

2025 specification  
first exams in 2026

# Course Companion

for Pearson Level 3 AAQ BTEC National  
in Applied Science (Extended Certificate)

*Unit 2 Principles and Applications of Chemistry*

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# Teacher's Introduction

Thank you for choosing this course companion which has been written specifically for the Level 3 BTEC National Extended Certificate in Applied Science (AAQ) qualification (first teaching from September 2025).

The theory notes and recap questions cover the essential knowledge and understanding prescribed in the BTEC Unit 2 specification.

## About Unit 2: Principles and Applications of Chemistry

Unit 2 <sup>(60 GLH)</sup> is assessed using a 1 hour (50-mark) written examination, which is set and marked by Pearson. There are two opportunities for assessment each year – in January and in May/June.

Unit 2 is a mandatory unit and will be assessed in a variety of styles, such as: multiple-choice questions, calculations, short-answer questions and extended-response questions.

Each of the five *learning aims* (A–E) is given its own section in the resource. These are as follows:

- A. Atomic and electronic structure
- B. Bonding and structure
- C. Periodicity
- D. Physical chemistry
- E. Organic chemistry

### Remember!

Always check the exam board website for new information, including changes to the specification and sample assessment material.

Within each section there are student notes covering the specification content and structure. These aim to break down the content into manageable chunks, further supported with diagrams, images and examples of how to structure answers. Questions are interspersed throughout the guide to test and develop understanding. Suggested answers are included at the back of this resource.

NB the intention of these is to save the teacher time, rather than to offer a comprehensive set of definite answers. In some cases, there are equally valid alternative answers to those that have been given.

Best wishes and good luck to you and your students!

April 2025



# A: Atomic and electronic s

## A1.1 Features of the periodic table



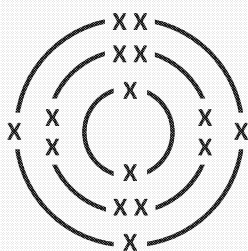
### Key points covered

- Use of symbol, atomic number and mass number to determine numbers of subatomic particles
- Use of groups and periods to determine arrangement of electrons
- Use of relative atomic mass to determine relative abundance of isotopes, and relative formula mass

### The periodic table

The periodic table is a first reference for chemists everywhere. It can be found in almost all science laboratories across the world, from teaching classrooms to research facilities. As of 2024, the periodic table consists of 118 elements arranged into **groups** and **periods** and ordered by increasing atomic number.

In your previous science studies you have learnt that the arrangements of electrons in an atom can be linked to its position within the periodic table. The number of electrons located in an atom's outer shell corresponds to the *group* you would find it in. The number of energy levels (shells) indicates the element's *period*.



#### Example:

The sketch of the atom shown can help you determine its position in the periodic table and therefore its identity.

The atom shown has five electrons on its outer shell, meaning it is in group 5. It has three shells in total, meaning it is in period 3. This element is phosphorus.

Each element on the periodic table is accompanied by select pieces of information:

- A chemical symbol
- The atomic (proton) number
- The mass number

mass  
number

atomic  
number

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### Test your knowledge

- What period would you find sulfur in?
- What group would you find boron in?
- Use its position in the periodic table to sketch the arrangement of electrons in an atom of sulfur.

**Discussion question:** despite having one electron in its outer shell, hydrogen is in group 1 of the periodic table. Suggest why.

## Subatomic particles

Atoms do not only consist of electrons. There are three subatomic particles which make up the atom: protons, neutrons and electrons. An atom is identified by the number of protons. All atoms of the same element will contain the *same number* of protons. Elements are arranged in ascending order of protons, and this is shown as the **atomic number**.

Whilst all atoms of magnesium (atomic number 12) will contain 12 protons, and all atoms of sulfur (atomic number 16) contain 16 protons, the number of neutrons found in atoms of the same element can vary. Elements usually consist of a mixture of **isotopes**. The number of neutrons in an atom can be calculated by subtracting the atomic number from the mass number.

$^{23}_{11}\text{Na}$

**Example:**

This atom of sodium has a mass number of 23 and an atomic number of 11. It has 11 protons and  $(23 - 11) = 12$  neutrons in the nucleus of this atom.

Atoms are electrically neutral due to an equal amount of positively charged protons and negatively charged electrons. **Ions** of an element will contain the same amount of protons as the original atom, but a different number of electrons due to a loss or gain during chemical reactions.

- **Cations** are positively charged ions. They have fewer electrons than protons, e.g.  $\text{Ca}^{2+}$  has two fewer electrons than protons.
- **Anions** are negatively charged ions. They have more electrons than protons, e.g.  $\text{N}^{3-}$  has three more electrons than protons.

### Test your knowledge

- State the number of subatomic particles in a neutral atom of oxygen-16 (protons, electrons and neutrons).
- Describe the differences in the physical properties of oxygen-16 and oxygen-18.

**Discussion question:** explain why different isotopes of an element have different physical properties but the same chemical properties.

## Relative atomic mass, $A_r$

The information given on the periodic table of elements includes a value for relative atomic mass. This number is often a decimal number – this is due to the fact that it is an *average* value of the mass of this element taking into account all isotopes of this element that exist and their relative abundances.

Relative atomic mass (RAM) is calculated using the following equation:

$$\text{RAM} = \frac{[(\text{mass of isotope 1} \times \text{abundance of isotope 1}) + (\text{mass of isotope 2} \times \text{abundance of isotope 2}) + \dots]}{\text{Total abundance}}$$

### Example:

Chlorine exists naturally as two main isotopes: chlorine-35 (75.8 %) and chlorine-37 (24.2 %). Calculate the relative atomic mass of chlorine.

$$\text{RAM} = \frac{[(\text{mass of isotope 1} \times \text{abundance of isotope 1}) + (\text{mass of isotope 2} \times \text{abundance of isotope 2})]}{\text{Total abundance}}$$

$$\text{RAM} = \frac{[(35 \times 75.8) + (37 \times 24.2)]}{100} = 35.484 = 35.5 \text{ to 1 decimal place}$$

The value of an element's relative atomic mass gives some indication of the relative masses of the isotopes that makes up the element. An element made from two main isotopes with a relative atomic mass of 35.5 suggests a 50 : 50 distribution of isotopes. If the relative atomic mass is closer to the mass value of one isotope than the other it suggests that this is the more natural isotope.

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## Relative formula mass

Two or more different elements chemically bonded together form a compound. If atoms within that compound are combined then you will have calculated the relative substance, as shown below.

- $K_2O = (A_r K \times 2) + A_r O = (39.1 \times 2) + 16.0 = 94.2$
- $Mg(NO_3)_2 = A_r Mg + 2 \times [A_r N + (A_r O \times 3)] = 24.3 + 2 \times [14.0 + (16.0 \times 3)] = 148.3$

?

### Recap questions: Features of the periodic table

- Sulfur is a mixture of four isotopes:  $^{32}\text{S}$ ,  $^{33}\text{S}$ ,  $^{34}\text{S}$  and  $^{36}\text{S}$ . Compare these isotopes. (3 marks)
- Determine the relative formula mass of ammonium carbonate,  $(\text{NH}_4)_2\text{CO}_3$ .
  - A group 1 sulfide,  $\text{M}_2\text{S}$ , has a relative formula mass of 267.2. Determine the relative atomic mass of M. (2 marks)
  - An unsaturated hydrocarbon,  $\text{C}_x\text{H}_y\text{O}_2$ , is analysed via a mass spectrometer. Determine the values of x and y in the chemical formula. (3 marks)
- A sample of potassium (atomic number = 19) was analysed in a mass spectrometer. The spectrum produced showed the following composition of isotopes:

Isotope	Abundance (%)
$^{39}\text{K}$	93.20
$^{40}\text{K}$	0.07
$^{41}\text{K}$	6.73

- Calculate the relative atomic mass of the potassium and give your answer to two decimal places. (2 marks)
  - Determine the number of each subatomic particle present in the  $^{40}\text{K}$  atom. (2 marks)
- Chlorine has a relative atomic mass of 35.5. Chlorine exists as two isotopes. Explain what information the relative atomic mass gives you about the abundance of the isotopes. (2 marks)

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# A1.2 Electronic structure



## Key points covered

- Use of shells, subshells and electronic orbitals in electronic structure
- Use of the rules around electronic filling in atoms
- Writing electronic notation and electron configuration
- Use of blocks to determine electronic structure in atoms and ions

## Electrons and shells

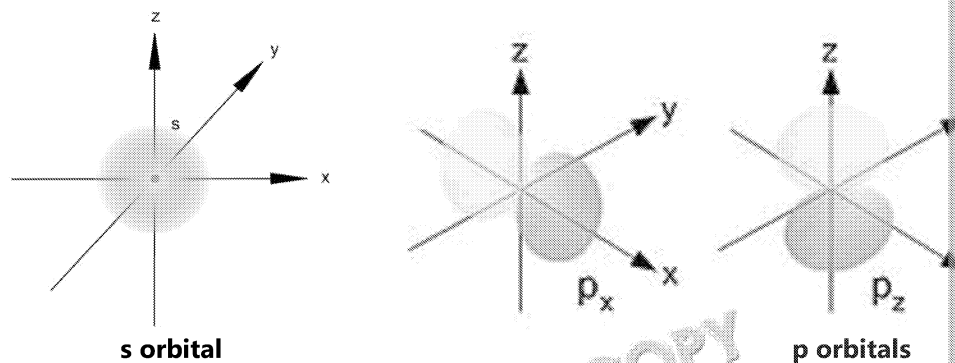
The nucleus of any atom is surrounded by shells of electrons. These shells can be regarded as energy levels, with the energy increasing as the shell number increases. Shells are made up of atomic **orbitals**. Orbitals can hold up to two electrons and can exist as different types: s, p, d and f. Within a shell, orbitals of the same type are grouped together as subshells.

Each shell contains a designated amount of electrons as shown in the table.

Shell number	Number of electrons
1	2
2	8
3	18
4	32

## Atomic orbitals

An atomic **orbital** is a region of space around the atom's nucleus that can hold up to two electrons. There are four different types of **orbital** and each one is a different shape. You should know about s orbitals and p orbitals.



Each shell contains a specific arrangement of orbitals and within each shell orbitals are grouped together as subshells. Whilst this is not confusing, it is easier to think of it as

Shell number	Subshells are present?	Number of each orbital type				Number of electrons in subshells
		s	p	d	f	
1	1s	1				2
2	2s + 2p	1	3			2 + 6
3	3s + 3p + 3d	1	3	5		2 + 6 + 10
4	4s + 4p + 4d + 4f	1	3	5	7	2 + 6 + 10 + 14

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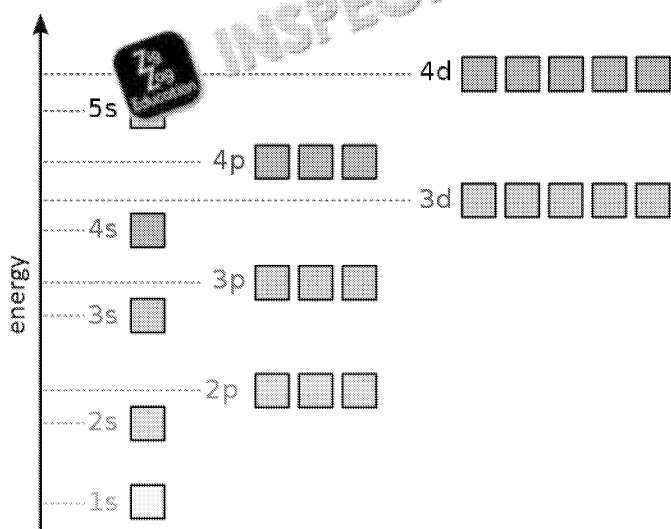
## Filling of orbitals

Electrons are placed into orbitals following a set of specific rules.

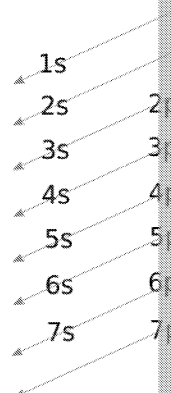
### Aufbau principle

Shells are made up of subshells and each set of subshells within an energy level has a slightly different energy level. Each time a new subshell is added it is slightly higher in energy than any subshells that were previously present. For example, in the second energy level the new subshell introduced is the 2p and it is at a higher energy level than the 2s. The Aufbau principle states that orbitals will fill up in order of increasing energy.

- In the second energy level shell the order of filling is 2s, 2p
- In the third energy level shell the order of filling is 3s, 3p, 3d
- In the fourth energy level shell the order of filling is 4s, 4p, 4d, 4f



Arrangement of orbitals according to energy levels



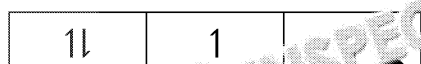
Order of filling of orbitals based on energy

Due to the fact that the highest energy level subshell in the third shell overlaps with the 4s subshell in the fourth energy level, you find that the 3d subshell is filled after the 4s subshell.

### Hund's law

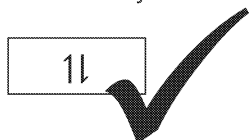
Within a subshell the orbitals are all equivalent in energy. When placing electrons in a subshell, Hund's law states that the orbitals must all be singly filled before any pairing occurs to minimise the effect of any repulsive forces coming from paired electrons until absolutely necessary.

For example, when placing four electrons into the 2p subshell, a single electron would be placed in each of the three orbitals (2p<sub>x</sub>, 2p<sub>y</sub>, and 2p<sub>z</sub>) before then pairing electrons in one of the orbitals.



### Pauli exclusion principle

Each orbital can hold a maximum of two electrons. Electrons have a property called spin. Spin is shown by an arrow pointing either up ↑ or down ↓. Electrons are fermions and two electrons in a closed space will repel each other. To help counteract the repulsive forces between charged electrons in an orbital they must have opposite spins.



### Test your understanding

- What is the order of filling of orbitals in the second energy level?
- What is the order of filling of orbitals in the third energy level?
- What is the order of filling of orbitals in the fourth energy level?

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## Electronic configurations

You are expected to be able to write out electronic configurations for all atoms and including krypton.

An atom of krypton has 36 electrons. The table below shows how these electrons

Energy level	1	2		3	
Subshell	1s	2s	2p	3s	3p
No. of electrons	2	2	6	2	6

As dictated by the Aufbau principle, the 4s subshell is filled before the 3d due to be

This filling of subshells can be shown in two ways: s, p and d notation or electron-in-

s, p and d notation of krypton's electronic configuration:  $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2$

It is worth noticing that although the 4s is filled first, it is written after 3d so that all

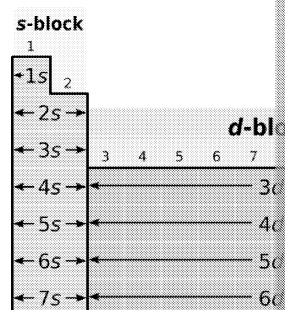
Electron-in-box diagram of krypton's electronic configuration:

↑↓	↑↓	↑↓ ↑↓ ↑↓	↑↓	↑↓ ↑↓ ↑↓	↑↓ ↑↓ ↑↓ ↑↓
1s	2s	2p	3s	3p	3d

When forming ions the electrons are lost from the highest energy orbital first. For example, sodium atoms form  $\text{Na}^+$  ions and oxygen atoms form  $\text{O}^{2-}$  ions as shown in the table on the right.

