the calibration curve to determine the corresponding concentration of the compound. This can be done by drawing a vertical line from the instrument response value, on the *x*-axis of the graph, to the calibration curve. From this point on the calibration curve, you can then draw a horizontal line to the *y*-axis to determine the concentration of the compound in the unknown sample. It is important to ensure that the calibration curve is linear within the range of concentrations used to prepare the standards, to ensure accurate quantification of the unknown sample.

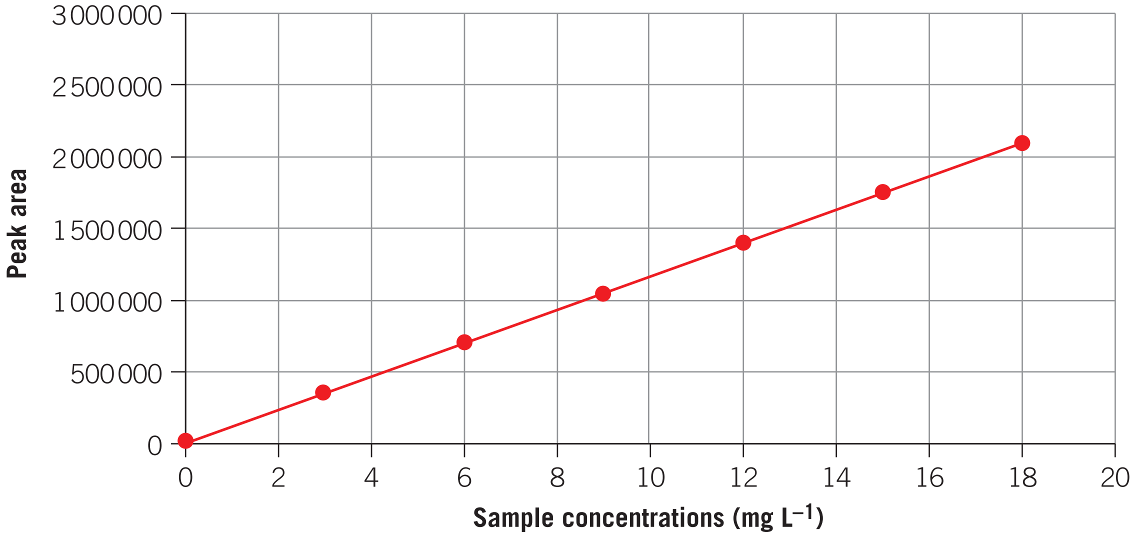

Figure 11D–2 A calibration curve uses standards with known concentration to determine a relationship between concentration and peak area in HPLC.

WORKSHEET 11D–2 USING CALIBRATION CURVES TO CALCULATE SAMPLE CONCENTRATIONS

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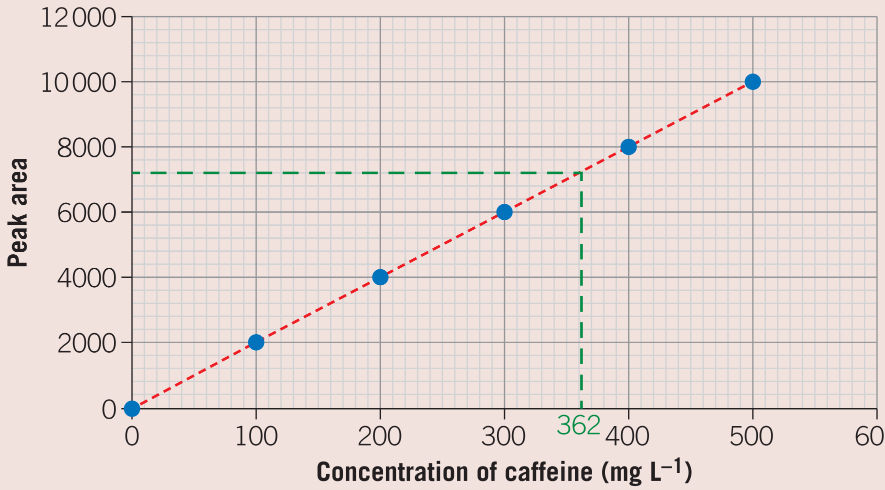
Worked example 11D–2: Determining unknown concentration of a sample using a calibration curve

VIDEO
WORKED
EXAMPLE 11D–2

Scientists want to measure the quantity of caffeine in a new energy drink, for which the label on a 250 mL can says contains 90 mg. To do this, they run six standards containing known concentrations of caffeine, ranging from 0 to 100 mg, and measure the peak area obtained on the chromatogram. Three samples of the energy drink are then also run and the peak areas calculated. The results are found in the table below. From these results, construct a calibration curve and determine if the label on the can is accurate.

Sample (mg L^{-1})	0.000	100.0	200.0	300.0	400.0	500.0	Energy drink #1	Energy drink #2	Energy drink #3
Peak area	0	1999	3978	6005	7986	10 022	7212	7198	7208

Solution



	Logic	Process
Step 1	Draw and label your axes for your calibration curve placing peak area on the *y*-axis and concentration on the *x*-axis.	*x*-axis = Concentration of caffeine (mg L^{-1}) *y*-axis = Peak area
Step 2	Place your data points on the graph.	Shown by the blue circles
Step 3	Draw a line of best fit for the data points to generate your calibration curve.	Shown by the dotted red line
Step 4	Calculate the average peak area for your energy drink samples.	Average peak area (energy drink samples) $= \frac{7212 + 7198 + 7208}{3} = 7206$
Step 5	Draw a line from the position on the *y*-axis of your calculated value in Step 4 to the calibration curve.	Shown by green horizontal dotted line
Step 6	Draw a line from the position on the calibration curve from Step 5 down to the *x*-axis and record the concentration value obtained.	Shown by green vertical dotted line
Step 7	Perform unit conversions to determine if the value on the can is accurate.	Concentration of caffeine in energy drink samples = 362.0 mg L^{-1} Therefore, a 250 mL can contains 90.50 mg of caffeine. This means the label is accurate.

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HPLC for identification and purity

As with the other analytical techniques described in this chapter, HPLC can also be used to gain an understanding of the purity and composition of a sample. The analysis of both these characteristics involves the use of the chromatogram, specifically through the use of the detected peaks and their retention times.

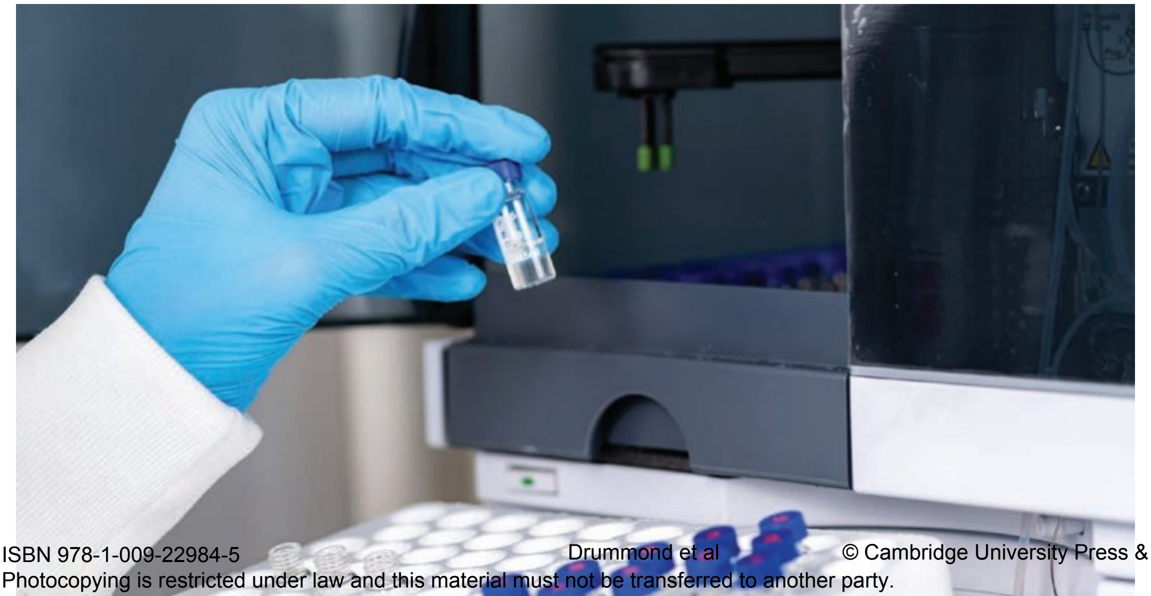
Identification

HPLC can be used to give an indication regarding the identity of components within a sample. The easiest way to do this is to compare the retention times of the observed peaks in the sample with those of known standards. If a particular compound is run through the same HPLC column under the same conditions, it will always have the same retention time. Importantly though, if the conditions are changed (such as a change in solvent for the mobile phase or temperature that the separation is conducted at), then the retention time will also change.

As an example, you may want to check whether there is vitamin C present in a new liquid multivitamin. To do this using HPLC, you would first run a sample of pure vitamin C through the column and measure its retention time. Following that, you would then run the multivitamin sample through the same column under the same conditions. If a peak was observed at the same retention time on both chromatograms, this would suggest that vitamin C is present in the multivitamin. However, it is important to note that this process only provides an indication as to the identity of the compound; it is not definitive. Multiple compounds can have the same retention time and so other techniques should be used to determine a conclusive identity.

Purity

Whereas the retention time is important for determining the identity of the components of a sample, the number of peaks is more relevant when analysing the purity. If a sample is expected to contain only one component, then it would be considered pure if only one peak was observed (at the correct retention time). Samples containing more than one compound can also be assessed for their purity using HPLC. In these instances, a pure sample would only have peaks corresponding to the expected components detected on the chromatogram. Additional peaks or peaks appearing at unexpected retention times would be indicative of impurities or the presence of contaminants within the sample. As mentioned in this section, a UV–visible spectrophotometer is often used as the detection method in HPLC. One limitation of this is that any impurities that don't absorb in this region of the electromagnetic spectrum won't be detected.



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VIDEO 11D–2
SKILLS:
USING KEY
TERMINOLOGY

11D SKILLS

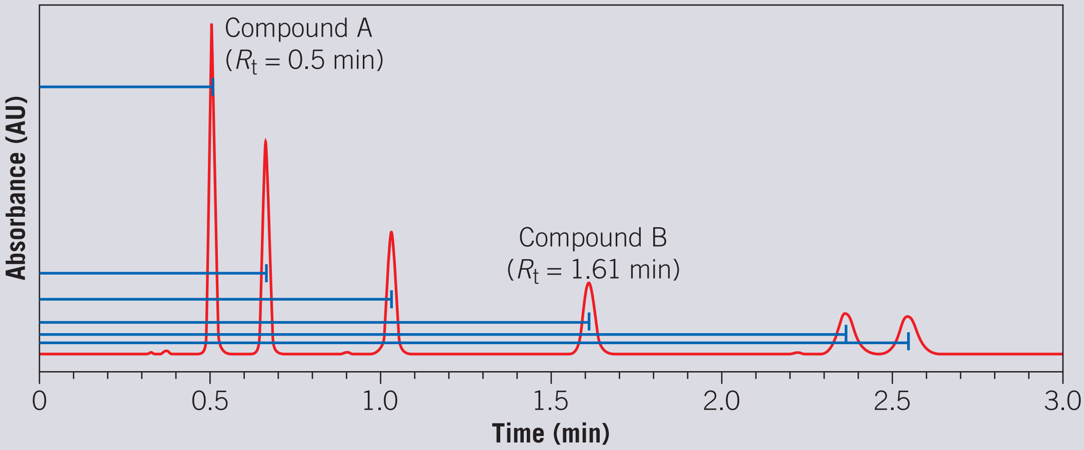
Using key terminology

When describing the separation of certain compounds or components of substances using HPLC, it is important to use precise key terminology and not oversimplify your language.

Take the following question as an example.

Question:

Explain the difference between compounds A and B, which have been separated by HPLC with a non-polar stationary phase and water as the solvent. The chromatogram is shown below.



Initial answer:

The two compounds separate during HPLC and are eluted at different times, with sample B having a longer time.

Comments:

While this is not wrong, the language used is not specific enough for the level expected in VCE. Before providing a more detailed answer to this question, it might be good to first list all the key terms that should be included in your answer.

HPLC
Mobile phase
Adsorption
Polar
Stationary phase
Desorption
Non-polar
Retention time

When it comes to writing your answer, you can use dot points if it is easier to keep it succinct, while still including the key terms that you identified.

Complete answer:

- Compounds A and B were separated using HPLC.
- The stationary phase of the HPLC was non-polar and the mobile phase, water, was polar.
- Compounds that are less polar (or more non-polar) experience more adsorption to the stationary phase and consequently take longer to elute. This can be seen with compound A.
- Compounds that are more polar tend to experience desorption from the stationary phase and interact more with the mobile phase. This can be seen with compound B.
- As such, compound B will have a longer retention time compared to compound A.

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Section 11D questions

1 Describe how the HPLC chromatogram can be used to help determine the identity of a compound in a sample.

2 Describe how the HPLC chromatogram can be used to help qualitatively determine the purity of a sample.

3 A reverse-phase HPLC column uses a non-polar stationary phase and a polar mobile phase.

  a Define 'stationary phase' and 'mobile phase'.

  b Describe how a mixture containing pentane, pentan-2-ol and pentanoic acid would separate in a reverse-phase HPLC column.

  c Define 'retention time'.

  d Place the three compounds listed in part **b** in the order that you would expect them to elute from the reverse-phase HPLC column, going from the lowest retention time to the highest.

4 You are hired to conduct an analysis of a commercial multivitamin.

  a To begin, you run a sample of pure vitamin D through a specific HPLC column and a peak is observed at a retention time of 4.6 minutes. A sample from the commercial multivitamin is run through the same column and a peak is observed at 4.6 minutes. Can you conclude that the commercial multivitamin contains vitamin D? Why or why not?

  b You want to run another sample of the commercial multivitamin to provide replicate data. However, someone else is using the HPLC column that you used initially. Being impatient, you decide to use a different column that is available and ready to go. The specific stationary phase and mobile phase used for this column are different from the previous one, but still one is polar and the other non-polar. No peak is observed at 4.6 minutes; however, you observe a peak at a retention time of 4.9 minutes. What can you conclude from this?

  c If you wanted to do further analysis on your result from part **b**, what would be a good additional experiment to run?

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Chapter 11 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
11A.1	Describe the principle of mass spectrometry (MS)	1☐
11A.2	Define 'base peak'	5☐
11A.3	Define 'molecular ion peak'	13☐
11A.4	Identify the base peak and molecular ion peak from a given mass spectrum	12☐
11A.5	State that the molecular ion peak corresponds to the molecular mass of the compound	13☐
11A.6	Determine the ions that correspond to fragments in a given mass spectrum	13☐
11A.7	Determine the identity of a compound from given mass spectrometry data	12☐
11B.1	Describe the principle of infrared (IR) spectroscopy	7☐
11B.2	Identify bond types present in a sample from given infrared spectroscopy data	2☐, 12☐
11B.3	Determine the identity of organic compounds from provided options using given infrared spectroscopy data	12☐
11C.1	Describe the principle of nuclear magnetic resonance (NMR) spectroscopy	8☐
11C.2	Determine the structure of an organic compound from given carbon-13 NMR data	9☐
11C.3	Determine the structure of an organic compound from given proton NMR data	3☐, 6☐
11C.4	Determine the structure of organic compounds using a combination of given MS, IR and NMR data	12☐
11D.1	Describe the principle of high-performance liquid chromatography (HPLC)	4☐
11D.2	Describe the qualitative purity of a substance from given HPLC data	11☐
11D.3	Describe how retention times from HPLC data can be used to help in the identification of organic compounds	10☐
11D.4	Construct a calibration curve from given HPLC data	11☐
11D.5	Calculate the concentration of an organic compound from a given calibration curve and HPLC data	11☐

Multiple-choice questions

1 In a mass spectrum, the *x*-axis shows the mass-to-charge ratio (*m*/*z*). What does the mass-to-charge ratio represent?

A the number of isotopes
B the abundance of each isotope
C the mass of the species divided by its net charge
D the net charge of the species divided by its mass

2 Which of the following families of organic compounds shows a strong absorption in the infrared region around 1700 cm^{-1} due to a C=O stretch?

A alkanes
B alkenes
C alkynes
D carboxylic acids

3 A compound shows a triplet signal in its ^{1}H NMR spectrum. What does this indicate about the protons causing this signal?

A They are in an aromatic ring.
B They are part of a triple bond.
C They are adjacent to two other protons.
D They are adjacent to three other protons.

4 In an HPLC set-up, the mobile phase is

A the sample to be separated.
B the liquid that carries the sample.
C the detector that captures the data.
D the stationary phase soaked in liquid.

5 What does the base peak represent in a mass spectrum?

A the most abundant ion
B the least abundant ion
C the ion with the lowest mass-to-charge ratio
D the ion with the highest mass-to-charge ratio

6 What does the integration (area under the peak) in a ^{1}H NMR spectrum represent?

A the charge on the protons
B the chemical shift of the protons
C the splitting pattern of the protons
D the relative number of protons that give rise to the peak

7 Infrared spectroscopy is often used to identify

A isotopes.
B atomic number.
C functional groups.
D molecular weight.

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8 The signal at 0 ppm in a ^{13}C NMR spectrum is

A an impurity.

B the solvent peak.

C a carbon–carbon double bond.

D the standard reference, often tetramethylsilane (TMS).

9 In a ^{13}C NMR spectrum, what does the chemical shift of a peak indicate?

A the number of carbon atoms

B the charge on the carbon atom

C the chemical environment of the carbon atom

D the number of bonds the carbon atom is making

10 An HPLC experiment is performed to separate a sample that contains ethane, ethanol and ethanoic acid. The HPLC column uses a silica stationary phase, which is polar, and hexane as the mobile phase, which is non-polar. Which answer below correctly predicts the order of elution from the HPLC column, going from shortest to longest retention time?

A ethanoic acid, ethanol, ethane

B ethane, ethanol, ethanoic acid

C ethanol, ethane, ethanoic acid

D ethane, ethanoic acid, ethanol

Short-answer questions

11 Phenol is an organic compound used in the production of plastic materials. There is a concern that a creek near a plastic manufacturer is contaminated with phenol, so an analytical chemistry laboratory is contracted to analyse samples of the creek water. The chemistry laboratory prepares standard solutions of phenol and analyses them using HPLC. The phenol standards produce a chromatogram with a single peak at a retention time of 2.78 minutes. The peak area for each of the standard solutions are shown in the table below.

Concentration of phenol standard (g L^{-1})	Peak area
0.100	103
0.200	198
0.300	304
0.400	410
0.500	497

a Use the data in the table to prepare a calibration curve. (3 marks)

Three samples of the creek water are prepared for HPLC by mixing 1.00 mL of creek water with 9.00 mL of distilled water. These diluted creek water samples are run on the HPLC under the same conditions as the standard solutions. The area under the peak with a retention time of 2.78 minutes on the chromatograms for the three creek water samples were 176, 182 and 179.

b The standard solutions result in chromatograms with just a single peak. However, the chromatograms from the creek water samples had multiple peaks. Suggest why this would be the case. (1 mark)

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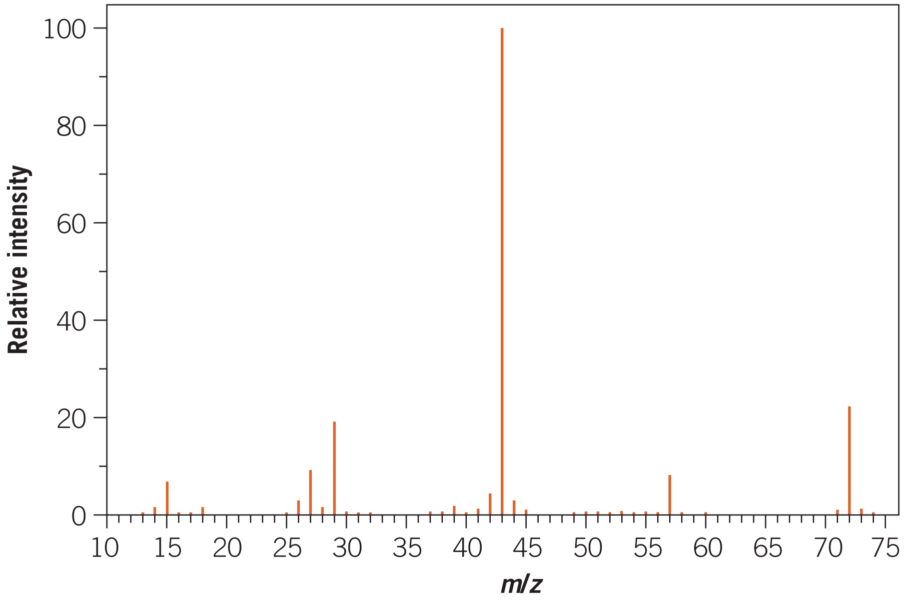
c Calculate the average peak area from the three creek water samples. (1 mark)

d Use the calibration curve to determine the concentration of phenol in the undiluted creek water samples. (2 marks)

12 An organic compound was known to have an empirical formula of C_4H_8O. It was analysed by various instruments to get information about its structure.

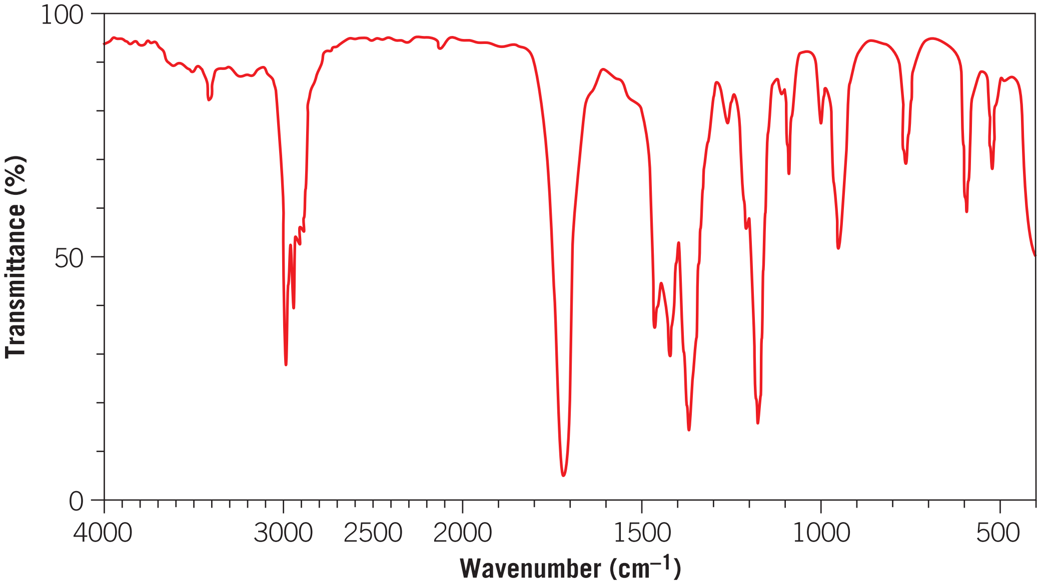
The mass spectrum of the compound is shown below.



a What is the *m*/*z* of the molecular ion peak? (1 mark)

b Use this molecular ion peak to determine the molecular formula of the compound. (1 mark)

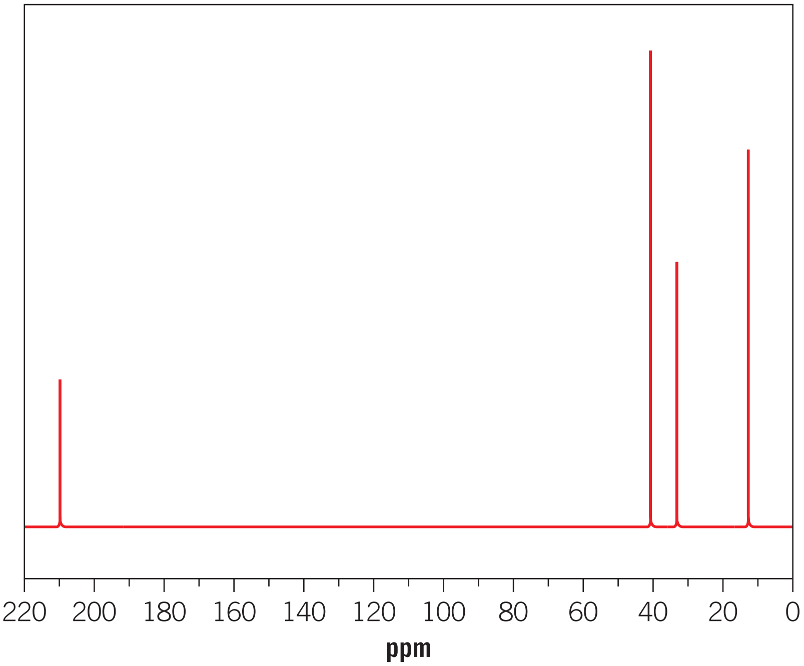
The infrared spectrum of the compound is shown below.



c What evidence is there from the infrared spectrum that the compound contains a C=O bond? (1 mark)

d What evidence is there from the infrared spectrum that the compound does not contain an O–H bond? (1 mark)

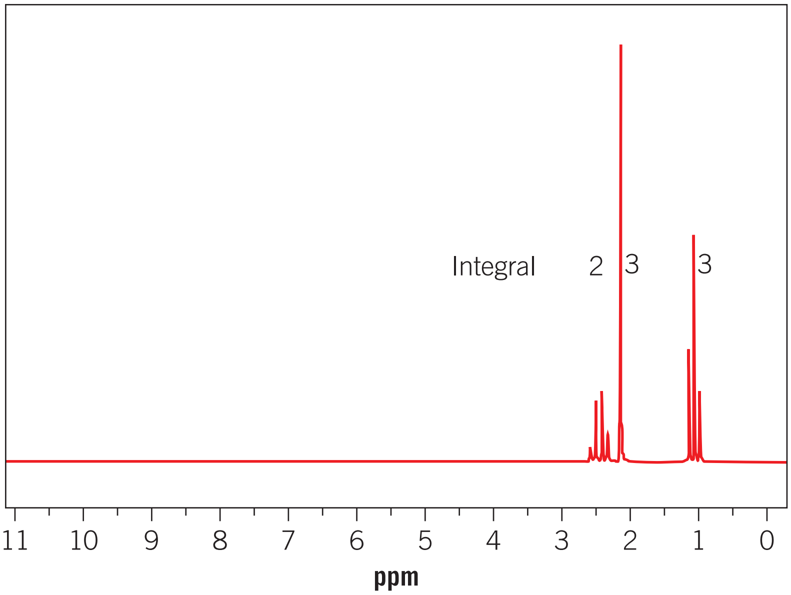
The ^{13}C NMR spectrum is shown below.



e How many different carbon environments are present in the molecule? (1 mark)

f What type of carbon environment produces the peak at 209 ppm? (1 mark)

The ^{1}H NMR spectrum is shown below.



g How many different hydrogen environments are present in the molecule? (1 mark)

h The peak at 2.5 ppm is a quartet. What does that tell you about the number of hydrogen atoms on neighbouring carbon atoms? (1 mark)

i Using information from all four spectra, give the structural formula of the compound. (1 mark)

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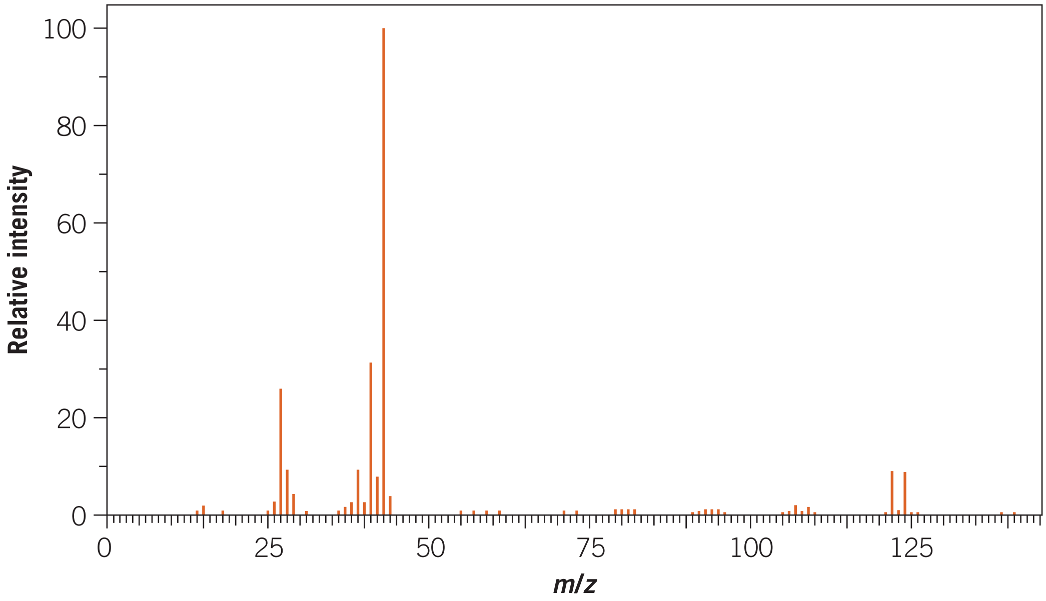
13 A compound with the molecular formula C_3H_7Br was analysed by mass spectrometry. Bromine has two stable isotopes: ^{79}Br with a natural abundance of 51% and ^{81}Br with a natural abundance of 49%. The mass spectrum of the compound is shown below.



a What is a molecular ion peak and what information does it tell you about the compound? (2 marks)

b The mass spectrum of this compound shows two molecular ion peaks at 122 and 124 *m/z*. Explain why there are two molecular ion peaks and give the molecular formula of the ion that produced the peak at 124 *m/z*. (2 marks)

c Give the likely structure of the ion that produced the base peak at 43 *m/z*. (1 mark)

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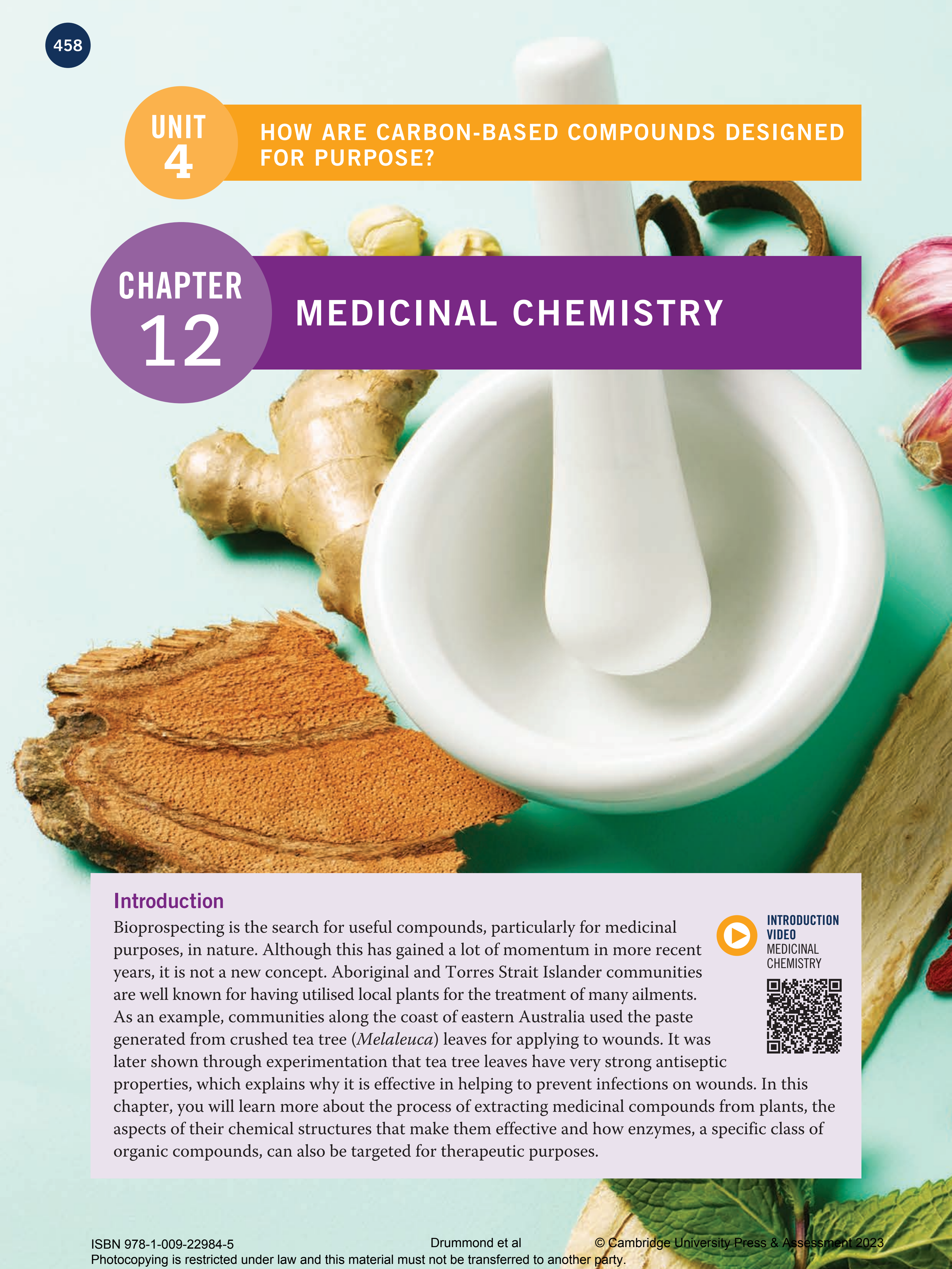

UNIT 4

HOW ARE CARBON-BASED COMPOUNDS DESIGNED FOR PURPOSE?

CHAPTER 12

MEDICINAL CHEMISTRY

Introduction

Bioprospecting is the search for useful compounds, particularly for medicinal purposes, in nature. Although this has gained a lot of momentum in more recent years, it is not a new concept. Aboriginal and Torres Strait Islander communities are well known for having utilised local plants for the treatment of many ailments. As an example, communities along the coast of eastern Australia used the paste generated from crushed tea tree (*Melaleuca*) leaves for applying to wounds. It was later shown through experimentation that tea tree leaves have very strong antiseptic properties, which explains why it is effective in helping to prevent infections on wounds. In this chapter, you will learn more about the process of extracting medicinal compounds from plants, the aspects of their chemical structures that make them effective and how enzymes, a specific class of organic compounds, can also be targeted for therapeutic purposes.