Species	Number of electrons
Na	11
$\text{Na}^+$	10
O	8
$\text{O}^{2-}$	10

When creating ions from d-block elements, the electron is removed from the 4s before the 3d, despite being filled first. This is due to the fact that once filled, the energy of the 3d subshell drops below that of the 4s and it is the higher energy subshells that are emptied first.



### Electronic configuration and the periodic table

The periodic table is divided into **blocks** as shown on the right:

The block an element is located in can be identified using the highest energy subshell.

- s-block elements have their highest energy electron in an s subshell
- p-block elements have their highest energy electron in a p subshell
- d-block elements have their highest energy electron in a d subshell

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### ? Recap questions: Electronic structure

- The number to each question below is a number.
  - The number of electrons a 3p orbital can hold. (1 mark)
  - The number of full shells in a krypton atom. (1 mark)
  - The maximum amount of electrons in the 3d subshell. (1 mark)
  - The number of unpaired electrons in a sulfur atom. (1 mark)
  - The maximum number of electrons in the third energy level. (1 mark)
- Draw out the electron-in-box diagram to show the electronic configuration of sulfur. (4 marks)
- Describe how the highest energy subshell is filled in an atom of sulfur. (4 marks)



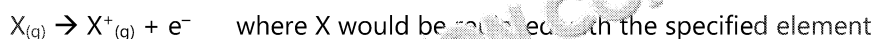
## A1.3 Ionisation energy



### Key points covered

- Definitions and equations to represent ionisation energies of atoms
- Use of ionisation energies to support ideas of electronic structure
- Exploring trends in period and down a group

**Ionisation energy** is a measure of how easily an atom loses an electron. It can be represented in equation form as follows:



An atom will have multiple ionisation energies, the total of which will be equal to the total amount of electrons the atom contains. Successive ionisation energies are defined in the same way as the first ionisation energy; however, you do need to be careful when identifying the species losing the electron. The number of the ionisation energy is the same as the charge formed on the resulting ion; for example, the third ionisation energy for an element will result in the 3+ ion being formed from a starting 2+ ion.

### Test your knowledge

- Give the definition of ionisation energy.
- Give the equation for ionisation energy.
- How many electrons would there be in a 3+ ion?

### Example:

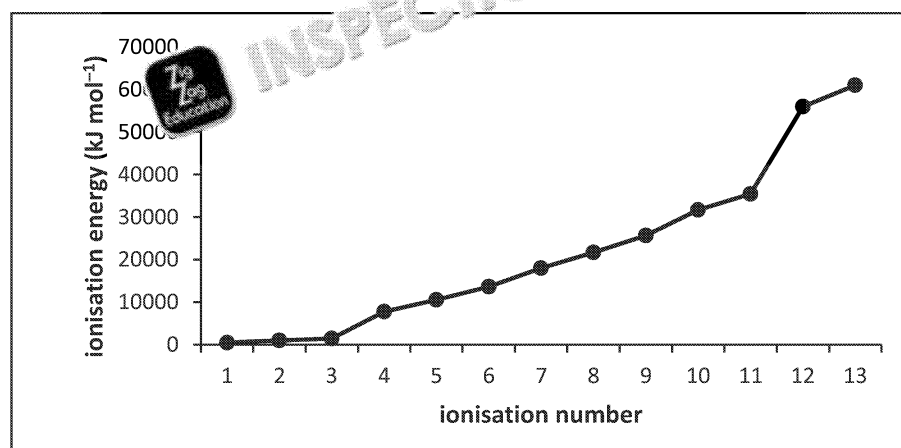
The equation representing the fourth ionisation energy for sodium would show the 3+ ion. It would be written as:  $Na^{3+}_{(g)} \rightarrow Na^{4+}_{(g)} + e^{-}$

## Making predictions using ionisation energies

Looking at the successive ionisation energies an atom has can tell you a variety of pieces of information regarding the electronic structure of that atom.

Each time a successive electron is removed from an atom, the ionisation energy always increases. This is due to the nuclear attraction on any remaining electrons increasing and therefore more energy being required to remove subsequent electrons. By studying the trends in how the ionisation energy increases in value you can determine:

- The amount of electrons in the outer shell
- The number of shells an atom has
- The group of the periodic table an atom is in
- The identity of the atom



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When analysing successive ionisation energies the key is to look for large jumps in energy values. Each large jump signifies a move into a new shell, with the electron in focus being closer to the nucleus and therefore more strongly attracted. The data shown on page 8 shows two such large jumps in ionisation energy, between ionisation 3 and 4 and then again between 11 and 12. This suggests that electrons 4 and 12 are being taken from new shells, closer to the nucleus and being held more tightly.

- Energy level 3 (the outer shell) contains three electrons
- Energy level 2 contains eight electrons
- Energy level 1 (closest to the nucleus) contains two electrons

All this evidence points to the atom being aluminium.

## Factors affecting ionisation energy

Electrons are held in their shell due to attraction from the nucleus. There are three factors which affect the strength of the nuclear attraction and subsequently the ionisation energy.

### Test yourself

Where would you expect to find the highest ionisation energies of the elements?

#### 1. Nuclear charge

As the number of protons in the nucleus increases, the strength of the nuclear attraction increases. Therefore the greater the attraction between nucleus and electron.

#### 2. Number of shells

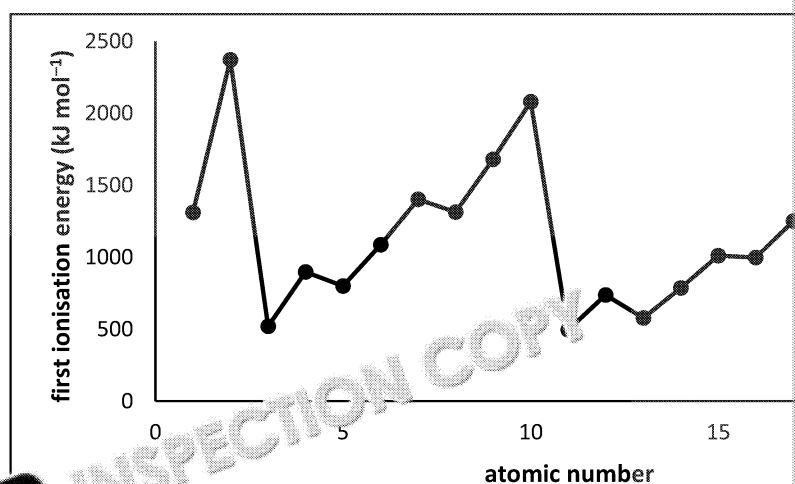
The larger the number of shells, the greater the distance between the nucleus and the outer electrons. Nuclear attraction will be weaker with increasing distance.

#### 3. Shielding

The more shells of electrons there are, the greater the effect of shielding of the outer electrons by the inner shell electrons. Shielding reduces the nuclear attraction between the nucleus and outer electron.

## Trends in ionisation energy

The graph below shows the first ionisation energy for the first 21 elements on the periodic table. You can see that there are repeating patterns in ionisation energy as you go down a group.



### Down a group

As you go down a group, the first ionisation energies decrease. Despite the increasing nuclear charge, down the group this is outweighed by the increasing distance from the nucleus of the outer electron and the increased shielding from inner shells.

### Across a period

As you go across a period, the first ionisation energy will generally increase. Each element has one more proton in its nucleus, increasing its nuclear charge. The outer shell electron is placed in the same shell as the previous element, therefore experiences the same level of shielding as the previous electron. This causes the nuclear attraction to increase and as a result the atomic radius decreases.

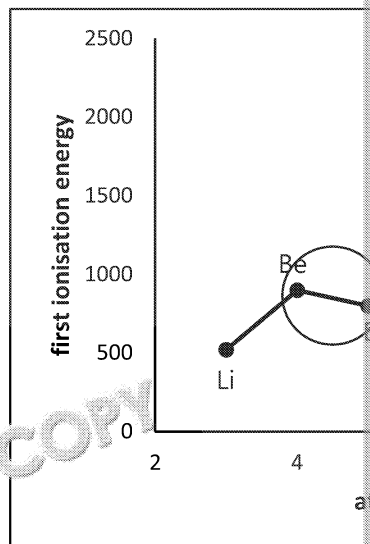
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### Subshells and first ionisation energies

Despite the general trend being an increase in ionisation energy as you go across a period, there are repeating patterns in the periodic table where anomalies seem to occur and ionisation energy falls. Considering period 2, these two anomalies can be observed between beryllium and boron and then between nitrogen and oxygen. Both of these can be explained by considering the subshells.



### Comparing beryllium to boron

The outer electron in boron is located in the 2p subshell. This subshell is higher in energy than the 2s containing the outer electron of beryllium and therefore the electron requires less energy to be removed.

### Comparing nitrogen to oxygen

Both nitrogen and oxygen have their outer shell electron in the 2p subshell. However, nitrogen is occupying singly filled orbitals. Oxygen's extra electron is placed into a half-filled orbital from the electron already in there which means oxygen's outer electron is lost more easily.



### Recap questions: Ionisation energy

- Write equations to represent the first two ionisation energies for oxygen, and state how ionisation energies always increase. (4 marks)
- The first six ionisation energies for a period 3 element are

Ionisation number	1	2	3	4
Energy (kJ/mol)	578	1817	2745	11 577

Suggest the identity of the element and give your reasoning. (3 marks)

- Explain why the first ionisation energy of Al is lower than that of Mg. (2 marks)
  - Explain why the first ionisation energy of S is lower than that of P. (2 marks)

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# B: Bonding and structure

## B1.1 Metallic bonding and giant metallic lattices

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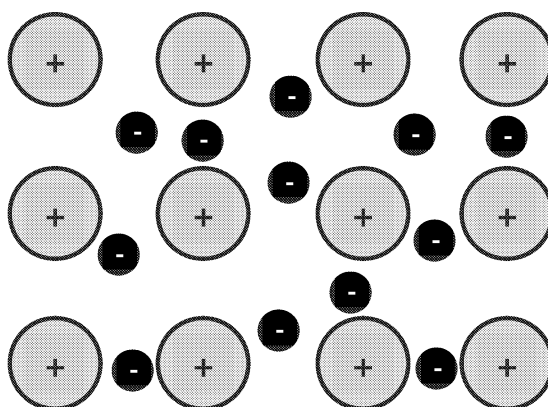
### Key points covered

- Description of metallic bonding in terms of the species involved
- Diagrammatic representation of metallic bonding

Metallic bonding is the strong electrostatic attraction between metal **cations** and a sea of **delocalised electrons**. The metal atoms are held together in a giant metallic lattice.

Each metal atom has its outer shell electrons to a shared pool of electrons; these are known as delocalised. The resulting cations are held in position while the delocalised electrons are mobile and free to move through the structure.

In the metal shown, the 12 cations are balanced by the 12 delocalised electrons present. In metals that form 2+ cations you would expect to see double the amount of delocalised electrons, resulting in a stronger electrostatic attraction.



### Test your knowledge

Use the idea of metallic bonding to explain why the bonding in aluminium metal is stronger than in sodium metal.

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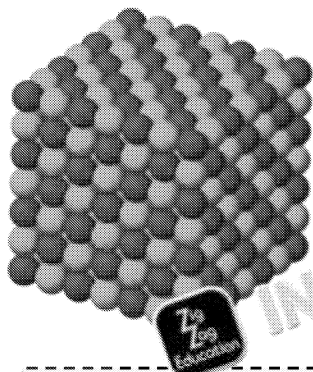
## B1.2 Ionic bonding and giant ionic structures

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### Key points covered

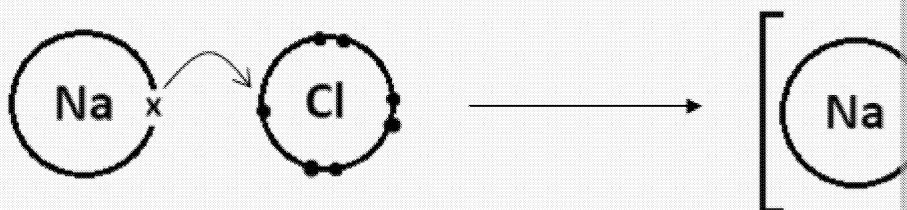
- Description of ionic bonding in terms of the species involved
- Diagrammatic representation of ionic bonding



Ionic bonding is the strong **electrostatic attraction** between oppositely charged ions. Each ion attracts oppositely charged ions in all directions and as a result a giant ionic lattice is formed.

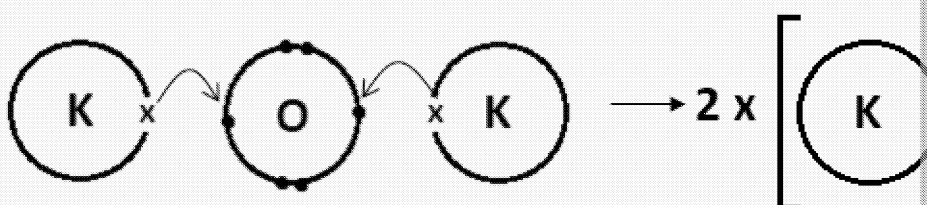
In most ionic compounds a metal atom transfers its outer electron to a non-metal atom so both resulting ions have full outer shells, i.e. noble gas configuration.

### Example 1 – Sodium chloride (NaCl)



A sodium atom contains one electron in its outer shell, whilst chlorine has seven. One electron is transferred from sodium to chlorine forming a positively charged sodium ion and a negatively charged chloride ion. The ratio of each ion in the resulting giant ionic lattice is 1 : 1 (NaCl).

### Example 2 – Potassium oxide (K<sub>2</sub>O)



A potassium atom contains one electron in its outer shell, whilst oxygen has six. Two electrons are transferred from potassium to oxygen forming a positively charged potassium ion and a negatively charged oxide ion. The ratio of each ion in the resulting giant ionic lattice is 2 : 1 (K<sub>2</sub>O).



### Test your knowledge

- Use a dot-and-cross ionic bonding diagram to determine the chemical formula of aluminium oxide.
- Draw a giant ionic lattice to show the arrangement of ions in magnesium oxide.

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# B1.3 Covalent bonding and molecules



## Key points covered

- Definition of covalent bonding
- Using dot-and-cross diagrams to represent single, multiple and dative covalent bonds
- Recognising and drawing simple covalent structures

Covalent bonding is the strong electrostatic attraction between a shared pair of electrons and the nuclei of the bonded atoms. Covalent bonding tends to happen between atoms of non-metals to form molecules.

Covalent bonds can be single, double, triple or dative.

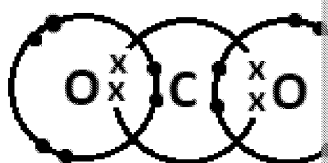
**Dative covalent bond**  
One atom provides both electrons involved in the bond.

**Double bond** – two shared pairs of electrons

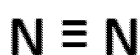
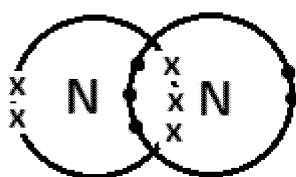
**Triple bond** – three shared pairs of electrons



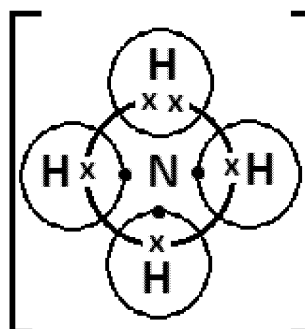
Single bond



Double bond



Triple bond



Dative bond

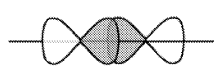
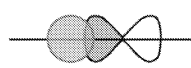
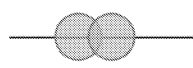
The strength of a covalent bond can be directly linked to its length; the longer the bond, the weaker it is.

Bond type	Bond strength ( $\text{kJ mol}^{-1}$ )	Bond length ( $\text{nm}$ )
O-H	464	0.096
C-C	348	0.154
C-I	238	0.238

In a covalent bond, the shared pair of electrons comes about due to an overlap of atomic orbitals. This results in two different types of covalent bonds.

## Sigma ( $\sigma$ ) bond

Formed by the overlap of one orbital from each atom in a bonding pair. The electron density is located directly between the nuclei of the two atoms.



## Pi ( $\pi$ ) bond

Formed by the sideways overlap of p-orbitals. The electron density is located above and below the plane of the bond.



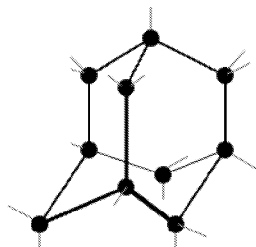
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## Allotropes of carbon

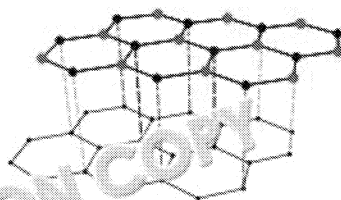
Most covalent molecules exist as simple substances where the individual molecules are held together by weak intermolecular forces. However, when carbon covalently bonds to itself, due to the four electrons it has in its outer shell, **giant covalent structures** can be formed.

**Diamond**



Each carbon atom forms four strong covalent bonds to its four neighbouring carbon atoms. The atoms arrange themselves in a tetrahedral structure with bond angles of  $109.5^\circ$ .

**Graphite**



Each carbon atom forms three strong covalent bonds and the final outer electron is added to a pool of delocalised electrons. The atoms are arranged in planar hexagonal layers with bond angles of  $120^\circ$ .

### Test your knowledge

Why do diatomic chlorine molecules contain single covalent bonds whereas oxygen molecules contain double covalent bonds?



### Recap questions: Types of bonding

- 1 Describe the type of bonding found in aluminium chloride ( $\text{AlCl}_3$ ). (4 marks)
- 2 In metallic bonding, what forms the 'sea of electrons' that allows metals to conduct heat? (2 marks)
- 3 Describe how simple covalent bonding occurs in a molecule of water ( $\text{H}_2\text{O}$ ). (4 marks)
- 4 Compare the bonding in graphite and diamond. (3 marks)

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## B1.4 Physical properties of substances



### Key points covered

- Describing and explaining the melting points of metallic, ionic and covalent substances
- Describing and explaining the boiling points of metallic, ionic and covalent substances

The physical properties of substances can be explained by looking at the structure.

### Melting points

#### Metallic

Most metals will have very high melting points. The melting point of a metal will depend on the strength of the attraction between the cations and the sea of delocalised electrons. These are strong, therefore high temperatures are needed to provide sufficient energy to overcome them.

#### Ionic

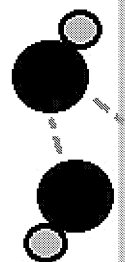
Almost all ionically bonded substances are solid at room temperature. This is due to the strong electrostatic attractions between the oppositely charged ions. A large amount of energy is needed to break the many strong electrostatic attractions between the oppositely charged ions. Therefore, high temperatures must be provided at lower temperatures. Ionic compounds will generally have high melting points. The strength of the ionic bond is affected by:

- The charge of the ion
- The size of the ion

Ions that have a larger **charge density** (larger charge, small **ionic radius**) will form stronger electrostatic attractions, and therefore have a higher melting point than those with a small charge density. For example, KCl has a lower melting point than  $\text{CaCl}_2$  due to potassium and calcium ions having a similar size but the calcium ion has a +2 charge and potassium only a +1 charge.

#### Simple covalent

When a simple covalent substance is melted or boiled it is not the strong covalent bonds between atoms that are required to be broken, but the weaker intermolecular forces that need to be overcome. The lower energy requirement of these weaker forces means that most simple covalent substances are liquid or gas at room temperature due to a low melting and boiling point.



#### Giant covalent

Unlike simple molecular substances, giant covalent structures do not require intermolecular forces to be broken during state change. In order to melt a giant covalent substance you would be required to break the strong covalent bonds between the atoms. This would require large amounts of energy and therefore substances such as diamond and graphite, have very high melting points.

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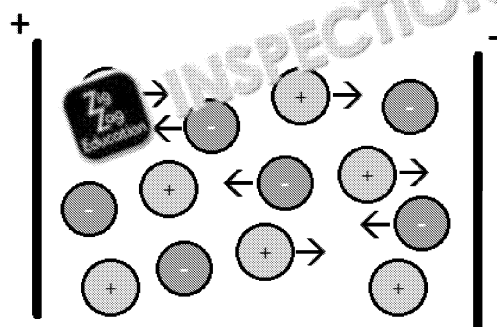
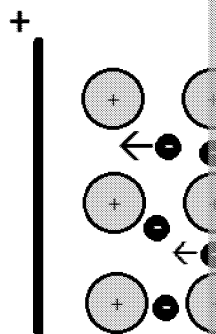
### Test your knowledge

Compare and explain the relative melting points of magnesium oxide and ammonia.

## Electrical conductivity

### Metallic

All metals can conduct electricity in any state. When a voltage is applied to a metal the delocalised electrons will carry the charge through the substance as they move.



### Ionic

In the solid state ionic substances do not conduct electricity. The ions are fixed in position in the lattice. There are no mobile charge carriers. However, if you melt the substance, the giant ionic lattice breaks down and the oppositely charged ions are free to move. Now the substance can conduct electricity.

### Simple covalent

Due to the absence of charge carriers, simple covalent substances are unable to conduct electricity.

### Giant covalent

The electrical conductivity of giant covalent structures varies depending on the substance. Most do not conduct electricity as all its outer shell electrons are involved in covalent bonding. However, in graphite and graphene there are three covalent bonds per carbon atom. The fourth electron is free to move and carry an electric current. These substances are electrical conductors.

?

### Recap questions: Physical properties of substances

Substance	Melting point / (°C)	Conductivity when solid
X	34	Poor
Y	1156	Poor
Z	987	Good

Identify, with reasons, the type of bonding in substance X, Y and Z. (6 marks)

2 Sodium has a melting point of 97.72 °C whereas magnesium melts at 650 °C. Use ideas of structure and bonding to explain the difference in these two melting points. (4 marks)

	Melting point (°C)	Conductivity at 25 °C
Aluminium oxide	2072	Poor

Use ideas of structure and bonding to help you explain the data in the above table.

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## B1.5 Molecular shape



### Key points covered

- Use of electron pair repulsion theory to determine the shape of molecules
- The names and any molecular shapes

Electron pair repulsion theory (VSEPR) is a model used in chemistry to help predict the shape of molecules. Electrons are negatively charged. When electrons are paired together, these pairs of electrons will repel one another.

- There will be a central atom and the arrangement of the electron regions around this atom will determine the shape of the molecule.
- Due to the repulsion of electron pairs, they will arrange themselves as far apart as possible to try to minimise this repulsion.
- The number of electron regions and the combination of bonding and lone pairs will result in different shapes.

It can be hard to represent a three-dimensional shape on a two-dimensional sheet of paper. A series of wedges has been created to help chemists portray and visualise molecular shapes.

A solid line represents a bond that lies in the same plane as the paper



A dotted wedge represents a bond that goes into the plane of the paper



A solid wedge represents a bond that comes out of the plane of the paper



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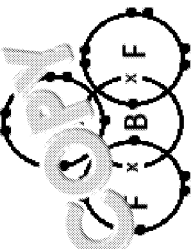
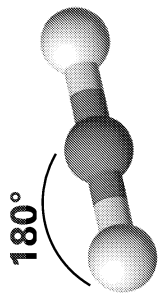
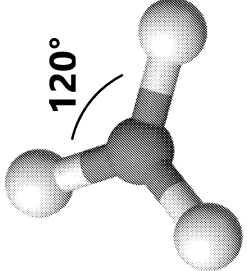
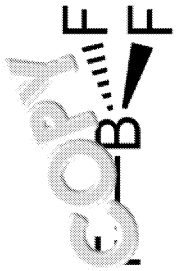


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The following table shows the main shapes, their names and the bond angles associated with 2, 3, 5 and 6

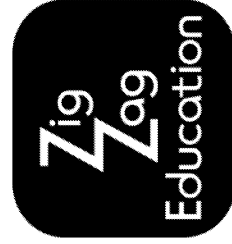
Dot-and-cross diagram	 <p>Carbon dioxide (<math>\text{CO}_2</math>)</p>	 <p>Boron trifluoride (<math>\text{BF}_3</math>)</p>	Phosph
Number of electron regions	2	3	
Shape and bond angles	 <p>180°</p>	 <p>120°</p>	
Name of shape	$\text{O}=\text{C}=\text{O}$ Linear	 <p>Trigonal planar</p>	

### Test your knowledge

Use dot-and-cross diagrams to help you predict the shape and bond an

- Sulfur trioxide ( $\text{SO}_3$ )
- Chlorine trifluoride, ( $\text{ClF}_3$ )

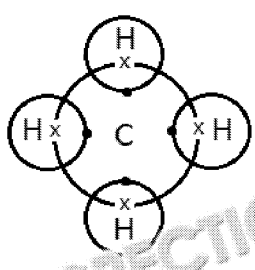
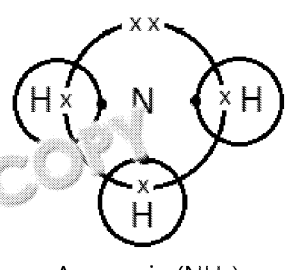
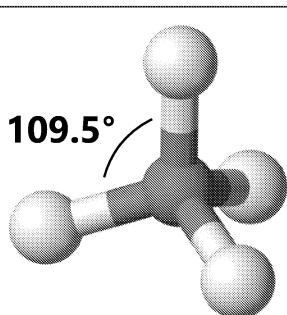
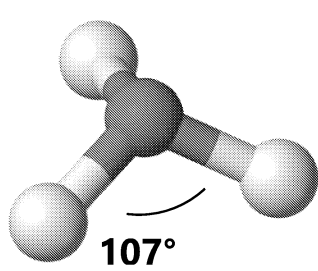
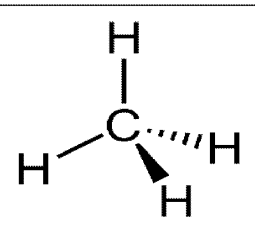
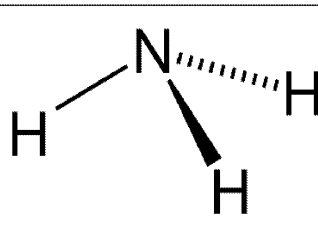
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There is a great variety of molecules which contain four regions of electron density. These regions can be bonding pairs or lone pairs. As lone pairs sit closer to the central atom and also take up more room, they will repel more strongly. Each additional lone pair repels the other regions by approximately  $2.5^\circ$ .

The different combinations of lone pairs and bonding pairs result in a variety of molecular shapes shown below.

Dot-and-cross diagram	 <p>Methane (<math>\text{CH}_4</math>)</p>	 <p>Ammonia (<math>\text{NH}_3</math>)</p>
Number of bonding pairs	4	3
Number of lone pairs	0	1
Shape and bond angles		
Name of shape	 <p>Tetrahedral</p>	 <p>Pyramidal</p>

?

### Recap questions: Molecular shapes

- For each molecule in the table below you should
  - Give the bond angle
  - Name the shape (10 marks)
  - $\text{CH}_4$
  - $\text{CO}_2$
  - $\text{PF}_3$
  - $\text{H}_2\text{O}$
  - $\text{SF}_6$
- Explain why  $\text{NH}_3$  is trigonal pyramidal whereas  $\text{BF}_3$  is trigonal planar. (5 marks)
- Antimony chloride,  $\text{SbCl}_3$ , exists as simple covalent molecules.
  - Draw the dot-and-cross diagram for this molecule. (1 mark)
  - Name the shape of this molecule. (1 mark)
  - Give the bond angles in this molecule. (1 mark)
  - Explain why it has this shape. (2 marks)

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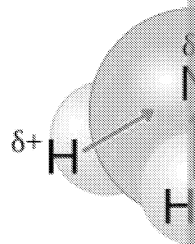
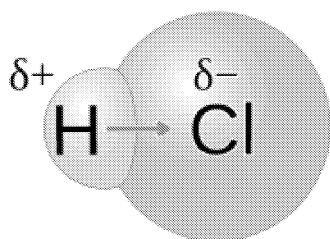
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### Key points covered

- Page 20 of 10

## Polar bonds

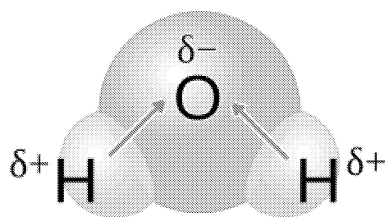
A **polar bond** is formed when a bonded pair of electrons is not equally shared between the two bonding atoms due to differing electronegativities. The atom with the greater electronegativity exerts a bigger force of attraction on the bonded electrons and will therefore experience a bigger proportion of negative charge.



Each bond shown above is polarised and contains a separation of charge. The  $\delta^-$  is the more electronegative atom in the bond and will have a partial positive charge, labelled as  $\delta^+$ . The less electronegative atom will have a partial negative charge,  $\delta^-$ . This separation of charges in a covalent bond is called a dipole. A dipole does not change and is called a permanent dipole.

## Polar molecules

If a molecule contains more than one **polar bond** the individual polar bonds can either work together to form one large overall dipole, or work against each other to cancel themselves out and leave the molecule with no dipole at all.