INTRODUCTION VIDEO
MEDICINAL CHEMISTRY

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Curriculum

Area of Study 2 Outcome 2
How are organic compounds analysed and used?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Extraction and purification of natural plant compounds as possible active ingredients for medicines, using solvent extraction and distillation • Identification of the structure and functional groups of organic molecules that are medicines • Significance of isomers and the identification of chiral centres (carbon atom surrounded by four different groups) in the effectiveness of medicines	**12A Organic compounds as medicines** **12A.1** Recall that natural plant compounds can contain active ingredients used for medicinal purposes **12A.2** Describe how solvent extraction can be used to extract and purify natural plant compounds for medicinal purposes **12A.3** Describe how distillation can be used to extract and purify natural plant compounds for medicinal purposes **12A.4** Recall some common classes of organic medicines and the key functional groups that characterise each class **12A.5** Explain why understanding how functional groups contribute to the mechanism of action of medicines will help guide future drug development **12A.6** Define 'chiral centre' and identify compounds that contain a chiral centre **12A.7** Describe how chiral centres can result in isomers and enantiomers **12A.8** Explain why the presence of isomers in compounds used as medicines can cause problems

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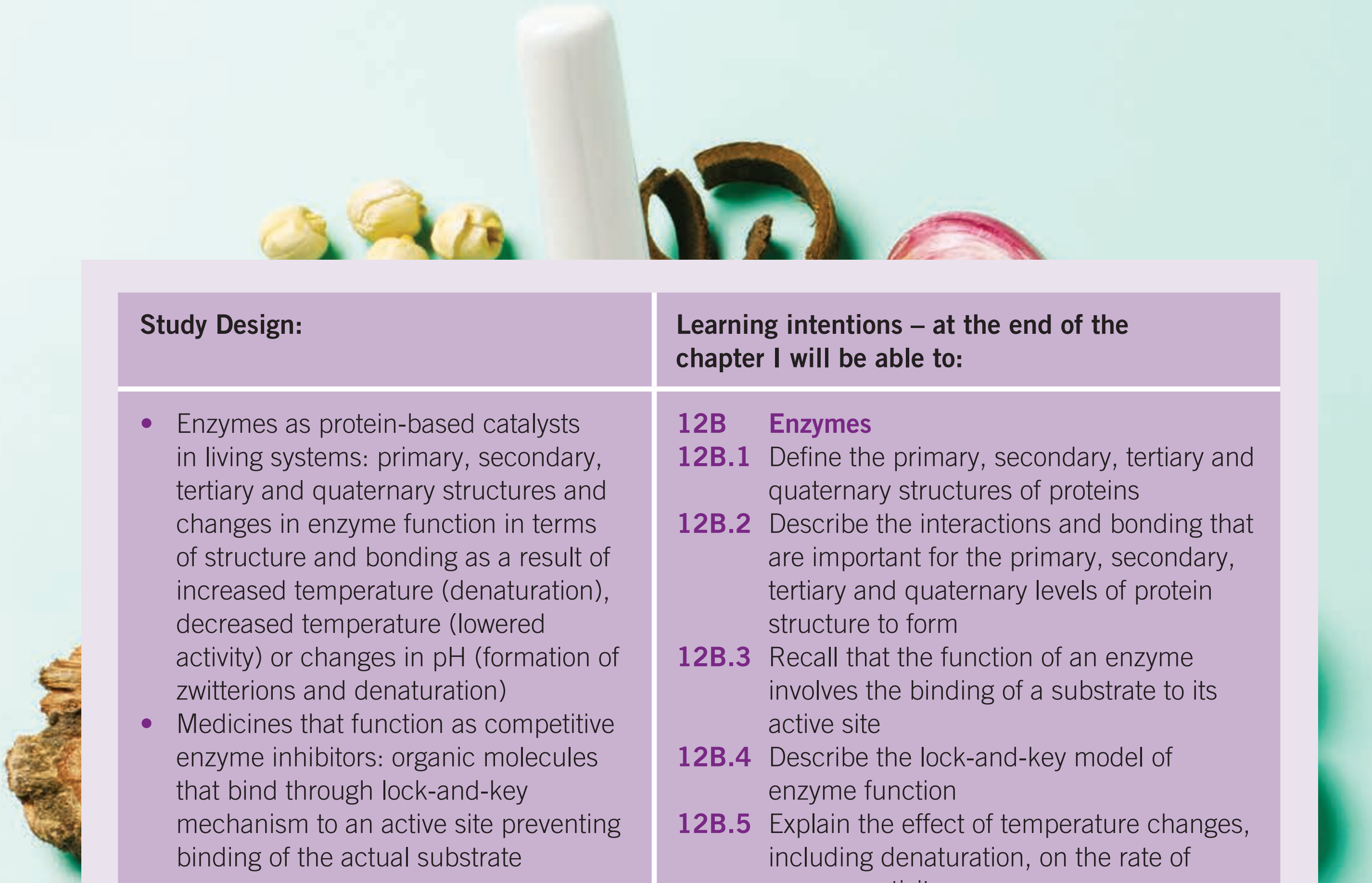

Study Design:	**Learning intentions – at the end of the chapter I will be able to:**
- Enzymes as protein-based catalysts in living systems: primary, secondary, tertiary and quaternary structures and changes in enzyme function in terms of structure and bonding as a result of increased temperature (denaturation), decreased temperature (lowered activity) or changes in pH (formation of zwitterions and denaturation) - Medicines that function as competitive enzyme inhibitors: organic molecules that bind through lock-and-key mechanism to an active site preventing binding of the actual substrate	**12B Enzymes** **12B.1** Define the primary, secondary, tertiary and quaternary structures of proteins **12B.2** Describe the interactions and bonding that are important for the primary, secondary, tertiary and quaternary levels of protein structure to form **12B.3** Recall that the function of an enzyme involves the binding of a substrate to its active site **12B.4** Describe the lock-and-key model of enzyme function **12B.5** Explain the effect of temperature changes, including denaturation, on the rate of enzyme activity **12B.6** Explain the effect of changes in pH on the rate of enzyme activity **12B.7** Define ‘zwitterion’ and explain how this forms in relation to amino acids **12B.8** Explain the effect of a competitive inhibitor on the rate of enzyme activity **12B.9** Describe how competitive inhibition can be used as a treatment approach

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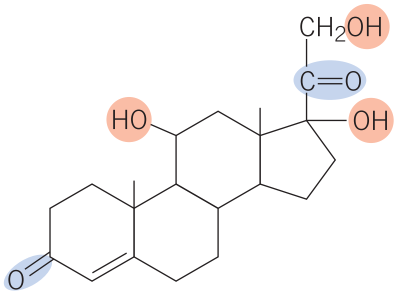
Glossary

Achiral
Active site
Chiral
Chiral centre
Competitive inhibition
Denatured
Enantiomer
Monomer
Peptide bond
Pharmacology
Polymer
Polypeptide
Solvent extraction
Substrate
Zwitterion

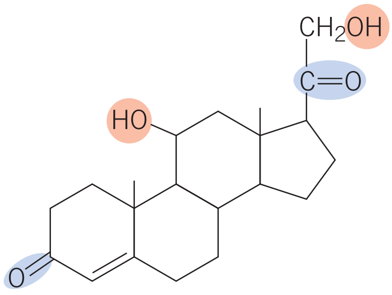
Concept map

12A Organic compounds as medicines

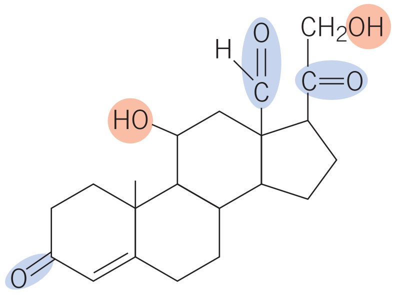
Developing medicine using compounds found in nature and identifying key functional groups that make medicine effective



Cortisol



Corticosterone

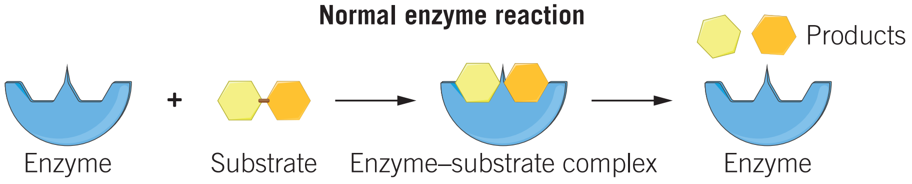


Aldosterone

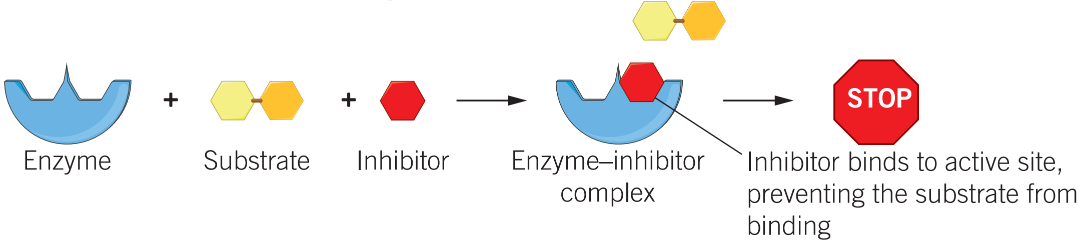
12B Enzymes

Biological catalysts that speed up chemical reactions and can be used as therapeutic targets

Normal enzyme reaction



Competitive inhibition



See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

12A Organic compounds as medicines

Study Design:

- Extraction and purification of natural plant compounds as possible active ingredients for medicines, using solvent extraction and distillation
- Identification of the structure and functional groups of organic molecules that are medicines
- Significance of isomers and the identification of chiral centres (carbon atom surrounded by four different groups) in the effectiveness of medicines

Glossary:

Achiral
Chiral
Chiral centre
Enantiomer
Pharmacology
Solvent extraction

ENGAGE

Mummy's medicine

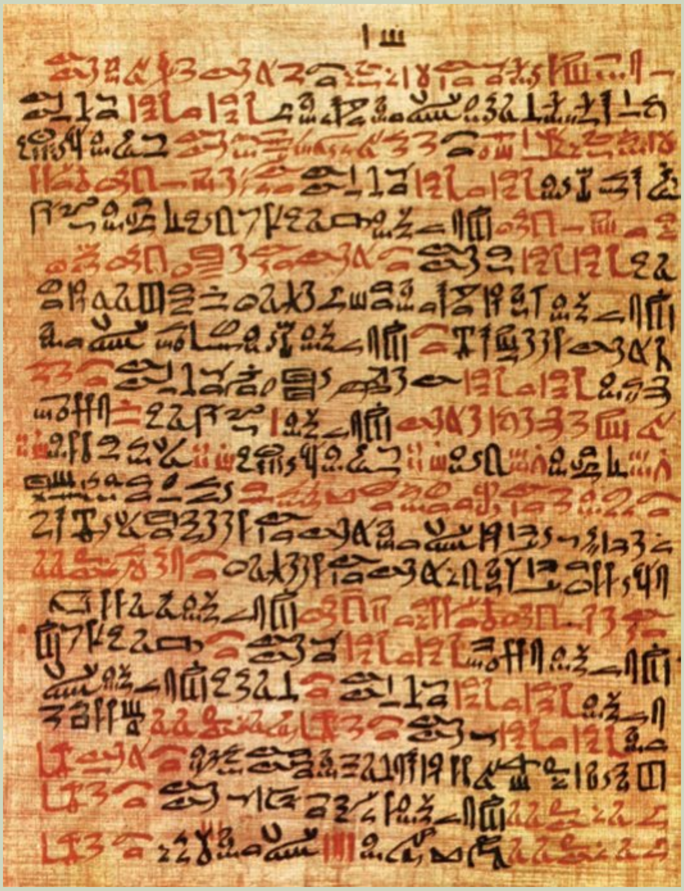


Figure 12A–1 The Ebers Papyrus is an ancient Egyptian medical scroll from around 1550 BCE written in hieroglyphics.

The image shown here is of Ebers Papyrus, which is an ancient text from around 1550 BCE. Written in hieroglyphics, it is one of the oldest medical scrolls from ancient Egypt and highlights many of the natural healing approaches that they believed worked at the time. As an example, the papyrus has information suggesting that a person suffering from asthma should be treated by inhaling the vapour produced by heating a mixture of herbs on a brick. The text also describes a potential treatment for diabetes, which involves drinking a concoction of plant fibres, beer, cucumber flowers, elderberry and green dates. Although some of these medicinal approaches may not be used today, Ebers Papyrus does provide a clear indication that humans were using compounds from nature as medicine even 3500 years ago. In this section, you will be exploring chemistry techniques that can be employed to extract and purify compounds from nature to be used as medicines. As well as this, you will also be learning about important properties of organic compounds that can determine their effectiveness as medicine.

EXPLAIN

Medicine from nature

In Australia, Aboriginal and Torres Strait Islander peoples have been using plant compounds for thousands of years to treat a variety of medical conditions. One example of this is the use of the *Pittosporum angustifolium*, or gumby gumby plant as it is more commonly known (Figure 12A–2), which is found all across mainland Australia.

> **NOTE**
>
> *P. angustifolium* is a medium-sized tree growing to approximately 10 m high, with yellow flowers and fragrant orange fruit in the winter and spring months. It most commonly grows in dry sandy inland areas, such as mallee country.

Figure 12A–2 The leaves, flowers, bark and fruit from *Pittosporum angustifolium*, or gumby gumby plant, have been used as medicine by Aboriginal and Torres Strait Islander peoples for a very long time.

While uses varied for different groups, a common traditional use involved the leaves being infused in hot water to provide treatment against colds and coughs. As well as this, the orange-coloured fruit has been mashed into a pulp and used as a balm to help treat muscle cramps and skin conditions like eczema. These traditional approaches, which have been claimed to be effective, have not yet been approved by the Therapeutic Goods Administration (TGA) for therapeutic use in humans; however, research into their potential is ongoing. These approaches are now being combined with modern chemistry to see if other methods can help extract highly purified versions of the active compounds. One of the techniques being assessed is solvent extraction.

Solvent extraction is a process used to separate compounds from mixtures by dissolving the desired compound in a solvent. This technique is commonly used in the purification of natural plant compounds for medicinal purposes. Plants contain a variety of compounds, such as alkaloids, flavonoids and terpenoids, that have medicinal properties.

Solvent extraction
a process used to separate compounds from mixtures by dissolving the desired compounds in a solvent, often with additional heating or agitation

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Table 12A–1 Examples of bioactive compounds present in *Pittosporum angustifolium* (gumby gumby)

Type of bioactive compound	Part of plant compound can be sourced from	Feature of compound	Ailments that are treated by *P. angustifolium*	Examples of this type of compound from other plants
Alkaloids	Leaves Bark	Nitrogen-containing compounds	Colds, coughs and cramps	Morphine, which is a pain-relieving drug (analgesic) found in opium poppies Quinine, which is used to treat malaria and is found in bark of the cinchona tree
Flavonoids	Fruit (and leaves)	Non nitrogen-containing pigments (15-carbon backbone consisting of two phenyl rings and a heterocyclic ring)	Eczema and muscle aches	Anthocyanins, which make up the red, blue or purple pigments in red cabbage. (You may have made a pH indicator with this.)
Terpenoids	Leaves and seeds	Five-carbon isoprene chains with additional oxygen-containing functional groups	Tumours, fungal infections and HIV	Limonene found in the rind of citrus fruit Cannabinoids found in cannabis

However, extracting these compounds from the plant material can be challenging due to the presence of unwanted materials or impurities. The steps involved in solvent extraction are listed below.

1. The initial sample of plant material is dried and ground in a mortar and pestle, and is then extracted with a polar solvent (for example, water, ethanol, methanol), including additional heating and agitation to help the dissolving process.

   Note: the appropriate solvent is chosen based on its selectivity towards the desired solute(s) rather than undesired compounds.

11D CHROMATOGRAPHY LINK

2. The solvent containing the dissolved plant compounds is passed through filter paper and then the solvent is removed under vacuum to give a crude extract. This is then redissolved in a mixture of de-ionised water and an organic solvent that is immiscible with water, and these liquid layers are separated in a separating funnel.
3. The denser aqueous phase can then be run off from the bottom of the separating funnel, leaving the organic layer in the funnel.
4. The solvent can be removed by evaporation and the residue further purified by techniques such as high-performance liquid chromatography (HPLC). Alternatively, distillation can be used to purify the compound of interest if it is a liquid.

LINK **10B** ANALYSIS OF PURITY AND CONCENTRATION

As you learned in Section 10B, simple distillation is a method used to separate solutes from solvents based on their different boiling points, and subsequently to purify different chemicals. Aboriginal and Torres Strait Islander peoples used this technique to place wet, ground plant matter over a controlled fire and the subsequent vapours were used to treat fever. The steps involved in the distillation process are as follows.

1. Begin circulating water in the condenser.
2. Using a water or oil bath for even heat distribution, begin heating the flask containing the solute(s) and solvent until the solution starts to boil. The substance with the lower boiling point will vaporise (turn into a gas) first and then travel up the cylinder and through the condenser.
3. In the condenser, this gas cools and turns back into the liquid state, where it is collected in a separate container as distillate.

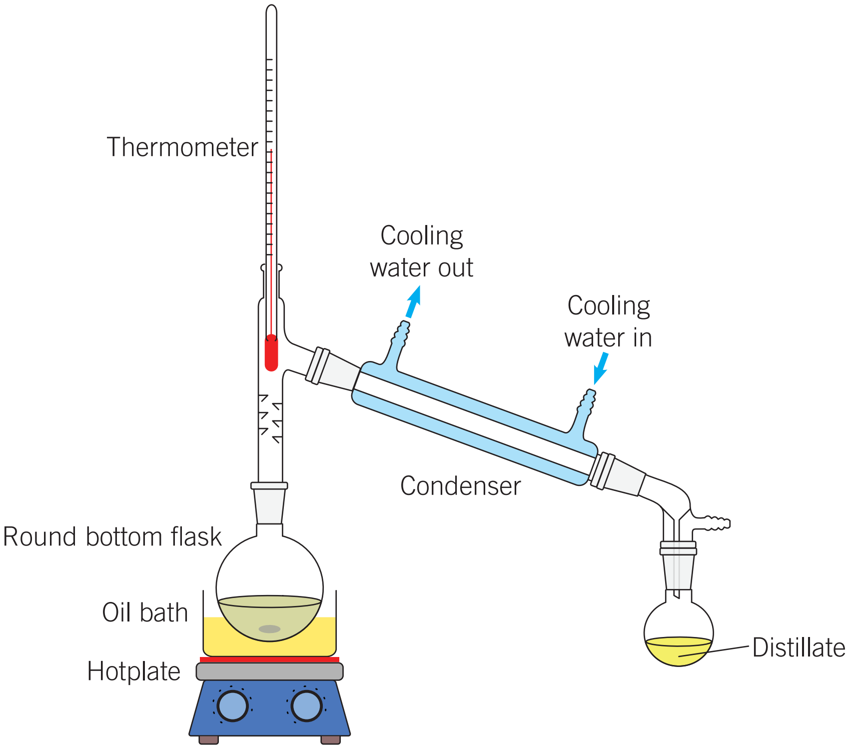

Figure 12A–3 The general set-up of a simple distillation experiment

Common structures and functional groups in medicines

Organic compounds are widely used as medicines due to their unique structures and functional groups that allow them to interact with biological systems in specific ways. The structure of organic compounds plays an important role in determining their properties and effects on the body.

As discussed in Sections 8C and 8D, the basic structure of organic compounds consists of a carbon backbone, which can be straight, branched, cyclic or aromatic, and with various functional groups attached to it. Functional groups are specific arrangements of atoms that give organic compounds their unique chemical properties. Examples include hydroxyl (–OH), carboxyl (–COOH), amino (–NH_2) and methyl (–CH_3) groups, among others. These functional groups play an important role in determining the biological activity of the organic compound.

LINK **8C** FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS

LINK **8D** FUNCTIONAL GROUPS: ALDEHYDES, KETONES, CARBOXYLIC ACIDS AND ESTERS

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Medicinal organic compounds can be categorised into several classes based on their biological effect. For example, analgesics are organic compounds that relieve pain and inflammation. Aspirin and ibuprofen are organic molecules, which contain a carboxyl functional group and act as analgesics. These two analgesics also contain a benzene ring, as is seen in Figure 12A–4.

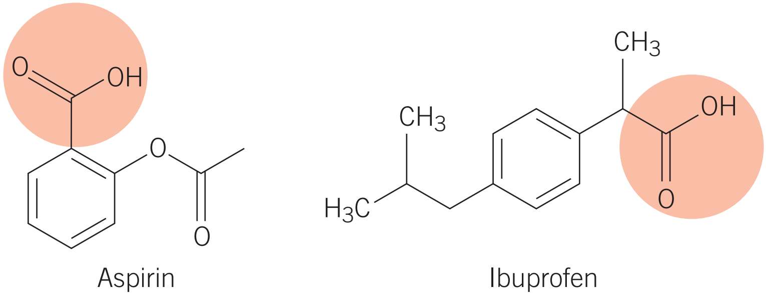


Figure 12A–4 Pain-relieving and anti-inflammatory medications, aspirin and ibuprofen, share a common carboxyl functional group (highlighted in red).

Another important class of organic compounds used as pain-relieving medication is the opioids, which are derivatives of the opium poppy plant. These compounds are highly addictive and are often used to treat pain. Opioids contain an amine functional group, causing some to be able to bind to specific receptors in the brain and block pain signals. All opioids also contain at least one hydroxyl group, which is important for forming interactions with proteins and improves their solubility in water. Lastly, opioids contain a benzene ring, like aspirin and ibuprofen, that helps maintain the structural stability of the drug. In Figure 12A–5, we can see the structure of two common pain-relieving opioids: morphine and codeine.

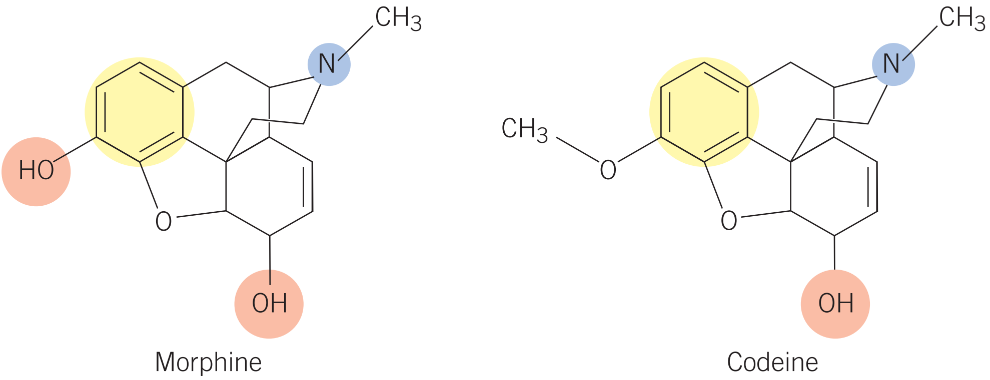
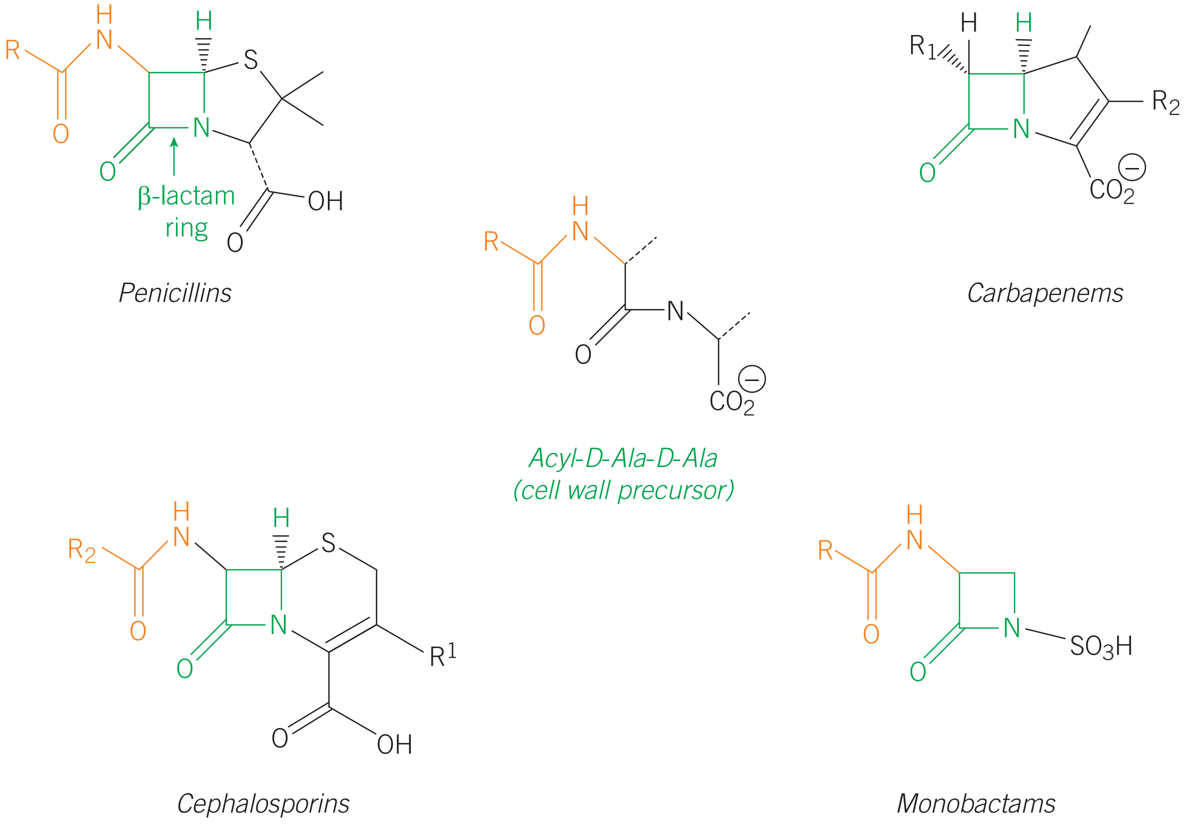


Figure 12A–5 Morphine and codeine are both pain-relieving medications from the opioid family and contain similar functional groups that help them achieve their desired function: hydroxyl groups (red), an amine group (blue) and a benzene ring (yellow).

While codeine can be found in prescription pain medication that can be self-administered, morphine is a more powerful drug that can only be administered by an authorised healthcare professional. Despite these differences, we can see that morphine and codeine both contain these similar functional groups, which are characteristic of the opioid family of drugs. These groups are important for these analgesics to be able to achieve their desired effect.

Antibiotics, such as penicillin, are organic compounds that can kill or inhibit the growth of bacteria. Penicillin contains a beta-lactam (β-lactam) ring structure, as shown in Figure 12A–6.



Penicillins

Acyl-D-Ala-D-Ala (cell wall precursor)

Carbapenems

Cephalosporins

Monobactams

Figure 12A–6 Classes of drugs that are used to treat bacterial infections, known as β-lactam antibiotics, all contain a characteristic β-lactam ring (green) and some another functional group containing an amide (orange).

In Figure 12A–6, it can be seen that all of these antibiotics contain structural similarities, which, importantly, mimic a compound found in the bacteria, acyl-D-Ala-D-Ala. By having the β-lactam ring (shown in green) and the amide group (shown in orange) in common with the bacterial compound, these drugs mimic this cell wall precursor and are able to form interactions with a bacterial enzyme to stop it from functioning. This mechanism of action of medicines, where enzymes are blocked from working, will be discussed in greater detail in Section 12B.

LINK **12B** ENZYMES

Another important class of organic compounds used as medicines is the steroids, which are examples of terpenoids. These compounds can be used to treat inflammation and immune system disorders. Steroids contain carbonyl and hydroxyl functional groups, which contribute to their anti-inflammatory activity (Figure 12A–7).

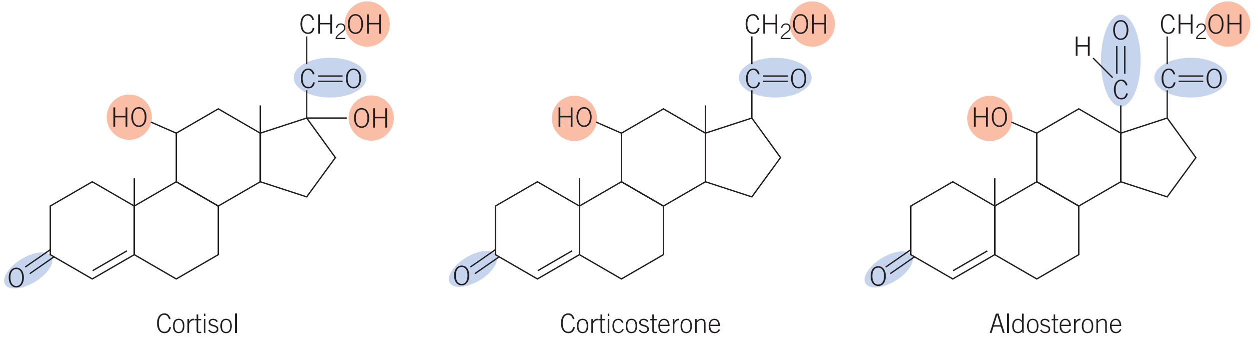


Figure 12A–7 Steroids, which form an important class of therapeutic agents, all contain a number of carbonyl (C=O, blue) and hydroxyl (–OH, red) functional groups.

Pharmacology the branch of medicine that studies the origin, chemistry and use of drugs with their associated effects on the body

Enantiomer a molecule that has the same chemical formula and similar physical and structural properties to another, but the two are mirror images of each other

8A STRUCTURAL DIVERSITY IN ORGANIC COMPOUNDS LINK

Chiral a shape or structure that cannot be superimposed on its mirror image. *Chiral* is from the Greek word for 'hand'

Achiral a shape or structure that can be superimposed on its mirror image

In summary, the unique structure and functional groups of organic compounds allow them to interact with biological systems in specific ways, making them valuable tools for medicinal purposes. Overall, the structure and functional groups of organic compounds used as medicines play a critical role in their biological activity and potential side effects. By understanding the biochemical properties of these compounds, scientists can design more effective and safer drugs to treat a variety of diseases and conditions.

Check-in questions – Set 1

1 Recall the main steps involved in solvent extraction.
2 Identify two functional groups that can be present in drugs or medication.

Isomers and chirality

Isomers are molecules that have the same molecular formula but different structural arrangements. They can have different physical and chemical properties, and this can alter the effectiveness of medicines significantly. For example, one isomer of a drug may be toxic, while another may be safe for use in humans. Therefore, it is crucial to understand the differences between isomers when developing drugs.

One type of isomer that is particularly important in **pharmacology** is the **enantiomer**. Enantiomers are molecules that have the same chemical formula and similar physical and structural properties, but are mirror images of each other. This means that they cannot be superimposed on each other, just like your left and right hand cannot be superimposed on each other, and they are said to be **chiral**, as represented in Figure 12A–8, which also shows the opposite term, **achiral**. Enantiomers can have very different biological activity, even though they have the same chemical formula. This is because many biological molecules, such as enzymes and receptors, are also chiral and can only interact with one of the enantiomers.

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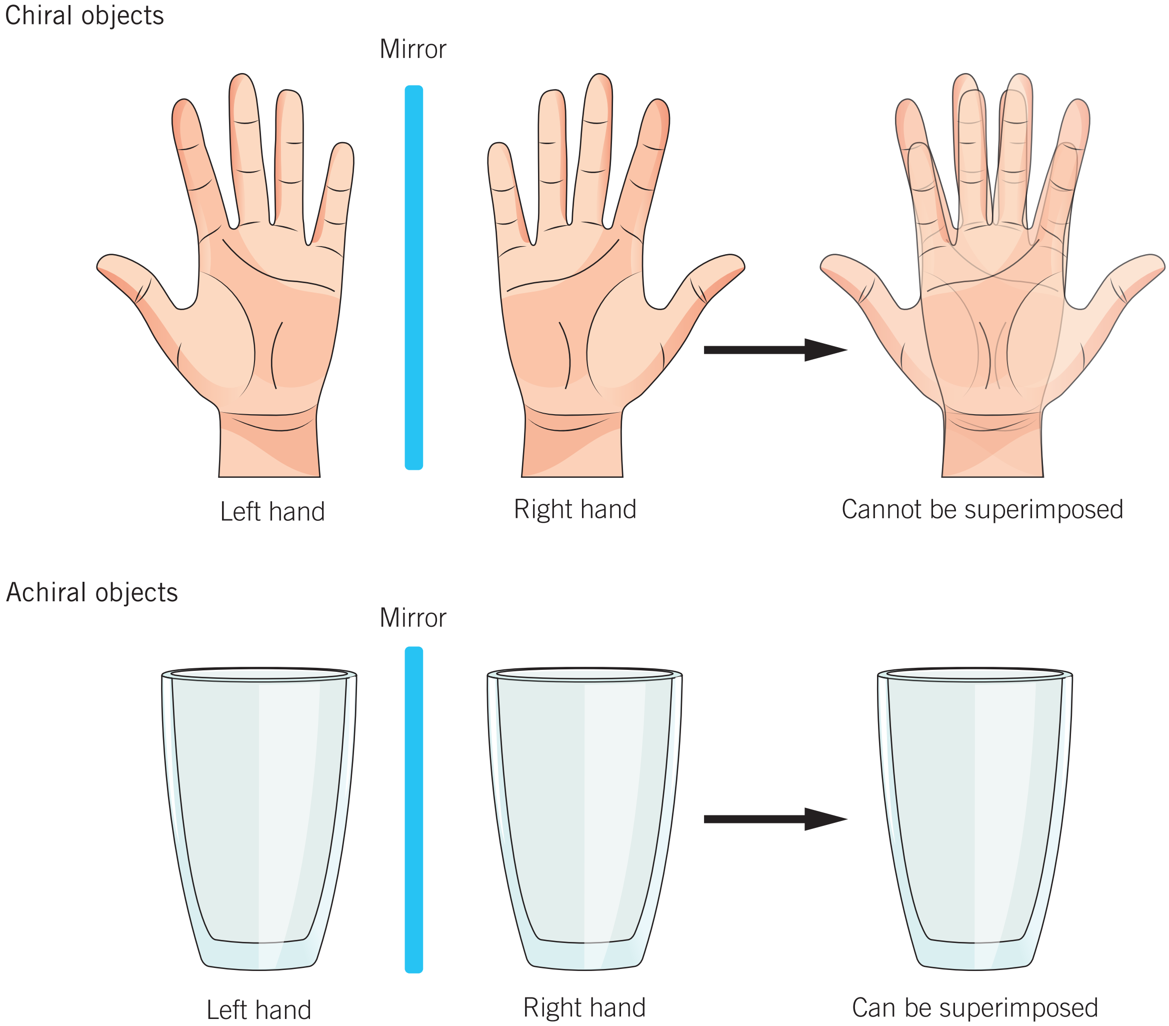

Figure 12A–8 Chiral objects (top) are mirror images that cannot be superimposed on each other, whereas achiral objects (bottom) can be superimposed on each other.

A **chiral centre** is an atom in a molecule that is bonded to four different groups (usually, though three and two are also possible), and these groups can be arranged in two different ways, resulting in two mirror image structures (Figure 12A–9). Chiral centres are important because they help to determine whether a molecule is chiral or achiral. Molecules that contain a chiral centre are usually chiral, while molecules that lack a chiral centre are usually achiral. If a molecule is being investigated for use as a possible medicine, then it is important to know whether the molecule is chiral or not. If it is chiral, then it is possible that one enantiomer may have a beneficial effect while the other may be ineffective or have a deleterious effect on the human body.

Chiral centre an atom in a molecule that is bonded to four different groups, and these groups can be arranged in two different ways, resulting in two mirror image structures

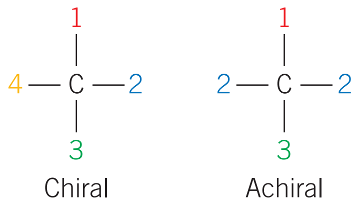

Figure 12A–9 Chiral carbons have four different groups bonded to them, whereas achiral carbons have three or fewer different groups.

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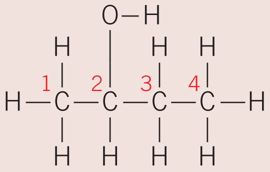
VIDEO
WORKED
EXAMPLE 12A–1

Worked example 12A–1: Identifying chiral centres of a molecule

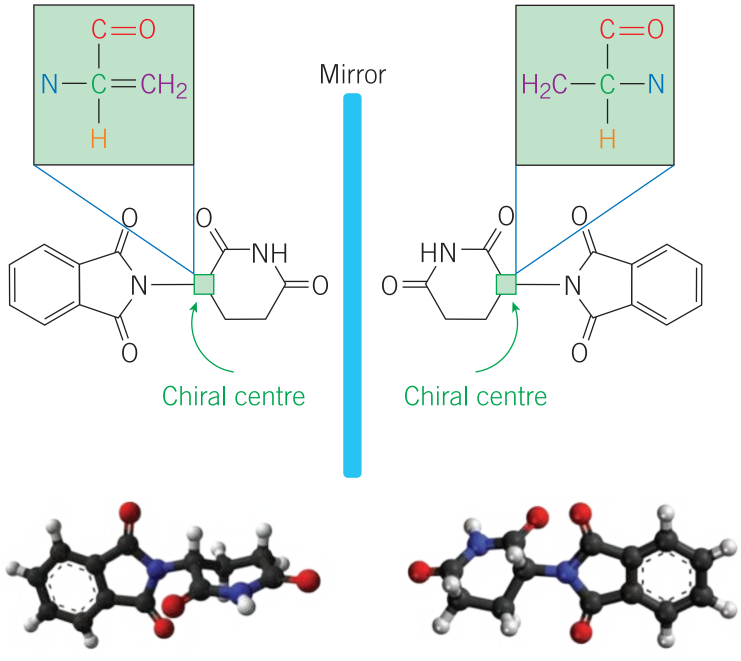
Determine if any of the carbons in the following molecule are chiral.



Solution

	Logic	Process
Step 1	Look at the first carbon and identify the atoms or groups that it is bonded to.	The first carbon is bonded to three hydrogen atoms and a $CHOHCH_2CH_3$ group.
Step 2	Look at the second carbon and identify the atoms or groups that it is bonded to.	The second carbon is bonded to a hydrogen atom, a hydroxyl group (–OH), a methyl group ($–CH_3$) and an ethyl group ($–CH_2CH_3$).
Step 3	Look at the third carbon and identify the atoms or groups that it is bonded to.	The third carbon is bonded to two hydrogen atoms, a methyl group ($–CH_3$) and a $CHOHCH_3$ group.
Step 4	Look at the fourth carbon and identify the atoms or groups that it is bonded to.	The fourth carbon is bonded to three hydrogen atoms and a $CH_2CHOHCH_3$ group.
Step 5	Determine if any of the carbons are chiral.	The first, third and fourth carbons do not have four different groups bonded to them and so are achiral. The second carbon does have four different groups bonded to it and so is chiral.

The significance of chiral centres in medicine can be illustrated by the example of thalidomide. Thalidomide was a drug that was widely used in the 1950s and 1960s and was effective as a sedative and in relieving nausea. As such, it was prescribed to pregnant women in the first three months of pregnancy to treat morning sickness. The structure of thalidomide is shown in Figure 12A–10. It can be seen that thalidomide contains a chiral centre, highlighted in green and shown in the inset.



***R*-thalidomide** ***S*-thalidomide**

Figure 12A–10 Thalidomide exists as two enantiomers, *R* and *S*, each with a chiral carbon atom at its centre, shown in green (top). Both enantiomers are shown as three-dimensional ball-and-stick models (bottom).

This chiral centre means that there are two enantiomers of thalidomide – *R*-thalidomide and *S*-thalidomide. While this may not seem like a major issue, considering the chemical composition and bonding is the same, it was later discovered that *R*-thalidomide was safe, while *S*-thalidomide caused severe birth defects. With even further research, it was then discovered that there was not really a safe enantiomer of thalidomide, as *R*-thalidomide gets converted to the *S* enantiomer, which is toxic to the foetus. This had devastating effects, with thousands of newborn children having missing or malformed limbs, and many dying in early infancy. This tragic episode highlights the importance of understanding the effects of chiral centres in drug development. Nowadays, if a new drug is planned to be marketed, testing is carried out on each enantiomer separately. Pharmaceutical companies will synthesise or separate the single enantiomer of the drug to ensure that a mixture of the two enantiomers (a racemic mixture) is not given.

WORKSHEET 12A–1 CHIRAL ATOMS AND CHIRAL CENTRES

VIDEO 12A–1 SKILLS: ANALYSING THE DIFFERENT TYPES OF EXAM QUESTIONS

12A SKILLS

Analysing the different types of exam questions

Think about what you have learned in this chapter so far. You've connected new knowledge related to various natural compounds found in plants and their role as active ingredients in medicines. You have hopefully clued in to the fact that this ties in neatly with previous knowledge about distillation for the separation and purification of compounds, as you learned in Section 10B. It also connects to knowledge you developed both in Unit 1 and earlier in Unit 4 around the various functional groups present in organic compounds, such as hydroxyl, carboxyl and amine groups.

LINK **10B** ANALYSIS OF PURITY AND CONCENTRATION

LINK **UNIT 1**

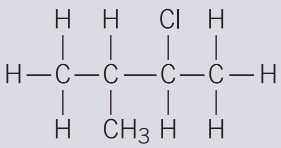
LINK **8C** FUNCTIONAL GROUPS: HALOALKANES, AMINES AND ALCOHOLS

LINK **8D** FUNCTIONAL GROUPS: ALDEHYDES, KETONES, CARBOXYLIC ACIDS AND ESTERS

However, there is now a new addition to your knowledge – the identification of chiral centres, where the carbon atom is surrounded by four different groups. While this is not a new addition to the Study Design, and has been present in previous versions, the context of this in relation to the effectiveness of medicines is new. But, don't let this scare you! Here, we provide examples of some questions you might see related to this topic.