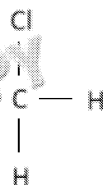
Water molecules contain two polar bonds. The bonds are acting in completely opposite directions to each other and do not cancel each other out. A water molecule is a polar molecule.

Carbon dioxide molecules also contain two polar bonds. However, these bonds are acting in completely opposite directions to each other. The effect of the dipoles is cancelled out and, despite having polar bonds, carbon dioxide is not a polar molecule.



### Recap questions: Electronegativity and polarity

- 1 Chlorine gas reacts with methane to form dichloromethane.



The Pauling value for each element in dichloromethane is shown below.

Element	Pauling value
Carbon	2.3
Hydrogen	2.1
Chlorine	3.0

Draw a 3D diagram, using dashes and wedges, to show the shape of dichloromethane. To represent any polar bonds. (3 marks)

- 2 Explain whether dichloroethane is a polar molecule. (1 mark)

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# B1.7 Intermolecular forces

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## Key points covered

- Identification of the three main types of intermolecular force
- Explaining how the three main types of intermolecular bonds are formed
- Relative strength of intermolecular forces

Intermolecular forces are responsible for the physical properties of covalent molecules. There are forces of attraction between dipoles of neighbouring molecules and these are divided into one of three categories:

1. London dispersion forces (temporary dipole-induced dipole forces)
2. Permanent dipole – permanent dipole forces
3. Hydrogen bonding

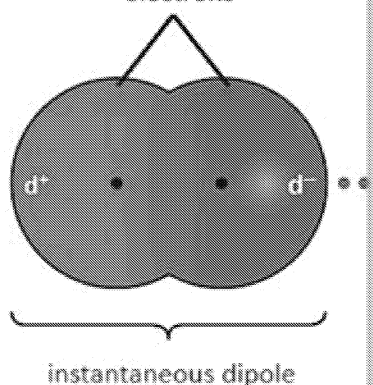
## London dispersion forces

London dispersion forces are the weakest types of intermolecular force and exist between all molecules, regardless of polarity. They are an interaction between instantaneous and induced dipoles in molecules.

### Instantaneous-induced dipoles

Electrons are not static in atoms, but instead are continuously moving. This constant movement means that at any one moment there will be an uneven proportion of the electron cloud density on one of the atoms in a bonding pair, causing an ever-changing dipole. This is known as an instantaneous dipole.

unsymmetrical distribution of electrons



The instantaneous dipole in one molecule causes a dipole to be induced in a neighbouring molecule, which then induces dipoles on other nearby molecules. These dipoles will then attract each other.

These attractions are only temporary and in the next moment will have disappeared and reformed in a different configuration.

The strength of a London force will depend on the number of electrons in the electron cloud. The larger the number of electrons, the larger the instantaneous dipole – induced dipole interaction and therefore the more energy is needed to overcome them. This will be observed as an increased boiling point.

### Permanent dipole – permanent dipole forces

When a molecule contains a permanent dipole, the attraction between the two opposite poles of the dipoles in neighbouring molecules forms an intermolecular force stronger than that of London dispersion forces.



It is important to remember that as well as having these permanent dipole – permanent dipole forces, polar molecules will also contain London dispersion forces.

#### Test yourself

Why do halogens have higher boiling points than the group 1 elements?

#### Test yourself

What is a permanent dipole – permanent dipole interaction?

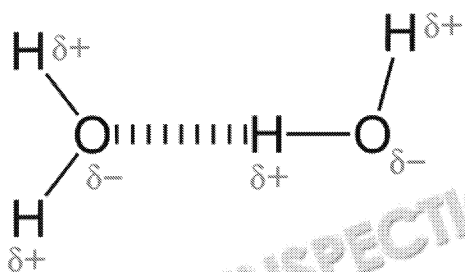
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## Hydrogen bonding

Hydrogen bonds are the strongest type of intermolecular attraction. A hydrogen bond is a permanent dipole – permanent dipole attraction formed between molecules which

- i) A highly electronegative atom which contains a lone pair of electrons (nitrogen, oxygen or fluorine)
- AND**
- ii) A hydrogen atom bonded to a highly electronegative atom (N–H, O–H or F–H)



The hydrogen bond forms between the lone pair on the electronegative atom and the  $\delta+$  hydrogen of a neighbouring molecule.

You represent hydrogen bonds using a dashed line. The geometry around the hydrogen bond is linear.

?

### Recap questions: Intermolecular forces

- 1 The boiling points of three molecules are shown in the table below.

Molecule	Boiling point
Chloromethane, $\text{CH}_3\text{Cl}$	-24
Fluorine, $\text{F}_2$	-188
Hydrogen fluoride, $\text{HF}$	20

Explain the difference in these boiling points. (5 marks)

- 2 Methanol,  $\text{CH}_3\text{OH}$ , is soluble in water as hydrogen bonds are able to form. Draw a diagram showing the hydrogen bond formed between these two molecules. Label the partial charges and lone pairs. (2 marks)

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## B1.8 Hydrogen bonding and properties of water

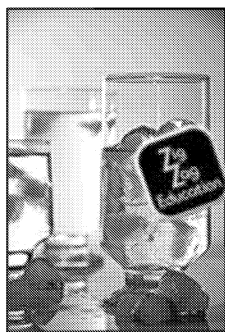


### Key points covered

- Explaining how hydrogen bonding affects the properties of water

The hydrogen bonding in water gives rise to some anomalous (unusual) properties

- Lower than expected density in the solid form
- Higher than expected melting and boiling points
- Higher than expected surface tension

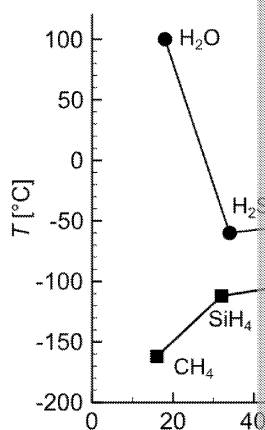


### Density

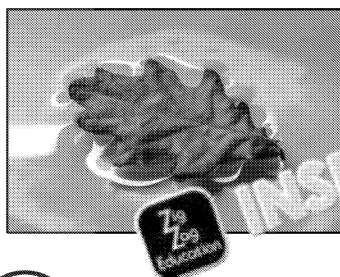
Solid water floats on top of liquid water. This is due to the ability of water molecules to form four hydrogen bonds per molecule – two from the hydrogen atoms and one from each of the lone pairs of electrons on the oxygen atoms. The hydrogen bonds that are formed extend out from the molecule, holding the molecules in an open tetrahedral lattice with large holes in. When the ice melts, the water molecules are able to move closer together again. This structure that decrease the density of the solid form of water.

### Melting and boiling point

If you were to consider the patterns and trends in boiling point of the hydrides, you would expect water to boil at  $-75^{\circ}\text{C}$  and be a gas at room temperature. But this is not the case; water boils at  $100^{\circ}\text{C}$ , considerably higher than expected. The reason for this, again, is hydrogen bonding. Like all simple covalent substances, when you try to melt or boil water it is the intermolecular forces you need to overcome and break. And just like all molecules, water has London dispersion forces that require breaking. However, water also contains hydrogen bonding and this type of intermolecular force requires a large amount of additional energy to overcome. This results in a much higher than expected melting and boiling point.



### Surface tension



Water droplets can be considered to be 'not wet' on water! This phenomenon is due to the fact that water molecules are more strongly attracted to each other than to the surface. Water on the top surface of a liquid forms hydrogen bonds to its neighbours, just like molecules in the bulk of the liquid. However, molecules on the top surface of the liquid have fewer neighbours with which to form hydrogen bonds, as they are only on the top half. This means that the hydrogen bonds that water molecules are even stronger than normal, resulting in a higher surface tension.



### Recap questions: Hydrogen bonding and properties of water

- What role does hydrogen bonding play in the density of water? (4 marks)
- How does hydrogen bonding contribute to the high melting and boiling points of water? (4 marks)
- What are the implications of water's high surface tension and how does hydrogen bonding contribute to this? (3 marks)

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! <i>Key points covered</i>	
<ul style="list-style-type: none"> <li>Describe and explain how atomic radius and ionic radius change across period 3</li> <li>Describe and explain how melting point changes across period 3</li> </ul>	<ul style="list-style-type: none"> <li>Describe and explain how electronegativity changes across period 3</li> </ul>

# Atomic Plus

Atomic radius (pm)

Element	Atomic radius (pm)
Na	160
Mg	140
Al	124
Si	114
P	109
S	104

## Ionic radius

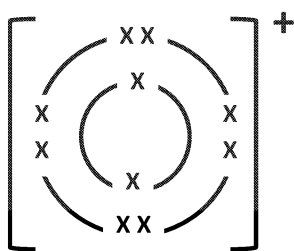
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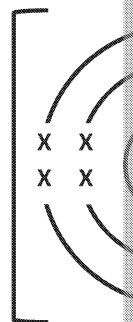




The large jump between positive and negative ions can be explained by considering the resulting ions.



Electronic structure of a positively charged ion in period 3



Electronic structure of a negatively charged ion in period 3

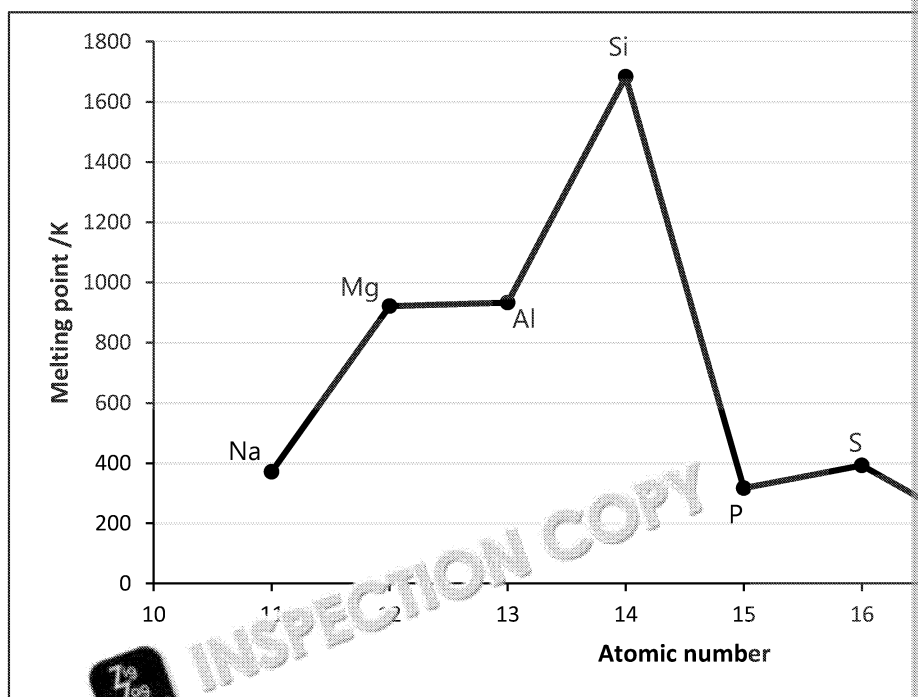
The negative ion contains an extra shell of electrons compared to the positively charged ion. This results in a large jump in ionic radius when the nature of the ion changes.

#### Test your knowledge

- Why do positively charged ions have a smaller radius than the atomic radius of the element?
- Why do negatively charged ions have a larger radius than the atomic radius of the element?

## Melting point

The melting point of a substance is linked to the strength of the attractive forces between its particles. The stronger the forces of attraction, the higher the amount of energy needed to break the bonds, resulting in a higher melting point.



It is easier to understand the reasons behind this variation in melting points if you consider the different types of bonding in these sections, based on the type of bonding the element contains.

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## Sodium – Aluminium

As you move across the first three elements of period 3 there is an increase in melting point. These elements are metals, containing metallic bonding, and therefore to make them melt you are overcoming the electrostatic forces of attraction between the sea of delocalised electrons and positive metal ions.

As you go from sodium to aluminium the amount of electrons donated to the sea of delocalised electrons increases, which also causes a greater charge on the positive metal ions. This results in a stronger electrostatic attraction which requires a larger amount of thermal energy to break.

## Silicon

Silicon is a covalent molecule with a giant structure, similar to that of diamond. The melting point is very high due to the fact that the forces between silicon atoms are strong covalent bonds that require breaking to melt.

## Phosphorus – Argon

The remaining elements in period 3 all consist of a simple covalent structure. When these elements melt, the intermolecular forces are broken and not the covalent bonds between atoms. For phosphorus and sulfur, the forces are very weak and only require small amounts of thermal energy to break.

The strength of a London dispersion force is related to the amount of electrons contained in the molecule. The more electrons, the stronger the force. Sulfur exists as  $S_8$  molecules, meaning it has a higher melting point than phosphorus,  $P_4$ , and consequently a higher melting point. Chlorine is found as  $Cl_2$  molecules.

## Electrical conductivity

Electrical conductivity is the measure of a material's ability to carry an electrical current. It depends on the presence of mobile charged particles, such as electrons and ions (see section B1.1).

As you go across period 3, the electrical conductivity of the elements initially increases to group 4 and then stays almost negligible until group 8. This trend is explained by the nature of each element.

Sodium	Magnesium	Aluminium	Silicon	Sulfur	Phosphorus
<b>Metals</b> Contain ionic bonding. As you go across the group, a further electron is donated to the sea of electrons, resulting in more electrons available to carry charge.			<b>Metalloid</b> Acts as a semi-conductor	<b>Non-metals</b> No charged particles in the elements to carry the electric current.	



### Recap questions: Properties of period 3 elements

- 1 Explain which element would have the smallest atomic radius in period 3. (4)
- 2 Describe and explain the trend in melting point for the first three elements. (4)
- 3 Explain the trend in the boiling points of phosphorus, chlorine and sulfur. (5)

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## C1.2 Oxidation numbers, oxidation and reduction



### Key points covered

- Assign oxidation numbers for elements in compounds and ions
- Define oxidation and reduction
- Write half-equations for redox reactions

A redox reaction is a reaction where both **oxidation** and **reduction** occur simultaneously. During this reaction one species will become oxidised (meaning it loses electrons) and a second species will be reduced (it gains electrons). When the redox reaction involves covalent compounds, **oxidation numbers** must be used in order to identify the oxidation and reduction processes.

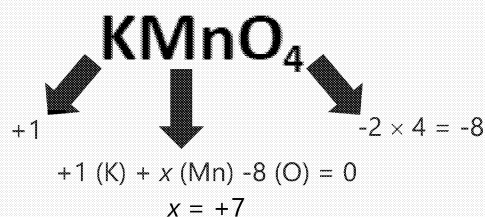
### Oxidation numbers

In order to assign an oxidation number to a species, a series of rules must be applied.

- Any element in its natural form will have an oxidation number of 0, e.g. Na, Al, O<sub>2</sub>.
- If an element is present as an ion, its oxidation number will be the same as the charge on the ion, e.g. Na<sup>+</sup> has an oxidation number of +1.
- Group 1, 2, 6 and 7 elements present in compounds will have oxidation ions matching their ionic charges.
- Oxidation numbers of species in a compound will add to a total of 0.
- Oxidation numbers in a polyatomic ion will add to a total of the charge on the ion.
- The oxidation number of oxygen in a compound is always -2 (except when in a peroxide).

#### Example 1: KMnO<sub>4</sub>

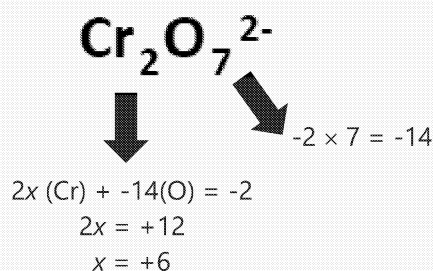
- This is a compound – the oxidation numbers of all species must add up to a total of 0.
- K is in group 1 of the periodic table, therefore in a compound it has an oxidation number of +1.
- O in a compound is always -2 (except when in a peroxide)
- Therefore Mn must have an oxidation number of +7



Oxidation numbers: K = +1, Mn = +7, O = -2

#### Example 2: Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup>

- This is a polyatomic ion – the oxidation numbers of all species must add up to a total of -2.
- O in a compound is always -2 (except when in a peroxide)
- Therefore Cr must have an oxidation number of +6



Oxidation numbers: Cr = +6, O = -2

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## Using oxidation numbers in naming

A characteristic property of transition metals is the ability to form ions with multiple oxidation numbers. When these ions then form compounds it is important to know which oxidation number they are in order to correctly determine the chemical formula.

Roman numerals are used to show the oxidation number of an element and will be placed at the end of any compound containing that species.

Number	1	2	3	4	5
Roman numeral	I	II	III	IV	V

- **KMnO<sub>4</sub>** – manganese can adopt multiple oxidation numbers. In this compound it is present in its +7 form. The systematic name is potassium manganate(VII).
- **CuO** – copper can adopt multiple oxidation numbers. In this compound it is present in its +2 form. The systematic name is copper(II) oxide.

### Test your knowledge

Can you explain the difference between an oxidation number and a charge? Can you explain the difference between a compound, a species, and an ion? Can you explain the exceptions to the rules?

## Identifying oxidation and reduction

The terms oxidation and reduction were originally used to describe reactions involving oxygen.

- A substance was said to be oxidised if it gained oxygen.
- A substance was said to be reduced if it lost oxygen.

The following equation shows both oxidation and reduction:

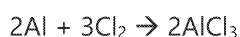


- Iron(II) oxide has lost oxygen and has therefore been reduced.
- Carbon monoxide has gained oxygen and has been oxidised.

## Redox in terms of electron transfer

A further example of redox involves the loss and gain of electrons: **OILRIG**.

The reaction below does not involve any oxygen but does involve electron transfer.



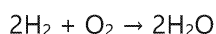
- **AlCl<sub>3</sub>** is made up of positive aluminium ions, **Al<sup>3+</sup>**, and negative chloride ions, **Cl<sup>-</sup>**.
- Aluminium atoms have lost three electrons to become **Al<sup>3+</sup>** and have therefore been oxidised.
- Chlorine atoms have gained one electron to become **Cl<sup>-</sup>** and have therefore been reduced.

## Redox in terms of oxidation numbers

In order to determine which species has been oxidised and which species has been reduced, the oxidation number of the element must be determined in both the reactants and the products.

- An increase in oxidation number between the reactant and the product indicates oxidation.
- A decrease in oxidation number between the reactant and the product indicates reduction.

Take the following reaction:

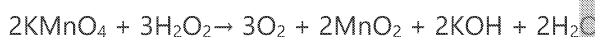


- Hydrogen starts with an oxidation number of 0 which has changed to +1 when it forms water. It has increased; hydrogen was oxidised.
- Oxygen starts with an oxidation number of 0 which has changed to -2 when it forms water. It has decreased; oxygen was reduced.

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A second, more complex example, including far more species would be:



Element	Oxidation number in reactant	Oxidation number in product
Potassium	+1	+1
Manganese	+7	+4
Oxygen	-2 (-1 in peroxide)	-2 (0 in O <sub>2</sub> )
Hydrogen	+1	+1

- Oxygen starts with an oxidation number of -1 in H<sub>2</sub>O<sub>2</sub> which has changed to 0 when in O<sub>2</sub>. The oxidation number has increased; oxygen was oxidised.
- Manganese starts with an oxidation number of +7 which has changed to +4. The oxidation number has decreased; manganese was reduced.

Potassium and hydrogen are acting as **spectator ions**.

## Disproportionation

In some chemical reactions an element is simultaneously oxidised and reduced to form two different products. A chemical reaction like this is known as disproportionation. Here is an example of involving chlorine:



In this reaction:

- Some chlorine (Cl<sub>2</sub>) is oxidised to chlorate ions (ClO<sub>3</sub><sup>-</sup>) with a +5 oxidation state.
- Some chlorine (Cl<sub>2</sub>) is reduced to chloride ions (Cl<sup>-</sup>) with a -1 oxidation state.

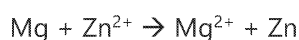
### Test your knowledge

The following reaction is a disproportionation reaction:  
 $\text{Ca} + 2\text{HCl} \rightarrow \text{CaCl}_2 + \text{H}_2$

Explain which species is oxidised and which species is reduced.

## Redox equations and half-equations

A redox equation gives the full, balanced equation for a redox reaction.



This equation can be separated out to show the oxidation and reduction processes

**Oxidation:**  $\text{Mg} \rightarrow \text{Mg}^{2+} + 2\text{e}^-$

**Reduction:**  $\text{Zn}^{2+} + 2\text{e}^- \rightarrow \text{Zn}$

If any spectator ions are present they will not appear in the half-equations, as seen in the following example:



Oxidation: Copper's oxidation number changes from 0 to +2;  $\text{Cu} \rightarrow \text{Cu}^{2+} + 2\text{e}^-$

Reduction: Silver's oxidation number changes from +1 to 0;  $\text{Ag}^+ + \text{e}^- \rightarrow \text{Ag}$

## Using half-equations to write redox equations

If you are provided with the equations that show the oxidation and reduction processes, you can combine them to give the overall, full balanced equation by following these steps:

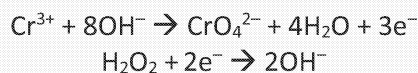
- Balance the electrons
- Combine equations and cancel out the electrons
- Cancel out any species that appear on both sides of the equation

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**Example:**

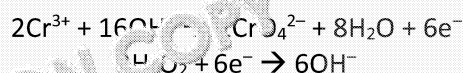
A redox reaction occurs with the following oxidation and reduction processes:



Use the half-equations to give the overall redox equation.

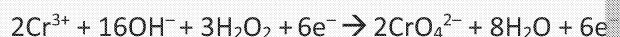
**1. Balance the electrons**

There are three electrons in the top equation (oxidation) and only two electrons (reduction). The oxidation equation needs to be multiplied by 2 and the reduction equation by 3 to give six electrons in each equation.

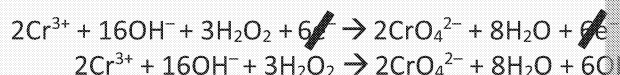
**2. Combine equations and cancel out the electrons**

Combining all products from the oxidation and reduction processes gives:  $2\text{CrO}_4^{2-} + 8\text{H}_2\text{O}$   
Combining all reactants from the oxidation and reduction processes gives:  $2\text{Cr}^{3+} + 16\text{OH}^- + 3\text{H}_2\text{O}_2$

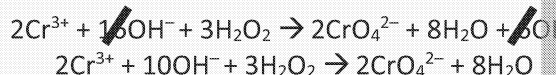
This gives the following equation:



The electrons can then be cancelled out to give:

**3. Cancel out any species that appear on both sides of the equation**

There are hydroxide ions on both the reactant and product sides of the equation. The product can be cancelled out from the 16 on the reactant side, leaving only 10.



This gives the final redox equation as being:

**Recap questions: Oxidation numbers, oxidation and reduction**

- Determine the oxidation numbers of each element in the species below. (5 marks)  
a)  $\text{Na}_2\text{CO}_3$       b)  $\text{Cr}_2\text{O}_3$       c)  $\text{CO}_3^{2-}$       d)  $\text{MnO}_4^{2-}$
- Use oxidation numbers to determine what has been oxidised and what has been reduced in the following equations. (6 marks)  
a)  $3\text{CuO} + 2\text{NH}_3 \rightarrow 3\text{Cu} + 3\text{H}_2\text{O} + \text{N}_2$   
b)  $\text{MnO}_2 + 4\text{HCl} \rightarrow \text{MnCl}_2 + \text{Cl}_2 + 2\text{H}_2\text{O}$   
c)  $\text{Mg} + \text{H}_2\text{SO}_4 \rightarrow \text{MgSO}_4 + \text{H}_2$
- Write half-equations for the following conversions and classify each change as oxidation or reduction. (10 marks)  
a)  $\text{Na} \rightarrow \text{Na}^+$       b)  $\text{Pb}^{4+} \rightarrow \text{Pb}^{2+}$       c)  $\text{H}_2 \rightarrow \text{H}^+$       d)  $\text{Br}^- \rightarrow \text{Br}_2$
- Combine the following half-equations to give the full, balanced redox equation. (6 marks)  
a)  $\text{MnO}_4^- + 8\text{H}^+ + 5\text{e}^- \rightarrow \text{Mn}^{2+} + 4\text{H}_2\text{O}$  and  $\text{Ce}^{3+} \rightarrow \text{Ce}^{4+} + \text{e}^-$  (2 marks)  
b)  $\text{H}_2\text{O}_2 \rightarrow 2\text{H}^+ + \text{O}_2 + 2\text{e}^-$  and  $\text{MnO}_4^- + 8\text{H}^+ + 5\text{e}^- \rightarrow \text{Mn}^{2+} + 4\text{H}_2\text{O}$  (2 marks)  
c)  $\text{C}_2\text{O}_4^{2-} \rightarrow 2\text{CO}_2 + 2\text{e}^-$  and  $\text{FeO}_4^{2-} + 8\text{H}^+ + 3\text{e}^- \rightarrow \text{Fe}^{3+} + 4\text{H}_2\text{O}$  (2 marks)

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## C1.3 Reactions of period 3 elements



### Key points covered

- Describe trends in the reaction of period 3 elements with oxygen
- Describe trends in the reaction of period 3 elements with water

### Reactions with oxygen

The reaction of a substance with the oxygen found in air is known as **combustion** or **oxidation**. The table below outlines the characteristics of some period 3 elements when reacting with oxygen, and the balanced chemical equations for the reactions that occur.

Element	Observations
Sodium, Na	Burns vigorously with an orange flame to produce a white solid, sodium oxide.
Magnesium, Mg	Burns vigorously with a bright white light to produce a white solid, magnesium oxide.
Aluminium, Al	Aluminium powder will burn quickly in oxygen with a white flame to produce white aluminium oxide. Sheets of aluminium will also slowly react with oxygen in the absence of a flame, to produce a layer of aluminium oxide on the surface of the metal.
Phosphorus, P	Phosphorus will ignite spontaneously in oxygen and burn with a white flame, producing white smoke. In an excess of oxygen the main product is phosphorus(V) oxide, a white solid.
Sulfur, S	Requires gentle heating to burn with a pale blue flame. A colourless, toxic gas, sulfur dioxide, is formed.

### Test your knowledge

Why does the reactivity of the period 3 metals decrease as you go across the group? Explain your answer.

**Discussion:** Phosphorus(III) oxide, a second oxide of phosphorus, phosphorus(III) oxide, is also formed when phosphorus reacts with oxygen. What conditions do you think would be required to form this oxide? What would be the formula of the oxide formed?

### Reactions with water

Period 3 elements react with water to varying degrees; however, non-metals such as silicon and phosphorus do not react with water under normal conditions. The table overleaf outlines the characteristics of some period 3 elements when reacting with water, and balanced chemical equations for the reactions that occur.

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Element	Observations
Sodium, Na	Will react with cold water in a highly <b>exothermic</b> reaction. Bubbles of hydrogen are generated and a colourless solution of sodium hydroxide.
Magnesium, Mg	Reacts much more slowly with cold water than sodium. Eventually the surface of the magnesium will become coated in bubbles of hydrogen gas and a thin layer of magnesium hydroxide is formed on the surface of the metal, causing the reaction to stop.
Aluminium, Al	Aluminium has very low reactivity with water due to the aluminium oxide coating and needs to lose three electrons. Aluminium powder will react with warm water slowly to produce aluminium hydroxide and hydrogen gas.

## Reactions with chlorine

When we mix chlorine gas with elements from the third period of the periodic table each element reacts uniquely. The products formed are known as chlorides. The table below outlines the characteristics of some period 3 elements when reacting with chlorine, and balanced chemical equations for the reactions that occur.

Element	Observations
Sodium, Na	Will burn easily in chlorine with an orange flame. The sodium chloride produced is a white solid.
Magnesium, Mg	Will burn easily in chlorine with a bright, white flame. The magnesium chloride produced is a white solid.
Aluminium, Al	Burns in a stream of dry chlorine to produce a pale yellow solid of aluminium chloride which quickly <b>sublimes</b> due to the high temperatures.
Silicon, Si	A colourless liquid, silicon tetrachloride, is formed which immediately vaporises due to the high temperatures.
Phosphorus, P	Will burn spontaneously in chlorine and form an off-white solid of phosphorus(V) chloride.

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### ? Recap questions: Reactions of period 3 elements

- Phosphorus reacts with oxygen to form phosphorus(V) oxide.
  - What do you see happening as phosphorus burns? (2 marks)
  - Write the balanced equation for phosphorus burning in oxygen. (2 marks)
- Name the two products formed when sodium reacts with water and write the balanced equation showing this reaction. (3 marks)
  - Explain why the reaction of aluminium with water is so slow and suggest how it could be increased. (2 marks)
- Give the chemical formula of the chlorides formed when sodium, aluminium and phosphorus react with oxygen and state the oxidation numbers of the non-chlorine elements in each compound.



# C1.4 Physical properties of period 3 oxide



## Key points covered

- Describe the differences in melting point for the period 3 oxides and chlorides
- Describe the differences in structure of the period 3 oxides and chlorides

As seen in section B, the properties of a substance are related to the structure and bonding. To understand the trends in the properties of the period 3 oxides and chlorides, you need to know how the particles within them are held together.