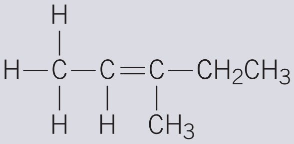
Firstly, you might be given a multiple-choice question and asked to identify which of the four molecules are chiral, as shown from the options below.

A



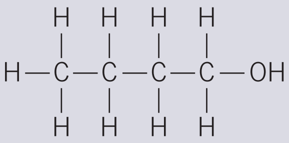
$$\begin{array}{ccccccccccc} & & H & & H & & Cl & & H & & \\ & & | & & | & & | & & | & & \\ H & - & C & - & C & - & C & - & C & - & H \\ & & | & & | & & | & & | & & \\ & & H & & CH_3 & & H & & H & & \end{array}$$

B



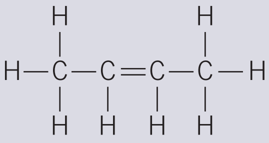
$$\begin{array}{ccccccccc} & & H & & & & & & \\ & & | & & & & & & \\ H & - & C & - & C & = & C & - & CH_2CH_3 \\ & & | & & | & & | & & \\ & & H & & H & & CH_3 & & \end{array}$$

C



$$\begin{array}{ccccccccccc} & & H & & H & & H & & H & & \\ & & | & & | & & | & & | & & \\ H & - & C & - & C & - & C & - & C & - & OH \\ & & | & & | & & | & & | & & \\ & & H & & H & & H & & H & & \end{array}$$

D



$$\begin{array}{ccccccccccc} & & H & & & & & & H & & \\ & & | & & & & & & | & & \\ H & - & C & - & C & = & C & - & C & - & H \\ & & | & & | & & | & & | & & \\ & & H & & H & & H & & H & & \end{array}$$

To be able to successfully complete this question, as opposed to simply guessing, you need to recall the following points.

1 What does chiral mean?

A molecule with a mirror image that cannot be superimposed onto it.

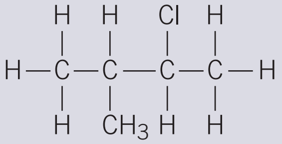
2 How do you determine which carbon atom could be a chiral centre?

Eliminate carbon atoms with the following:

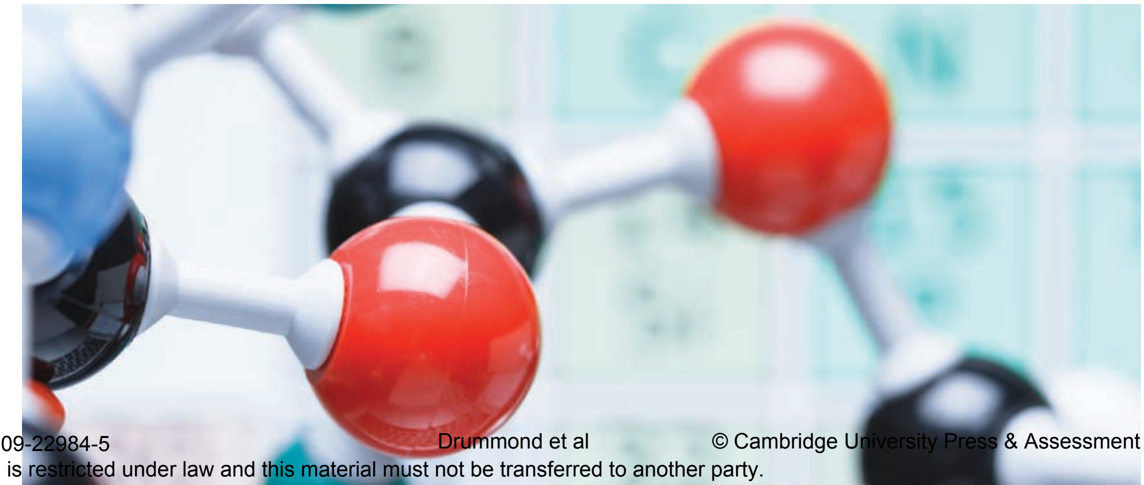
- *CH_3 group*
- *CH_2 group*
- *C atoms involved in a double or triple intramolecular covalent bond.*

Applying these rules quickly eliminates A, C and D, leaving only B as the correct option, where the chiral centre carbon atom is the one with the chlorine bonded to it.

Secondly, you might instead get a short-answer question that asks you to *draw* a named molecule (for example **2-chloro-3-methylbutane**) and *identify* the carbon atom at its chiral centre with a *justification* of your choice. It is likely that a question such as this would be broken up into parts and even include different molecules or cues for each part so that you don't lose all available marks by not knowing one step. For the sake of this question, let's complete this.

	Logic	Process
Step 1	Draw the molecule 2-chloro-3-methylbutane.	 $\mathrm{H-\underset{H}{\overset{H}{C}}-\underset{CH_3}{\overset{H}{C}}-\underset{H}{\overset{Cl}{C}}-\underset{H}{\overset{H}{C}}-H}$
Step 2	Identify the carbon atom that is the chiral centre.	The two terminal carbon atoms (carbon atoms at each end) and the methyl group off the third carbon atom in the main chain can be ruled out as they are all $–CH_3$ groups. This leaves only the second and third carbon atoms in the main chain. In this example, both of these atoms are chiral centres.
Step 3	Justification of these carbon atoms being the chiral centres.	The reason why each of these carbon atoms are chiral centres is because they are not carbon atoms with either three hydrogen or two hydrogen atoms attached, and the molecule is an alkane, so it has no double or triple bonds like those seen in alkenes and alkynes, respectively. As each of these carbon atoms is covalently bonded to four different groups, each could be the chiral centre.

The key to improving, if you are struggling, is to use the questions in this textbook and in the exam generator online, which has past VCAA exam questions with solutions, to further hone your skills. Make sure you target specific areas by selecting from the various topics present, reading through the worked solutions and using the experience and support of your teacher and peers.



Section 12A questions

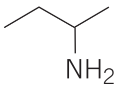
1 Explain the basis of separation in the purification of natural plant compounds by

- **a** solvent extraction.
- **b** distillation.

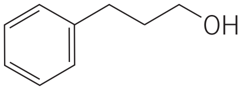
2 Define 'chiral' and 'achiral'.

3 Indicate whether or not each of the following molecules exists as a pair of enantiomers.

a



b



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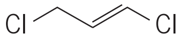

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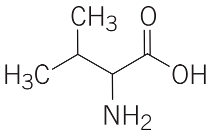
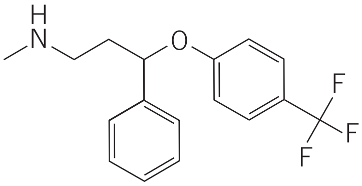


4 A synthetic chemist is interested in modifying a functional group of an antibacterial drug molecule to create a derivative. The original drug molecule has a hydroxyl group (–OH) attached to a specific position. The chemist modifies this functional group to a methyl group ($-CH_3$).

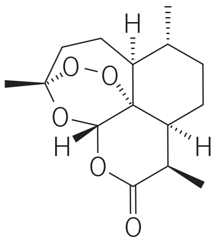
- **a** Explain how the modification of the functional group might affect the solubility of the drug.
- **b** Explain how the modification of the functional group might affect the antibacterial activity of the drug.

5 The structure of fluoxetine, an antidepressant belonging to the selective serotonin re-uptake inhibitor (SSRI) class, is shown below.



- **a** Identify the chiral centre(s) in the structure of fluoxetine.
- **b** Based on the presence of chiral centres in fluoxetine, discuss whether it exists as a pair of enantiomers.
- **c** Explain how enantiomers can have different biological activities despite having the same chemical formula.

6 Artemisinin is an antimalarial drug derived from the plant *Artemisia annua*, commonly known as sweet wormwood. It is a key component in the treatment of malaria, particularly for drug-resistant strains. The structure of artemisinin is shown below.



- **a** Describe two advantages of obtaining artemisinin from natural sources (*Artemisia annua*) compared to synthetic production.
- **b** Identify two functional groups present in the structure of artemisinin.
- **c** Discuss the potential significance of the functional groups in the mechanism of action of artemisinin against malaria.
- **d** Is artemisinin a chiral molecule? Provide a justification for your answer.

12B Enzymes

Study Design:

- Enzymes as protein-based catalysts in living systems: primary, secondary, tertiary and quaternary structures and changes in enzyme function in terms of structure and bonding as a result of increased temperature (denaturation), decreased temperature (lowered activity) or changes in pH (formation of zwitterions and denaturation)
- Medicines that function as competitive enzyme inhibitors: organic molecules that bind through lock-and-key mechanism to an active site preventing binding of the actual substrate

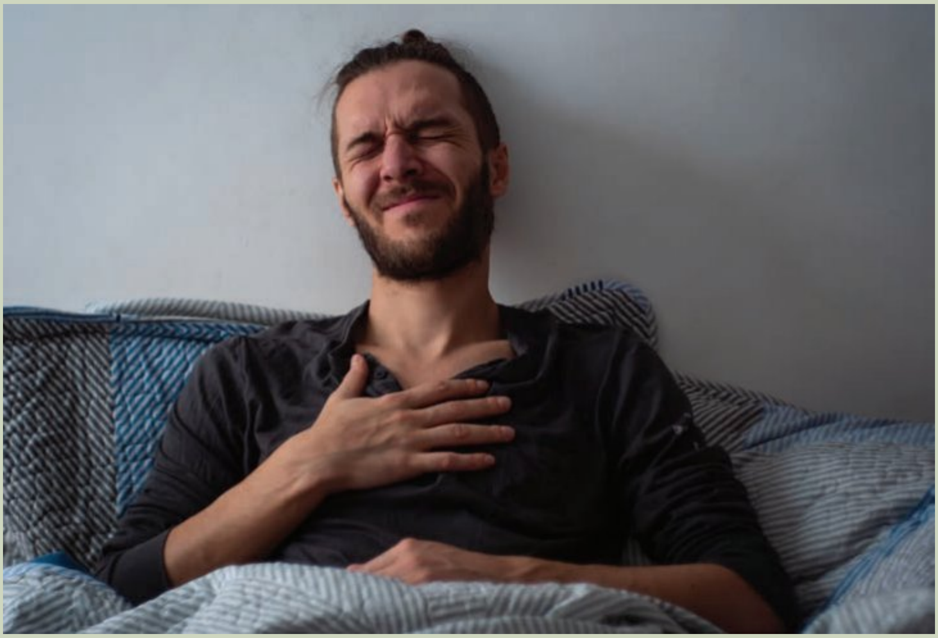
Glossary:

Active site
Competitive inhibition
Denatured
Monomer
Peptide bond
Polymer
Polypeptide
Substrate
Zwitterion

ENGAGE

The connection between heartburn and enzymes

Heartburn, caused by acid reflux, is a medical condition that is estimated to affect around 20% of the population worldwide. This occurs when acid from the stomach escapes and travels back up the oesophagus, which leads to a burning sensation in the chest (that is, heartburn), nausea, vomiting and a sensation of constantly having a lump in the throat. Medications, such as omeprazole, have been developed that can help reduce the production of stomach acid and decrease the symptoms that people experience. Omeprazole, as well as other treatments for reflux, often target an important step in the process involving a special type of protein known as an enzyme. In this section, you are going to learn about enzymes as catalysts in the body, as well as how they can be targeted and disrupted for the treatment of disease.



EXPLAIN

Amino acids

Many molecules in the body are present as **polymers**, that is, they are composed of a series of repeating subunits known as **monomers**. Proteins are an example of biological polymers. The building blocks (monomers) of proteins are known as α-amino acids. The generalised structure of an α-amino acid is illustrated in Figure 12B–1. An α-amino acid molecule has a central carbon atom to which is attached an amine functional group ($-NH_2$), a carboxyl functional group ($-COOH$), a hydrogen atom (H) and a group (R) that varies from one α-amino acid molecule to another. If R is not a hydrogen atom, the central carbon atom is chiral and the α-amino acid molecule will be chiral.

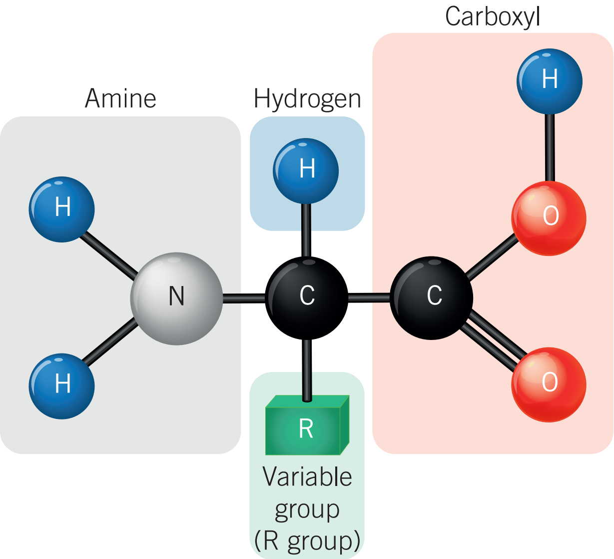


Figure 12B–1 The generalised structure of an α-amino acid, the building blocks of proteins

LINK UNIT 1

Polymer
a long-chain molecule made up of a large number of smaller repeating units (monomers)

Monomer
a molecule that forms bonds with other identical molecules as the repeating units that make up a polymer

LINK **12A** ORGANIC COMPOUNDS AS MEDICINES

The other important feature of an α-amino acid is the variable group, or R group (highlighted in green). All the α-amino acids are identical in all other parts of their structure – that is, they all have exactly the same amine group (grey), hydrogen (blue) and carboxyl group (red). The only thing that differentiates the 20 α-amino acids found in the body is the variable group.

Peptide bonds

As already mentioned, α-amino acids are the monomers that make up proteins. For this to occur, the α-amino acids need to join to each other to make a long chain, known as the **polypeptide** chain. This occurs through the formation of the **peptide bond**.

Polypeptide
a long chain of α-amino acids forming part of a protein

Peptide bond
a chemical bond between two amino acids

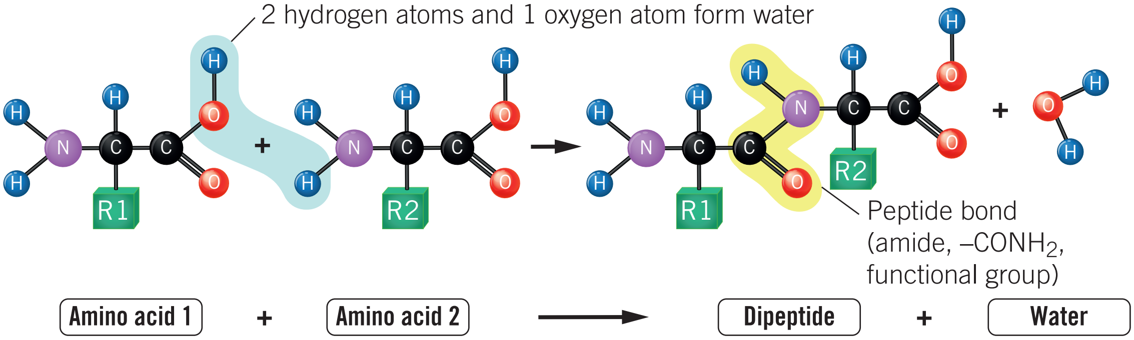


Figure 12B–2 A condensation reaction between two α-amino acids to form a dipeptide with a peptide bond. This reaction is repeated numerous times to form a polypeptide chain.

There are a couple of aspects of the reaction illustrated in Figure 12B–2 that should be highlighted. Firstly, the reaction to link two amino acids together is a condensation reaction – a second, small product is generated in the form of water. Secondly, the peptide bond is an example of an amide functional group ($-CONH_2$), highlighted in yellow.

LINK **9B** ORGANIC REACTIONS: CONDENSATION AND HYDROLYSIS

Proteins

After these amino acids have bonded together to form long polypeptide chains, they begin to fold and adopt unique structures. These unique structures are critical for being able to perform their function in the body. There are four levels of protein structure, each building on the foundation laid by the previous level.

Primary structure

Primary structure is defined as the sequence of α-amino acids joined by peptide (amide) bonds that make up a single polypeptide chain, as shown in Figure 12B–3. Each R group, which is different for each of the 20 α-amino acids, is represented in a different colour, with the amide bond connecting amino acids shown in yellow highlight.

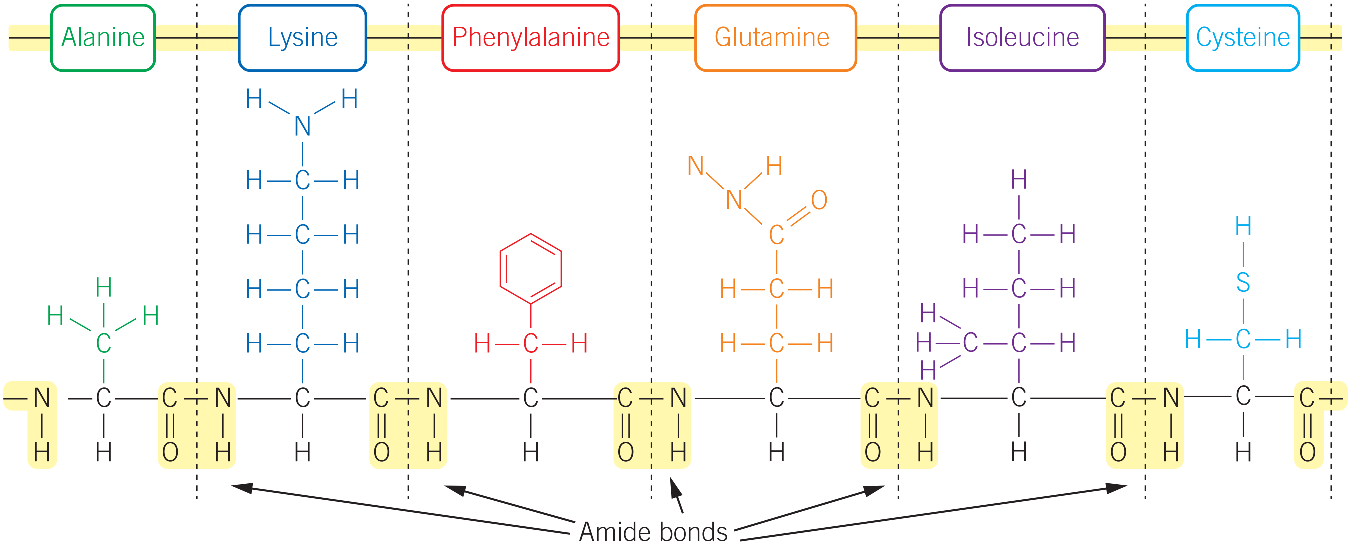


Figure 12B–3 Primary structure of a six α-amino acid sequence composing part of a single polypeptide chain

Secondary structure

This is the level of protein structure one level up from the primary structure, where sections of a single polypeptide chain fold into specific structures called alpha helices and beta-pleated sheets. These specific structures, shown in Figure 12B–4, are held together by hydrogen bonds between the polar –NH group in one amide functional group (peptide bond) and the polar –C=O group in a different amide functional group (peptide bond). Alpha helices form when an amino acid chain forms a three-dimensional spiral shape, whereas beta-pleated sheets form when two amino acid chains line up parallel to each other.

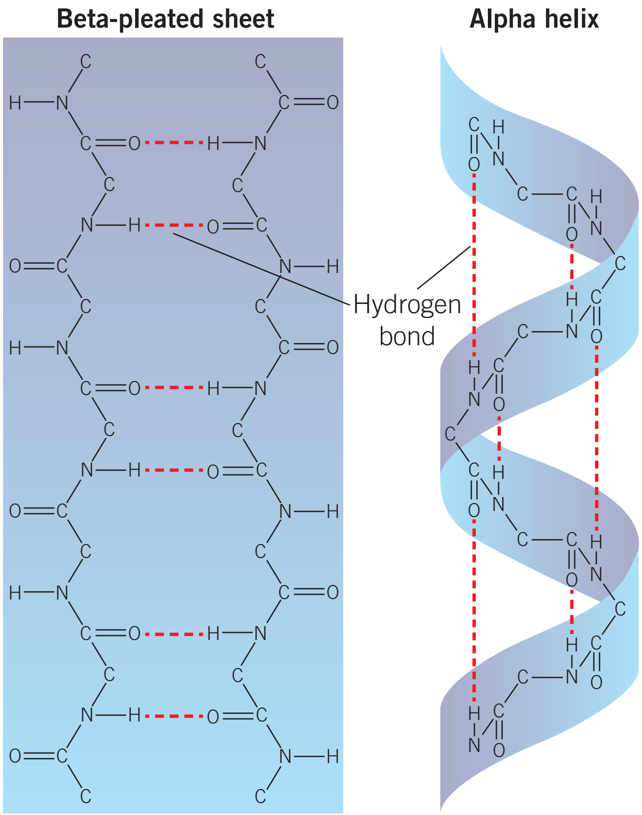


Figure 12B–4 Regions of polypeptide chains folded into specific secondary structures; alpha helices (right) and beta-pleated sheets (left) are held together through hydrogen bonding between amine and carboxyl functional groups of different amino acids.

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Tertiary structure

This level of protein structure is one level up from the secondary structure and is the overall functional three-dimensional structure of an entire single polypeptide chain due to folding of the respective alpha helices and beta-pleated sheets. There are examples of proteins that are completely functional as a single polypeptide chain, such as myoglobin, present in heart and skeletal muscles. This overall three-dimensional structure is formed through many types of bonds and interactions between the R groups (or side chains) of separate α-amino acids. The types of bonds involved are shown in Figure 12B–5 and summarised in Table 12B–1.

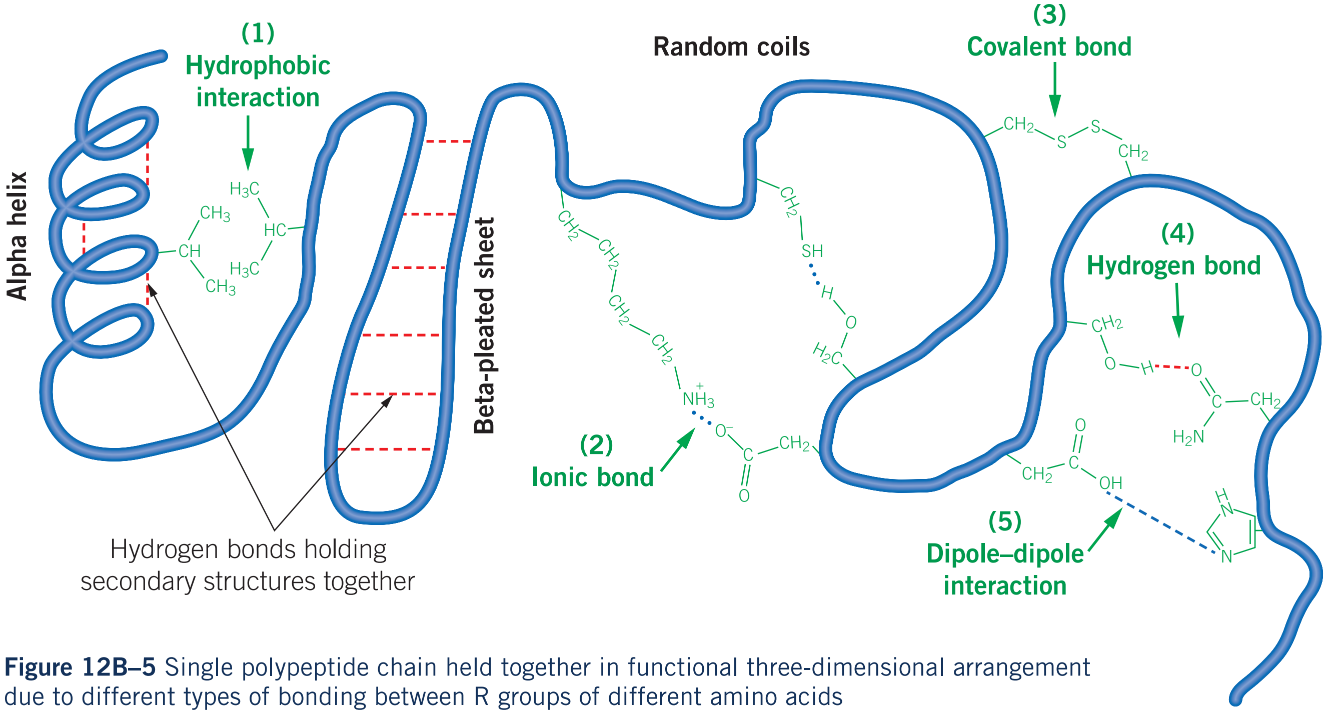


Figure 12B–5 Single polypeptide chain held together in functional three-dimensional arrangement due to different types of bonding between R groups of different amino acids

Table 12B–1 Different types of bonds associated with tertiary structure of proteins

Type of bond/interaction present in tertiary structure	Explanation	Example from Figure 12B–5
Hydrophobic interactions	Dispersion forces acting between different non-polar R groups	Between two valine α-amino acids (1)
Ionic interaction	Between $-NH_3^+$ part of one R group and $-COO^-$ part of a different R group	Between lysine and aspartic acid α-amino acids (2)
Covalent bonding	Disulfide bridge, –S–S–	Between two cysteine α-amino acids (3)
Hydrogen bonding	Between –O–H, –N–H, –C=O part of one R group and any one of these in a part of a different R group	Between serine and asparagine α-amino acids (4)
Dipole–dipole interaction	Between partially charged parts, such as –S–H, –N–H or –O–H, of polar R groups	Between aspartic acid and histidine α-amino acids (5)

Quaternary structure

Some proteins, such as enzymes, which you will learn about later in this chapter, are composed of two or more polypeptide chains. These proteins are referred to as having a quaternary structure. One example is an antibody, shown in Figure 12B–6, which is produced within the immune system to combat pathogens. The quaternary structure is held together by the same types of bonds and interactions that are present within the tertiary structure, however, here they occur between different polypeptide chains to shape them into a functional three-dimensional shape, as opposed to the single polypeptide chain (tertiary structure).

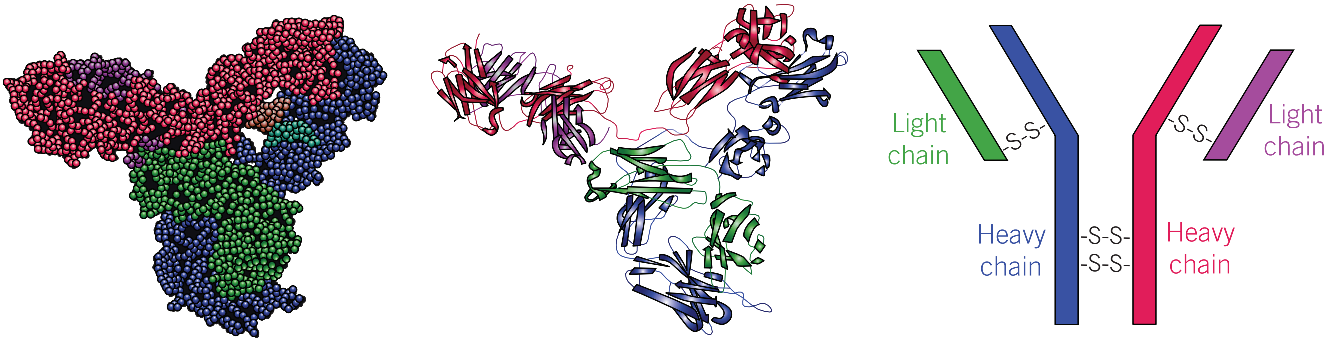


Figure 12B–6 Quaternary structure of an antibody represented as a computer-generated space-filling model (left), crystal structure (middle) and simplified diagram (right). The four polypeptides are represented here as different colours.

VIDEO 12B–1 BONDING AND INTERACTIONS PRESENT IN PROTEINS

WORKSHEET 12B–1 COMPARING THE LEVELS OF PROTEIN STRUCTURE

As can be seen in Figures 12B–3 to 12B–6, the four levels of protein structure all involve interactions between various parts of the amino acids. The types of bonds involved in each level are summarised in Table 12B–2.

Table 12B–2 Bonds associated with the different levels of protein structure

Levels of protein structure	Types of bonds involved
Primary	Peptide/amide bond between α-amino acids
Secondary	Hydrogen bonding between the oxygen in the C=O of an amide functional group at one site in the polypeptide chain and a hydrogen in the N–H of an amide functional group at a different site in the polypeptide chain
Tertiary	Hydrogen bonding, ionic bonding, covalent bonding, hydrophobic interactions, disulfide bonding and dipole–dipole interactions between the R groups of the α-amino acids
Quaternary	Same as tertiary structure, but happening between multiple polypeptide chains

Enzymes

1C EXOTHERMIC AND ENDOTHERMIC REACTIONS LINK

Enzymes are a class of proteins known as biological catalysts. As you learned in Section 1C, all chemical reactions have an energy threshold that needs to be overcome for the reaction to occur. This threshold is known as the activation energy. As was discussed previously with catalysts, enzymes speed up (catalyse) chemical reactions within organisms by lowering this activation energy. This means that less energy is required for the reaction to take place, and therefore, the reaction can occur more frequently. This is illustrated in Figure 12B–7.

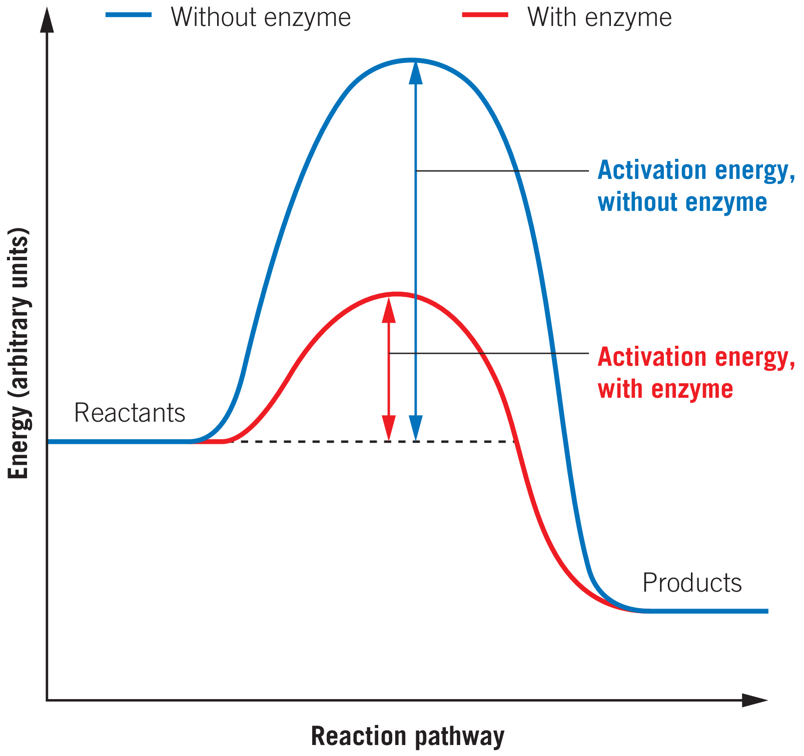


Figure 12B–7 Enzymes speed up biological reactions by lowering the activation energy.

The functional three-dimensional structures of proteins are particularly important for them to be able to perform their desired function. This is no different for enzymes because they are proteins. Proteins with a functional three-dimensional tertiary or quaternary structure are chiral molecules. They have a pocket, called the **active site**, which is complementary to the stereochemistry of their specific reactant(s), known as **substrate(s)**. Referring back to Section 12A, take the example of thalidomide. An enzyme may bind specifically to *R*-thalidomide but not *S*-thalidomide, which are enantiomers. For the reaction to occur, the substrate must successfully bind to the enzyme at its active site. It is important to realise that the shape and charge of the active site are unique to each enzyme and are complementary to the shape and charge of the enantiomer that binds to it. This feature is what provides enzymes with their high level of specificity in terms of what they will bind to. It also explains why one enantiomer is biologically active but its mirror image enantiomer is not: the first will bind to an enzyme but the second won't. Earlier, we discussed the general structures of α-amino acids. The R group is the part of the α-amino acid structure that makes each amino acid unique. These R groups are very important during the interaction of an enzyme's active site with its substrate. The specific α-amino acids found in the active site help to determine the specificity of the enzyme, through having R groups that will only interact and bind with that substrate.

Active site
the region of an enzyme where the substrate(s), also known as reactants, bind for a chemical reaction to take place

Substrate
reactant molecule(s) that binds to the active site of an enzyme and then takes part in a reaction

LINK **12A** ORGANIC COMPOUNDS AS MEDICINES

As represented in Figure 12B–8, the interaction between the substrate(s) and the enzyme active site occurs via a lock-and-key mechanism. Essentially, this means that the substrate(s) (the key) has a complementary shape to the active site (the lock). As this interaction requires the shapes of both the substrate(s) and the active site to align, this feature means that enzymes have a very high specificity. The active site allows more successful collisions between substrates in a reaction than would normally occur without the presence of an enzyme.

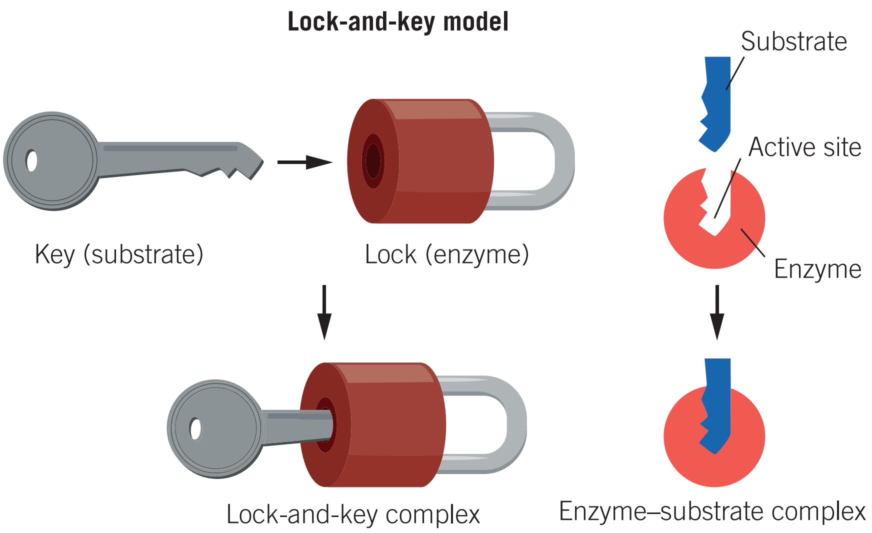
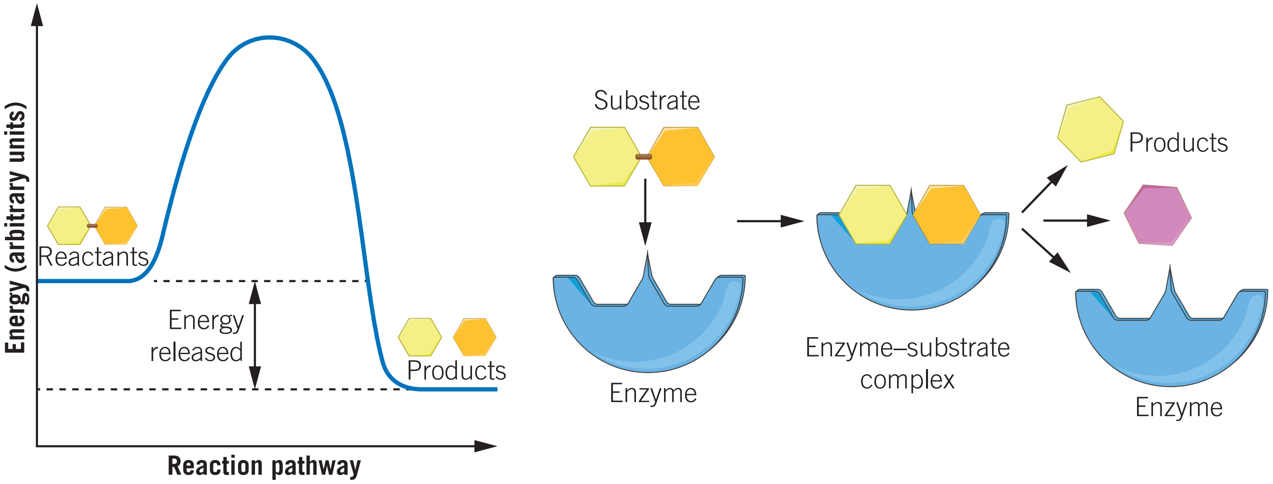


Figure 12B–8 The lock-and-key model describes the interaction between a substrate and an enzyme.

Once the substrate(s) has bound to the active site, there are two main categories of reaction that can take place, as shown in Figure 12B–9.

Exothermic reactions: breaking down large molecules into smaller ones with the release of energy



Endothermic reactions: building larger molecules from smaller ones, requiring energy input

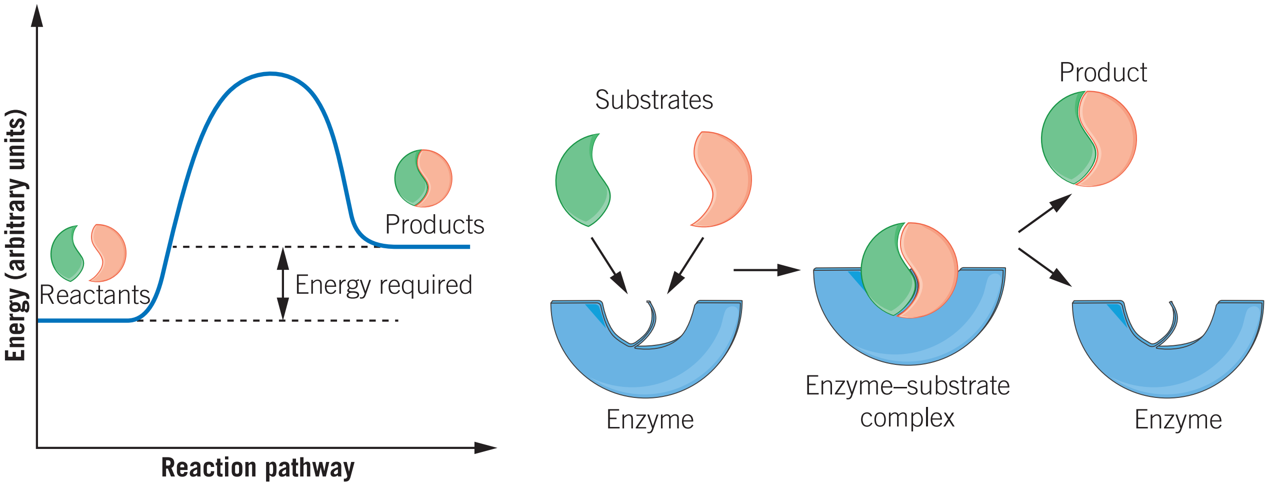


Figure 12B–9 Reactions catalysed by enzymes can either be exothermic (top) or endothermic (bottom) depending on whether they are breaking down molecules or building them.