Period 3 oxide	Na <sub>2</sub> O	MgO	Al <sub>2</sub> O <sub>3</sub>
Chemical bonding	Ionic	Ionic	Ionic
Structure	Giant ionic	Giant ionic	Giant ionic

Period 3 chloride	NaCl	MgCl <sub>2</sub>	Al <sub>2</sub> Cl <sub>6</sub>
Chemical bonding	Ionic	Ionic	Covalent
Structure	Giant ionic	Giant ionic	Simple molecular

As you go across period 3, the bonding within the oxides and the chlorides becomes more covalent. The structure changes from giant ionic to simple molecular.

## Physical properties of the period 3 oxides

### Melting point

Period 3 oxide	Melting point °C
Na <sub>2</sub> O	1132
MgO	2852
Al <sub>2</sub> O <sub>3</sub>	2072
P <sub>4</sub> O <sub>10</sub>	340
SO <sub>2</sub>	-76

The metallic oxides are all ionic in nature. They have very high melting points due to the strong attractions between oppositely charged ions which require large amounts of energy to overcome.

The remaining oxides are simple covalent substances. When melting they require the weak intermolecular attractions to be overcome and this does not need as much energy.

### Electrical conductivity

In solid form, none of the period 3 oxides have free ions or delocalised electrons available to carry the current.

However, if the metallic oxides are molten or dissolved in water, the ionic lattice will break down into positively and negatively charged ions to move independently of each other, resulting in electrical conductivity.

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## Physical properties of the period 3 chlorides

### Melting point

Period 3 chloride	Melting point °C
NaCl	801
MgCl <sub>2</sub>	714
Al <sub>2</sub> Cl <sub>6</sub>	sublimes
SiCl <sub>4</sub>	-69
PCl <sub>5</sub>	160

The melting points of sodium chloride and magnesium chloride are very high due to the amount of energy needed to overcome the strong electrostatic attractions between the ions.

The melting points of the other chlorides are so much lower due to their covalent nature and the requirement to overcome the weaker intermolecular attractions.

### Electrical conductivity

Both sodium and magnesium chloride have a giant ionic structure which means they do not conduct electricity when solid as the ions are held firmly in position and unable to move. However, in aqueous solution the ions become mobile and are therefore free to carry an electrical charge.

The other chlorides are unable to conduct in any state due to their covalent nature and the lack of mobile electrons and so an electrical charge cannot be transferred.



### Recap questions: Physical properties of period 3 oxides and chlorides

- 1 The melting point of magnesium oxide is 2852 °C, whereas that of sodium chloride is 801 °C. Account for this large difference in melting point in terms of their bonding.
- 2 P<sub>4</sub>O<sub>10</sub> has a low melting point. Account for the low melting point in terms of its structure.
- 3 Compare the electrical conductivity of magnesium chloride with phosphorus pentachloride.

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# C1.5 Acid-base behaviour of period 3 oxides and hydroxides



## Key points covered

- Explain how period 3 oxides and hydroxides act in water
- Describe whether a period 3 oxide acts as an acid or a base in chemical reactions
- Describe whether a period 3 hydroxide acts as an acid or a base in chemical reactions

When placed in water, period 3 oxides and hydroxides can act as either acids (donate  $H^+$  ions and react with bases) or bases (accept  $H^+$  ions and react with acids).

The nature of the period 3 oxides is summarised below.

Period 3 oxide/hydroxide	$Na_2O$	$MgO$	$Al_2O_3$	$SiO_2$
Acid/basic nature	Basic	Basic	Amphoteric	Acidic

The reason behind the acidic/basic nature of the oxide is dependent on the way it reacts with water.

## Basic oxides

When sodium and magnesium oxide are placed in water the ions dissociate and the  $O^{2-}$  ions interact with the water molecules. This forms an alkaline solution which is basic.

Period 3 oxide	Reaction with water	Example
$Na_2O$	The ionic lattice dissolves in water to form $Na^+$ and $O^{2-}$ ions. The $O^{2-}$ ions then react with water: $O^{2-} + H_2O \rightarrow 2 OH^-$ Overall the process is $Na_2O + H_2O \rightarrow 2 NaOH$	e.g. $Na_2O + H_2O \rightarrow 2 NaOH$
$MgO$	The ionic lattice dissolves in water to form $Mg^{2+}$ and $O^{2-}$ ions. The $O^{2-}$ ions then react with water: $O^{2-} + H_2O \rightarrow 2 OH^-$ Overall the process is $MgO + H_2O \rightarrow Mg(OH)_2$ The resulting solution is less alkaline than the one formed from sodium oxide as magnesium oxide has a lower solubility in water due to the stronger electrostatic forces between the oppositely charged ions.	e.g. $MgO + H_2O \rightarrow Mg(OH)_2$

## Amphoteric oxides

Aluminium oxide is amphoteric when placed in water as the electrostatic forces between the ions are strong enough to overcome the hydration energy. Aluminium oxide has the ability to react with both acids and hot, concentrated alkalis.

Reaction with acid	Reaction with alkali
$Al_2O_3 + 6H^+ \rightarrow 2Al^{3+} + 3H_2O$ e.g. $Al_2O_3 + 6HCl \rightarrow 2AlCl_3 + 3H_2O$ $Al_2O_3 + 3H_2SO_4 \rightarrow 2Al_2(SO_4)_3 + 3H_2O$ $Al_2O_3 + 6HNO_3 \rightarrow 2Al(NO_3)_3 + 3H_2O$	$Al_2O_3 + 2OH^- + 3H_2O \rightarrow 2[Al(OH)_4]^-$ e.g. $Al_2O_3 + 2NaOH + 3H_2O \rightarrow 2Na[Al(OH)_4]$

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## Acidic oxides

The covalently bonded period 3 oxides all dissolve in water to produce acids which when reacting with bases.

Period 3 oxide	Reaction with water	
$P_4O_{10}$	When put into water $P_4O_{10}$ reacts violently to form phosphoric acid $P_4O_{10} + 6H_2O \rightarrow 4H_3PO_4$	$P_4O_{10}$ or in its $OH$
$SO_2$	Sulfur dioxide dissolves when placed into water and forms sulfurous acid $SO_2 + H_2O \rightarrow H_2SO_3$ <i>A second oxide of sulfur, <math>SO_3</math>, also does this, but when placed in water, except this time sulfuric acid is formed</i> $SO_3 + H_2O \rightarrow H_2SO_4$	$SO_2$ $2OH$

Other acidic oxides not covered here include silicon dioxide and various chlorine

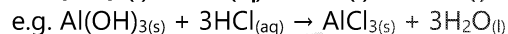
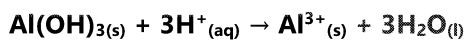
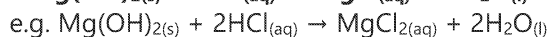
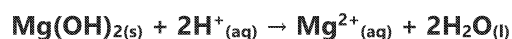
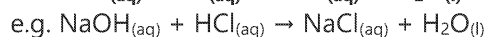
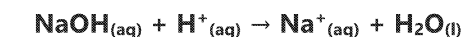
Period 3	Reaction with water	
$SiO_2$	No reaction due to the giant covalent network structure adopted by silicon dioxide	$SiO_2$ (the base)
$Cl_2O_7$	When dissolved in water the very strong acid, perchloric acid, is formed $Cl_2O_7 + H_2O \rightarrow 2HClO_4$	$OH$
$Cl_2O$	When dissolved in water, the weak acid, hypochlorous acid, is partially formed $Cl_2O + H_2O \rightleftharpoons 2HClO$	$OH$

### Test your knowledge

What are the oxidation numbers of chlorine in each of the oxides given?

## Period 3 hydroxides

All three metallic period 3 hydroxides act as bases and will react with acids to form



As with its oxide, aluminium hydroxide is amphoteric but when in the presence of an acid it acts as a base:



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Recall the acid-base behaviour of period 3 oxides and hydroxides.

- The oxides of the elements of the third period were added to water and the pH of the solutions formed recorded. What general trend in pH would be observed? (1 mark)
  - Which two of the oxides of the period 3 elements sodium to sulfur are acidic? (2 marks)
- Suggest a value for the pH of the solution formed when magnesium oxide is added to water. Give the formula of the compound formed which is responsible for the change in pH. (2 marks)
  - Sulfur dioxide reacts readily with water. Suggest a value for the pH of the solution formed. Give the formula of the compound which is responsible for the change in pH. (2 marks)
- Aluminium hydroxide will react with both nitric acid and sodium hydroxide. Write balanced equations for these reactions. (4 marks)

# C1.6 Reaction of water and period 3 chlorides

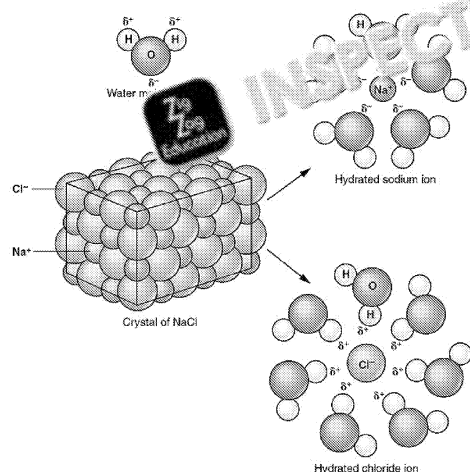


## Key points covered

- Describe the interaction of period 3 chlorides with water
- State the pH of solutions of period 3 chlorides in water

The reaction of a substance with water is known as hydrolysis. The period 3 chlorides react in different ways depending on their structure and bonding. As a result, the solutions formed have different pH values.

Period 3 chloride	NaCl	MgCl <sub>2</sub>	Al <sub>2</sub> Cl <sub>6</sub>	SiCl <sub>4</sub>	PCl <sub>5</sub>	PCl <sub>3</sub>
pH of solution	7	5	3	0	0	0



## Sodium and magnesium chlorides

When placed in water, both sodium chloride and magnesium chloride dissolve, rather than react. They form separate down and independent ions are formed in the water molecules.

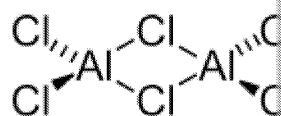
The higher charge of the magnesium ion attracts a small amount of the polar water molecules, resulting in the slightly more acidic solution.

## Aluminium chloride

Aluminium chloride, Al<sub>2</sub>Cl<sub>6</sub>, exists as a **dimer**.

When this substance is placed in water the dimer breaks down and produces hydrated Al<sup>3+</sup> and Cl<sup>-</sup> ions.

As with magnesium chloride, the high charge on the positive aluminium ion causes a water molecule to lose an H<sup>+</sup> ion and make the solution acidic.



This H<sup>+</sup> ion is able to then react with the Cl<sup>-</sup> ions to produce hydrogen chloride gas, which escapes from the solution.

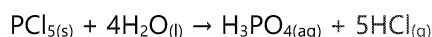
## Silicon chloride

When reacting with water, silicon chloride again produces white fumes of hydrogen chloride gas. A white **precipitate** of silicon dioxide is formed and some of the hydrogen chloride produced dissolves in the water to form a strongly acidic solution.



## Phosphorus chloride

PCl<sub>5</sub> is hydrolysed in water in a violent reaction to form two very acidic substances: phosphoric acid and hydrogen chloride gas.



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## Recap questions: Reaction of water and period 3 chlorides

- Describe the trend in pH of the solutions formed as a result of hydrolysis of period 3. (1 mark)
- What observations are recorded when silicon chloride is placed in water? Write a balanced equation to represent this reaction. (3 marks)
- Name the two substances formed when phosphorus(V) chloride is placed in water. (2 marks)

## C1.8 Predicting physical and chemical properties



### Key points covered

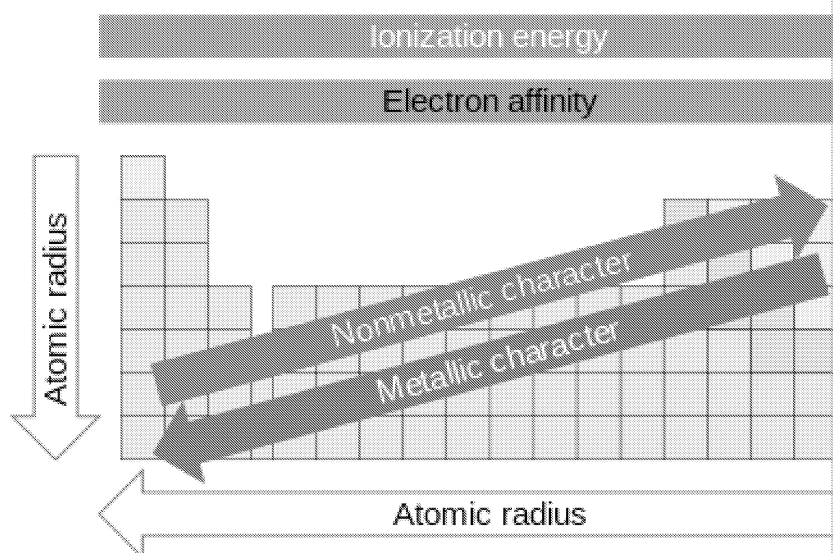
- Use of periodicity to predict physical properties of period 2 elements
- Use of periodicity to predict chemical properties of period 2 elements

Periodicity is a useful tool that can be used by chemists to predict **physical and chemical properties** of other elements based on their location within the periodic table. As previously discussed, the periodic table arranges elements based on their electronic structure. All elements in the same group as each other will have similar electronic configurations, with the exception of an extra shell added as you progress down the group. All elements in the same period as each other will follow the same pattern in electronic configuration as the group before, but with an extra shell further from the nucleus.

Physical properties affected by electronic structure

Chemical properties affected by electronic structure

The following properties can be predicted using periodicity: ionisation energy, atomic radius, electronegativity, and metallic nature. The image below shows the trends followed by these properties in the periodic table.



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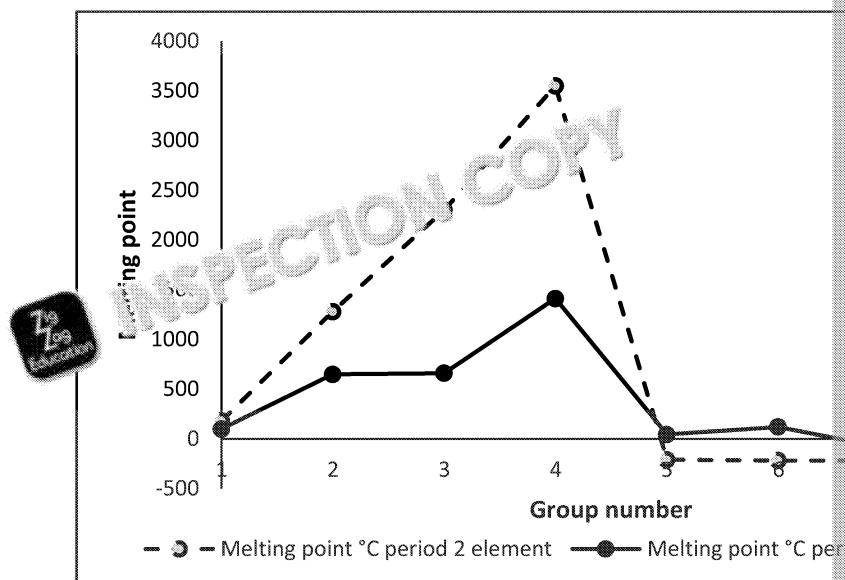


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Other properties of elements can also be predicted using the trends previously met elements. Consider the data shown below in both tabulated and graphical form, fo

Group number	1	2	3	4	5
Melting point °C period 2 element	181	1278	2300	3547	-21
Melting point °C period 3 element	98	649	660	1410	44



Despite the values between the period 2 elements and the equivalent period 3 elements, see that the trend for both periods is the same. As you move across the metallic elements, the melting point rises, peaking at the group 4 giant covalent substance. The remaining elements in the period show a sharp drop in melting point due to their simple covalent nature.

?

### Recap questions: Predicting physical and chemical properties

- In period 2, which substance, out of the following pairs, would you expect to have the highest melting point, and why? (3 marks)
  - lithium and carbon
  - neon and beryllium
  - lithium and beryllium
- Rewrite the following list in order of decreasing electronegativity: fluorine (F), boron (B). (1 mark)
- Based on the periodic trends for ionisation energy, which period 2 element has the highest ionisation energy? Explain your answer. (4 marks)
- True or false? Nitrogen has a larger atomic radius than oxygen. Explain your answer. (2 marks)

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## C1.9 Uses of period 3 elements and compounds

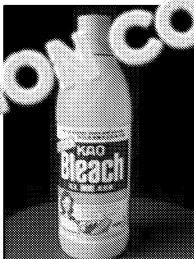
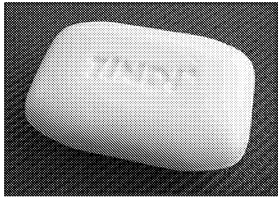
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### Key points covered

- Applications of period 3 elements
- Applications of period 3 compounds

The table below outlines uses and applications of period 3 elements and their compounds. This is not exhaustive and there are many more uses out there.

Element	
<p>Chlorine – disinfectant due to its ability to kill bacteria</p> <p>Argon – at pressure for welding due to its inert nature</p> 	<p>Sodium oxide – glassmaking</p> <p>Magnesium oxide – fireproof materials</p> <p>Silicon dioxide – construction industry</p> <p>Phosphorus oxide – dry</p>
Hydroxides	
<p>Sodium hydroxide – soap production</p> <p>Magnesium hydroxide – antacid due to its ability to neutralise acids</p> <p>Aluminium hydroxide – treat heartburn</p> 	<p>Sodium chloride – food</p> <p>Magnesium chloride – dietary supplement</p> <p>Silicon chloride – chemical</p>



### Recap questions: Uses of period 3 elements and compounds

- 1 Stomach acid can be thought of as HCl. With the use of an equation, explain how it can be used as an antacid. (2 marks)
- 2 Silicon dioxide can be used in the construction industry due to its high melting point. Use structure and bonding to explain the reason for these two properties.

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# D: Physical chemistry

## D1.1 Moles

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### Key points covered

- Use of the mole to calculate mass and relative formula mass of substances
- Use of mole calculations to determine ratios of atoms in a compound and substances in a reaction
- Use of the mole to calculate the number of particles in a substance
- Use of moles to calculate the mass of substances in chemical reactions

### The mole

When chemists carry out chemical reactions the substances involved are usually measured by volume. However, chemistry is the study of atoms and therefore chemists need a way to convert the relative quantities of chemicals into the actual number of particles that have

**Avogadro constant,  $N_A$**  – a numerical value equivalent to  $6.02 \times 10^{23}$ . This is the amount of particles in one mole of a substance.

Due to the small size of atoms, huge amounts of a substance are involved in a chemical reaction. The units used to measure the amount of a substance are moles, and one mole of a substance contains the same number of particles as one mole of any other substance.

Carbon-12 is the standard for measuring atomic mass, and if you were to take the mass of one mole of carbon-12 you would find that they weigh a total of 12 g. This means it is very easy to measure the mass of any substance; it is the relative atomic mass of that element, expressed in grams.

One mole of oxygen atoms, O, would have a mass of 16 g

One mole of magnesium atoms, Mg, would have a mass of 24 g

Two moles of oxygen atoms, O, would have a mass of  $(2 \times 16)$  32 g

Four moles of magnesium atoms, Mg, would have a mass of  $(4 \times 24)$  96 g

The idea of the mole gives us a way to take something that is too small to be seen and yet know exactly how many particles there are present; as long as you know which element you have and how much of this substance you have.

### Test your knowledge

- What is the molar mass of  $\text{BeO}$ ?
- Calculate the mass in grams of 0.125 moles of  $\text{H}_3\text{PO}_4$ .

### Molar mass

Relative atomic mass can only be used in relation to elements. However, moles can refer to anything, not just elements. **Molar mass** is a way of linking moles with mass for any chemical substance. The molar mass of carbon is  $12 \text{ g mol}^{-1}$ , whereas the molar mass of carbon dioxide,  $\text{CO}_2$ , is  $44 \text{ g mol}^{-1}$  ( $12 + (2 \times 16)$ ).

Moles, molar mass and mass can be linked using the equation:  $\text{moles} = \frac{\text{mass in g}}{\text{molar mass}}$

### Test your knowledge

- What is the molar mass of  $\text{BeO}$ ?
- Calculate the mass in grams of 0.125 moles of  $\text{H}_3\text{PO}_4$ .

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## Empirical formula

Empirical formula is the simplest whole number ratio between the different elements useful for chemical substances that are not molecular and exist in giant structures. Millions of oppositely charged ions, with no set amount; the number of ions present is proportional to the size of the crystal studied. However, what will not change is the ratio between the

Empirical formula for substances can be calculated using one of two methods: through analysis of percentage composition. Both methods involve the following steps:

**Step 1** – calculate moles of each element using  $\text{moles} = \frac{\text{mass in g}}{\text{molar mass}}$

**Step 2** – divide by the smallest amount to find the simplest whole number ratio

**Step 3** – write the empirical formula

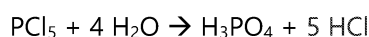
Empirical formula using mass data	Empirical formula using percentage data
A student carried out an experiment where 0.6 g of calcium reacted with 1.05 g of chlorine. Use the given mass data to determine the empirical formula of the resulting compound.	An organic chemical compound was found to have the following composition: carbon 40.00 %, hydrogen 6.71 %, oxygen 53.29 %. Determine the empirical formula.
<p><b>Step 1 –</b>  Moles of calcium = <math>0.6 \div 40 = 0.015</math> mol  Moles of chlorine = <math>1.05 \div 35.5 = 0.03</math> mol</p> <p><b>Step 2 –</b>  Moles of calcium is the smallest value  Mol Ca = <math>\frac{0.015}{0.015}</math> Mol Cl = <math>\frac{0.03}{0.015}</math>  1 : 2</p> <p><b>Step 3 –</b>  Empirical formula = <math>\text{CaCl}_2</math></p>	<p>Before following the steps, convert the percentages given into masses using the process as for mass data.</p> <p><b>Step 1 –</b>  Moles of carbon = <math>40 \div 12 = 3.33</math>  Moles of hydrogen = <math>6.71 \div 1 = 6.71</math>  Moles of oxygen = <math>53.29 \div 16 = 3.33</math></p> <p><b>Step 2 –</b>  Moles of carbon/oxygen = <math>\frac{3.33}{3.33}</math> Mol H = <math>\frac{6.71}{3.33}</math>  1 : 2 : 1</p> <p><b>Step 3 –</b>  Empirical formula = <math>\text{CH}_2\text{O}</math></p>

### Test your knowledge

**Discussion question:** if you were told the mass of substance used to give the data in example 2, could you suggest a way to determine its molecular formula?

## Balancing equations

Due to the **conservation of mass**, all chemical equations that are written must be balanced; this is to say that they must have the same type and amount of atoms on the reactant side as they do on the product side. These atoms, however, will be arranged and bonded differently depending on the substance they are found in.



In the balanced equation above, the conservation of mass is illustrated

Number present on reactant side	Element	Number present on product side
1	P	1
5	Cl	5
8	H	8
4	O	4

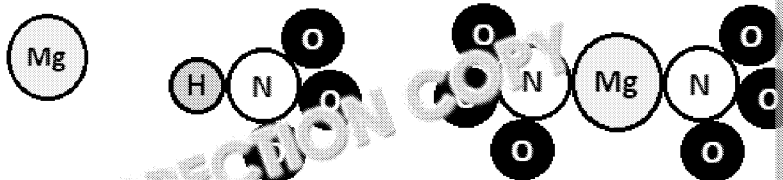
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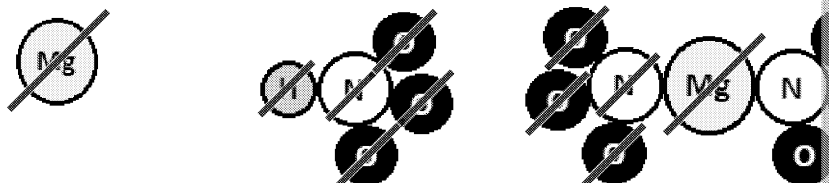
**Stoichiometric** – the required relationship between substances in a balanced equation

When balancing equations you need to remember you numbers in front of each species. These numbers indi relationship between the substances involved in the cl the small, subscript numbers, you are changing the be molecules and therefore changing the nature of the cl

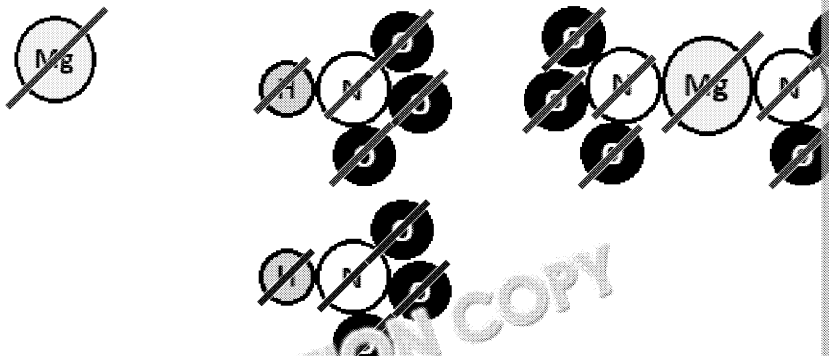
It is important that you consider the substances in their entirety, i.e. as compounds individual atoms. Drawing particle diagrams of the chemical formula can sometime




Once you a  of how many atoms and what types you have on each side of the cancelling out any that are accounted for on each side of the equation.



Once all existing atoms have been accounted for, you then add extra species to help the example above you can see that there is an absence on the reactant side of one and three oxygens. By introducing a second  $\text{HNO}_3$  molecule you can address this



Now all atoms have been crossed out and there is no surplus on either side. The last thing  required is to add in the large numbers showing how many of each species are required for balancing. Using the particle diagrams to help, you can see that only one of each species ( $\text{HNO}_3$ ), was needed. Two nitric acid molecules were required. This equation would



**Test your**

- Balance the following equations:
- $\text{Na} + \text{Cl}_2 \rightarrow \text{NaCl}$
  - $\text{Li} + \text{H}_2\text{O} \rightarrow \text{LiOH} + \text{H}_2$

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## Gas volumes

In the previous section you saw that the number of moles of a substance can be related to its mass. Whilst this works well for solids, in practice it is very hard to measure the mass of a gas.

Particle theory tells us that gas particles will spread out and fill all the space available to them in a container. As all gases will behave in this way, equal volumes of different gases will contain the same amount of molecules. This means that you indirectly have a method to count the number of molecules in your sample. We can refer to this standard as the **molar volume**.

Generally speaking, most chemical reactions are carried out under a standard set of conditions. These are known as room temperature and pressure (RTP). Under these conditions a volume of  $24 \text{ dm}^3$  ( $24\,000 \text{ cm}^3$ ). At RTP the molar volume of gas is  $24 \text{ dm}^3 \text{ mol}^{-1}$ .

### Converting between volume of gas and moles

The volume of a gas and the number of moles it contains can be linked using the formula:



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

Volume can be measured in either  $\text{cm}^3$  or  $\text{dm}^3$ . When using this equation it is important that the quantities are in the same units.

$$1 \text{ dm}^3 = 1000 \text{ cm}^3$$

When converting from  $\text{cm}^3$  to  $\text{dm}^3$  you would divide the volume by 1000. If converting from  $\text{dm}^3$  to  $\text{cm}^3$ , you multiply by 1000.

#### Example 1

How many moles of  $\text{O}_2$  gas are present in  $360 \text{ cm}^3$ , measured at room temperature and pressure? (molar volume is  $24 \text{ dm}^3 \text{ mol}^{-1}$ )

Before carrying out the calculation, convert both volumes into the same units.

$$360 \text{ cm}^3 \rightarrow \text{dm}^3 = \div 1000 \rightarrow 0.360 \text{ dm}^3$$

$$\text{Moles} = \frac{\text{volume}}{\text{molar volume}} = \frac{0.360}{24} = 0.015 \text{ moles}$$

#### Example 2

What volume, in  $\text{cm}^3$ , would be occupied by 1.25 moles of methane ( $\text{CH}_4$ ) gas? (molar volume is  $24 \text{ dm}^3 \text{ mol}^{-1}$ )

Before carrying out the calculation, convert both volumes into the same units.

$$24 \text{ dm}^3 \rightarrow \text{cm}^3 = \times 1000 \rightarrow 24\,000 \text{ cm}^3$$

$$\text{Volume} = \text{moles} \times \text{molar volume} = 1.25 \times 24\,000 = 30\,000 \text{ cm}^3$$

#### Test your knowledge

- How many moles are present in  $56 \text{ cm}^3$  of nitrogen gas?
- What volume would be occupied by  $2.5 \times 10^{-3}$  moles of ethane gas?

**Discussion question:** if a set mass of solid is heated to vaporise it and the volume of the gas is then measured, how could you determine the relative formula mass of the compound?

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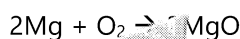
## Yield

The yield of a reaction is a description applied to how much desired product has been produced. There are three specific types of yield you are expected to be familiar with:

- Theoretical yield – the expected mass of product, based on the mass of reactants
- Actual yield – the mass of product physically obtained at the end of a reaction
- Percentage yield – a comparison between the theoretical yield and the actual yield

## Theoretical yield

If you have a balanced equation and know how much starting reactant you are using, you can calculate the amount of product you would expect to make.



In the equation above, the molar relationship between the different substances – and the ratio of moles – is given by the large coefficients. Therefore see that for every two moles of magnesium, two moles of magnesium oxide will be produced. It is a 1 : 1 ratio between magnesium and magnesium oxide.



3 moles of magnesium makes 3 moles of magnesium oxide  
0.125 moles of magnesium makes 0.125 moles of magnesium oxide

The ratio between oxygen and magnesium oxide is 1 : 2.