If a larger substrate is broken down into smaller products, the reaction is exothermic. Exothermic reactions release energy, so the products have less energy than the reactants. An example of a biological reaction that is exothermic is cellular respiration, which you studied in Section 1B. On the other hand, if the reaction involves smaller substrates being built up into larger products, the reaction is endothermic. Endothermic reactions require energy, so the energy of the products is greater than the reactants. An example of an endothermic reaction is the formation of a dipeptide from two amino acids, which was discussed earlier in this section.

LINK **1B** PRODUCTION OF CHEMICAL ENERGY IN NATURE

Check-in questions – Set 1

1 What are the four levels of protein structure?
2 How does an enzyme speed up biological reactions?
3 Draw an energy profile diagram for an enzyme reaction in which a single substrate is broken down into two products.

Factors affecting enzyme activity

As discussed, enzymes function to increase the rate of biological reactions. However, there are a number of factors that can affect their ability to do this, such as temperature, pH and the presence of inhibitors.

Temperature

Temperature is one of the most important factors that control the activity of an enzyme. All enzymes have an optimal temperature – that is, the temperature at which they function best. For most enzymes within the human body, it makes sense that this temperature is around 37°C. The effect of temperature on enzyme activity differs depending on whether it is above or below the optimal temperature. This is highlighted in Figure 12B–10, which shows the rate of reaction for a typical human enzyme across a temperature range.

Next, we will consider how the shape of this curve can be explained in terms of what is happening with the chemistry of enzymes at a molecular level.

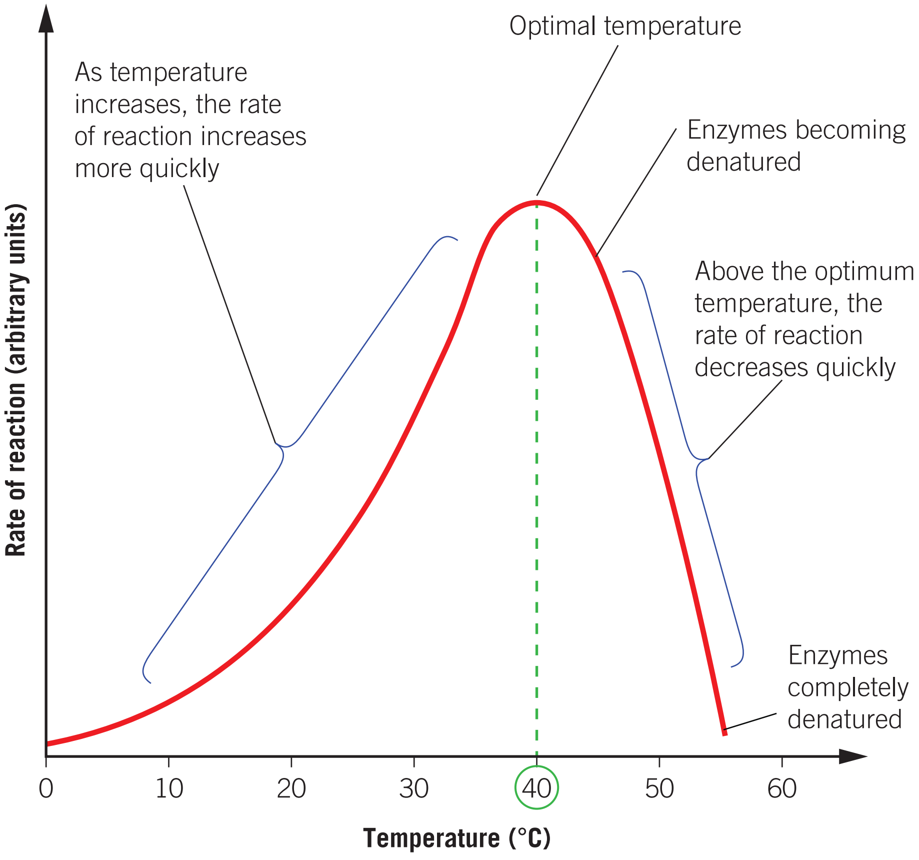


Figure 12B–10 The rate of reaction for a typical human enzyme across a range of temperatures

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Enzyme activity below optimal temperature

5A WHAT CAUSES A CHEMICAL REACTION? LINK

Figure 12B–10 shows that at low temperatures the enzyme activity is reduced. As the temperature increases from 0°C towards the optimal temperature, the enzyme activity (and so the rate of reaction) also increases. The explanation for this involves understanding the relationship between temperature and the kinetic energy (related to speed of vibration or other movement) that molecules have, which was discussed earlier in Section 5A. The faster something is moving or vibrating, the more kinetic energy it has. Temperature is a measure of the average kinetic energy of atoms and molecules, and adding heat energy raises their speed, kinetic energy and therefore temperature (Figure 12B–11).

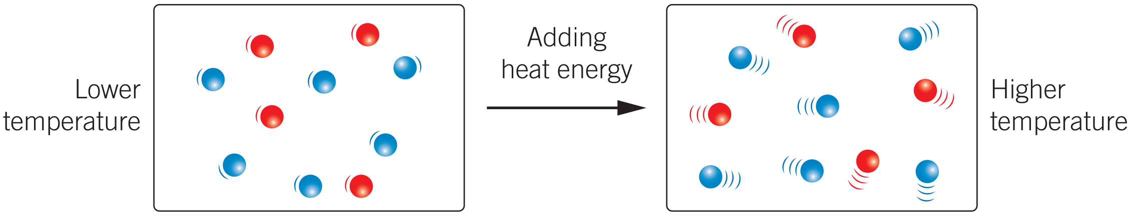


Figure 12B–11 At higher temperatures, particles have more kinetic energy. As the particles are moving around more quickly, there will be more successful interactions between the enzyme's active site and substrates, leading to an increased rate of reaction.

However, how is the speed at which these molecules are moving around related to the rate at which they function? Imagine that you and a friend are in your chemistry laboratory, are blindfolded and told to walk around for a 10-minute experiment. You are told to keep count of the number of times you collide with each other, as this will represent every time that a substrate and enzyme active site interact with each other. Now imagine doing this experiment a second time, but instead of walking, you are told to run around as fast as you can. In which experiment do you think you would bump into each other more often? The most likely answer would be experiment number 2.

By thinking about it this way, you can appreciate why an increase in temperature may lead to an increase in enzyme activity. For this to happen, the molecules first need to collide, but they also need to interact in such a way that the substrate binds successfully with the active site of the enzyme. From this you may realise that, while many things need to go right for an enzyme reaction to occur, the greater the kinetic energy of both the enzyme and the substrate, the more likely it is to occur. This is exactly the same concept that was discussed in collision theory and rates of reaction in Section 5A.

5A WHAT CAUSES A CHEMICAL REACTION? LINK

Enzyme activity above optimal temperature

As can be seen in Figure 12B–10, when the temperature exceeds the optimal temperature, there is a sharp decrease in the rate of reaction. To understand what is happening under these conditions, it is important to remember this important fact: enzymes are proteins.

At higher temperatures, the bonds and interactions that form the tertiary and quaternary structures, specifically the hydrophobic interactions, ionic interactions, hydrogen bonding and dipole–dipole interactions (intermolecular interactions), of a protein begin to break down due to increasing vibrations in the molecules. Additionally, the hydrogen bonds holding the alpha helix and beta-pleated sheet secondary structures together also break.

When this occurs, we say that the enzyme is being **denatured** and the process is called denaturation. Unlike reversible reduced enzyme activity due to temperatures lower than optimal, this process is permanent, so once an enzyme is denatured it will not function properly again. So why does this process have such a profound effect on the activity of an enzyme?

Denatured refers to an enzyme that has lost its conformational three-dimensional structure and hence cannot function as a catalyst

It is easier to illustrate this by looking at what happens in a series of steps.

Step 1: At the optimal temperature, binding of the substrate to the enzyme active site occurs normally.

Step 2: As the temperature increases beyond the optimum, the enzyme's three-dimensional conformational shape changes.

Step 3: The specific structure of the active site begins to disappear, which means that the substrate is no longer complementary and cannot bind.

Step 4: Enzyme activity becomes zero, as substrate interaction is no longer possible.

This process is shown in Figure 12B–12.

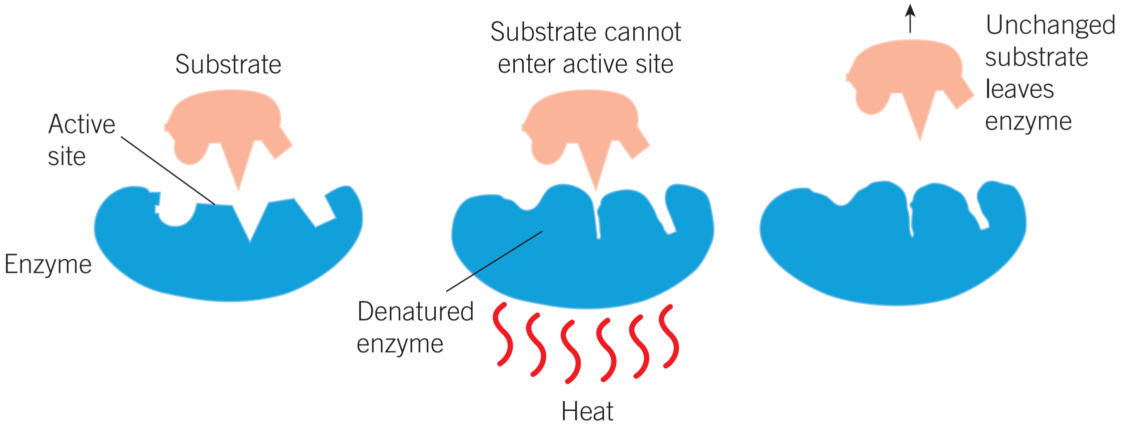


Figure 12B–12 An increase in temperature denatures the enzyme, which leads to a change in the conformation of the active site, so the substrate is unable to bind and the enzyme is unable to function.

pH

pH is another factor that can affect the function of an enzyme. Figure 12B–13 shows a summary of how a number of enzymes in the body function at different pH levels.

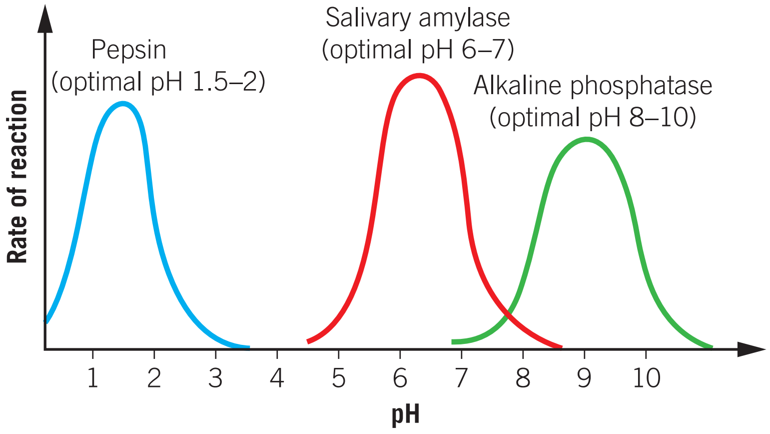


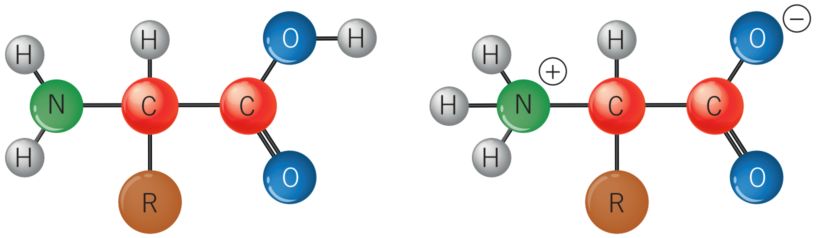
Figure 12B–13 The effect of pH on the rate of reactions catalysed by different enzymes within the human body

Firstly, different enzymes within the body function at different optimal pH values. pH values of different environments within organisms can vary greatly. Therefore, it is not surprising that enzymes have an optimal pH that suits the environment that they function in. For example, pepsin (an enzyme found in the stomach) has an optimal pH of 1.5–2, which suits the acidic nature of gastric juices. In contrast, salivary amylase works best at a pH of around 6.5, which is appropriate for the neutral pH environment of the mouth.

UNIT 2 LINK

Secondly, the rate of reaction on either side of the optimal pH changes quickly. You may recall from Unit 2 that as the pH decreases (becomes more acidic), hydrogen ion concentration increases, and when the pH increases (becomes more basic), hydrogen ion concentration decreases. You should also recall from earlier in this section that amino acids contain polar carboxyl (–COOH) and polar amine (–NH_2) groups. In aqueous solutions the amine functional group can accept a hydrogen ion, or proton, and therefore act as a base. Alternatively, the carboxyl functional group can donate a hydrogen ion, or proton, therefore acting as an acid. Consequently, amino acids in solution may be in the form of a **zwitterion**, as shown in Figure 12B–14.

Zwitterion a molecule with equal positive and negative charges, giving it an overall neutral charge; also called a dipolar ion



Non-ionised form of amino acid

Ionised form of amino acid (zwitterion)

Figure 12B–14 Comparison between the non-ionised (left) and ionised, or zwitterion (right), forms of an α-amino acid

Therefore, changes to pH can affect some of the R groups of α-amino acids. As a result, the conformational shape of an enzyme changes due to disruptions of the interactions between α-amino acids' R groups within the tertiary and quaternary levels of protein structure. An example of this can be seen in Figure 12B–5 on page 477, and the ionic interaction between lysine and glutamic acid α-amino acids. A zoomed-in version of this interaction is shown in Figure 12B–15.

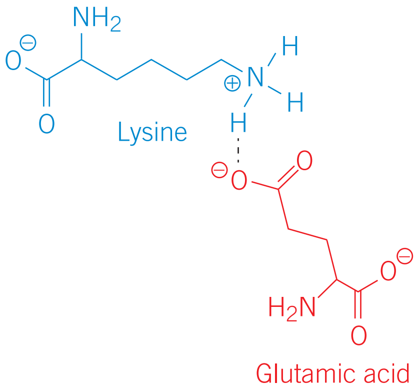


Figure 12B–15 The ionic interaction between the α-amino acids, lysine (left) and glutamic acid (right). Note, lysine is present as a zwitterion in this interaction.

In neutral pH ranges, this interaction is likely to occur. However, as the pH decreases and becomes more acidic, the carboxyl functional group in each glutamic acid molecule is less likely to ionise (donate its hydrogen ion), meaning it will not possess a negative charge. Therefore, this ionic interaction will not occur and the tertiary (or quaternary) structure of the enzyme will be affected. Likewise, if the pH increases and becomes more basic, the amine functional group in lysine is less likely to ionise (accept a hydrogen ion). Therefore, it will not possess a positive charge. Again, the ionic interaction will be disrupted.

As you can see, changes in pH have a drastic effect on the stability of an enzyme's tertiary and quaternary (if present) structures. This would consequently affect the enzyme's active site, causing the rate of reaction or enzyme activity to decrease quickly.

Changes in pH, in a similar way to an increase in temperature above an enzyme's optimal temperature, can also lead to denaturation. Remember that denaturation is a permanent process due to disruption of the hydrogen bonds holding alpha helices and beta-pleated sheets (secondary structures) together, as well as the interactions and bonding within the tertiary and quaternary levels of protein structure. It is important to note that the strong covalent bonds (amide, or peptide bonds) between amino acids in the polypeptide chain (primary structure) are not disrupted. So, even though the conformational three-dimensional shape of the enzyme, and as such its active site, is altered, the specific sequence of amino acids comprising the protein is not.

Competitive inhibition

An enzyme's active site is critical to its ability to function. The active site is the location where the substrate binds to the enzyme, allowing the reaction to take place (Figure 12B–16). Previously, you learned how this mechanism is often described as being like a lock and a key. If this analogy is taken further, imagine that a person returned home one day and found that someone had jammed something into the lock of their front door. In this case, the key would no longer be able to fit and the person wouldn't be able to unlock and open their door.

The same principle governs **competitive inhibition**. In competitive inhibition, an inhibitor binds to the active site of the enzyme instead of the substrate. It is able to do this because it has a shape and charge that mimic the substrate (or a complementary shape and charge to the active site), thus fitting the active site. In this situation, the inhibitor and the substrate compete with each other to bind to the active site, which is why this process is referred to as competitive inhibition. With the inhibitor bound, the substrate is unable to access the active site and the enzyme cannot function.

Competitive inhibition the process of disrupting the function of an enzyme by blocking its active site with a molecule other than the substrate

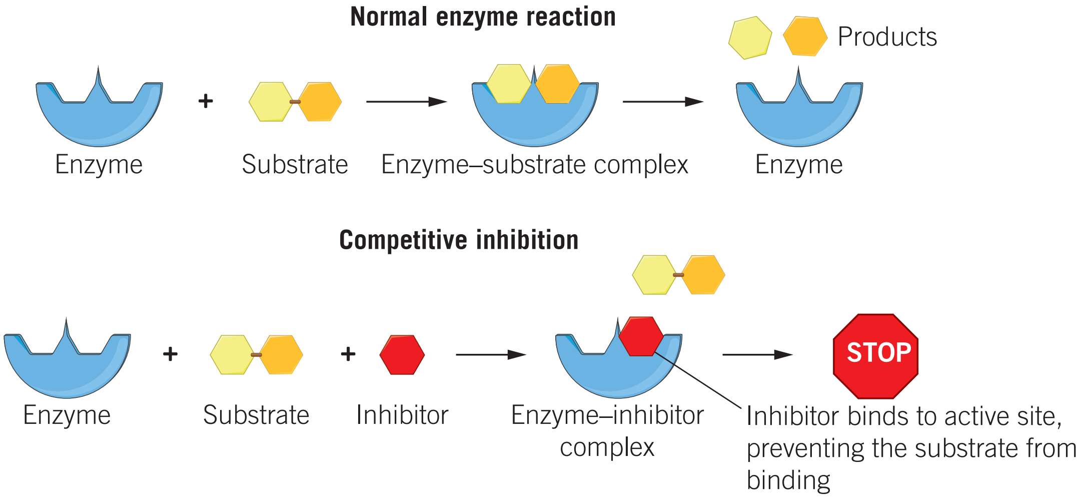


Figure 12B–16 The normal function of an enzyme can be blocked through competitive inhibition, where an inhibitor interacts with the active site, preventing the substrate from binding.

As enzymes play a vital role in almost all biological processes in organisms, competitive enzyme inhibitors have become a valuable therapeutic option. These inhibitors work as a type of medicine (or drug) by blocking the activity of specific enzymes in the body. These enzymes are responsible for carrying out a wide range of biochemical reactions, from breaking down food to producing essential molecules for the body. By inhibiting these enzymes, competitive inhibitors can help to regulate or reduce the activity of certain biochemical pathways, which can lead to therapeutic benefits.

One example of a competitive enzyme inhibitor used as a medicine is the drug Simvastatin, which is used to lower high blood cholesterol levels in patients (Figure 12B–17). Simvastatin works by blocking the active site, and therefore the activity, of an enzyme called HMG–CoA reductase, responsible for producing cholesterol in the liver. By inhibiting this enzyme, simvastatin can reduce the amount of cholesterol produced by the liver, leading to a decrease in blood cholesterol.

Figure 12B–17 The drug Simvastatin is taken by people with high blood cholesterol to block HMG-CoA reductase, an enzyme in the biochemical pathway responsible for cholesterol produced by the liver.

Simvastatin is a great example of how competitive enzyme inhibitors can be used to reduce the natural activity of enzymes within the body. However, foreign organisms, such as viruses and bacteria, also rely on enzymes for a number of their processes. Therefore, these enzymes can also be a target for treatments against infections. Indeed, many antibiotics treat bacterial infections by inhibiting the function of enzymes needed by the bacteria to survive.

Another famous example of a competitive enzyme inhibitor that has been incredibly successful as a medication is Relenza. Relenza is a medication developed to treat influenza, a highly contagious respiratory infection caused by the influenza virus. Relenza is a type of antiviral medication known as a neuraminidase inhibitor. Taken orally, the drug travels down into the the lungs where it binds to the active site of the neuraminidase enzyme on the surface of the influenza virus particles. By blocking this enzyme, the virus is unable to be released from the host cell it has infected and therefore does not spread to infect new uninfected cells in the body. This can help to reduce the severity and duration of influenza symptoms, as well as prevent complications from the virus.

WORKSHEET 12B–2
FACTORS AFFECTING ENZYME ACTIVITY

VIDEO 12B–2
SKILLS: STRUCTURAL DIAGRAMS AND SPECIFICITIES OF THE 20 DIFFERENT AMINO ACIDS

12B SKILLS

Structural diagrams and specificities of the 20 different amino acids

In this section, you learned that there are 20 different α-amino acids, each of which has a different R, or variable, group. These 20 α-amino acids with their R groups are shown in Figure 12B–18.

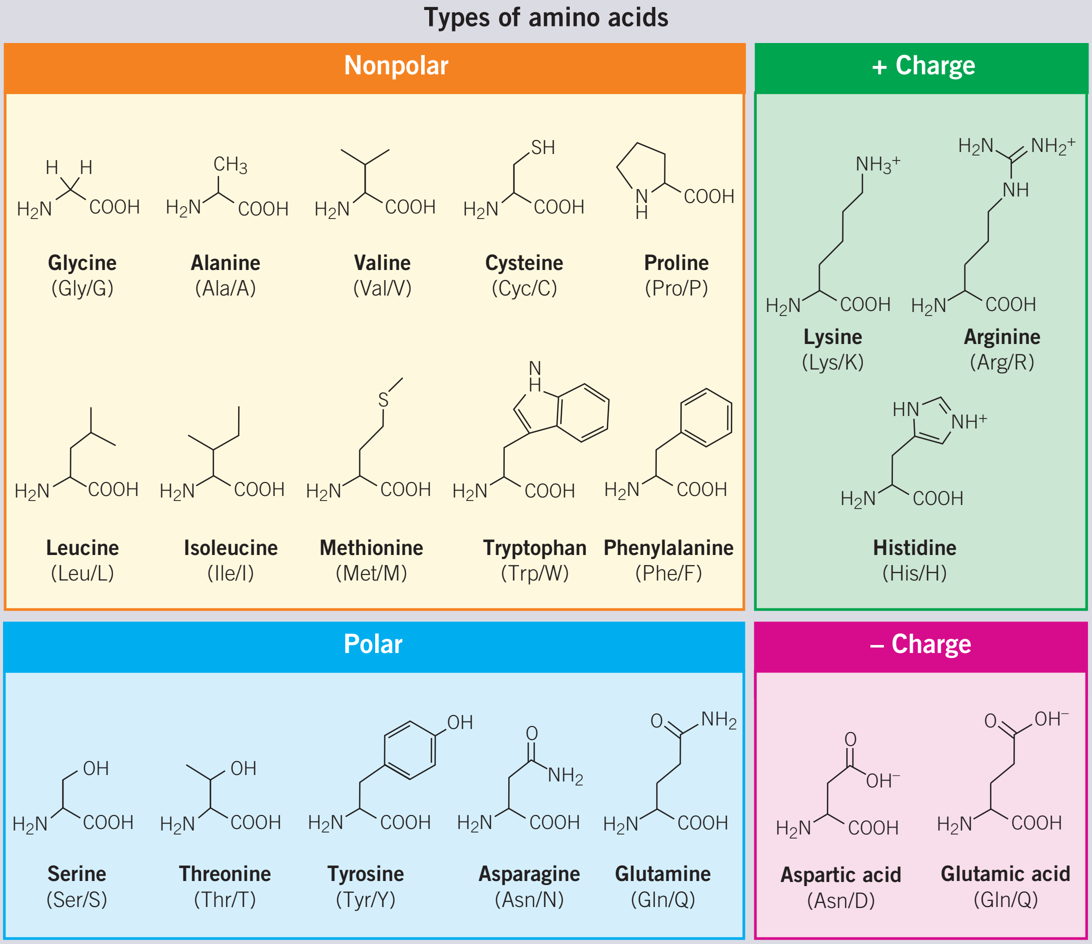


Figure 12B–18 The structural formulas of the 20 different α-amino acids at neutral pH, categorised by the properties based on their R groups

As VCE students, it is not important for you to memorise the specific structure of each R group and which α-amino acid it belongs to. In previous Study Designs, these amino acids have all been provided in the VCAA Chemistry Data Book, which you have available for School-Assessed Coursework and Examinations. It is anticipated you will continue to be provided with these.

LINK UNIT 1

However, what you are not provided with is the breakdown of which α-amino acids are polar, non-polar, positively or negatively charged, which is shown in Figure 12B–18. You must use your knowledge established back in the covalent molecules chapter in Unit 1 to identify key features of these that could characterise them as polar or non-polar. The presence of –O–H and –N–H polar bonds should indicate that an α-amino acid will be polar due to the formation of partial charges, which allow it to form either dipole–dipole interactions or hydrogen bonds. α-Amino acids that display the presence of a full negative charge on the $-COO^-$ carboxyl functional group in their R group would be capable of forming an ionic interaction with the R group of another α-amino acid that has a full positive charge. This should bring you back to your understanding of ionic bonding, which you developed in Unit 1. It is these types of interactions that are key to you understanding the formation of primary, secondary, tertiary and quaternary levels of protein structure, and subsequently your ability to anticipate and explain effects on each of these structural levels based on pH or temperature changes.

Section 12B questions

1 Amino acids are the building blocks of proteins, with just 20 different amino acids making up thousands of proteins in the human body.
  a Describe the similarities shared by the 20 α-amino acids.
  b What differentiates the 20 α-amino acids from each other?
  c Explain how two proteins composed of the same set of α-amino acids can exhibit drastic differences in their properties.

2 What kind of bond links α-amino acids together in a polypeptide chain?

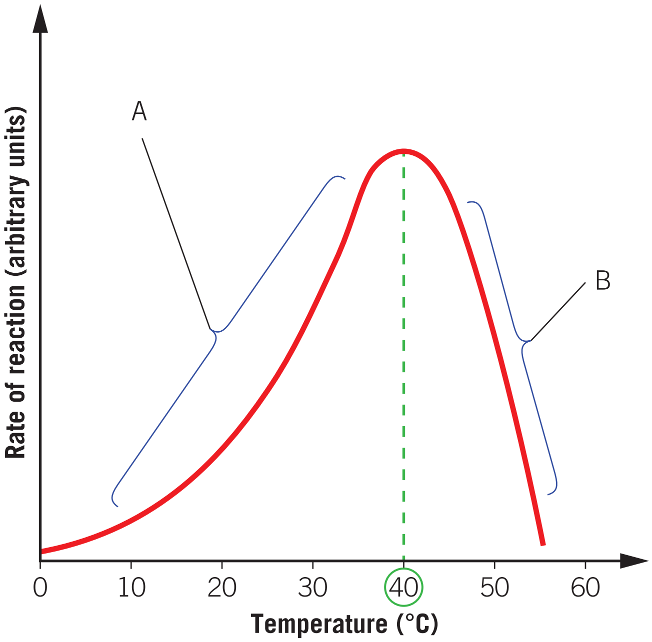
3 Identify two common types of secondary structures found in proteins.

4 Match each of the following statements with the appropriate level of protein structure (primary, secondary, tertiary or quaternary). Multiple options may apply in some cases.
  a the linear sequence of α-amino acids in a polypeptide chain
  b alpha helices and beta-sheets formed by hydrogen bonding between α-amino acid residues
  c the overall three-dimensional folding of a single polypeptide chain
  d the interaction of multiple polypeptide chains to form a functional protein
  e disulfide bridges between cysteine residues
  f interactions between R groups of α-amino acids

5 Define the following terms.
  a enzyme
  b substrate
  c active site

6 Indicate whether each of the following statements is true or false. For those that are false, rewrite the statement to make it true.
  a Enzymes increase the activation energy required for a chemical reaction.
  b Enzymes are specific in their substrate recognition.
  c The lock-and-key model suggests that enzymes change their shape to accommodate the substrate.
  d Denaturation of an enzyme alters its primary structure.
  e Enzymes can only function optimally at a narrow range of pH and temperature.
  f Competitive inhibitors bind to the active site of an enzyme.
  g Enzymes can be reused and are not consumed in a reaction.
  h All enzymes function optimally at a pH of 7.
  i Enzymes are capable of turning an endothermic reaction into an exothermic reaction.

7 The rate of reaction for a typical human enzyme across a temperature range is shown below. Explain the trends observed in the regions labelled A and B and compare the processes happening there.



8 One example of an α-amino acid that exists mostly as a zwitterion is aspartic acid, which has the R group, CH_2COOH.

a Draw the structural formula for aspartic acid, clearly labelling the following in your structure:

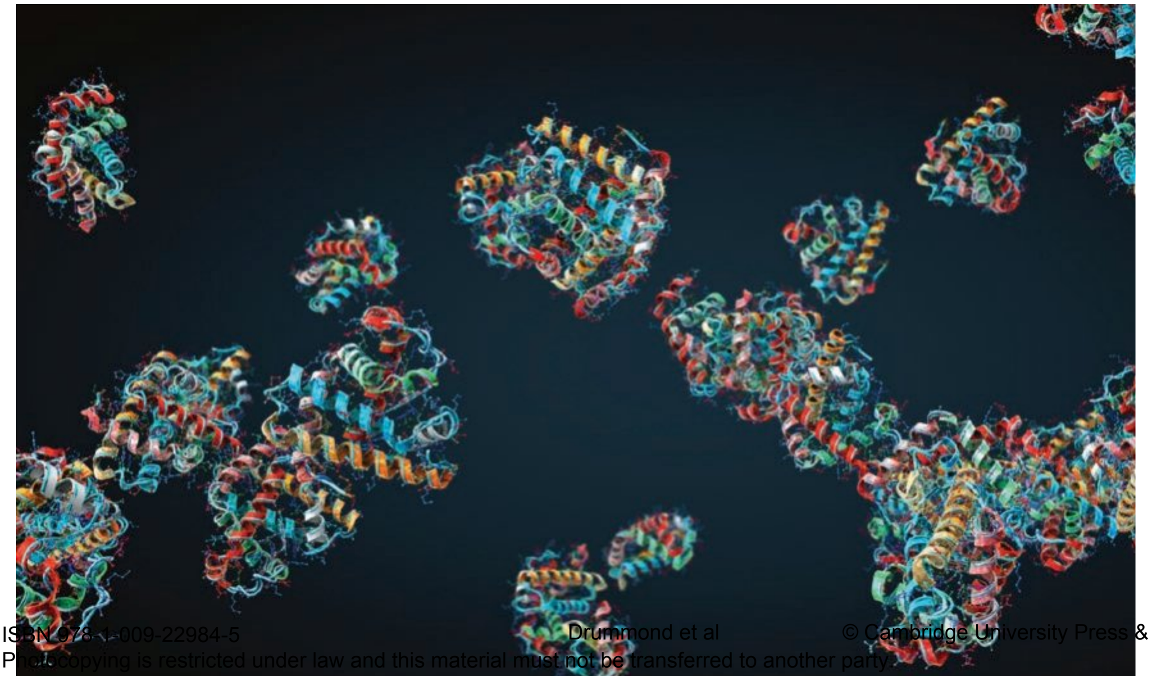
amine group carboxyl group chiral carbon atom R group

b Explain how and why the structure of the zwitterion you drew in part **a** changes if an aqueous solution containing the amino acid was at each of the following pH values. In your answer, draw the structure that would form, making sure to include the correct charges that would be present.

i pH 7

ii pH 3

iii pH 11



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Chapter 12 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
12A.1	Recall that natural plant compounds can contain active ingredients used for medicinal purposes	11☐
12A.2	Describe how solvent extraction can be used to extract and purify natural plant compounds for medicinal purposes	1☐, 2☐, 13☐
12A.3	Describe how distillation can be used to extract and purify natural plant compounds for medicinal purposes	3☐
12A.4	Recall some common classes of organic medicines and the key functional groups that characterise each class	12☐
12A.5	Explain why understanding how functional groups contribute to the mechanism of action of medicines will help guide future drug development	14a☐, 14b☐
12A.6	Define 'chiral centre' and identify compounds that contain a chiral centre	5☐, 14c☐, 15a☐
12A.7	Describe how chiral centres can result in isomers and enantiomers	4☐, 15b☐, 15c☐
12A.8	Explain why the presence of isomers in compounds used as medicines can cause problems	16☐
12B.1	Define the primary, secondary, tertiary and quaternary structures of proteins	7☐
12B.2	Describe the interactions and bonding that are important for the primary, secondary, tertiary and quaternary levels of protein structure to form	6☐
12B.3	Recall that the function of an enzyme involves the binding of a substrate to its active site	10☐, 17a☐
12B.4	Describe the lock-and-key model of enzyme function	17b☐
12B.5	Explain the effect of temperature changes, including denaturation, on the rate of enzyme activity	8☐, 17c☐
12B.6	Explain the effect of changes in pH on the rate of enzyme activity	8☐, 17c☐
12B.7	Define 'zwitterion' and explain how this forms in relation to amino acids	18a☐, 18b☐
12B.8	Explain the effect of a competitive inhibitor on the rate of enzyme activity	17d☐
12B.9	Describe how competitive inhibition can be used as a treatment approach	9☐

Multiple-choice questions

1 The process of solvent extraction is primarily used for
  - **A** increasing the shelf life of medicines.
  - **B** synthesising new organic compounds.
  - **C** changing the physical properties of organic compounds.
  - **D** purifying natural and synthesised compounds.

2 What is the most important factor to consider when choosing a solvent for extraction?
  - **A** cost-effectiveness
  - **B** availability in the laboratory
  - **C** environmental sustainability
  - **D** solubility of the desired compound

3 What is the basis for separation in distillation?
  - **A** differences in solubilities
  - **B** differences in boiling points
  - **C** differences in molecular weights
  - **D** differences in chemical reactions

4 Enantiomers can have different biological activities. What is the primary reason for this difference?
  - **A** Enantiomers have different physical states.
  - **B** Enantiomers have different functional groups.
  - **C** Enantiomers have different molecular weights.
  - **D** Enantiomers interact differently with chiral biological molecules.

5 Which of the following is true about chiral carbons in organic compounds?
  - **A** Chiral carbons can be found at any position within the carbon chain.
  - **B** Chiral carbons are always located in the middle of the carbon chain.
  - **C** A carbon bonded to four other carbon atoms cannot be chiral.
  - **D** Chiral carbons have one or more identical substituents.

6 Which levels of protein structure can involve hydrogen bonding?
  - **A** secondary only
  - **B** secondary and tertiary only
  - **C** secondary, tertiary and quaternary only
  - **D** primary, secondary, tertiary and quaternary

7 Which of the following statements regarding the levels of protein structure is false?
  - **A** The tertiary structure represents the overall three-dimensional shape of a single polypeptide chain.
  - **B** Primary structure refers to the linear sequence of amino acids that make up a polypeptide chain.
  - **C** Quaternary structure describes the interactions between multiple polypeptide chains.
  - **D** The secondary structure involves interactions between side chains of amino acids.

8 Which of the following statements accurately describes the effect of pH and temperature on enzyme activity?
  - **A** Increasing temperature always leads to increased enzyme activity, while decreasing temperature slows down enzyme reactions.
  - **B** Enzymes are unaffected by pH and temperature variations, as they can function under a wide range of conditions.
  - **C** Increasing both pH and temperature can lead to loss of enzyme activity due to denaturation.
  - **D** Increasing pH generally enhances enzyme activity, while decreasing pH can denature enzymes.

9 Competitive enzyme inhibitors may act as therapeutic agents because they
- **A** reduce the activity of specific enzymes.
- **B** enhance the activity of specific enzymes.
- **C** promote the breakdown of specific substrates.
- **D** increase the production of essential molecules.

10 Which of the following statements accurately describes the interaction between an enzyme and its substrate?
- **A** The substrate binds irreversibly to the enzyme's active site.
- **B** The substrate and enzyme undergo covalent bonding to form a new compound.
- **C** The enzyme modifies the chemical structure of the substrate to enhance its reactivity.
- **D** The enzyme and substrate form a temporary enzyme-substrate complex held together by non-covalent interactions.

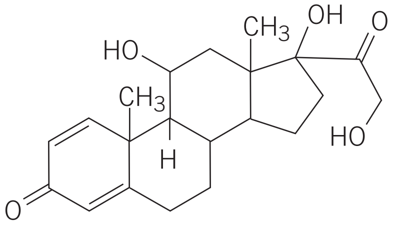
Short-answer questions

11 Provide one example of a natural compound used for medicinal purposes. (1 mark)

12 Provide an example of a class of organic medicines and identify one functional group that is commonly shared throughout the class. (2 marks)

13 Imagine you are extracting a medicinal compound from a plant using a solvent extraction process. Briefly explain the purpose of each of the following steps involved in the extraction process.
- **a** Plant material is ground into smaller pieces. (1 mark)
- **b** The ground plant material is mixed with a suitable solvent and left to soak for a period of time. (1 mark)
- **c** The mixture is filtered. (1 mark)
- **d** The solvent extract is evaporated to remove the solvent. (1 mark)

14 Prednisolone, a member of a group of medicines called corticosteroids, is used for the treatment of various inflammatory and autoimmune conditions. Answer the following questions about prednisolone, referring to its structure shown below.



- **a** Identify three different functional groups, by writing their chemical elements and general name, present in prednisolone. (3 marks)
- **b** Identify three properties of prednisolone that may be affected if the functional groups were modified. (3 marks)
- **c** Determine the location and number of chiral carbons in prednisolone and explain what makes a carbon atom chiral. (Hint: You might want to draw the full structural formula for prednisolone to answer this.) (2 marks).

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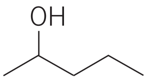
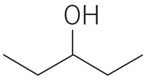
15 Consider the following structural isomers of pentanol.

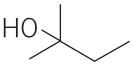
A



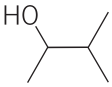
B



C



D



a Determine the number of chiral carbons present in each structural isomer. (4 marks)

b Based on the presence of chiral carbons, determine whether each structural isomer exists as a pair of enantiomers or not. Justify your answer. (2 marks)

c Explain how enantiomers differ in terms of their structural formula and spatial arrangement. (2 marks)

16 An organic chemist successfully synthesises a pharmaceutical compound through a series of reactions and purification steps. However, during chemical analysis, the presence of two enantiomeric forms is detected in the purified product. Outline any challenges that this may pose in the development and use of the drug. (2 marks)

17 Enzymes are essential for accelerating chemical reactions in biological systems.

a Describe how enzymes facilitate and speed up chemical reactions within organisms. (2 marks)

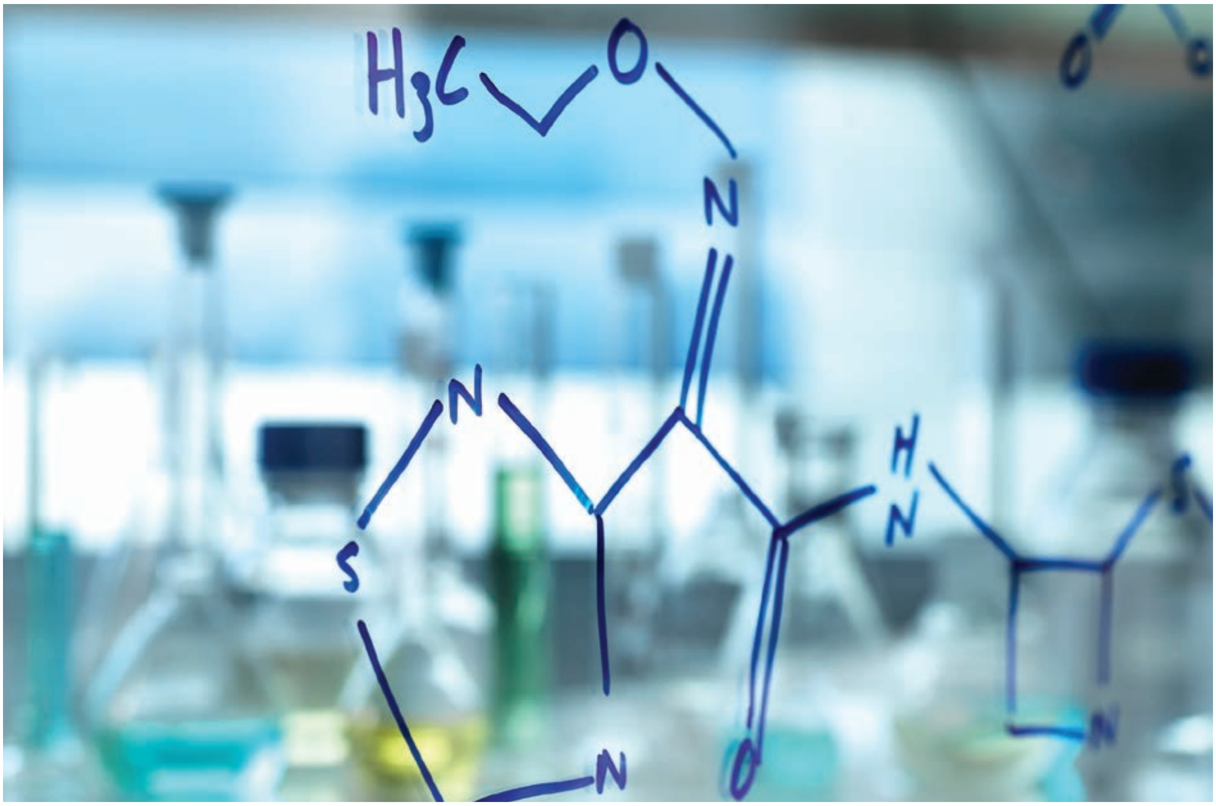
b Explain the concept of the 'lock-and-key' model of enzyme activity. (3 marks)

c The denaturation of enzymes affects their activity.

  i Define 'denaturation'. (1 mark)

  ii Identify and describe two possible causes of denaturation, highlighting the mechanism through which denaturation occurs and the levels of protein structure affected by denaturation. (6 marks)

d Define a 'competitive inhibitor' and describe its impact on the rate of enzyme activity. (3 marks)



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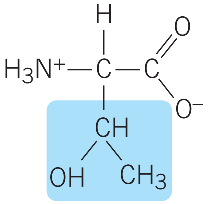
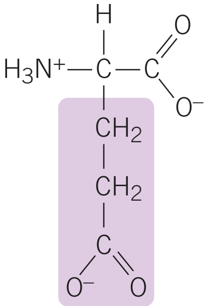
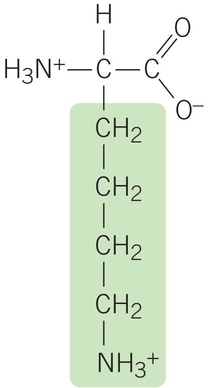
18 As well as being affected by temperature, enzyme activity can also be affected by changes in pH. The R groups of α-amino acids are important in helping to form the tertiary and quaternary levels of enzyme structure. The charge of the R group can change due to changes in pH.

a Copy and complete the table below to outline the differences expected due to pH changes in each of the α-amino acids. (3 marks)

α-amino acid (with highlighted R group)	Is R group neutral, or negatively or positively charged at each pH? pH 3	pH 7	pH 12
 Threonine			
 Glutamic acid			
 Lysine			

b Which of the above α-amino acids is present as a zwitterion? Justify your answer by explaining what a zwitterion is. (2 marks)

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UNIT 4 HOW ARE CARBON-BASED COMPOUNDS DESIGNED FOR PURPOSE?

CHAPTER 13 SCIENTIFIC INVESTIGATIONS

Introduction

Scientific investigation skills and understanding are fundamental to the daily work of a scientist. As a component of your assessment for Units 3 and 4, you will be required to design an investigation, generate primary data and report on the findings. The focus can be on content from across Units 3 and/or 4 related to the production of energy or chemicals or the synthesis or analysis of organic compounds. You will be required to conduct an investigation, followed by the production of a scientific poster, as this is a key requirement for School-assessed Coursework (SAC) in Unit 4. As many VCAA exam questions focus on practical understanding and skills, this is also an opportunity for you to develop your knowledge and skills in this area.

This chapter outlines how to plan, conduct and present the results of a scientific investigation, and provides useful tips and examples along the way. The digital resource contains additional information about alternative formats for demonstrating your understanding of chemicals and the analysis and synthesis of organic compounds, which may be used as the basis for different assessments.

Curriculum

Area of Study 3 Outcome 3
How is scientific inquiry used to investigate the sustainable production of energy and/or materials?

Study Design:	Learning intentions – at the end of the chapter I will be able to:
Scientific evidence • Authentication of generated primary data through the use of a logbook	**13A** **Investigative planning and design** **13A.1** Document investigations appropriately using a logbook
Investigation design • Chemical concepts specific to the selected scientific investigation and their significance, including definitions of key terms	**13A.2** Define key terms related to scientific skills

Study Design:	Learning intentions – at the end of the chapter I will be able to:
- Characteristics of the selected scientific methodology and method, and appropriateness of the use of independent, dependent and controlled variables in the selected scientific investigation	**13A.3** Define ‘controlled experiment’ **13A.4** List the features that a controlled experiment includes **13A.5** Understand the meaning of single-variable exploration **13A.6** Define and identify independent, dependent and controlled variables **13A.7** Select and use the procedures and equipment appropriate to an investigation
Scientific evidence - The nature of evidence that supports or refutes a hypothesis, model or theory	**13A.8** Distinguish between an aim and a hypothesis **13A.9** Construct aims and questions for investigations **13A.10** Formulate hypotheses and predict possible outcomes based on models or theory
Investigation design - The accuracy, precision, repeatability, reproducibility, resolution and validity of measurements	**13A.11** Define ‘reproducibility’, ‘repeatability’ and ‘validity’, and distinguish between these **13A.12** Design an investigation that is valid **13A.13** Design an experiment that is fully repeatable and reproducible by others
- The health, safety and ethical guidelines relevant to the selected scientific investigation	**13A.14** Determine potential ethical issues with investigation design **13A.15** Identify how bias can be minimised in an investigation **13A.16** Follow clear guidelines for health and safety when undertaking practical investigations
Investigation design - Techniques of primary quantitative data generation relevant to the selected scientific investigation - The accuracy, precision, repeatability, reproducibility, resolution and validity of measurements	**13B** **Scientific evidence** **13B.1** Define ‘qualitative’ and ‘quantitative’ **13B.2** Distinguish between qualitative and quantitative data **13B.3** Include appropriate units of measurement for quantitative data
Scientific evidence - Authentication of generated primary data through the use of a logbook - Ways of organising, analysing and evaluating primary data to identify patterns and relationships, including sources of error and uncertainty	**13B.4** Transform primary data into an appropriate format of results (table, flow chart, bar and/or line graph) **13B.5** Identify trends in data **13B.6** Define the different types of errors (random and systematic) **13B.7** Identify sources of error and outliers from primary data **13B.8** Use evidence to determine whether an investigation supports or discounts a hypothesis, scientific model or theory

Study Design:	Learning intentions – at the end of the chapter I will be able to:
• Assumptions and limitations of investigation methodology and/or data generation and/or analysis methods	**13B.9** Identify areas for improvement in investigation design and analysis to increase accuracy and precision and reduce the likelihood of errors
Science communication • Conventions of science communication: scientific terminology and representations, symbols, formulas, standard abbreviations and units of measurement	**13C** **Scientific communication** **13C.1** Appropriately communicate all aspects of a scientific investigation **13C.2** Apply correct abbreviations to chemical terminology **13C.3** Recall and convert between different units of measurement in chemistry **13C.4** Determine the correct number of significant figures to use in answers to questions
• Conventions of scientific poster presentation, including succinct communication of the selected scientific investigation, and acknowledgements and references	**13C.5** Know and demonstrate how scientific investigations are presented succinctly on a poster **13C.6** Recall how and what to acknowledge and/or reference in correct format
• The key findings and implications of the selected scientific investigation	**13C.7** Justify conclusions and evaluate whether evidence supports or refutes the hypothesis **13C.8** Interpret investigation outcomes in terms of broader chemical concepts

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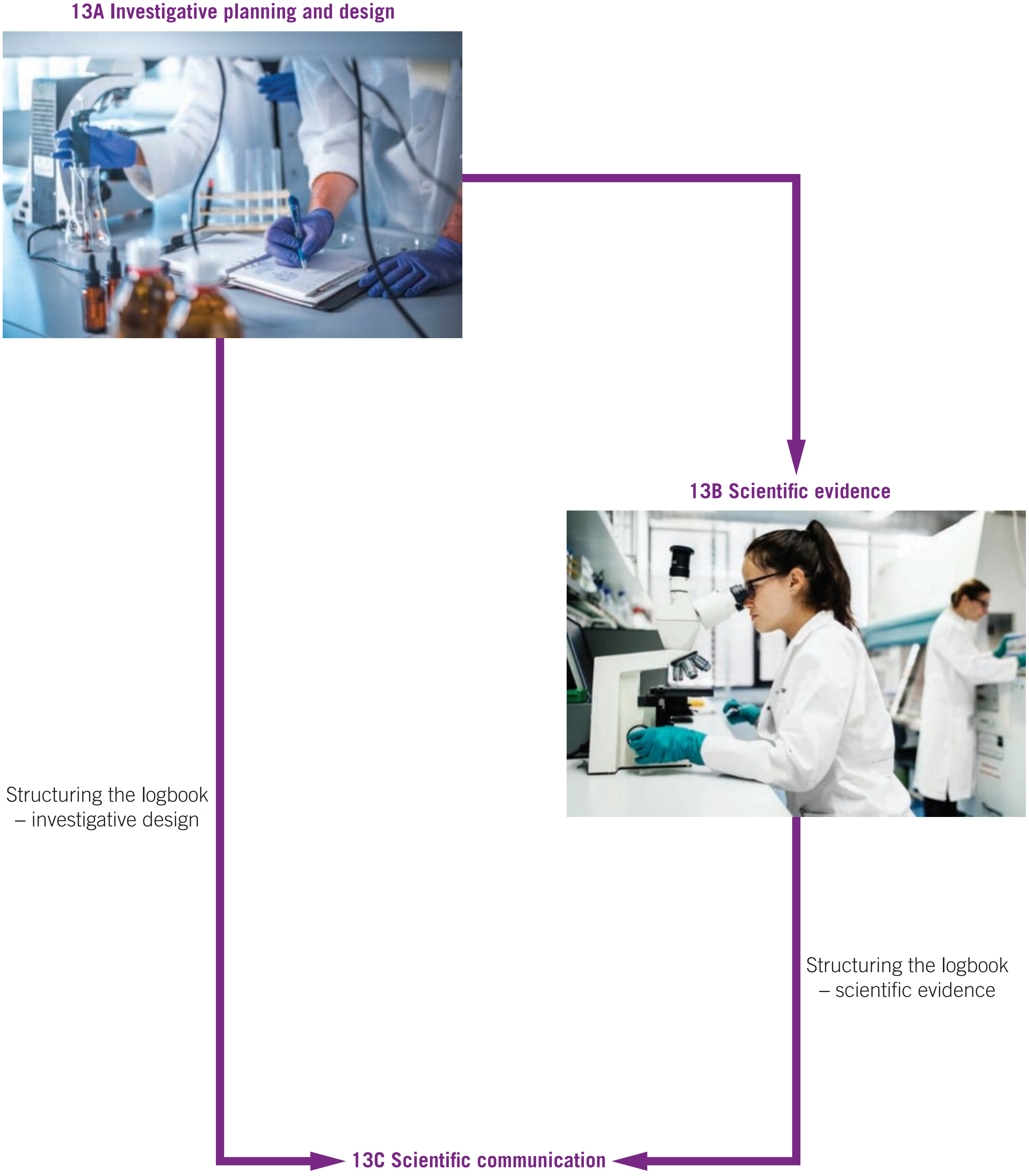
Glossary

Aim
Accuracy
Conclusion
Continuous data
Controlled variable
Dependent variable
Discrete data
Hypothesis
Independent variable
Introduction
Line of best fit
Method
Outlier
Precision
Primary data
Qualitative data
Quantitative data
Random error
Reliability
Repeatability
Reproducibility
Resolution
Secondary data
Single-variable exploration
Systematic error
Title
True value
Validity

Concept map



13A Investigative planning and design

13B Scientific evidence

Structuring the logbook – investigative design

Structuring the logbook – scientific evidence

13C Scientific communication

See the Interactive Textbook for an interactive version of this concept map interlinked with all concept maps for the course.

13A Investigative planning and design

Study Design:

Scientific evidence

- Authentication of generated primary data through the use of a logbook
- The nature of evidence that supports or refutes a hypothesis, model or theory

Investigation design

- Chemical concepts specific to the selected scientific investigation and their significance, including definitions of key terms
- Characteristics of the selected scientific methodology and method, and appropriateness of the use of independent, dependent and controlled variables in the selected scientific investigation
- The accuracy, precision, repeatability, reproducibility, resolution and validity of measurements
- The health, safety and ethical guidelines relevant to the selected scientific investigation

Glossary:

Aim
Controlled variable
Dependent variable
Hypothesis
Independent variable
Introduction
Method
Primary data
Reliability
Repeatability
Reproducibility
Secondary data
Single-variable exploration
Title
Validity

ENGAGE

Scientific breakthroughs

Scientists ask questions and plan investigations to learn more about the world around us and help develop solutions for real-world problems. They work both individually and in teams to share knowledge for the greater good of humans and the existence and survival of many other species. If you consider the rapid rise in the production and generation of new forms of energy across the last century, we have seen the following:

- The solar cell, which was the first device able to convert light into electrical energy by the photovoltaic effect, was developed in 1954.
- The world's first onshore wind farm opened in the United States in 1980, followed some 11 years later by the first offshore wind farms in Denmark.
- The first commercial operating plant for manufacturing biodiesel opened in Austria in 1991.
- The Three Gorges Dam in China, which was the world's largest hydroelectric power plant, opened in 2012.

Figure 13A–1 The Three Gorges Dam, the world's largest hydroelectric power plant

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EXPLAIN

Structuring a logbook – investigative design

A logbook allows a scientist to keep track of the specific dates of their investigation ideas, planning, questions, important results, errors and any modifications required, thereby maintaining a record of all work and experimentation conducted. Information recorded in a logbook is an original source of the information, written, processed or collected by the experimenter(s) or researcher(s) themselves. In doing so, a clear record of all information and data can be authenticated, meaning it is true or valid. A requirement of the VCE is that each student must maintain a logbook of practical activities in Units 1–4 for assessment purposes. The need for a printed logbook, rather than an online or digital logbook, removes the likelihood of any tampering with results. Of course, this will depend on your school and your teacher's authentication practices, so it is best to work within your school's guidelines.

Primary data refers to any data source that is obtained firsthand by a researcher for their project. Primary data can be collected through many means, including experiments, interviews and field observations. While more time-consuming and expensive than collecting **secondary data** (already existing collected data), in many instances primary data collection is the best suited for your research.

Primary data sourced data that is collected firsthand by the researcher for a specific purpose; commonly collected through investigations, observations, interviews, field work or surveys

In this section, you will learn how to develop a logbook for your own practical investigation and the importance of each section in contribution to the end report. This is usually in the form of a practical report or scientific poster (outlined in Section 13C).

LINK **13C** SCIENTIFIC COMMUNICATION

The best way to record an investigation in a logbook is demonstrated in the example below, which shows two logbook entries written by different students:

- Investigation ① is written by a student who has completed the task to a satisfactory standard.
- Investigation ② is written by a student who has completed the task to a very high standard.

Secondary data existing data that is collected and/or utilised by someone other than the primary investigator. Common examples include published journal articles, books or websites

The investigation involved determining the effect of the addition of invertase on the production of glucose, which can then be used as a reactant for the production of bioethanol, a renewable fuel. The differences between Investigation 1 and Investigation 2, as well as tips on what to include in each of the key sections, are included to assist you with your own logbook development.

ISBN 978-1-009-22984-5 Drummond et al

Logbook

Title
the research question under investigation; includes information about what is being tested

Title

① Determine the effect of a catalyst on the rate of a chemical reaction.

② Does the addition of invertase result in an increased rate of glucose production through its function as a catalyst on the hydrolysis of sucrose?

Notes
The title should include reference to the variables being changed (independent variable) and measured (dependent variable).

Introduction
a detailed, but succinct, explanation of the reason for undertaking the investigation; includes key chemical concepts, aim and hypothesis

Introduction

① Enzymes are substances essential to help reactions proceed more efficiently for these chemical reactions to actually occur. They are made of key chemical elements, such as carbon, hydrogen, oxygen, nitrogen and sulfur. Enzymes are specific to the substance that they act on.

② Enzymes are catalysts that increase the rate of chemical reactions by lowering the activation energy for that reaction to occur by providing an alternate reaction pathway. Invertase, the focus of this investigation, is an enzyme present in plants and yeast that catalyses the hydrolysis of sucrose into fructose and glucose.

Hydrolysis reactions involve the addition of water, as shown for this reaction below:

$$\begin{array}{ccccccc} \text{sucrose} & + & \text{water} & \rightarrow & \text{glucose} & + & \text{fructose} \\ C_{12}H_{22}O_{11}(aq) & + & H_2O(l) & \rightarrow & C_6H_{12}O_6(aq) & + & C_6H_{12}O_6(aq) \end{array}$$

The progress of this reaction can therefore be measured by the formation and concentration of glucose, determined using glucose test strips. The more glucose present, the darker the colour displayed on the test strip will be. This detects concentrations of glucose between 0 mg mL^{-1} and 30 mg mL^{-1}.

Glucose produced in yeast and plants can be further broken down with the aid of anaerobic bacteria to form ethanol (bioethanol) via fermentation, according to the following chemical equation:

$$C_6H_{12}O_6(aq) \rightarrow 2C_2H_5OH(aq) + 2CO_2(g)$$

Bioethanol as a fuel is a renewable source of energy that results in less greenhouse gas emissions compared to fossil fuels.

In the introduction (to a poster) it can also be appropriate to present a labelled diagram of the concept/idea being investigated.

Aim
the main purpose of an investigation

Aim

① To determine whether the presence of an enzyme increases the rate of a chemical reaction.

② To determine whether the presence of the enzyme invertase increases the rate of hydrolysis of sucrose by measuring the concentration of glucose produced using glucose test strips.

The aim includes explicit reference to the independent and dependent variable. This will be included in your introduction for the final scientific poster presentation.

Hypothesis a prediction of the outcomes, which are testable experimentally and form the basis of the methodology

Hypothesis

① The enzyme will increase the rate of reaction.

② The presence of invertase will increase the rate of the hydrolysis reaction of sucrose, producing an increased concentration of glucose, when compared to the reaction occurring without invertase. This will occur due to the ability of invertase to catalyse the hydrolysis of sucrose by lowering the activation energy of the reaction by providing an alternate reaction pathway.

The hypothesis is a prediction of what you think will occur. It does not have to be correct but should be supported by your knowledge of the theory, which is the difference between Investigations 1 and 2.

Independent variable the variable for which quantities are changed by the experimenter

Independent variable

① The presence of the enzyme

② The presence of invertase

The independent variable should be specific and list all quantities or changes being investigated. It should also list the control group, if one is included in the investigation.

Dependent variable the variable that changes in response to changes in the independent variable; the experimenter measures these changes

Dependent variable

① The hydrolysis of sucrose

② The concentration of glucose produced at 40°C over time as detected with the use of glucose test strips

State how the dependent variable will be measured in your experiment. This will likely involve using an instrument and units of measurement.

Controlled variable anything kept constant, or monitored, so it does not affect the independent and dependent variables, and therefore the validity of experimental results

Controlled variables

① Environmental conditions

Equipment

Invertase

② Same initial concentration of sucrose (50.0 mg mL^{-1})

Same volume of sucrose added (3.00 mL)

Same initial concentration of invertase (5.0×10^{-2} mg mL^{-1})

Same volume of invertase added (3.00 mL)

Same temperature of all solutions (40.0°C)

There will always be more than one controlled variable in any investigation. List as many as you can for your investigation. The word 'same' is used for each variable, to show that the variables have been kept constant, and so the results are valid.

WORKSHEET 13A–1 IDENTIFYING VARIABLES

Method a series of numbered steps describing the procedure

Method

①

1 Place sucrose into a test tube and incubate in water bath.
2 Add water to the test tube.
3 Allow the chemical reaction time to occur.
4 Measure the presence of glucose using glucose test strips to confirm chemical reaction occurred.
5 Repeat steps 1–4 but add enzyme instead of water.

The method must contain enough information for the investigation to be repeated by yourself (repeatability) and others (reproducibility). Therefore it must include specific quantities of any substances and specific equipment used.

②
1. Six different test tubes were set up, each containing 3.00 mL of 50.0 mg mL^{-1} sucrose aqueous solution.
2. One of the test tubes was placed in a water bath at 40°C for 30 seconds.
3. 3.00 mL of distilled water was added to the test tube, the stopwatch started and the solution was immediately tested using a glucose test strip for the 0 second timepoint.
4. After 60 seconds, the solution from the test tube was tested using the glucose test strips. This was repeated at the 120 s, 180 s, 240 s and 300 s timepoints.
5. Results were recorded in the results table.
6. Steps 2–5 were repeated a further two times and the average across the three trials was recorded.
7. Steps 2–6 were repeated but with 3.00 mL of invertase solution added instead of 3.00 mL of distilled water..

Health, safety and ethical considerations

① Wearing of lab coat, safety glasses and gloves.

There are no ethical issues to consider.

② For this experiment, wearing of personal protective equipment (lab coat, safety glasses and gloves) is required.

While yeast is commonly found in nature on plant leaves, flowers, fruits and in soil, the yeast from which the invertase was extracted for this experiment was manufactured by a company that sells it to commercial bread producers. Therefore, no plants or animals were harmed in obtaining the yeast for this investigation. Therefore, this choice of using the manufactured yeast in preference to a plant-based yeast is the resolution for any potential ethical considerations around the use of living organisms by chemists, general public and/or consumers.

Some schools have access to an online risk assessment program that allows you to input equipment and any chemicals specific to your own investigation, which generates safety requirements to be followed. With the use of living organisms, ethical integrity when using data and reporting on outcomes should be clearly considered and outlined.

Repeatability

① Repeat experiment three times to determine the effect of invertase on the chemical reaction.

② This experiment was conducted three times to increase the sample size and ensure repeatability (or reliability) of results.

Repeatability the ability to produce the same results when the experiment is repeated in one lab by one operator under the same conditions

Without repeating your experiment, your results are potentially valid but not reliable (representative of normal conditions). It is important in any investigation to have a large sample size.

Reproducibility when the same results are obtained for the same experiment by different operators using different equipment

Reliability the extent to which an experiment always yields the same results under the same conditions

Reproducibility

① Someone else repeats experiment three times to determine the effect of invertase on the chemical reaction.

② The experiment could be repeated by other investigators using a different technique for measuring glucose concentrations or a different concentration of invertase. Results could then be compared based on the similarity of experimental set-up and aim of the investigation.

Other experimenters achieving the same result as you after conducting the same investigation further strengthens the validity and **reliability** of your results. It is worth researching if others have done your experiment previously, or getting your peers to perform your experiment using your method, to see if they achieve the same results. It is important not to confuse reproducibility and repeatability.

Validity the extent to which all variables in the experiment have been controlled, so that the independent variable is the only factor that changes

Single-variable exploration an investigation that contains only one independent and one dependent variable

Validity

① All variables are controlled in the experiment, and therefore it is a valid test.

② This experiment contains one independent variable (the presence of invertase) and one dependent variable (concentration of glucose produced), where all other factors in the experimental design have been controlled (same volume of invertase, same concentration and volume of sucrose, same temperature of solutions). Hence, it is a single-variable exploration.

It is crucial to ensure that the independent variable is the only aspect changing in your investigation (**single-variable exploration**), and that all other variables are controlled. If this is not done or noted, then it is impossible to draw meaningful conclusions from your results.

13A SKILLS

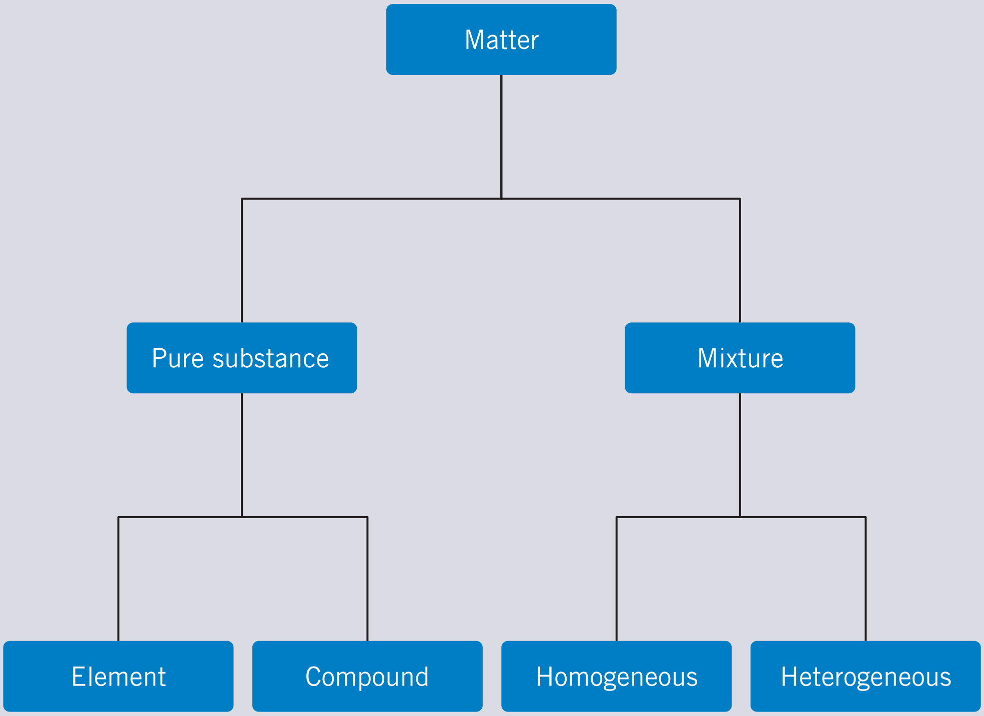
Scientific methodologies

In this chapter, you have seen how the scientific investigation process is used to establish facts or acquire knowledge. It involves formulating a hypothesis, collecting data, analysing the data and drawing conclusions. These principle steps of the scientific process can be applied across all disciplines of science; however, the specifics of each step may change depending on the aim of the investigation and what is being examined. In this ‘scientific skills’ section, you will learn about different scientific methodologies that may be applied to investigations.

Classification and identification

Classification is the arrangement of phenomena, objects or events into groups or categories based on their relationships. Identification involves allocating unidentified objects to the correct category once a classification has been established.

Classification can involve a simple set of categories (for example, acids and bases) or can be performed using a tree structure to show how some classes can be further divided into more specific groups. For example, matter may be classified as follows:



Observations from scientific investigations can be used to identify an unknown object or event. Using the classifications examples above, we could make the following identifications based on observations:

Observations	Identification
• Does not separate into components • Made up of more than one element	Compound
• Liquid appears uniform • Separates into multiple components when analysed by TLC	Homogeneous mixture

Think about some of the other classification systems in chemistry that you have come across in Units 3 and 4.

Fieldwork

Fieldwork involves collecting data at a specific location, rather than in the semi-controlled environment of a lab or classroom. Environmental chemists often perform fieldwork, travelling to locations to collect and analyse samples to investigate the effects that chemicals have on the air, water and soil.

13B SCIENTIFIC EVIDENCE LINK

The generation of site-specific data should be recorded in your logbook. An example of a portion of a logbook entry for a fieldwork investigation is shown below. Section 13B further explores how to present results of your investigations in your logbook.

Aim: To investigate the water quality of Lake Daylesford

Location: End of Lake Daylesford jetty

Date: 9/10/2022

Results:

Test	Result	Units
1. Temperature	12	°C
2. pH	6.8	pH units
3. Dissolved oxygen	7.1	mg L^{-1}
4. Total phosphates	0.4	mg L^{-1}
5. Nitrates	8.9	mg L^{-1}
6. Total solids	5.5	mg L^{-1}

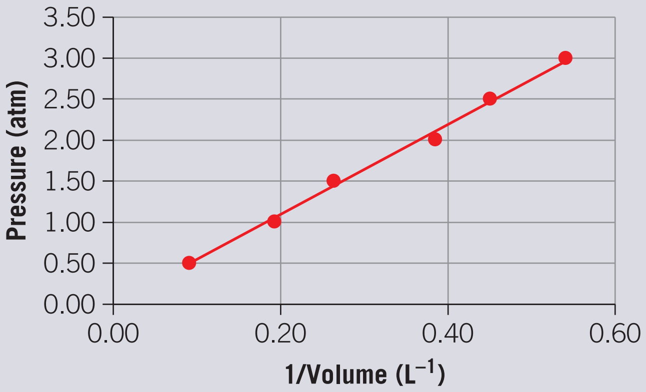
Modelling and simulation

Scientific modelling involves the construction of a physical, conceptual or mathematical model, which represents a real phenomenon. Models provide a visual way of linking theory with experiment and provide a way to explain or predict behaviour of objects or systems. Simulation involves using a model to study the behaviour of a real or theoretical system. Performing simulations can overcome experimental limitations; for example, a system may be too complex, too large or small, too fast or slow, inaccessible or too dangerous.

One model that you will have already come across is Bohr's model of the structure of the atom, which was primarily based on the emission spectrum of hydrogen.

An example of a simple mathematical model is shown below. In this investigation, a student examined the relationship between volume and pressure using a gas syringe and a pressure gauge. An inverse relationship between volume and pressure was observed. Further analysis involved mathematical modelling of the data by fitting to a linear function.

Volume (L)	1/Volume (L^{-1})	Pressure (atm)
11.0	0.09	0.50
5.20	0.19	1.00
3.80	0.26	1.50
2.60	0.38	2.00
2.22	0.45	2.50
1.85	0.54	3.00



Based on the mathematical model determined, can you predict what the volume of the system would be if the pressure is 0.75 atm?

Far more complicated models have been developed by scientists to identify and understand patterns in our world. For example, mathematical models have been used to simulate future temperature increases due to climate change.

Product, process or system development
Some scientific investigations involve the design of a product, process or system to meet a particular need. This may involve technological applications in addition to scientific knowledge and procedures.

You will have encountered many examples where scientific knowledge has been used to generate a range of everyday products, such as:
- knowledge of measurement of pH to design kits for testing the acidity of swimming pools and aquariums
- knowledge of removal of impurities from water to build industrial water treatment and sewerage plants
- knowledge of redox reactions to generate batteries and power sources that produce greener, cleaner energy.

Section 13A questions

1 What features does a controlled experiment include?

2 Define the following terms: independent variable, dependent variable, controlled variable.

3 Compare validity and reliability.

4 Outline the difference between repeatability and reproducibility.

5 Explain what single-variable exploration means.

6 When aqueous hydrogen peroxide, H_2O_2, is heated, it decomposes, resulting in the production of both water and oxygen as per the chemical equation below:

$$2H_2O_2(aq) \rightarrow 2H_2O(l) + O_2(g)$$

This decomposition reaction can also occur at SLC if a catalyst, such as manganese(IV) oxide or lead(IV) oxide, is added. Both of these catalysts are poisonous if ingested or inhaled and can also cause skin irritation.
A chemist is given a 0.500 M solution of hydrogen peroxide and a syringe with a 100 mL capacity and is planning to investigate the effects of adding manganese(IV) oxide on the rate of reaction.

a Write a suitable aim for this investigation.

b Identify the independent and dependent variables in this investigation.

c Draw a fully labelled diagram of the set-up, including all equipment to be used, to ensure that no oxygen could be lost when the investigation was conducted.

d Determine two features of a catalyst that would need to be controlled in this investigation.

e List and justify two safety precautions that need to be carried out when conducting this investigation.

f Describe what the chemist would need to measure to achieve the desired aim from your answer to part **a** above.

g Determine one aspect of this investigation that would potentially influence its repeatability. Justify your response.

7 The material safety data sheet (MSDS) for an organic powder includes the following precaution:
'Warning! This substance causes skin, eye and respiratory irritation.'

a Identify three pieces of personal protective equipment (PPE) that should be used by students conducting an experiment using this powder.

b Justify the need for each of the PPE items in your answer to part **a** above.

13B Scientific evidence

Study Design:

Investigation design

- Techniques of primary quantitative data generation relevant to the selected scientific investigation
- The accuracy, precision, repeatability, reproducibility, resolution and validity of measurements

Scientific evidence

- Authentication of generated primary data through the use of a logbook
- Ways of organising, analysing and evaluating primary data to identify patterns and relationships, including sources of error and uncertainty
- Assumptions and limitations of investigation methodology and/or data generation and/or analysis methods

Glossary:

Accuracy
Conclusion
Continuous data
Discrete data
Line of best fit
Outlier
Precision
Qualitative data
Quantitative data
Random error
Resolution
Systematic error
True value

EXPLAIN

Structuring a logbook – scientific evidence

This section discusses how to represent the results of your investigation in your logbook, including: drawing up tables and graphs, analysing the data collected, commenting on any errors, ensuring the precision and accuracy of the data, and noting areas for improvement.

Before recording your results, it is important to understand the difference between **qualitative data** and **quantitative data**. Qualitative data is *descriptive* – this means it is in the form of words, not numbers. For example, it could be the appearance of something (for example, ‘cloudy’ or ‘clear’) or colour (for example, ‘red’ or ‘yellow’). Quantitative data is *numerical* – this means it is in the form of numbers, based on counting or measuring. For example, it could be volume (for example, 25 mL) or pH recorded on a scale of 0 to 14.

Knowing this difference is important when determining what type of graph should be used to represent the data you have generated.

When collecting quantitative data using measuring equipment or devices, it is important to also consider the **resolution** of this data. Resolution refers to the smallest change in the quantity being recorded that results in a noticeable change in the value shown on the measuring equipment. For example, if the gas syringe shown in Figure 13B–1 has a resolution of 1.0 mL and is used to record the volume of carbon dioxide gas produced, then the experimenter can only estimate the volume between the two marked intervals on the syringe. It is accepted that with graduations like this, an estimate to the nearest 0.1 mL can be made. This means that a data reading of 11.1 mL or 11.7 mL is possible, but a reading of 11.15 mL would not be possible. Alternatively, if you were using the burette shown in Figure 13B–1, where the resolution is 0.1 mL, then the experimenter can estimate the volume to the nearest 0.01 mL. For example, a volume recorded could be 40.51 mL or 40.73 mL.

Qualitative data
data that is descriptive (not numeric)

Quantitative data
data that is measured and represented numerically

Resolution
the smallest change in the quantity being measured that results in a noticeable change in the value shown on the piece of measuring equipment

Consequently, when recording primary data – that is, data collected firsthand by the experimenter in their results table – the number of decimal places recorded is dependent on the instrumentation used.

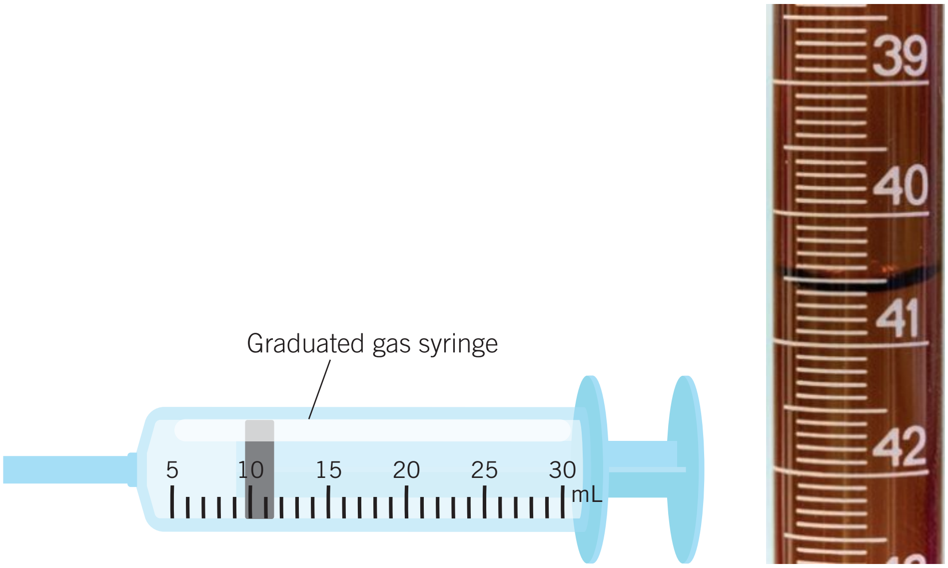


Figure 13B–1 Different pieces of equipment will have different resolutions, depending on their graduated markings. The gas syringe (left) has markings every 1 mL and therefore has a resolution of 1.0 mL, whereas a section of the burette (right) has markings every 0.1 mL and therefore has a resolution of 0.10 mL. Instruments such as these affect the number of decimal places data can be recorded to.

Results – table

①

	Glucose concentration				
	1 min	2 min	3 min	4 min	5 min
Without enzyme	0	1	1.5	3	3
With enzyme	6.5	10	20	20	20

② Title: Concentration of glucose produced from the hydrolysis of sucrose over time without the presence of invertase.

Results – table

Time after reaction started (s)	Concentration of glucose produced recorded using glucose test strips (mg mL^{-1})			
	Trial 1	Trial 2	Trial 3	Average
0.0	0.00	0.00	0.00	0.00
60	0.00	0.00	0.00	0.00
120	1.00	1.50	1.00	1.20
180	1.00	1.50	1.50	1.30
240	3.00	3.00	3.00	3.00
300	3.00	6.50	3.00	4.20

A results table should include a title with both variables (independent and dependent) mentioned.

All columns/rows must be labelled with an appropriate heading and relevant units. It is good to include an average, or a percentage, from multiple repeats. The table can be drawn by hand or generated digitally.

Title: Concentration of glucose produced from the hydrolysis of sucrose over time in the presence of invertase.

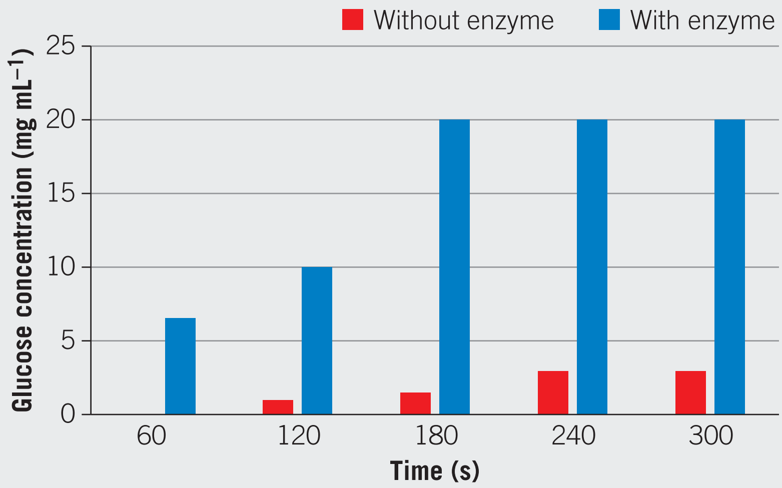
Time after reaction started (s)	Concentration of glucose produced recorded using glucose test strips (mg mL^{-1})			
	Trial 1	Trial 2	Trial 3	Average
0.0	0.00	0.00	0.00	0.00
60	10.0	6.50	6.50	7.70
120	20.0	10.0	10.0	13.3
180	20.0	20.0	20.0	20.0
240	20.0	20.0	20.0	20.0
300	20.0	20.0	20.0	20.0

WORKSHEET 13B–1
REPRESENTING DATA

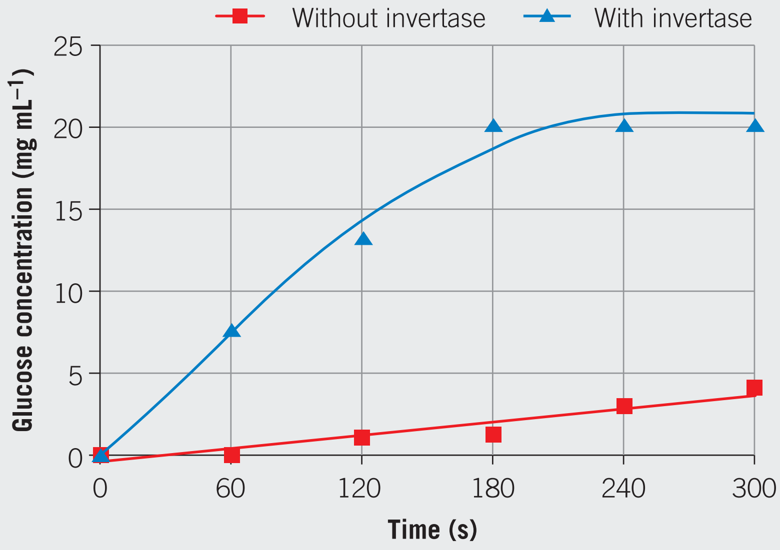
Discrete data data that is countable and in discrete categories; contains distinct or separate values; best represented by a bar graph

Continuous data data that is measurable and continuous, with infinite possible values; best represented by a line graph

① *Results – graph*



② *Results – graph*



Graphs should include a main title and have both *x*- and *y*-axes labelled with units (if required). The *x*-axis is for the independent variable and the *y*-axis is for the dependent variable.

The correct type of graph must be used. **Discrete data** (based on counting), should be represented as a bar graph. If data is **continuous** (based on measuring, for example, changing time, temperature, volume, concentration, pH), the data should be represented as a line graph.

Accuracy
how close the measurements are to the 'true' value of the quantity being measured

True value
the value or range of values that would be obtained if the quantity could be measured perfectly

Accuracy

① This experiment is accurate, as data was generated using correct experimental procedure.

② To fully determine the accuracy of this experiment, the experimentally achieved results for the concentration of glucose as measured by the glucose test strips would need to be compared to the concentration of glucose measured with a more accurate technique. As it stands, no conclusion can be drawn about the accuracy of the experiment.

The accuracy of an experiment is not always known. It depends on how unique your investigation is. Most experiments you perform will have been completed by others previously, so you are just reproducing results. In those cases, a **true value** is known and you can compare your own results to it.

Systematic error
when the readings obtained from measurements differ from the 'true' value consistently in one direction every time

Systematic errors

① For each test tube for which the concentration of glucose produced was recorded, the measurements were compared to a set value on the test strips so was only an approximate value.

② The most likely source of systematic error in the experiment may result from the colour of the glucose test strip incorrectly corresponding to the glucose concentration. To minimise the chance of this, the glucose test strips could be first calibrated against a series of standards that contain known concentrations of glucose. This should be done across the range of detection of the test strips, which is 0 mg mL^{-1} to 30 mg mL^{-1}.

A systematic error cannot be improved by repeating measurements, having a larger sample size or taking a mean. As the results are always out by a consistent value, they will always be inaccurate. Therefore, a change in the method or equipment must occur in order to eliminate the error.

Random error
an unpredictable variation in the readings obtained due to variables not all being controlled (extraneous variables), resulting in the readings being higher or lower than expected

Outlier
a reading that is very different from other results obtained for the same measurement

Random errors

① There were no random errors because the experiment was only conducted once for each condition tested.

② Random errors would be associated with all of the measurements in this experiment, such as the added volumes of sucrose solution and invertase solution, the timepoints that measurements were taken at and the reading of the glucose test strips. Repeating and averaging helps minimise the impact of these random errors..

The effect of a random error can be reduced by repeating measurements, having a larger sample size and/or finding the mean. As results are equally likely to be high or low, averaging can improve the precision of results. For most experiments in a laboratory where multiple trials are conducted, you will need to account for the effect of these errors on your investigation. You may need to also account for **outliers** by repeating measurements.

Precision
how close all the measurements are to each other

Precision

① *The results were not precise as the amount of glucose produced was only recorded once for each experimental condition.*

② *The precision of this experiment is likely limited by the glucose test strips, which just have five reference colours corresponding to five different glucose concentrations. A more precise way of measuring glucose concentration might be to use a glucometer, which has a numerical display.*

Precision can be improved by selecting more precise measuring tools for your experiment. In many cases, this will mean measuring tools that allow a number to be reported to more significant figures. With more precise measuring tools, repeated measurements will be closer together.

Discussion

The discussion is the most crucial aspect of the investigation. Use your logbook to write down any notes about what you plan to address in this section. The discussion should include the following key content.

- Interpret and evaluate the *trends and patterns in your data.* It is important here to also quote relevant data from the table/graph when referring to trends in the data.
- Acknowledge any *deviations (outliers) in the data from the results that were expected.* Relate the results to the relevant chemistry or scientific theory and key terms. This is very important, as this outlines how well you understand your results and can interpret them based on your knowledge of the theory. Therefore, use the knowledge in previous chapters of this text to help with the topic you are investigating.
- State whether the data you collected *supports or doesn't support the hypothesis.*
- Identify any *limitations in the data or the method.* Refer to random and systematic errors, and accuracy and precision, as discussed earlier in this chapter.
- Suggest *future improvements to the investigation* if it were to be performed again. This means referring to experimental errors, not human errors (for example, incorrect measuring of volume or not calibrating electronic balances). If your experiment is performed correctly, there should be no human errors.

NOTE

Avoid terms such as 'proved', 'disproved', 'correct' and 'incorrect' in relation to your hypothesis, as it is unlikely that you can be this certain from a single investigation. Instead use terms such as 'supported', 'not supported', 'indicated' and 'suggested'. If your results contradict your predictions, this would warrant repeating the experiment, if you have time. If you cannot repeat the experiment, then your report should include a discussion of flaws in the design or method, and suggestions for how the investigation could be altered to minimise or eliminate these.

Conclusion

The main purpose of the **conclusion** is to briefly summarise the position of the experiment in the wider understanding of the chemistry topic(s). You need to state the important overall trend of the data (referring specifically to data from your results) and whether or not the results support the tested hypothesis. The conclusion should assess whether the results

Conclusion
a summary of what you can deduce from the results of the investigation, including whether the tested hypothesis was supported

of the experiment have contributed new information to what is known about the topic, and any further investigations that need to be undertaken. The conclusion should not introduce any information that has not already been discussed in the results and discussion sections.

For example, in the experiment described in this chapter, the conclusion might read like this:

> In conclusion, the results indicate that the presence of invertase increased the rate of the hydrolysis of sucrose from ________ to ________. As such, the results support the hypothesis.

Investigation extension

Sometimes, your practical investigation needs to include a possible extension. This should be based directly on your results with a view to what could be tested further. It should either focus on the same independent variable with more variations tested to provide a more detailed set of results, or a different independent variable that will add value and further clarification to your initial question. Ultimately, it should have specific reference to real-world applications, green chemistry principles or sustainability goals.

In the experiment presented in this chapter, it was mentioned that systematic errors and the lack of precision could both be attributed to the use of glucose test strips. To improve the experiment, a calibrated glucometer could be employed, allowing for more precise measurements to be made.

Check-in questions – Set 1

1. What is the difference between qualitative data and quantitative data?
2. What is the appropriate method of representing continuous data?
3. Compare random and systematic errors, including what results from each type of error.
4. What is the difference between accuracy and precision?

13B SKILLS

VIDEO 13B–1 SKILLS: RECORDING RESULTS IN A TABLE

When completing work within this 'scientific skills' section, you will draw upon some very important skills. Many of these you will have learned in previous years of studying science, but it is particularly important to highlight some here, to ensure that you maximise your performance on any given assessment.

Recording results in a table

When constructing and recording your results in a table:

- Rule the table in pencil, so any amendments can be made easily.
- Give each column a clear heading, including both the quantity and the unit in which it is measured. Do not enter the units in the table along with each numerical value – the units go in the heading only.

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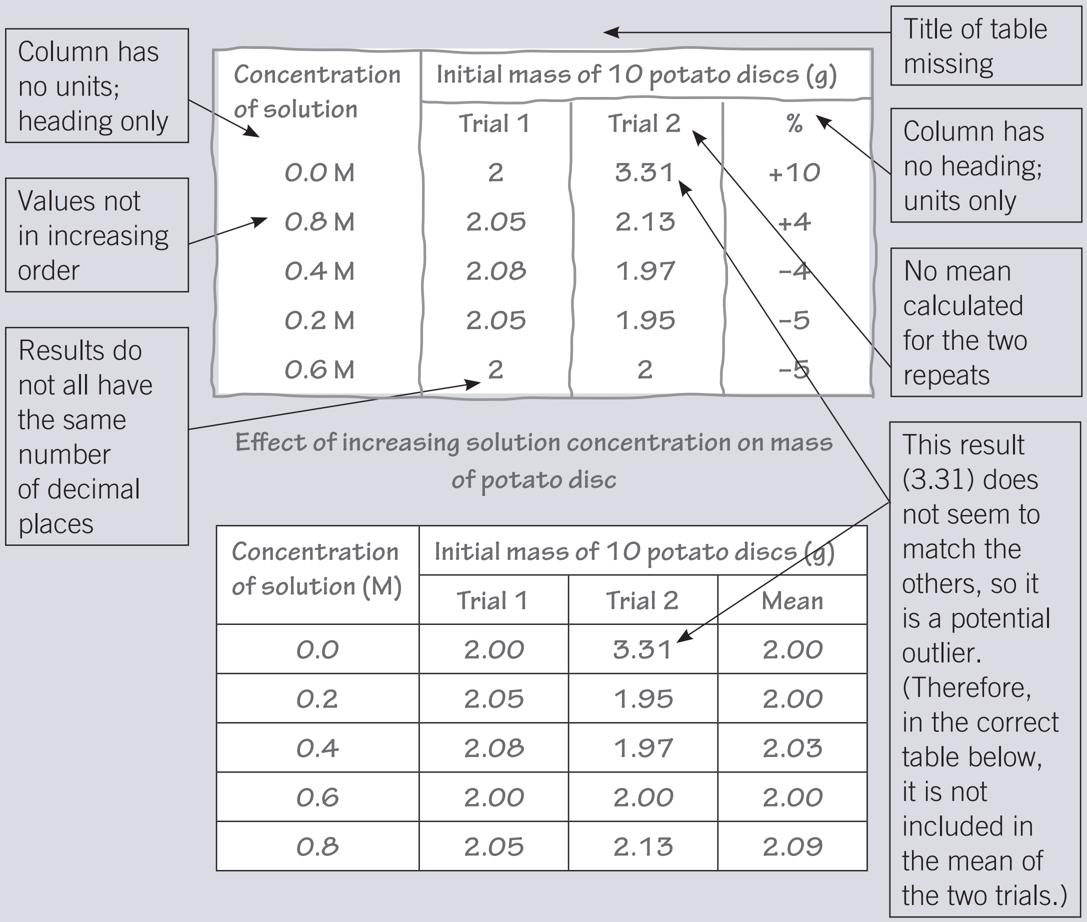
- The independent variable is usually placed in the first column, with the dependent variable to follow in the other columns.
- Organise the results appropriately. For example, if your experiment involved testing an increasing concentration of a solute solution, your results should start with the lowest concentration and continue to the highest concentration.
- If recording quantitative results, all values should have the same number of decimal points.
- Include results for all repeats in the table and the mean (average) calculated for these.
- Any results that are outliers should be recorded again (repeat the measurement). If there is no time to repeat the experiment, include the outliers but ignore them when calculating the mean.
- Give the table an overall title. This should include mention of both the independent and dependent variables.
- In most cases, data from a table also need to be displayed as a graph: a line graph for continuous data, a bar graph for discrete data.



Concentration of solution	Initial mass of 10 potato discs (g)		
	Trial 1	Trial 2	%
0.0 M	2	3.31	+10
0.8 M	2.05	2.13	+4
0.4 M	2.08	1.97	−4
0.2 M	2.05	1.95	−5
0.6 M	2	2	−5

Column has no units; heading only

Values not in increasing order

Results do not all have the same number of decimal places

Title of table missing

Column has no heading; units only

No mean calculated for the two repeats

This result (3.31) does not seem to match the others, so it is a potential outlier. (Therefore, in the correct table below, it is not included in the mean of the two trials.)

Effect of increasing solution concentration on mass of potato disc

Concentration of solution (M)	Initial mass of 10 potato discs (g)		
	Trial 1	Trial 2	Mean
0.0	2.00	3.31	2.00
0.2	2.05	1.95	2.00
0.4	2.08	1.97	2.03
0.6	2.00	2.00	2.00
0.8	2.05	2.13	2.09

The top table lacks ruled lines, and there are errors in the representation of data. A corrected version is shown in the table below it.

Drawing graphs

When constructing a graph:

- Use pencil, as this will allow you to make any amendments easily.
- Put the independent variable on the x-axis (horizontal axis) and the dependent variable on the y-axis (vertical axis).

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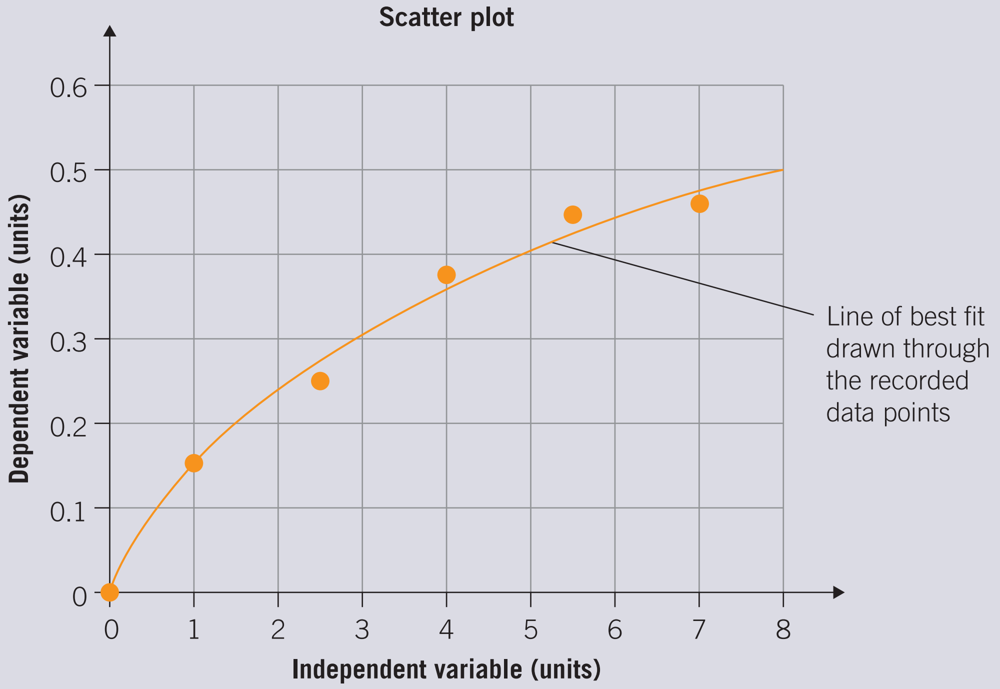
- Fully label both axes and include units (units should be the same as the results table if headings are correct there).
- The scale on the axes should have increasing values spaced at equal intervals, and it should be easy to read values between these intervals. Do not extend the scales too far beyond the recorded data values. Note: *You do not have to begin your scale at 0.*
- Make the graph as large as possible, so it is easy to read precise values.

When drawing *scatter plots:*

- Use a scatter plot to represent continuous data.
- Plot data points as crosses (×) or dots (•). If using dots, be sure to draw them large enough so that they are not covered by the line drawn in the next step.
- Draw a **line of best fit**. This does not need to go through the first and last point, nor does it need to be a straight line (both common mistakes made by students).
- If constructing your line of best fit digitally, software will have functions that allow you to select 'line of best fit' when plotting data. If constructing this by hand, you will need to do this by eye, which can be quite difficult. The line can be linear or nonlinear. Your aim here is to ensure that if you were to measure the distance between the data points below the line of best fit and the line itself, they would be equal to the distance between the data points above the line of best fit and the line itself. As you are unlikely to get this perfect on your first attempt, it is crucial you draw this line of best fit in pencil (as you should for all graphs anyway!).

Line of best fit a line on a graph that shows the general trend of the data points; the distance to the points above the line should equal the distance to the points below the line

VIDEO 13B–2 DRAWING GRAPHS



When drawing *bar graphs*:

- Use a bar graph to represent discrete data, and draw the bars with gaps between them.
- However, for a histogram, a special type of bar graph showing the distribution of numerical data, the rules are different. It displays the frequency of values on the vertical axis that fall into defined ranges called 'bins' marked on the horizontal axis.

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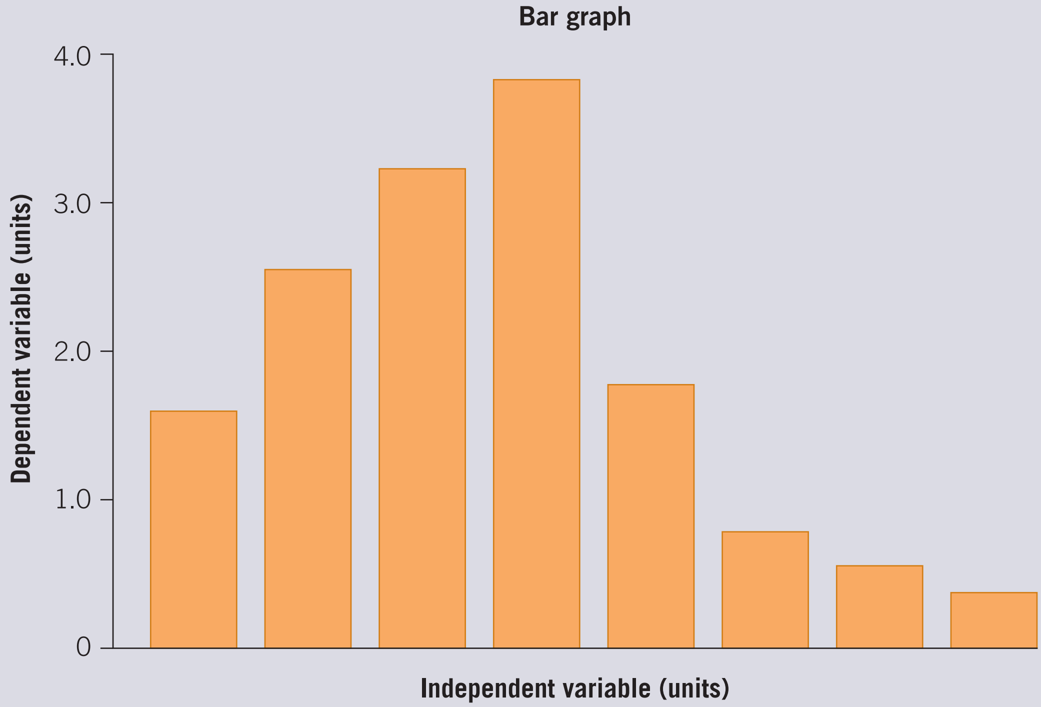

Ordering your discussion

When choosing an order for all the points to talk about in your discussion, follow this sequence.

1. Describe the overall trend (overall relationship between the independent and dependent variable).
2. Describe any changes in the gradient of the graph, particularly focusing on sharp changes and where they occur.
3. Quote data from the graph.
4. Explain the results using your scientific knowledge of the key concepts studied in your investigation.
5. Identify sources of errors in the experiment. Begin this section with any *systematic errors* and how these affected the accuracy of your measurements due to limitations in the apparatus, experimental technique or experimental design. Do not include human errors (for example, incorrectly measuring an exact volume of solution). Then identify any *random errors* and how these affected the precision of your measurements.
6. Identify areas for improvement. Focus on how to reduce the errors mentioned in step 5. This could include things such as:
   - using better techniques for measuring the dependent variable
   - using equipment that is more likely to keep controlled variables constant and therefore make your data valid, as well as more precise and accurate
   - repeating the investigation to increase reliability.

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Section 13B questions

1 A year 12 student is designing a practical investigation based on the question: 'How does half-cell concentration affect the potential difference of galvanic cells?'

   a For this investigation, identify at least four concepts that would be important for a student to include in their introduction to their research report.

   b Sketch a potential results table the student would need to set up to collect their results.

   c For this investigation, how should the student present their results graphically? Explain.

   d Using your knowledge of how a voltmeter works, determine the resolution of the instrument shown on the right. Explain your answer, including defining what resolution is.

   e If the student is using this voltmeter and has recorded the reading shown for one of their trials of varying concentrations of the half-cells, determine one random and one systematic error that may have occurred.

2 The specific heat capacity of a substance is a measure of the amount of energy required to raise the temperature of one gram of a substance by one degree Celsius. Different substances have different specific heat capacities. Specific heat capacity can be determined using the following equation:

$$c = \frac{q}{m\Delta T}$$

where c is the specific heat capacity (measured in $\mathrm{J\,g^{-1}\,{}^\circ C^{-1}}$), q is the energy (measured in joules, J), m is the mass (measured in grams, g) and ΔT is the change in temperature (measured in °C).

A trio of students planned to measure the specific heat capacity of four different substances – water, ethanol, sand and iron.

The internationally accepted values for the specific heat capacity of these substances are:

water = $4.18\ \mathrm{J\,g^{-1}\,{}^\circ C^{-1}}$
ethanol = $2.46\ \mathrm{J\,g^{-1}\,{}^\circ C^{-1}}$
sand = $0.830\ \mathrm{J\,g^{-1}\,{}^\circ C^{-1}}$
iron = $0.450\ \mathrm{J\,g^{-1}\,{}^\circ C^{-1}}$

The students completed five trials with one of their samples, recording the following results.

Trial	Calculated specific heat capacity ($\mathrm{J\,g^{-1}\,{}^\circ C^{-1}}$)
1	0.460
2	0.455
3	0.458
4	0.460
5	0.462

- a Determine the average calculated specific heat capacity from the trials recorded in the table.
- b Based on the average from your answer to part **a**, what is the likely substance from the four the students were testing?
- c Using your determination of the substance in part **b** above, discuss both the precision and accuracy of the students' results.
- d The students later suspected that the digital scales they were using to record the mass of the sample was not previously calibrated with a substance of known mass. They predicted that the mass reading was incorrect and underestimated the actual value.

  Would this be classified as a systematic, random or human error? Justify your answer.
- e For this experimental investigation, identify the independent and dependent variables.

3 A chemistry class was committed to determining the concentration of a specific compound in a mixture of substances using high-performance liquid chromatography (HPLC). The class ran four standard solutions containing different concentrations of the substance under identical conditions. The areas under the peak were measured from the chromatogram and are shown in the table below.

Standard solution (ppm)	Peak area
0.00	20
0.20	1000
0.40	2040
0.50	2950
1.00	6100

- a Use the data in the table above to graph the calibration curve for the specific compound's standard solutions. Be sure to label your axes correctly and carefully plot the data.
- b Are the results collected by the class to generate the calibration curve from the different standard solution concentrations repeatable or reproducible? Comment on each of these.

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13C Scientific communication

Study Design:

Science communication

- Conventions of science communication: scientific terminology and representations, symbols, formulas, standard abbreviations and units of measurement
- Conventions of scientific poster presentation, including succinct communication of the selected scientific investigation, and acknowledgements and references
- The key findings and implications of the selected scientific investigation

ENGAGE

Communicating your work

Think about how you've presented your experimental work in science in previous years. You would have written up your planning stages and presented your results in a typical scientific report. These types of scientific report are similar to journal articles, which are a common format that researchers use to publish their work for peers. However, when they want to share their research at conferences, scientists often communicate their findings in the form of a scientific poster. This type of format requires scientists to be able to communicate their ideas in a way that is clear, concise and engaging.

Producing a scientific poster involves developing skills and is not easy. It often requires a lot of thought and preparation.

Figure 13C–1 A poster session at a General Meeting of the American Society for Microbiology.

EXPLAIN

Scientific poster template

A key part of the School-assessed Coursework in Units 3 & 4 Chemistry is a student-designed practical investigation presented in the format of a poster, using the following template:

<table>
<tr><td colspan="3">Title
Student name</td></tr>
<tr><td>Introduction
Methodology and methods
Results</td><td>Communication statement reporting the key finding of the investigation as a one-sentence summary</td><td>Discussion
Conclusion</td></tr>
<tr><td colspan="3">References and acknowledgements</td></tr>
</table>

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This template is the same as the one provided in the VCAA Chemistry Study Design. You'll notice from the template that the heading of each section correlates closely with the information that is recorded in your logbook from Sections 13A and 13B. This should highlight the importance of the way the information is structured in your logbook. The VCAA has stipulated that the poster should not exceed 600 words, meaning that you may have to summarise the information from your logbook in a more succinct fashion. The communication statement occupies approximately one quarter of the page and needs to be one sentence summarising the main outcomes of your investigation. This should be engaging to encourage any reader to want to read the other sections of your poster.

LINK **13A** INVESTIGATIVE PLANNING AND DESIGN

LINK **13B** SCIENTIFIC EVIDENCE

While the aim and hypothesis aren't specifically mentioned in the template, they are often included in the introduction, following a brief explanation of the reasons for conducting your investigation, and link to the relevant chemical concepts. The rubric provided by your school will likely give more information about what should be included in your introduction and the other sections of the poster.

References and acknowledgements

In the poster, you should include the sources of information (references) that you used when planning and conducting the investigation. You can also acknowledge those who supported your investigation, such as peers and your teacher.

VIDEO 13C–1 SCIENTIFIC POSTER EXAMPLE

A bibliography, or reference list, appears at the bottom of your poster and contains items that you have directly referenced in your investigation. If you are referencing a website, the reference must include the URL and the date on which the website was accessed.

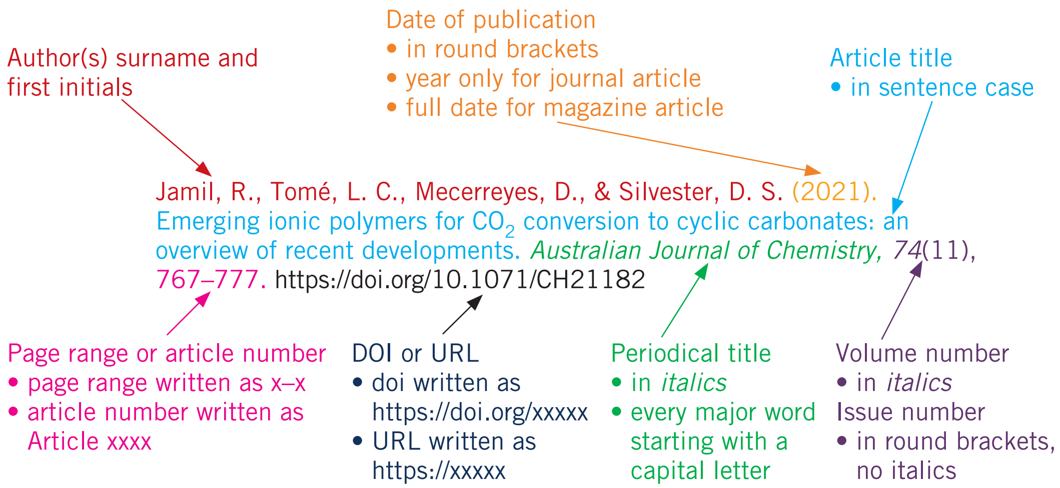
There are a few common formats used for referencing sources of information. This textbook will focus on the Harvard referencing format.

Reference lists

All sources cited in text, such as in the introduction section of a scientific poster, must be included in the reference list. References should be listed in alphabetical order by author surname or organisation name. There are very specific formatting rules for reference lists, and different source materials require different details. In general, four elements are included in a reference: author, date, title and source. The examples below show a reference entry for a journal article, a book and a website. For more examples and explanations of how to reference other sources, such as Wikipedia, organisational reports, films, YouTube clips, TED talks and podcasts, a referencing quick guide is provided in the Interactive Textbook.

DOCUMENT 13C–1 APA-STYLE REFERENCING

Periodical (journal, magazine or newspaper article; print or online)



Date of publication
- in round brackets
- year only for journal article
- full date for magazine article

Author(s) surname and first initials

Article title
- in sentence case

Jamil, R., Tomé, L. C., Mecerreyes, D., & Silvester, D. S. (2021). Emerging ionic polymers for CO_2 conversion to cyclic carbonates: an overview of recent developments. *Australian Journal of Chemistry, 74*(11), 767–777. https://doi.org/10.1071/CH21182

Page range or article number
- page range written as x–x
- article number written as Article xxxx

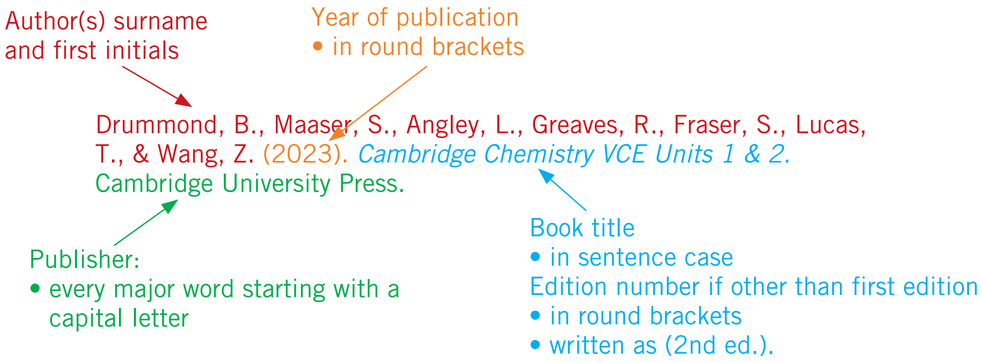
DOI or URL
- doi written as https://doi.org/xxxxx
- URL written as https://xxxxx

Periodical title
- in *italics*
- every major word starting with a capital letter

Volume number
- in *italics*

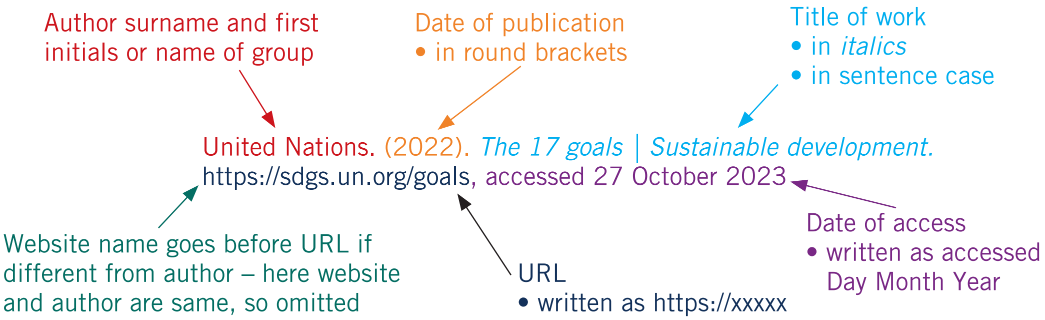
Issue number
- in round brackets, no italics

Book



Drummond, B., Maaser, S., Angley, L., Greaves, R., Fraser, S., Lucas, T., & Wang, Z. (2023). *Cambridge Chemistry VCE Units 1 & 2.* Cambridge University Press.

Website



United Nations. (2022). *The 17 goals | Sustainable development.* https://sdgs.un.org/goals, accessed 27 October 2023

13C SKILLS

Validity and reliability of information

When completing your background planning for your practical investigation to complete your introduction, you should use sources of information that are reputable. To determine if a source is reputable, a number of factors must be considered.

1. **Author credentials:** A reputable source should have a clear and identifiable author or group of authors. In the case of scientific information, this would typically be a scientist or a group of researchers who are experts in the field they're writing about. The authors' credentials, affiliations and academic backgrounds should be available, showing that they have the necessary knowledge and expertise to be considered trustworthy on the subject.
2. **Citations and references:** Reputable sources usually have a list of references or citations at the end. These references indicate that the authors have done a comprehensive review of existing literature on the topic and are acknowledging the work of other scientists where it is due.
3. **Publication date:** In science, recent sources can often be more reliable because they account for the latest research and advancements in the field. This is not to say older sources cannot be reputable, but it's always important to check the timeliness of the source.
4. **Objective and unbiased:** Good scientific writing should always be objective, meaning it should present the facts without bias or personal opinion. If a source seems to be pushing a certain viewpoint without providing evidence or seems overly biased, it might not be the most reliable.

5 **Supported by evidence:** Reputable sources should always back up their claims with empirical evidence, such as data, results from experiments or references to other scientific research.

Plagiarism and referencing

Plagiarism is where you directly use another author's writing or images without acknowledging them. Even if you're paraphrasing pieces of information or changing it into your own words, it is still important to include a reference as to where you sourced this information.

Figure 13C–2 Plagarism involves passing someone else's work off as your own.

This is why as you source information, you must ensure that you record (reference) accurately the sources you have read and accessed for information. Referencing is necessary to avoid plagiarism. Remember, your final written investigation will be a form of secondary source, and if your reader is interested in finding out more about your question, they may want to locate the primary source.

Section 13C questions

1 Where should you draw information from to complete your scientific poster?
2 What is included in the introduction section of the scientific poster?
3 What are the key sections of a scientific poster?
4 What is the purpose of the communicating statement in the centre of the poster?
5 What are some other ways of presenting the results of an investigation in chemistry and, in general, to the scientific community?

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Chapter 13 review

Summary

Create your own set of summary notes for this chapter, on paper or in a digital document. A model summary is provided in the Teacher Resources and can be used to compare with yours.

Checklist

In the Interactive Textbook, the success criteria are linked from the review questions and will be automatically ticked when answers are correct. Alternatively, print or photocopy this page and tick the boxes when you have answered the corresponding questions correctly.

Success criteria – I am now able to:		Linked questions
13A.1	Document investigations appropriately using a logbook	11☐
13A.2	Define key terms related to scientific skills	12☐
13A.3	Define ‘controlled experiment’	13☐
13A.4	List the features that a controlled experiment includes	12☐
13A.5	Understand the meaning of single-variable exploration	1☐
13A.6	Define and identify independent, dependent and controlled variables	7☐, 12☐, 13☐
13A.7	Select and use the procedures and equipment appropriate to an investigation	5☐, 12☐, 13☐
13A.8	Distinguish between an aim and a hypothesis	10☐
13A.9	Construct aims and questions for investigations	12☐
13A.10	Formulate hypotheses and predict possible outcomes based on models or theory	12☐
13A.11	Define ‘reproducibility’, ‘repeatability’, ‘resolution’ and ‘validity’, and distinguish between these	6☐, 8☐, 13☐
13A.12	Design an investigation that accounts for accuracy and precision and is valid	2☐, 12☐
13A.13	Design an experiment that is fully repeatable and reproducible by others	12☐
13A.14	Determine potential ethical issues with investigation design	12☐
13A.15	Identify how bias can be minimised in an investigation	16☐
13A.16	Follow clear guidelines for health and safety when undertaking practical investigations	5☐, 12☐
13B.1	Define ‘qualitative’ and ‘quantitative’	13☐
13B.2	Distinguish between qualitative and quantitative data	4☐, 13☐
13B.3	Include appropriate units of measurement for quantitative data	13☐
13B.4	Transform primary data into an appropriate format of results (table, flow chart, bar and/or line graph)	9☐, 12☐
13B.5	Identify trends in data	12☐
13B.6	Define the different types of errors (random and systematic)	12☐, 13☐

Success criteria – I am now able to:		Linked questions
13B.7	Identify sources of error and outliers from primary data	3☐, 12☐
13B.8	Use evidence to determine whether an investigation supports or discounts a hypothesis, scientific model or theory	12☐, 15☐
13B.9	Identify areas for improvement in investigation design and analysis to increase accuracy and precision and reduce the likelihood of errors	12☐, 15☐
13C.1	Appropriately communicate all aspects of a scientific investigation	12☐
13C.2	Apply correct abbreviations to chemical terminology	12☐
13C.3	Recall and convert between different units of measurement in chemistry	14☐
13C.4	Determine the correct number of significant figures to use in answers to questions	14☐
13C.5	Know and demonstrate how scientific investigations are presented succinctly on a poster	14☐
13C.6	Recall how and what to acknowledge and/or reference in correct format	14☐
13C.7	Justify conclusions and evaluate whether evidence supports or refutes the hypothesis	12☐, 13☐, 15☐
13C.8	Interpret investigation outcomes in terms of broader chemical concepts	12☐

Multiple-choice questions

1 A year 12 student is designing a practical investigation based on the question:

'How does temperature and concentration affect the potential difference of galvanic cells?'

If the student is planning to conduct a single-variable exploration as part of their experiment, what is the issue with their investigation question?

A They have two dependent variables.

B They have two independent variables.

C They have two controlled variables.

D Both temperature and concentration are control groups and not experimental groups.

2 Each piece of chemistry equipment has an inherent uncertainty with using it to take measurements. This uncertainty affects which of the following?

A accuracy

B precision

C repeatability

D resolution

The following information relates to Questions 3–5.

A group of students was completing a titration to determine the concentration of potassium permanganate, $KMnO_4$, using an oxalic acid, $C_2H_2O_4$, standard solution.

They prepared a standard oxalic acid solution of total volume 250 mL.

Aliquots of 10.00 mL of the potassium permanganate solutions were added to conical flasks and titrated with the oxalic acid using the burette.

The student recorded the following results.

Final burette reading (mL)	49.80	27.50	45.90	23.60
Initial burette reading (mL)	27.50	5.35	23.60	0.00

Permanganate ions are a purple colour. Therefore, in this redox titration reaction, potassium permanganate is reduced from purple to a colourless solution.

3 Why did the students record four readings for the titre volume?

- **A** Four readings create a larger sample size, allowing them to calculate an average and improve the accuracy of their results.
- **B** Four readings increase the reproducibility of their results as all four readings are within the required concordant range.
- **C** Four readings remove any outliers, ensuring only concordant results are used to determine an average, giving more precise results.
- **D** Four readings ensure that through each trial any random and systematic errors could be removed and thus not affect the results.

4 What type of data is being recorded by the students in this experiment?

- **A** qualitative
- **B** quantitative
- **C** both qualitative and quantitative
- **D** neither qualitative nor quantitative

5 One safety measure that would need to be followed by the students while performing this redox titration is

- **A** ensuring that distilled water is used when preparing the standard solution so it is not contaminated with other ions present in the tap water.
- **B** wearing gloves to prevent any irritation that may be caused from spillage of the potassium permanganate solution or oxalic acid solution.
- **C** wearing safety glasses to reduce the risk of them falling if liquid was accidentally spilled onto the floor.
- **D** wearing a lab coat to prevent any glassware that is chipped or broken cutting their face.

6 A teacher was performing an experiment for a group of students testing their own collected sample of water, repeating their quality-testing technique five times.

Which aspect of their experiment was improved by repeating the procedure five times?

- **A** accuracy
- **B** reproducibility
- **C** validity
- **D** repeatability

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7 Linsey performs a series of tests in conical flasks that were placed in a water bath to ensure the flasks and the liquid inside them was kept at a constant temperature of 40°C.

In this experiment, the temperature at which this series of tests is conducted is the

A control group.
B independent variable.
C dependent variable.
D controlled variable.

8 The validity of experimental data depends mostly on

A the reproducibility of data recorded within the experiment.
B how close the averaged set of data is to the true value.
C whether the recorded data for the dependent variable is generated using only one independent variable.
D the data being recorded using measurements that have limited random and systematic errors.

9 If a student was to graph the effect of change in concentration of a reactant on the rate of a chemical reaction, the best type of graph used to present the data would be a

A line graph.
B column graph.
C pie chart.
D histogram.

10 A hypothesis is best described as

A a statement describing what the investigation hopes to determine.
B a series of steps involved in planning an investigation.
C clear ethical guidelines for how any living organisms should be handled in the experiment.
D a prediction of what will be observed.

11 Which of the following statements would be appropriate in the 'method' section of a logbook?

A Exactly 50 mL of solution was measured using a measuring cylinder.
B Exactly 50 mL of solution was measured using a beaker.
C Solution was measured and placed in a tube.
D Add solution to a measuring cylinder.

Short-answer questions

12 A student was investigating the following research question:

How do the concentrations of sodium hydroxide (NaOH) and hydrochloric acid (HCl) reagents affect the rate of their neutralisation reaction, assessed by measuring the increase in temperature from the exothermic reaction?

a The student tested concentrations of 0.10 M, 0.50 M, 1.0 M and 2.0 M. Identify the independent, dependent and controlled variables for this student's investigation. (4 marks)

b Using your chemistry knowledge, write an aim and a hypothesis for this student's investigation. (4 marks)

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The student followed the method outlined below.

1. Label four beakers with the following concentrations, respectively: 0.10 M, 0.50 M, 1.0 M and 2.0 M. Then label two pipettes 'HCl' and 'NaOH', respectively.
2. Label two other beakers 'HCl stock solution (0.10 M)' and 'NaOH stock solution (0.10 M)', respectively. Into the beaker labelled 'HCl stock solution (0.10 M)', pour 200 mL 0.10 M HCl, and into the beaker labelled 'NaOH stock solution (0.10 M)', pour 200 mL 0.10 M NaOH.
3. Using the pipette labelled 'HCl', draw up 25 mL of the 0.10 M HCl stock solution and dispense it into the beaker labelled '0.10 M'. Wait for the solution to reach room temperature if it has not yet done so, then record the temperature.
4. Using the pipette labelled 'NaOH', draw up a 25 mL aliquot of the 0.10 M NaOH stock solution.
5. Prepare a stopwatch and dispense the NaOH aliquot into the beaker labelled '0.10 M'. Then immediately start the stopwatch.
6. After one minute, record the temperature change of the combined solution.
7. Safely dispose of the solution and clean the thermometers and beakers with distilled water.
8. Repeat steps 2–7 seven more times so there are eight trials at this concentration of HCl and NaOH.
9. Repeat steps 2–8 of the experimental method for the remaining concentrations: 0.50 M, 1.0 M and 2.0 M.

c Using your understanding of the reagents used in this experiment, list the safety precautions required for the student and explain why these are important to follow. (4 marks)

d Draw a fully labelled diagram to represent the set-up of the experiment. (3 marks)

The student recorded the following results from the investigation.

	Change in temperature (ΔT)							
Initial concentration of NaOH and HCl solution	***T*1**	***T*2**	***T*3**	***T*4**	***T*5**	***T*6**	***T*7**	***T*8**
0.10 M	1.5°C	1.0°C	1.0°C	1.0°C	0.50°C	1.0°C	1.0°C	0.50°C
0.50 M	2.0°C	1.0°C	3.0°C	3.5°C	3.5°C	3.0°C	3.5°C	3.0°C
1.0 M	6.0°C	6.0°C	5.5°C	5.5°C	6.5°C	6.5°C	6.5°C	6.5°C
2.0 M	12.5°C	12.0°C	12.0°C	11.5°C	13.0°C	12.5°C	12.5°C	12.0°C

e The student has forgotten to write a title for their table of results. Write an appropriate title for them that includes reference to the independent and dependent variables. (2 marks)

f Identify two different things that the student could improve to follow correct conventions with their table of results. (2 marks)

g For which concentration of NaOH and HCl tested were the recorded results most precise? Explain. (2 marks)

h Based on the results above, what type of graph should be used to represent the student's results recorded? Explain your reasoning, referring specifically to the type of data collected. (3 marks)

i Plot a graph to represent the results recorded in the table above by the student. Remember to include an appropriate title for the graph and properly labelled axes. (4 marks)

j Synthesise the data from your graph in part **i** by describing the trend observed in your results. Ensure you refer to data, including any outliers, in your discussion. (4 marks)

k Compare the results to the hypothesis you wrote for this student's investigation in part **b**. Do the results support or not support this hypothesis? Justify your answer. (2 marks)

The student's analysis of their data connected to theory is included below.

> 'For chemical reactions to occur, particles must undergo a successful collision with other particles so that new particles can be formed. This is referred to as the collision theory, and in relation to this experiment, when concentration increased, the frequency of successful collisions increased, and thus reaction rate increased. This is because as concentration increases, the molarity of the solution is subsequently increased. Molarity is the amount of moles per litre, so as molarity increases, the moles per litre increases. For example, in this experiment, the increase in concentration from 1.0 M to 2.0 M, the 2.0 M would have a greater number of moles of reactants present to react. Subsequently, the probability of a successful collision increases, leading to an increase in the amount of successful collisions between reactants. This will result in more energy released into solution and to the nature of the exothermic reaction, thus increasing temperature by a larger amount and therefore improving the rate of reaction.'

l Reading this and using your knowledge of the relevant theory, what changes would you make to this analysis? (2 marks)

m Identify one random and one systematic error that could have occurred in this experiment. In your answer, also include a way that the student could modify the experiment to improve the results obtained. (4 marks)

n Compare the terms 'repeatability' and 'reproducibility', and outline which one has been achieved in this student's investigation. (3 marks)

o Using your knowledge of rates of reaction, suggest a future research question that could be explored by the student. (1 mark)

p Clearly outline the difference between accuracy, precision and validity in relation to the different types of errors that exist in an experimental investigation. (3 marks)

13 Using a calorimeter, the energy content of an oat bar was determined by the following procedure.

1. A sample of the oat bar was placed onto the digital scales and accurately weighed.
2. The calorimeter was filled with a known volume of water and the temperature recorded with a thermometer.
3. The power pack was turned on, igniting the wires in the calorimeter. The change in temperature was recorded.
4. Steps 1–3 of the procedure were repeated.

a Looking more closely at step 2 in the method above, identify two ways in which this step could be written more clearly in order for the experiment to be reproducible. (2 marks)

b Explain the purpose of step 4 in the method above. (1 mark)

c Identify one potential systematic error with this calorimetry experiment and the effect it would have on the results if not removed. (2 marks)

A 10.00 g sample of two different oat bars was burned separately in the calorimeter using an electrical current passed through a heating coil inside the calorimeter. Each sample was burned completely. The results of this experiment are shown below.

	Oat bar 1	Oat bar 2
Initial temperature (°C)	21.0	20.5
Final temperature (°C)	22.4	22.1

d In this specific experiment, identify the independent, dependent and two controlled variables. (4 marks)

e Is there a control group for this experiment? Justify your decision by explaining what the control group is or why there is no control group. (2 marks)

f Are the results obtained qualitative or quantitative? Explain by comparing these two terms. If the results are numerical, include the units of the measured results. (2 marks)

g Write a suitable conclusion for this investigation, based on the results presented in the table on the previous page. (2 marks)

14 The following questions relate to specific skills in the context of chemistry and are regularly part of scientific investigations and calculations in experiments.

a Explain how to convert between mL and L when required to convert volume values for calculations involving gas laws or moles. (1 mark)

b Explain how to convert concentrations in molarity to concentrations in grams per litre. (1 mark)

c Identify how many significant figures are represented by the following numbers:

i 34.980

ii 10.0

iii 0.0034 (3 marks)

d What is the benefit for scientists in presenting their investigation results in the form of a scientific poster? (1 mark)

e Explain in which ways the following reference source is presented in the appropriate format and identify what further information can be provided that is currently not included. (2 marks)

> Drummond, B., Maaser, S., Angley, L., Greaves, R., Fraser, S., Lucas, T., & Wang, Z. (2023). *Cambridge Chemistry VCE Units 1 & 2.* Cambridge University Press.

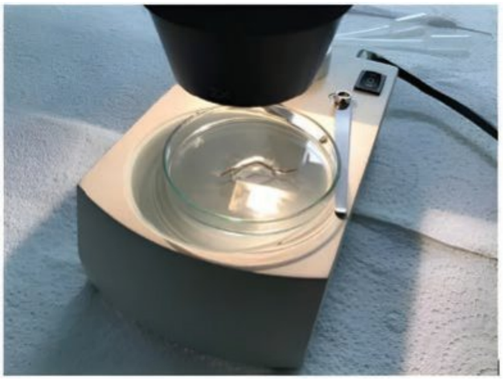
15 A student was completing a practical investigation to determine the rate of reaction between calcium and sulfuric acid. The method for their investigation is shown below.

1. A 2.0 M solution of sulfuric acid was prepared using a plastic pipette and distilled water.
2. A 100 mL flask was attached to a corresponding gas syringe.
3. Using a beaker, 25.0 mL was added to the flask.
4. 1 teaspoon of calcium metal was added to the flask and the stopper immediately placed on quickly to trap any of the gas produced.
5. The volume of gas produced was recorded using the graduations on the syringe.

a Describe two steps of the method above that would limit the accuracy of the results that would be obtained by the student. (2 marks)

b The student hypothesised that the rate of reaction would decrease as the concentration of acid decreased. Can the student conclude this from their experiment, if only the steps in the method were conducted? Explain. (2 marks)

16 Fatima investigated whether a displacement reaction occurred using combinations of different metals and ionic compound (salt) solutions. She used a stereomicroscope to observe the outcomes of the different reactions as shown below.



The method for the experiment is written below.

1. After your teacher has demonstrated how to set up and focus the stereomicroscope, place a Petri dish on the platform and use the forceps to place a piece of copper wire in the centre of dish. Focus the stereomicroscope on the wire. Then place two or three drops of the $AgNO_3$ solution over the centre of the wire and observe the changes. You will notice them immediately.
2. After a few minutes, carefully remove the Petri dish from the platform so that the crystals that have formed are not disturbed and place it next to the stereomicroscope for further observations. Record your observations in the table below.
3. Place a fresh clean Petri dish on the platform. Carefully place a small iron nail in the centre of the dish. Focus the stereomicroscope on the nail. Then place two or three drops of the $CuCl_2$ solution over the centre of the nail and observe the changes. You will notice them immediately.
4. Continue observing both reactions, swapping them out of the stereomicroscope carefully so that the crystals and solutions are not disturbed. If practicable, observe the crystals again on the following day. Record your observations in the table below.

Fatima recorded her results in a table, as shown below.

Mixture	Initial appearance of metal	Initial colour of salt solution	Changes observed
$Cu + AgNO_3$	Shiny bronze colour	Clear transparent solution	Brown substance was deposited on the metal. Solution turned slightly blue in colour
$Fe + CuCl_2$	Shiny silver colour	Light-blue coloured transparent solution	Solution became clear over time and the metal had growth of black crystals on the outside

a What type of data did Fatima collect? Explain. (1 mark)

b What is missing from Fatima's results table? (1 mark)

Answer the following questions in relation to the chemical concepts covered by Fatima in this experiment.

c Give the formulas of the species that were present before each reaction started (this should include any charged ions). (4 marks)

d Based on Fatima's observations and given that in a chemical reaction, no new elements are created and none are destroyed, what must be the products of both reactions? State their formulas. (2 marks)

e How can these changes be explained? What must have moved between the reactants? (2 marks)

f Why do metals react in this way? (2 marks)

g From the reactions that took place in this experiment, what can be determined about the reactivity of copper, iron and silver? Explain your reasoning. (3 marks)

h From your answer to part **g** above, predict what would happen if you were to add some silver nitrate solution to an iron nail. State your reasoning. (1 mark)

i What safety requirements would Fatima have needed to implement in this experiment? Explain why, in relation to the reactants that were used in the displacement reactions. (4 marks)

j Identify an aspect of Fatima's method that could be adjusted to increase both the accuracy and the precision of her results. Explain how making such an adjustment would improve the results by reducing the chance of bias or errors in Fatima's measurements. (4 marks)

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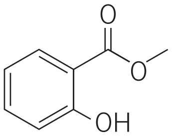
Unit 4 Revision exercise

Multiple-choice questions

1 Methyl salicylate is used as an ingredient in mint-flavoured lollies and also for pain relief for aching muscles and joints. The structure is shown below.



What is the molecular mass of methyl salicylate in $g\,mol^{-1}$?

A 137

B 148

C 152

D 154

2 Esters are formed from the reaction between primary alcohols and carboxylic acids. One ester has the semi-structural formula, $CH_3CH_2COOCH_2CH_3$. The name of this ester is

A ethyl propanoate.

B propyl ethanoate.

C ethyl butanoate.

D propyl propanoate.

3 The reaction between chlorine gas and pent-2-ene will produce which of the following organic products?

A 2-chloropentane

B 1,2-dichloropentane

C 2,2-dichloropentane

D 2,3-dichloropentane

4 The complete hydrolysis of three triglyceride molecules results in the production of how many water molecules?

A 1

B 3

C 6

D 9

5 The following equation shows how ethyl ethanoate, an ester, can be produced from the reaction between ethanol and ethanoic acid.

$$C_2H_6O(l) + C_2H_4O_2(l) \rightarrow C_4H_8O_2(l) + H_2O(l)$$

Determine the percentage yield for the reaction if 14.7 g of the ester, $C_4H_8O_2$, is produced from the reaction of 9.20 g of C_2H_6O with excess $C_2H_4O_2$.

A 6.25%

B 28.1%

C 62.6%

D 83.5%

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6 The reaction of an organic compound with bromine water would be most useful to distinguish between

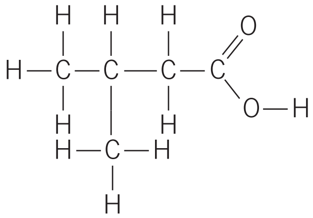
A alkane versus alkene.

B alcohol versus carboxylic acid.

C aldehyde versus carboxylic acid.

D primary alcohol versus secondary alcohol.

7 The following structure is 3-methylbutanoic acid.



Which of the following combinations below correctly predicts the number of peaks that would be observed in both ^{13}C NMR and low-resolution ^{1}H NMR?

	^{13}C NMR	^{1}H NMR
A	4	3
B	5	4
C	4	4
D	5	3

8 In an HPLC chromatogram of a mixture containing compounds A, B and C, compound A has a retention time of 3 minutes, compound B has a retention time of 6 minutes and compound C has a retention time of 9 minutes. If compound A is more polar than B, and compound B is more polar than C, what does this tell you about the stationary phase being used?

A It is relatively polar.

B It is relatively non-polar.

C It interacts most strongly with compound A.

D It has the same polarity as the mobile phase.

9 You perform mass spectrometry analysis of an organic compound. The molecular ion peak occurs at an m/z of 105. You observe a peak with greater intensity at an m/z of 103. Which of the following could potentially explain this observation?

A The compound contains one bromine atom.

B The compound contains one chlorine atom.

C The compound contains two bromine atoms.

D The compound contains two chlorine atoms.

10 An IR spectrum shows strong absorptions at 1710 cm^{-1} and 3300 cm^{-1}. What functional group is most likely present in the molecule?

A ether

B alcohol

C aldehyde

D carboxylic acid

11 Which of the following compounds contains a chiral carbon atom?

- **A** propane
- **B** propan-1-ol
- **C** propane-1,2-diol
- **D** propane-1,2,3-triol

12 The level of protein structure that is stabilised by hydrogen bonding between atoms in the R groups is the

- **A** primary structure.
- **B** secondary structure.
- **C** tertiary structure.
- **D** quaternary structure.

13 Which of the following is most true about the function of an enzyme at a temperature lower than its optimal?

- **A** The enzyme will have an altered primary structure.
- **B** All enzyme molecules will be denatured at this temperature.
- **C** The enzyme will not be able to catalyse the reaction at this temperature.
- **D** The enzyme will bind less frequently to its substrate at this temperature.

14 Repeating an experiment multiple times and averaging the findings will help to

- **A** generate a hypothesis.
- **B** improve the precision of results.
- **C** reduce the effect of random errors.
- **D** reduce the effect of systematic errors.

15 A conclusion should **not**

- **A** state key data from results.
- **B** summarise the key findings of an investigation.
- **C** state whether the hypothesis was supported.
- **D** introduce new information relevant to the investigation.

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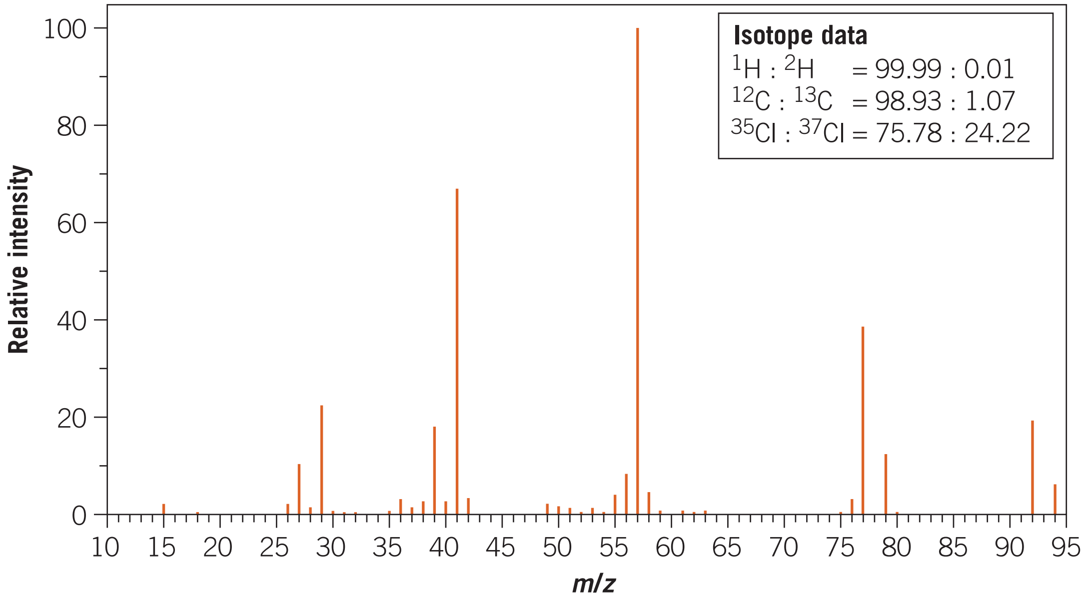
Short-answer questions

1 The reaction of 2-chloro-2-methylpropane with potassium hydroxide produces 2-methylpropan-2-ol. (9 marks)

a The mass spectrum for 2-chloro-2-methylpropane is shown below. The inset shows isotope data for the elements present in the molecule.



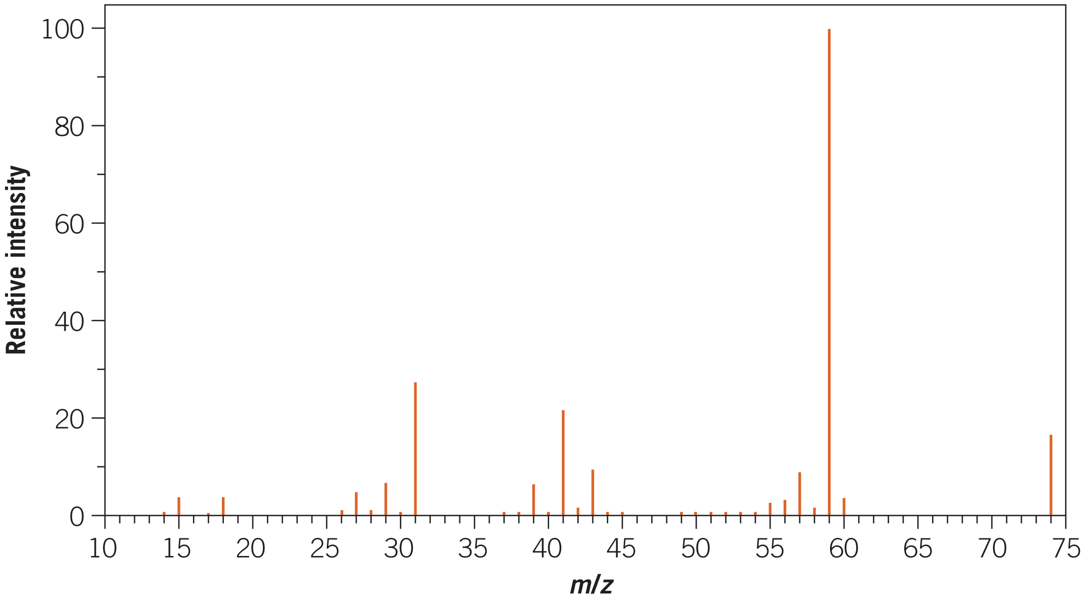
i Define m/z as used in mass spectrometry. (1 mark)

ii Give a reason why the mass spectrum shows two molecular ion peaks at $m/z = 92$ and 94, rather than just one. (1 mark)

iii Identify the fragment that produces the peak at $m/z = 94$. (1 mark)

iv Identify the fragment that produces the peak at $m/z = 57$. (1 mark)

b The mass spectrum for 2-methylpropan-2-ol is shown below.



i Label the base peak on the spectrum. (1 mark)

ii Write an equation to show the formation of the molecular ion from 2-methylpropan-2-ol. (1 mark)

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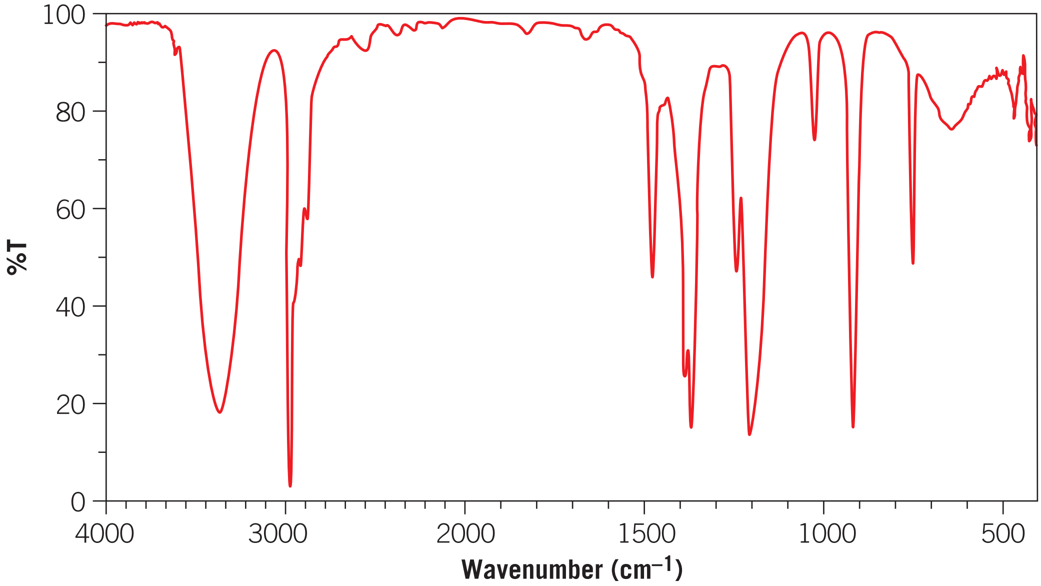
c After enough time passed for the reaction to occur, the organic product was isolated and analysed with an infrared spectrometer. The resulting spectrum is shown below.



Consider the region of the IR spectrum in the region 400–1500 cm^{-1}.

i Name this region. (1 mark)

ii Explain why this region, and not the region 1500–4000 cm^{-1}, is used to identify the molecule. (1 mark)

iii Is this spectrum consistent with the organic product being 2-methylpropan-2-ol? Use evidence from the IR spectrum in the region 1500–4000 cm^{-1} in your response. (1 mark)

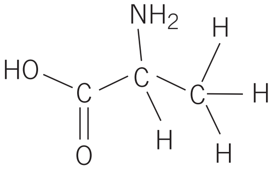
2 Refer to the following molecules in your responses to this question. (8 marks)

4-methylpentan-1-ol

Molecule 1

4-bromo-3-methylpent-2-ene

Molecule 2



Molecule 3

a Write the semi-structural formula of Molecule 1. (1 mark)

b Draw the structural formula of Molecule 2. (1 mark)

c Write the IUPAC name of Molecule 3. (1 mark)

d 4-Methylpentan-1-ol (Molecule 1) and hexan-1-ol are structural isomers. Explain why hexan-1-ol is expected to have a higher boiling point than 4-methylpentan-1-ol. (3 marks)

e Using the skeletal representation, draw and name a positional isomer of Molecule 3. (2 marks)

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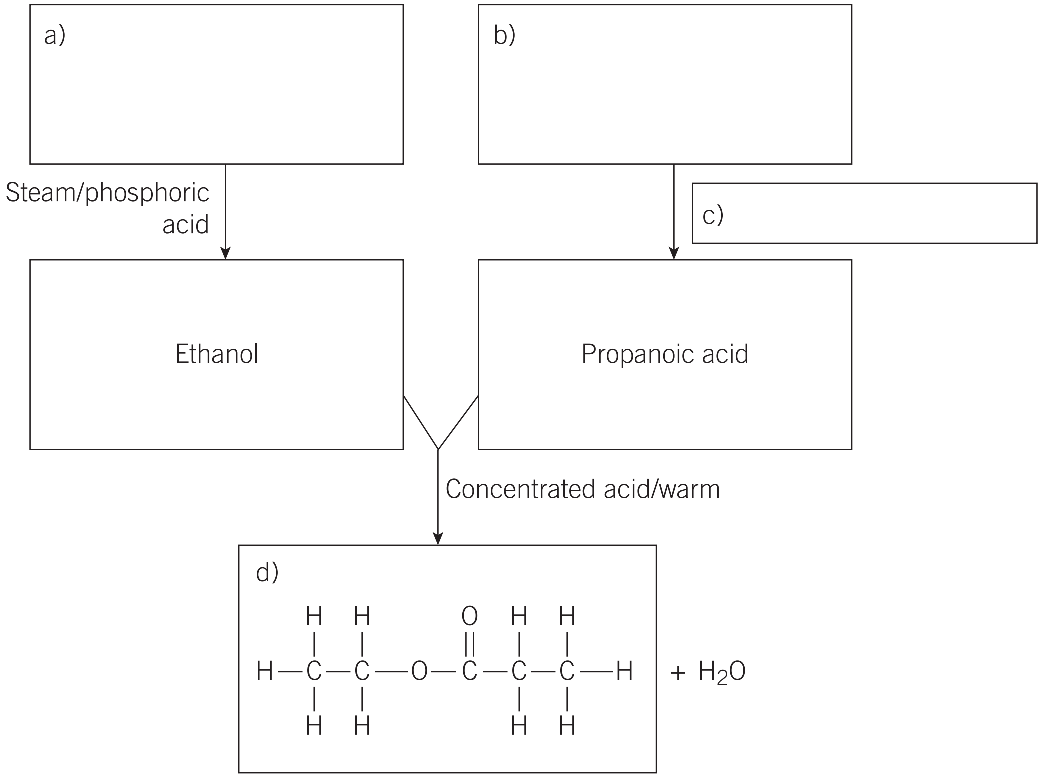
3 The diagram below represents the reaction pathway for the synthesis of an ester.



(7 marks)

a Draw the structural formula of the molecule in the box labelled **a)**. (1 mark)

b Draw the skeletal formula of the molecule in the box labelled **b)**. (1 mark)

c List any reagents and any specific conditions required in the box labelled **c)**. (2 marks)

d Write the name of the ester formed. (1 mark)

e Calculate the atom economy of the reaction involving ethanol and propanoic acid to form the ester. (2 marks)

4 Amylase is an enzyme found in various organisms, including animals and plants. It plays a key role in the digestion of starch, a carbohydrate, into sugars. (8 marks)

a The secondary structure of amylase consists of alpha-helices and beta-sheets. Describe the bonding that maintains the secondary structure of amylase. (2 marks)

b Explain why amylase selectively catalyses the breakdown of starch but is not effective in catalysing the breakdown of other carbohydrates. (2 marks)

c Alpha-amylase is a class of amylase found in the salivary glands that operates at an optimal pH of 6.7–7.0. Explain how the activity of alpha-amylase would change outside this pH range. (2 marks)

d Acarbose is a drug used for managing type 2 diabetes by inhibiting the action of enzymes involved in carbohydrate digestion, including amylase. Explain how competitive inhibitors such as acarbose affect enzyme activity. (2 marks)

5 A student has a sample of an organic compound with the molecular formula $C_4H_4O_2$. The student performs some tests on the compound and records their observations in the table below. (8 marks)

	Observation	Conclusion
Test 1	Adding the compound to bromine water causes a colour change from orange to colourless.	
Test 2	Blue litmus turns red.	
Test 3	2 moles of NaOH reacts completely with 1 mole of the compound.	

a For each test, write a conclusion about the structure of the compound. (3 marks)

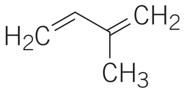
b Identify the type of reaction that occurred in Test 1. (1 mark)

c Write a balanced chemical equation for the reaction taking place in Test 3. (2 marks)

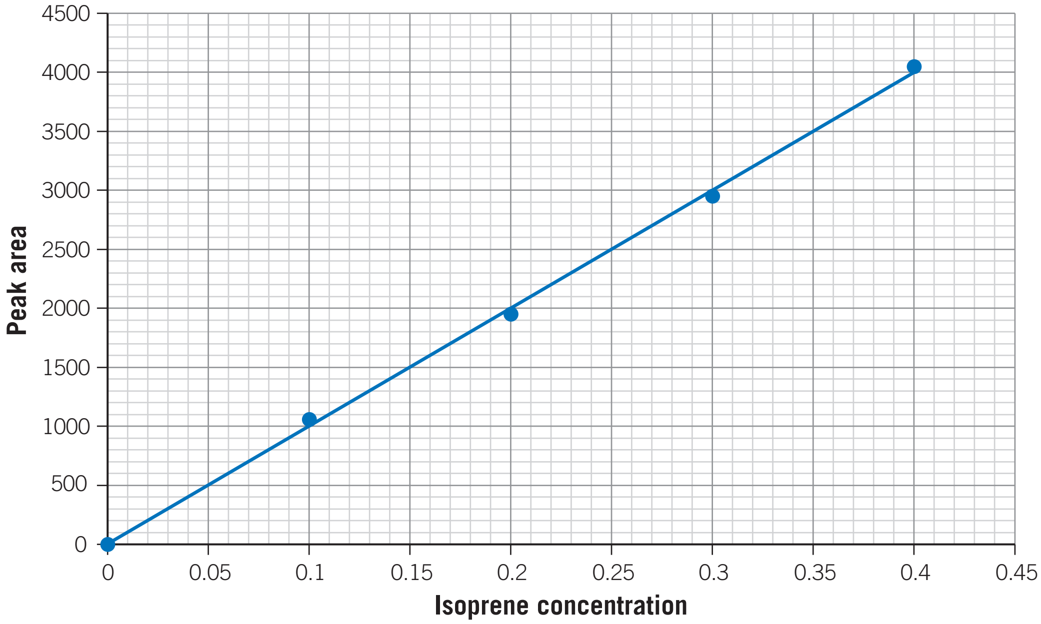
d Draw the structural formula of the initial compound. (1 mark)

e Describe an additional test that could be performed to confirm the purity of the sample. (1 mark)

6 Isoprene is a naturally occurring organic compound that is found in essential oils. The structure of isoprene is shown below.



High-performance liquid chromatography was used to determine the concentration of isoprene in a sample of eucalyptus oil. Standard solutions of pure isoprene were prepared, and a 2.0 mL sample of each standard solution was injected into the HPLC column. The calibration graph of the peak area versus concentration is shown below. A 2.0 mL sample of eucalyptus oil was injected into the HPLC column. The peak area of the sample was found to be 2400.



(5 marks)

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a Determine the concentration of isoprene in eucalyptus oil, in mg L^{-1}. (1 mark)

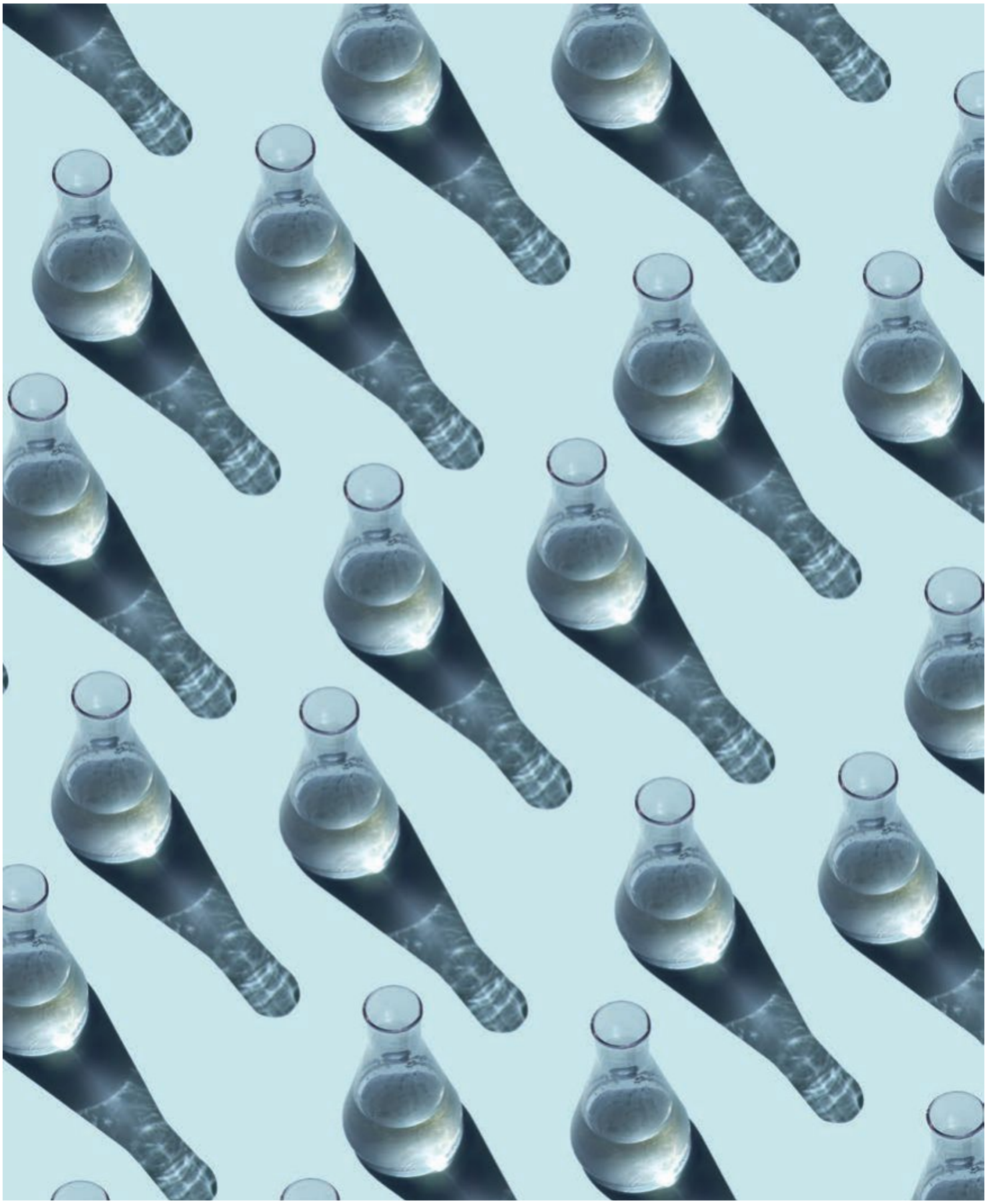
b What volume of eucalyptus oil would be required to extract 1 mg of isoprene, assuming an extraction yield of 90% could be achieved? (1 mark)

c ^{1}H and ^{13}C NMR spectroscopy were run on a sample of isoprene extracted from eucalyptus oil.

  i How many peaks would appear in the low-resolution ^{1}H NMR spectrum of pure isoprene? (1 mark)

  ii Give the integration ratio of the peaks in the ^{1}H NMR spectrum. (1 mark)

  iii How many peaks would appear in the ^{13}C NMR spectrum of pure isoprene? (1 mark)



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Appendix: Data

Periodic table

Atomic number
Relative atomic mass
Chemical symbol
Name of element

79 **Au** 197.0 Gold

GROUP

PERIOD	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 **H** 1.0 Hydrogen																	2 **He** 4.0 Helium
2	3 **Li** 6.9 Lithium	4 **Be** 9.0 Beryllium											5 **B** 10.8 Boron	6 **C** 12.0 Carbon	7 **N** 14.0 Nitrogen	8 **O** 16.0 Oxygen	9 **F** 19.0 Fluorine	10 **Ne** 20.2 Neon
3	11 **Na** 23.0 Sodium	12 **Mg** 24.3 Magnesium											13 **Al** 27.0 Aluminium	14 **Si** 28.1 Silicon	15 **P** 31.0 Phosphorus	16 **S** 32.1 Sulfur	17 **Cl** 35.5 Chlorine	18 **Ar** 39.9 Argon
4	19 **K** 39.1 Potassium	20 **Ca** 40.1 Calcium	21 **Sc** 45.0 Scandium	22 **Ti** 47.9 Titanium	23 **V** 50.9 Vanadium	24 **Cr** 52.0 Chromium	25 **Mn** 54.9 Manganese	26 **Fe** 55.8 Iron	27 **Co** 58.9 Cobalt	28 **Ni** 58.7 Nickel	29 **Cu** 63.5 Copper	30 **Zn** 65.4 Zinc	31 **Ga** 69.7 Gallium	32 **Ge** 72.6 Germanium	33 **As** 74.9 Arsenic	34 **Se** 79.0 Selenium	35 **Br** 79.9 Bromine	36 **Kr** 83.8 Krypton
5	37 **Rb** 85.5 Rubidium	38 **Sr** 87.6 Strontium	39 **Y** 88.9 Yttrium	40 **Zr** 91.2 Zirconium	41 **Nb** 92.9 Niobium	42 **Mo** 96.0 Molybdenum	43 **Tc** (98) Technetium	44 **Ru** 101.1 Ruthenium	45 **Rh** 102.9 Rhodium	46 **Pd** 106.4 Palladium	47 **Ag** 107.9 Silver	48 **Cd** 112.4 Cadmium	49 **In** 114.8 Indium	50 **Sn** 118.7 Tin	51 **Sb** 121.8 Antimony	52 **Te** 127.6 Tellurium	53 **I** 126.9 Iodine	54 **Xe** 131.3 Xenon
6	55 **Cs** 132.9 Caesium	56 **Ba** 137.3 Barium	**57–71** Lanthanides	72 **Hf** 178.5 Hafnium	73 **Ta** 180.9 Tantalum	74 **W** 183.8 Tungsten	75 **Re** 186.2 Rhenium	76 **Os** 190.2 Osmium	77 **Ir** 192.2 Iridium	78 **Pt** 195.1 Platinum	79 **Au** 197.0 Gold	80 **Hg** 200.6 Mercury	81 **Tl** 204.4 Thallium	82 **Pb** 207.2 Lead	83 **Bi** 209.0 Bismuth	84 **Po** (210) Polonium	85 **At** (210) Astatine	86 **Rn** (222) Radon
7	87 **Fr** (223) Francium	88 **Ra** (226) Radium	**89–103** Actinoids	104 **Rf** (261) Rutherfordium	105 **Db** (262) Dubnium	106 **Sg** (266) Seaborgium	107 **Bh** (264) Bohrium	108 **Hs** (267) Hassium	109 **Mt** (268) Meitnerium	110 **Ds** (271) Darmstadtium	111 **Rg** (272) Roentgenium	112 **Cn** (285) Copernicium	113 **Nh** (280) Nihonium	114 **Fl** (289) Flerovium	115 **Mc** (289) Moscovium	116 **Lv** (292) Livermorium	117 **Ts** (294) Tennessine	118 **Og** (294) Oganesson

57 **La** 138.9 Lanthanum	58 **Ce** 140.1 Cerium	59 **Pr** 140.9 Praseodymium	60 **Nd** 144.2 Neodymium	61 **Pm** (145) Promethium	62 **Sm** 150.4 Samarium	63 **Eu** 152.0 Europium	64 **Gd** 157.3 Gadolinium	65 **Tb** 158.9 Terbium	66 **Dy** 162.5 Dysprosium	67 **Ho** 164.9 Holmium	68 **Er** 167.3 Erbium	69 **Tm** 168.9 Thulium	70 **Yb** 173.1 Ytterbium	71 **Lu** 175.0 Lutetium
89 **Ac** (227) Actinium	90 **Th** 232.0 Thorium	91 **Pa** 231.0 Protactinium	92 **U** 238.0 Uranium	93 **Np** (237) Neptunium	94 **Pu** (244) Plutonium	95 **Am** (243) Americium	96 **Cm** (247) Curium	97 **Bk** (247) Berkelium	98 **Cf** (251) Californium	99 **Es** (252) Einsteinium	100 **Fm** (257) Fermium	101 **Md** (258) Mendelevium	102 **No** (259) Nobelium	103 **Lr** (262) Lawrencium

Electrochemical series

Reaction	Standard electrode potential (E^0) in volts at 25°C
$F_2(g) + 2e^- \rightleftharpoons 2F^-(aq)$	+2.87
$H_2O_2(aq) + 2H^+(aq) + 2e^- \rightleftharpoons 2H_2O(l)$	+1.77
$Au^+(aq) + e^- \rightleftharpoons Au(s)$	+1.68
$Cl_2(g) + 2e^- \rightleftharpoons 2Cl^-(aq)$	+1.36
$O_2(g) + 4H^+(aq) + 4e^- \rightleftharpoons 2H_2O(1)$	+1.23
$Br_2(l) + 2e^- \rightleftharpoons 2Br^-(aq)$	+1.09
$Ag^+(aq) + e^- \rightleftharpoons Ag(s)$	+0.80
$Fe^{3+}(aq) + e^- \rightleftharpoons Fe^{2+}(aq)$	+0.77
$O_2(g) + 2H^+(aq) + 2e^- \rightleftharpoons H_2O_2(aq)$	+0.68
$I_2(s) + 2e^- \rightleftharpoons 2I^-(aq)$	+0.54
$O_2(g) + 2H_2O(l) + 4e^- \rightleftharpoons 4OH^-(aq)$	+0.40
$Cu^{2+}(aq) + 2e^- \rightleftharpoons Cu(s)$	+0.34
$Sn^{4+}(aq) + 2e^- \rightleftharpoons Sn^{2+}(aq)$	+0.15
$S(s) + 2H^+(aq) + 2e^- \rightleftharpoons H_2S(g)$	+0.14
$2H^+(aq) + 2e^- \rightleftharpoons H_2(g)$	0.00
$Pb^{2+}(aq) + 2e^- \rightleftharpoons Pb(s)$	–0.13
$Sn^{2+}(aq) + 2e^- \rightleftharpoons Sn(s)$	–0.14
$Ni^{2+}(aq) + 2e^- \rightleftharpoons Ni(s)$	–0.25
$Co^{2+}(aq) + 2e^- \rightleftharpoons Co(s)$	–0.28
$Cd^{2+}(aq) + 2e^- \rightleftharpoons Cd(s)$	–0.40
$Fe^{2+}(aq) + 2e^- \rightleftharpoons Fe(s)$	–0.44
$Zn^{2+}(aq) + 2e^- \rightleftharpoons Zn(s)$	–0.76
$2H_2O(l) + 2e^- \rightleftharpoons H_2(g) + 2OH^-(aq)$	–0.83
$Mn^{2+}(aq) + 2e^- \rightleftharpoons Mn(s)$	–1.18
$Al^{3+}(aq) + 3e^- \rightleftharpoons Al(s)$	–1.66
$Mg^{2+}(aq) + 2e^- \rightleftharpoons Mg(s)$	–2.37
$Na^+(aq) + e^- \rightleftharpoons Na(s)$	–2.71
$Ca^{2+}(aq) + 2e^- \rightleftharpoons Ca(s)$	–2.87
$K^+(aq) + e^- \rightleftharpoons K(s)$	–2.93
$Li^+(aq) + e^- \rightleftharpoons Li(s)$	–3.04

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Glossary

Absorption band
a range of wavelengths in the IR spectrum where absorption of infrared light occurs

Accuracy
how close the measurements are to the ‘true’ value of the quantity being measured

Achiral
a shape or structure that can be superimposed on its mirror image

Activation energy
the minimum quantity of energy required so that a chemical reaction can proceed

Active site
the region of an enzyme where the substrate(s), also known as reactants, bind for a chemical reaction to take place

Actual yield
the actual quantity of product obtained from a reaction

Addition reaction
a reaction in which two or more reactants combine to form a larger product. Addition reactions require an unsaturated reactant

Aerobic
an organism or process that requires the presence of free oxygen

Aim
the main purpose of an investigation

Alcohol
a family of organic compounds characterised by a hydroxyl (–OH) functional group

Aldehyde
a molecule containing a carbonyl group where the carbon atom of the carbonyl group is bonded to a hydrogen atom. It has the general formula RCHO

Alkanol
an alkane in which a hydroxyl group (–OH) has replaced a hydrogen atom

Alkyl group
a group that is part of a larger molecule and is represented as an alkane minus a hydrogen atom, e.g. methyl ($-\mathrm{CH_3}$)

α-Glucose
a form of glucose in which the hydroxyl group on carbon 1 is on the same side of the six-membered ring as the hydroxyl group on carbon 4

Amide functional group
a functional group consisting of $-\mathrm{CONH_2}$

Amine
a family of organic compounds characterised by an amino ($-\mathrm{NH_2}$) functional group

Amino functional group
a functional group consisting of $-\mathrm{NH_2}$

Ampere
the unit used for measuring electric current; also known as amp

Amylose
a type of starch made from α-glucose units bonded to each other through α-1,4-glycosidic bonds

Anabolic
a biochemical process requiring energy, where simple molecules combine to generate complex molecules

Anaerobic
an organism or process that does not require oxygen

Analyte
a solution of unknown concentration in titration that is the subject of analysis

Anode
the electrode at which oxidation occurs. In a galvanic cell, the anode is negative

Aromatic compound
a cyclic molecule with a ring of delocalised electrons

Baeyer’s test
a test for an unsaturated carbon–carbon bond, such as an alkene

Base peak
the highest intensity peak in a mass spectrum

Biodiesel
a type of biofuel composed of the esters of fatty acids

Bioethanol
a type of biofuel produced by fermentation in plants and yeast

Biofuel
a renewable energy source produced from biological matter called biomass

Biogas
a type of biofuel formed from the breakdown of organic waste by anaerobic bacteria

Biomass
renewable organic matter that comes from plants, animals and other living organisms

Boiling point
the temperature at which a substance begins to boil, which occurs when the vapour pressure of the substance equals the atmospheric pressure

Bond strength
the amount of energy required to break apart one mole of a covalent bond in the gas state, measured in kJ mol^{-1}; also referred to as average bond energy

Branched isomer
a molecule in with the same molecular formula but different arrangement of alkyl branches

By-product
a product of a chemical reaction or industrial process that is produced as a direct result of the desired reaction, and so appears as part of the fully balanced chemical equation

Calorimetry
an experimental method by which the heat energy of food or a fuel is measured

Carbohydrate
a sugar or a saccharide, ranging from simple sugars (monosaccharides) to complex sugars (polysaccharides)

Carbonyl group
a functional group consisting of $-C=O$

Carboxyl group
a functional group consisting of $-COOH$. It consists of a carbonyl group bonded to a hydroxyl group

Carboxylic acid
a family of organic molecules characterised by the presence of a carboxyl group

Catabolic
a biochemical process releasing energy, in which complex molecules are broken down into simple molecules

Catalyse
to speed up a reaction

Catalysis
a process in which a catalyst is used to speed up a reaction

Catalyst
a substance that increases the rate of a chemical reaction by lowering the activation energy by providing an alternative reaction pathway and is itself not consumed as part of the reaction

Catalytic electrode
an electrode made from or coated with a substance that acts to speed up the rate of a reaction in an electrolytic cell

Cathode
the electrode at which reduction occurs. In a galvanic cell, the cathode is positive

Cellular respiration
the transformation of the chemical energy stored in glucose into usable energy (ATP) for cells

Chain isomer
see Skeletal isomer

Chemical energy
energy stored within the bonds between atoms

Chemical shift
the position of a signal in the nuclear magnetic resonance (NMR) spectrum relative to the signal produced by a reference compound, usually tetramethylsilane (TMS); measured in parts per million, ppm

Chiral
a shape or structure that cannot be superimposed on its mirror image. *Chiral* is from the Greek word for 'hand'

Chiral centre
an atom in a molecule that is bonded to four different groups, and these groups can be arranged in two different ways, resulting in two mirror image structures

Closed system
an environment where energy can be transferred between the reaction and the surroundings, but matter cannot

Coal
sedimentary rock containing plant remains formed over millions of years

Collision theory
the principle that allows for the prediction of the success and rate of a chemical reaction

Competitive inhibition
the process of disrupting the function of an enzyme by blocking its active site with a molecule other than the substrate

Complete combustion
a combustion reaction of organic fuel that takes place in the presence of excess oxygen gas to produce carbon dioxide and water

Complex half-equation
either the reduction or oxidation component of a redox reaction involving more than one element

Conclusion
a summary of what you can deduce from the results of the investigation, including whether the tested hypothesis was supported

Concordant
in titration, the volume of two or more titres that are within 0.10 mL of each other

Condensation reaction
a type of chemical reaction where two molecules combine to form a larger molecule with the release of a small molecule, usually water

Condensed formula
see Semi-structural formula

Conjugate redox pair
a reducing agent and its corresponding conjugate oxidising agent

Continuous data
data that is measurable and continuous, with infinite possible values; best represented by a line graph

Controlled variable
anything kept constant, or monitored, so it does not affect the independent and dependent variables, and therefore the validity of experimental results

Constitutional isomer
see Structural isomer

Coulomb
the unit used to measure the amount of electric charge something has

Crude oil
a naturally occurring mixture of liquid hydrocarbons that can be used as a fuel source

Current
the rate at which electrons flow within a circuit

Cyclic alkane
a molecule with one or more rings of saturated carbons in its structure

Cycloalkane
see Cyclic alkane

Degree of unsaturation
a calculation of the number of ring systems and double bonds (and triple bonds) in a molecule; can be shortened to DoU

Delocalised electron
an electron that is not associated with any particular atom and is free to move

Denatured
refers to an enzyme that has lost its conformational three-dimensional structure and hence cannot function as a catalyst

Dependent variable
the variable that changes in response to changes in the independent variable; the experimenter measures these changes

Dimer
a complex in which two identical or similar molecules are linked together

Disaccharide
a compound consisting of two sugar units linked by a glycosidic bond

Discharge cycle
when spontaneous chemical reactions occur converting chemical energy into electrical energy

Discrete data
data that is countable and in discrete categories; contains distinct or separate values; best represented by a bar graph

Dynamic equilibrium
when the forward and reverse reactions are occurring at the same non-zero rate

Electric charge
the amount of energy electrons carry; symbol Q

Electrical energy
energy that involves the flow of electrons and/or charged particles

Electrochemical cell
a system where electrical energy can be converted to chemical energy or vice versa

Electrochemical series
series of reduction half-cell reactions and their corresponding standard electrode potentials in order of strongest oxidising agent to weakest oxidising agent listed on the left-hand side

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Electrode
solid conducting material that can carry electric current; a connecting terminal that allows current to flow

Electrode polarity
the positive or negative charge associated with electrodes in an electrochemical cell because of reduction or oxidation occurring on their surface. In a galvanic cell, the cathode is positive and the anode is negative

Electrolysis
the process of forcing a redox reaction to occur by passing an electric current through an electrolyte

Electrolyte
a non-reactive solution or paste that enables the flow of charged particles and helps to facilitate the redox reactions

Electrolytic cell
a system in which electrical energy is converted to chemical energy

Electron transfer
the exchange of electrons that occurs during a redox reaction. Electrons are transferred from the reducing agent to the oxidising agent

Electroplating
an application of electrolysis, whereby electrical energy is used to deposit a coating of one metal onto the surface of another substance

Enantiomer
a molecule that has the same chemical formula and similar physical and structural properties to another, but the two are mirror images of each other

End point
the point in titration when the indicator changes colour

Endothermic
a reaction that has a positive enthalpy change value and absorbs heat from the environment

Enhanced greenhouse effect
the change of the normal climate equilibrium on Earth, primarily increased global temperatures; caused by increased emissions of greenhouse gases; also known as global warming

Enthalpy
the internal energy of a chemical system (plus the product of pressure and volume)

Enthalpy change
the difference in enthalpy between reactants and products in a chemical reaction; symbol ΔH

Enzyme
a protein molecule that acts as a catalyst in a specific biochemical reaction

Equilibrium
the state in which the concentration of reactants and products does not change

Equilibrium constant
the value of the reaction quotient at equilibrium; symbol K

Equivalence point
the point in a titration when the amount, in moles, of reactants is present in the stoichiometric ratio that achieves neutralisation

Ester
a molecule containing the ester functional group with the general formula RCOOR’

Ester functional group
a functional group consisting of –COO–

Esterification reaction
a type of condensation reaction that forms an ester from a carboxylic acid and an alcohol

Exothermic
a reaction that has a negative enthalpy change value and releases heat to the environment

Extent of reaction
the degree to which a reaction goes to completion

Faraday’s constant
the amount of charge that 1 mole of electrons carries ($F = 96\,500\ \mathrm{C\,mol^{-1}}$)

Fatty acid
a compound consisting of a carboxyl group with a long non-polar hydrocarbon chain, which can either be saturated or unsaturated

Fermentation
the process by which glucose is broken down in the absence of oxygen to produce energy (ATP); also called anaerobic cellular respiration

Fingerprint region
the part of an infrared spectrum that is found between 500 cm^{-1} and 1500 cm^{-1}, which, like a fingerprint, is unique and characteristic of a compound

First-generation feedstock
a biofuel produced from edible feedstocks (starch, glucose) from plants such as corn and wheat

Fluid
a substance that has no fixed shape and gives way to external pressure. Liquids and gases are considered fluids

Fossil fuel
a source of fuel made from decomposing plants and animals over hundreds of millions of years. It consists mainly of carbon and hydrogen atoms

Fracking
a process in which fluid is injected at high pressure, fracturing sedimentary rocks, releasing gas or oil

Fractional distillation
separation of a mixture of liquids into separate fractions based on their boiling points

Free radical
a short-lived uncharged molecule with an unpaired valence electron

Fuel
any substance that stores chemical energy

Fuel cell
a type of electrochemical cell that produces electrical energy from chemical energy, requiring a continuous supply of reactants

Functional group
an atom or a group of atoms in an organic molecule that largely determines the molecule's properties and reactions

Functional group isomer
a molecule with the same molecular formula and parent hydrocarbon but different types of functional groups

Galvanic cell
a system in which a spontaneous redox reaction takes place, converting chemical energy to electrical energy

Gasification
the process through which carbon-based material is converted into gas products that can be used for fuel

Global warming
the long-term warming of Earth's surface temperature, observed since the pre-industrial period

Glycerol
a compound containing three hydroxyl groups, with the chemical formula $C_3H_8O_3$

Glycogen
a highly branched polysaccharide of α-glucose joined by α-1,4 glycosidic bonds and α-1,6 glycosidic bonds. Glycogen is made by animals as a storage of energy

Glycosidic bond
the C–O–C linkage between two monosaccharide units; also called an ether bond

Green chemistry
the design of chemical products and processes that reduce or eliminate the use and generation of hazardous substances

Green hydrogen
hydrogen generated by renewable energy with lower carbon emissions than other sources of hydrogen

Greenhouse gas
a gas that absorbs and emits infrared radiation in the atmosphere, causing warming of Earth's surface

Half-cell
one half of a galvanic cell that contains an electrode submerged in a solution of ions

Half-equation
either the reduction or oxidation part of a redox reaction

Haloalkane
an alkane in which one or more halogen atoms has replaced a hydrogen atom or atoms

Halogenation reaction
a chemical reaction that involves the incorporation of one or more halogen atoms into a compound

Hazardous substance
a substance that can cause harm to your health or the environment

Heterogeneous
a mixture composed of substances in different states or phases

Homogeneous
a mixture composed of substances in the same state or phase

Homogeneous equilibrium
an equilibrium system where all of the reactants and products are in the same phase

Homologous series
a sequence of compounds that have identical functional groups and similar chemical properties but differ by a $–CH_2–$ group in their structure

Hydration reaction
a reaction in which a water molecule is added to an unsaturated molecule

Hydrogenation reaction
a reaction in which a hydrogen molecule is added to an unsaturated molecule

Hydrohalogenation reaction
a reaction in which a hydrogen halide molecule is added to an unsaturated molecule

Hydrolysis reaction
a type of chemical reaction involving the addition of water to break a larger molecule into smaller products; *hydro* refers to ‘water’, *lysis* refers to ‘breaking apart’

Hydroxyl group
a functional group characterised by –OH bonded to a carbon atom

Hypothesis
a prediction of the outcomes, which are testable experimentally and form the basis of the methodology

Incomplete combustion
a combustion reaction of organic fuel that takes place when oxygen is the limiting reagent to produce carbon monoxide and water

Independent variable
the variable for which quantities are changed by the experimenter

Inert
largely non-reactive; does not take part in a reaction

Inorganic
a chemical that does not contain both carbon and hydrogen or contains substances obtained from minerals

Integration curve
the area under a peak that directly correlates to the number of protons producing that particular signal in the spectrum

Intermediate compound
a chemical compound that is synthesised from a simpler compound and intended to be used for preparation of more complex molecules

Introduction
a detailed, but succinct, explanation of the reason for undertaking the investigation; includes key chemical concepts, aim and hypothesis

Ion
a positively or negatively charged atom that has either lost or gained electron(s)

Irreversible reaction
a unidirectional reaction where the reactants are converted to products, which cannot react further to produce the starting compounds again

Ketone
a molecule containing a carbonyl group where the carbon of the carbonyl group is bonded to two other carbon atoms. It has the general formula RCOR’

Kinetic energy
the energy an object or particle has due to its motion

Le Châtelier’s principle
If an equilibrium system is subjected to a change, the system will adjust itself to partially oppose that change and restore equilibrium

Limiting reagent (or **reactant)**
the reagent that is completely used up in a reaction and therefore limits the amount of product that can be formed

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Line of best fit
a line on a graph that shows the general trend of the data points; the distance to the points above the line should equal the distance to the points below the line

Lipid
a substance found in living systems that is derived from fatty acids. Common examples include fats and oils

Melting point
the temperature range from which a solid first starts to transition to a liquid state until this process has finished (i.e. all of the solid has become liquid or completely melted)

Method
a series of numbered steps describing the procedure

Mobile phase
the liquid or gas that flows during a chromatography experiment, which transports the compounds to be separated at different rates over the stationary phase

Molar volume
a measure of how much product is formed in a reaction, which can be calculated quantitatively

Molecular formula
the chemical formula that gives the total number of atoms of each element within a compound

Molecular ion peak
the ion peak that represents the molecular weight of the compound

Molten electrolyte
a chemical substance made from a hot liquified salt heated to over 100°C

Monomer
a molecule that forms bonds with other identical molecules as the repeating units that make up a polymer

Monosaccharide
a single sugar unit

Monounsaturated
an organic compound that contains one carbon-carbon double bond

Multiplet
the resulting peaks when peak splitting occurs in an NMR spectrum, which can provide important information about molecular structure

***n*-Alkane**
a straight-chain (unbranched) alkane

Natural gas
a fossil fuel formed when layers of decomposing plant and animal remains experience high temperatures and pressures

Non-renewable
limited or not capable of being replenished at a rate equal to consumption

Non-spontaneous redox reaction
a reaction that transforms electrical energy into chemical potential energy and has a negative cell potential (i.e. $E < 0$)

Open system
an environment where both energy and matter can be transferred between the reaction and the surroundings

Organic
a chemical that contains both carbon and hydrogen (hydrocarbons) or substances obtained from plants and animals

Outlier
a reading that is very different from other results obtained for the same measurement

Oxidation
a loss of electrons

Oxidation number
a measure of the degree of oxidation of an atom in a substance; defined as the charge an atom might have when electrons are counted to help identify redox reactions, oxidising agents and reducing agents

Oxidised
describes a chemical species that has undergone oxidation – that is, it has lost electrons in a reaction

Oxidising agent
the reactant in a redox reaction that causes oxidation. It is itself reduced and therefore will gain electrons – its oxidation number will decrease

Parent hydrocarbon
the longest continuous carbon chain in a molecule

Peak splitting
the division of a signal into several smaller peaks due to interactions with adjacent nuclei

Peptide
a short sequence of 2-amino acids joined by peptide bonds. Two 2-amino acids joined together by a peptide bond is called a dipeptide; three 2-amino acids make a tripeptide. A longer sequence is called a polypeptide. Proteins are polypeptides containing tens or thousands of 2-amino acids

Peptide bond
a chemical bond between two amino acids

Percentage atom economy
a measure of the percentage of the atoms in the reactants that are incorporated into the desired product

Percentage yield
a measure of the amount of product obtained as a percentage of the theoretical maximum amount of product that could be obtained from a reaction

Pharmacology
the branch of medicine that studies the origin, chemistry and use of drugs with their associated effects on the body

Photosynthesis
a chemical reaction in which light energy is used to convert the inorganic compounds carbon dioxide, CO_2, and water, H_2O, into the organic compound glucose; *photo* = light, *synthesis* = build or put together

Polymer
a long-chain molecule made up of a large number of smaller repeating units (monomers)

Polypeptide
a long chain of α-amino acids forming part of a protein

Polysaccharide
a compound consisting of many sugar units linked by glycosidic bonds

Polyunsaturated
an organic compound that has two or more $C{=}C$ double bonds or $C{\equiv}C$ triple bonds

Porous electrode
an electrode with tiny spaces or holes through which substances, in particular gases, can diffuse easily

Position of equilibrium
a quantitative measure of the relative amounts of reactants and products in an equilibrium system

Positional isomer
a molecule with the same molecular formula and parent hydrocarbon but different positions of functional groups

Potential difference
a difference in the amount of energy that the valence electrons have in atoms of different reactants used in galvanic cells. The greater the potential difference, the greater the voltage produced

Precision
how close all the measurements are to each other

Primary alcohol (1° alcohol)
an alcohol molecule in which the carbon bonded to the hydroxyl group is also bonded to (at most) one alkyl group

Primary amide
a molecule containing an amide functional group with the general formula $RCONH_2$

Primary cell
a type of electrochemical cell that spontaneously produces electrical energy from chemical energy; also referred to as a voltaic cell or battery

Primary data
sourced data that is collected firsthand by the researcher for a specific purpose; commonly collected through investigations, observations, interviews, field work or surveys

Protein
a polymer that consists of amino acids linked by peptide bonds

Purity
the degree to which a substance or compound is free from contaminants or other unwanted materials

Qualitative
the non-numerical characterisation of a substance or sample based on its observable properties

Qualitative data
data that is descriptive (not numeric)

Quantitative
the numerical determination of the quantity or concentration of a substance or component in a sample

Quantitative data
data that is measured and represented numerically

Random error
an unpredictable variation in the readings obtained due to variables not all being controlled (extraneous variables), resulting in the readings being higher or lower than expected

Reaction pathway
a sequence of reactions that convert a simple starting material into a desired product

Reaction quotient
the measurement of the relative amounts of products and reactants in a given reaction; symbol Q

Reagent
a chemical compound or mixture, typically inorganic, introduced to cause the desired change in an organic substance

Recharge cycle
when electrical energy is used to force a non-spontaneous redox reaction that converts electrical energy into chemical energy

Redox couple
a reducing agent, which donates electrons, and its corresponding oxidising agent, which accepts electrons

Redox reaction
a reaction involving a transfer of electrons. Both reduction and oxidation occur simultaneously

Reducing agent
the reactant in a redox reaction that causes reduction. It is itself oxidised and therefore will lose electrons – its oxidation number will increase

Reduction
a gain of electrons

Reliability
the extent to which an experiment always yields the same results under the same conditions

Renewable
a resource that can be replenished at an equal or higher rate than it is consumed

Renewable feedstock
raw material that is used to supply an industrial process and can be readily replenished

Repeatability
the ability to produce the same results when the experiment is repeated in one lab by one operator under the same conditions

Reproducibility
when the same results are obtained for the same experiment by different operators using different equipment

Resolution
the smallest change in the quantity being measured that results in a noticeable change in the value shown on the piece of measuring equipment

Retention time
the time taken from when the sample is added to the column to when it is eluted; symbol R_t

Reversible reaction
a reaction that can proceed in both directions: from reactants to products and from products to reactants

Salt bridge
connects the circuit in a galvanic cell and contains ions that balance the charges formed from each half-cell

Saponification reaction
a reaction that hydrolyses an ester under basic conditions

Saturated
an organic molecule in which all C–C bonds are single bonds

Secondary alcohol (2^o alcohol)
an alcohol molecule in which the carbon bonded to the hydroxyl group is also bonded to two alkyl groups

Secondary cell
a type of electrochemical cell that can undergo charge and discharge cycles; therefore, it can be recharged and reused

Secondary data
existing data that is collected and/or utilised by someone other than the primary investigator. Common examples include published journal articles, books or websites

Semi-structural formula
a representation of organic molecules that shows the order in which atoms or groups of atoms are connected; also called condensed formula

Simple half-equation
either the reduction or oxidation part of a redox reaction involving only one element

Single-variable exploration
an investigation that contains only one independent and one dependent variable

Skeletal formula
a representation of molecular structure in which covalent bonds are shown as zigzag lines. The symbol for all elements other than C and H are always drawn. Carbon and hydrogen are often omitted

Skeletal isomer
a molecule with the same molecular formula but differing in the arrangement of its carbon structure; also referred to as a chain isomer

Solution calorimeter
an instrument used to measure the heat absorbed or released during a chemical reaction, dissolution or neutralisation occurring in a liquid solution

Solvent extraction
a process used to separate compounds from mixtures by dissolving the desired compounds in a solvent, often with additional heating or agitation

Species
any reactant or product in a chemical reaction

Specific heat capacity
the amount of energy required to raise the temperature of one gram of a substance by one degree Celsius; symbol c

Spectator ion
a cation or anion that is present on both sides of a chemical equation and remains unchanged during the reaction

Spontaneous reaction
a reaction that takes place without the input of external energy

Standard cell potential
the theoretical amount of voltage that a galvanic cell can produce under standard conditions; also referred to as electromotive force (emf)

Standard electrode potential
the amount of voltage that can be produced by a half-cell, with reference to the standard hydrogen electrode

Standard hydrogen electrode
the hydrogen half-cell consisting of hydrogen gas, $H_2(g)$, and hydrogen ions, $H^+(aq)$. It is used as a reference against which the standard electrode potentials for all other half-cells are determined

Standard laboratory conditions
refers to the standard laboratory conditions (SLC) of 25°C and 100 kPa, as specified by the International Union of Pure and Applied Chemistry (IUPAC)

Standard solution
a solution that contains a precisely known concentration; often used in volumetric analysis

Starch
a polysaccharide of α-glucose joined by glycosidic bonds. Starch is made by plants as a storage of energy

Stationary phase
a solid, liquid or gel that remains static during a chromatography experiment

Stoichiometric
the quantity of reagents, as a molar ratio, as prescribed by the balanced equation of a reaction

Stoichiometry
the quantitative relationship between two or more substances during a reaction, based on the ratio in which they react

Straight-chain alkane
an alkane consisting of a continuous chain of carbon atoms

Structural formula
a representation of how the individual atoms of the compound may be arranged in three-dimensional space

Structural isomer
a molecule with the same molecular formula but different connectivity of atoms; also referred to as a constitutional isomer

Substitution reaction
a reaction in which an atom or group of atoms is replaced by another atom or group of atoms

Substrate
reactant molecule(s) that binds to the active site of an enzyme and then takes part in a reaction

Surface area
a measure of the area of a solid that is exposed and able to react

Systematic error
when the readings obtained from measurements differ from the ‘true’ value consistently in one direction every time

Tertiary alcohol (3^{o} alcohol)
an alcohol molecule in which the carbon bonded to the hydroxyl group is also bonded to three alkyl groups

Theoretical yield
the theoretical maximum quantity of product that could be obtained from a reaction if all the limiting reagent is converted to the product

Title
the research question under investigation; includes information about what is being tested

Titrant
a solution of known concentration that is added in titration

Transesterification
a reaction involving an ester and an alcohol to form a new ester. The alcohol involved becomes the new alkyl group of the ester product

Triglyceride
an organic compound in which the three hydroxyl groups of glycerol form esters with three fatty acid molecules

True value
the value or range of values that would be obtained if the quantity could be measured perfectly

Ultraviolet light
a form of electromagnetic radiation with wavelengths shorter than those of visible light and hence is invisible to most humans

Unsaturated
a molecule that has one or more $\mathrm{C=C}$ double bonds or $\mathrm{C\equiv C}$ triple bonds

Valence electron
an electron found in the outermost shell of an atom

Valence shell
the outermost shell of an atom

Valence shell electron pair repulsion (VSEPR)
a model used to predict the geometric shape of molecules based on the number of valence shell electron pairs surrounding the central atoms in molecules

Validity
the extent to which all variables in the experiment have been controlled, so that the independent variable is the only factor that changes

Vapour pressure
the pressure exerted by the gas particles of a substance just above its liquid or solid phase

Viscosity
a measure of a fluid’s resistance to flow

Voltage
the amount of electrical potential that exists between two points

Voltmeter
an instrument used for measuring electrical potential

Waste
unwanted substances that have no further value in production

Wavenumber
a measure of frequency denoting the number of wavelengths per unit distance, usually in reciprocal centimetres (cm^{-1}), with higher values corresponding to higher energy transitions in a molecule

Zwitterion
a molecule with equal positive and negative charges, giving it an overall neutral charge; also called a dipolar ion

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