This means that for every one mole of oxygen used, two moles of magnesium oxide will be produced.

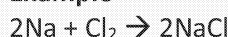
2 moles of oxygen makes 4 moles of magnesium oxide  
6 moles of oxygen makes 12 moles of magnesium oxide

As it is impossible to measure out chemicals using the value of moles, an initial conversion of mass in grams to moles is needed followed by converting the amount of moles made back into a mass once the ratio between the substances has been calculated.

### Test your knowledge

2Na + Cl<sub>2</sub> → 2NaCl  
Using the equation, calculate the number of moles of sodium chloride produced from:  
 • Hydrogen gas  
 • water is used  
 • Sodium hydroxide  
 moles of sodium chloride

### Example



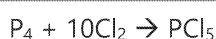
Calculate the theoretical yield of sodium chloride produced if 0.142 g of chlorine gas is used.

A<sub>r</sub>: Na = 23 g mol<sup>-1</sup>, Cl = 35.5 g mol<sup>-1</sup>

M<sub>r</sub>: NaCl = 58.5 g mol<sup>-1</sup>

- **Step 1:** Convert mass of chlorine gas into moles  
Moles =  $\frac{\text{mass}}{\text{M}_r} = \frac{0.142}{71} = 0.002$  moles
- **Step 2:** Use the balanced equation to predict the moles of sodium chloride produced  
1 mole of Cl<sub>2</sub> makes 2 moles of NaCl  
0.002 moles of Cl<sub>2</sub> makes 0.004 moles of NaCl
- **Step 3:** Convert moles of sodium chloride into a mass  
Mass = moles × M<sub>r</sub> = 0.004 × 58.5 = 0.234 g

### Test your knowledge



Using the above equation, calculate the theoretical yield of phosphorus(V) pentachloride if:

- 6.2 g of phosphorus is used
- 2.1 g of chlorine is used

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## Percentage yield

The percentage yield for a reaction is calculated using the following equation:

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

The closer to 100 % yield that is achieved, the more successful the reaction has been for a 100 % yield to be obtained. This is due to:

- impurities in your starting reagents
- unexpected side reactions
- a reversible reaction occurring
- not removing all product from the reaction vessel

### Example 1:

When magnesium and chlorine gas are reacted together it is expected you would get magnesium chloride. The reaction itself produced 3.7 g. Calculate the percentage yield.

$$\text{Percentage yield} = \frac{\text{actual yield}}{\text{theoretical yield}} \times 100 = \frac{3.7}{5.4} \times 100 = 68.5 \%$$

### Example 2:

The reaction between aluminium and chlorine has a percentage yield of 76 %. The theoretical yield is 9.5 g. Calculate the amount of aluminium chloride actually obtained.

$$\text{Actual yield} = \frac{\text{percentage yield} \times \text{theoretical yield}}{100} = 7.14 \text{ g}$$



## Recap questions: Moles

- Give balanced equations for the following reactions. (4 marks)
  - $\text{Mg} + \text{HNO}_3 \rightarrow \text{Mg}(\text{NO}_3)_2 + \text{H}_2$
  - $\text{CuCl}_2 + \text{NaOH} \rightarrow \text{Cu}(\text{OH})_2 + \text{NaCl}$
  - sodium + oxygen  $\rightarrow$  sodium oxide
  - calcium + hydrochloric acid  $\rightarrow$  calcium chloride + hydrogen
- How many moles are there in each of the following? (4 marks)
  - 72.0 g of Mg
  - 4.00 kg of CuO
  - 39.0 g of  $\text{Al}(\text{OH})_3$
  - 20.0 g of  $\text{Cu}(\text{NO}_3)_2$
- What mass of iron is produced when 32 kg of iron(III) oxide is heated?  
 $\text{Fe}_2\text{O}_3(\text{s}) + 3 \text{CO}(\text{g}) \rightarrow 2 \text{Fe}(\text{s}) + 3 \text{CO}_2(\text{g})$  (3 marks)
  - What mass of oxygen is needed to cause 102 g of ammonia to revert to nitrogen and water?  
 $4 \text{NH}_3(\text{g}) + 3 \text{O}_2(\text{g}) \rightarrow 2 \text{N}_2(\text{g}) + 6 \text{H}_2\text{O}(\text{l})$  (3 marks)
- Aluminium is extracted from aluminium oxide in the following reaction:  
 $2 \text{Al}_2\text{O}_3 \rightarrow 4 \text{Al} + 3 \text{O}_2$ 
  - Calculate the maximum theoretical mass of aluminium that can be made from 1020 g of aluminium oxide. (3 marks)
  - In the reaction, only 500 g of aluminium was made. Calculate the percentage yield. (3 marks)
- 3.53 g of iron reacts with chlorine to form 10.24 g of iron chloride. Find the relative formula mass of iron chloride. (5 marks)
  - A compound contains 40.0 g of carbon, 6.7 g of hydrogen and 53.5 g of oxygen. The relative formula mass of the compound is 180. Find both the empirical formula and the molecular formula. (5 marks)
- What volume of oxygen reacts with 100 cm<sup>3</sup> of but-1-ene?  
 $\text{C}_4\text{H}_{10}(\text{g}) + 6 \text{O}_2(\text{g}) \rightarrow 4 \text{CO}_2(\text{g}) + 5 \text{H}_2\text{O}(\text{l})$  (2 marks)
  - 1 dm<sup>3</sup> of but-1-ene is reacted with 10 dm<sup>3</sup> of oxygen. What volume of carbon dioxide is produced? (3 marks)

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## D1.2 Chemical kinetics



### Key points covered

- Use of collision theory and activation energy to explain factors that affect rate of reaction
- Use of Maxwell–Boltzmann distribution curves to explain the effect of temperature, concentration and catalyst on rate of reaction
- Understanding of rate equations and rate constants

### Chemical reactions

The rate of a chemical reaction is considered to be the speed at which reactants are consumed or products are formed. The average rate of a reaction can be calculated using:

$$\text{Rate (mol dm}^{-3} \text{ s}^{-1}) = \frac{\text{change in concentration (or reactant or product) (mol dm}^{-3})}{\text{Time (s)}}$$

In your previous science studies you will have been introduced to the fact that there are several factors that can have an effect on the rate of a chemical reaction:

- **Concentration** (or **pressure** if considering gaseous reactants) – the higher the concentration/pressure, the faster the rate
- **Temperature** – the higher the temperature, the faster the rate
- **Surface area** (for solid reactants) – the larger the surface area, the faster the rate
- **Catalysts** – the use of a **catalyst** will increase the rate

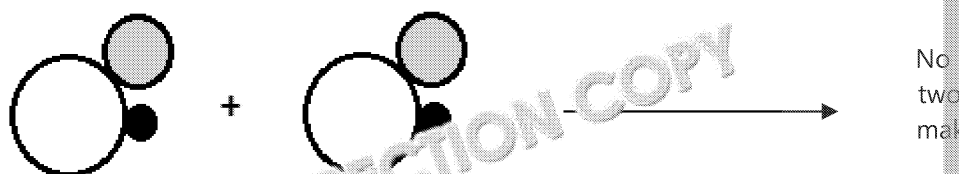
In order to explain the reasons behind each effect above you need to consider the collision theory.

### Collision theory

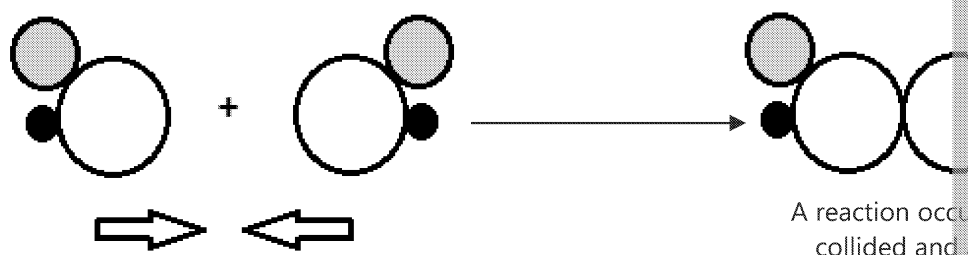
The chemical idea of collision theory states that in order for a reaction to occur the particles must come into contact with each other and collide. Usually when particles collide, the collision is unsuccessful and the particles simply bounce off each other but remain chemically unchanged. In order for a reaction to be successful a collision must fulfil two criteria:

1. The particles collide with the correct orientation
2. The particles collide with sufficient energy to exceed the **activation energy**

#### Unsuccessful collision



#### Successful collision



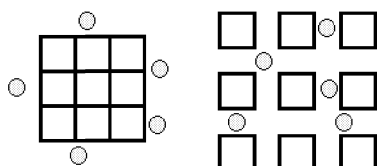
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## Factors affecting rate of reaction and collision theory

### Concentration

An increase in concentration of a solution results in a larger amount of particles in the same volume and therefore an increased frequency of collisions. As more collisions are now occurring per unit time, the probability of a successful collision increases and the rate of reaction increases.



### Surface area

When a solid reactant is broken up into smaller pieces, the total surface area increases, and therefore the available space for collisions increases. This means the frequency of collisions increases and the rate of reaction is faster.

### Pressure

An increase in pressure means the particles present are now occupying a smaller volume and, as such, have an increased concentration. The increased rate of reaction is explained in exactly the same way as for concentration.

### Temperature

When the temperature of a reaction is increased, the amount of kinetic energy the particles have increases and they move around the reaction faster. This will then increase the rate of reaction in two ways:

- The frequency of collisions increases.
- The probability of the energy of the collision meeting or exceeding the activation energy increases.

### Catalysts

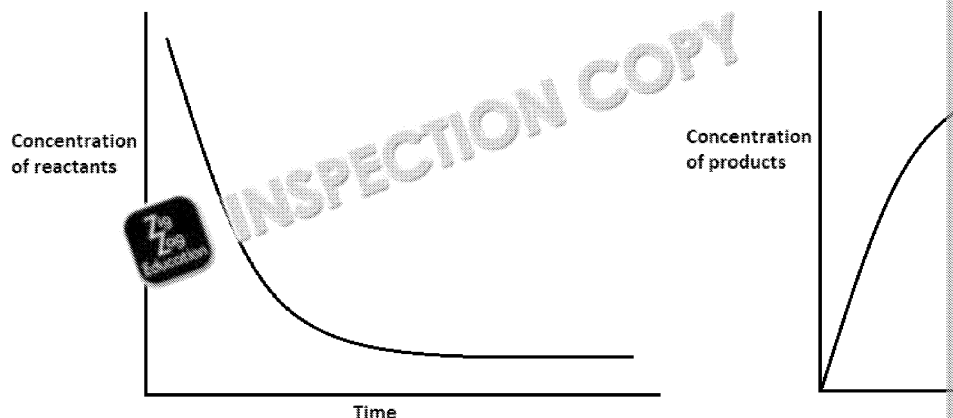
The addition of a catalyst to a chemical reaction will cause the rate of reaction to increase whilst the catalyst itself remains unchanged at the end. Catalysts are specific to their individual reaction and work by providing an alternative route with a lower activation energy.

#### Test your knowledge

1. State four factors that affect the rate of reaction.
2. Use collision theory to explain how each factor affects the rate of reaction.

### Concentration vs time graphs

The progress of a reaction can be followed by monitoring the decrease in reactants or the increase in products as a function of time. Graphical representation of this concentration data gives a quick insight into how the rate of reaction changes as a reaction progresses. The rate of reaction is shown by the **gradient** of the graph. The steeper the **gradient**, the faster the rate.



In both graphs you can see an initial high **gradient** as the rate of reaction is very fast at the start. A large number of reactant particles are present, colliding frequently and therefore a high probability of a successful collision occurring, resulting in a reaction.

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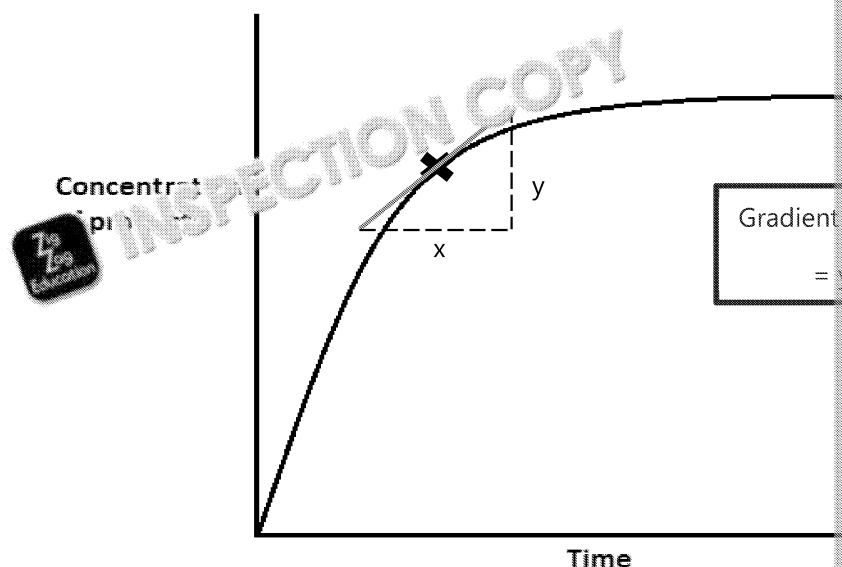




As the reaction progresses the **gradient** decreases. This indicates the reaction is becoming slower as the number of reactant particles being converted into products and less frequent collisions occur.

Eventually both graphs have a **gradient** of 0 showing that the reaction has stopped because the reactants have been used up and no further collisions are taking place.

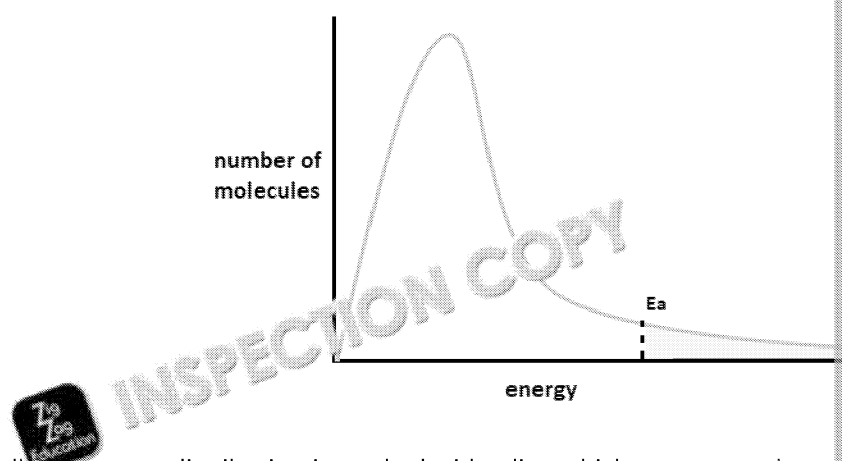
As well as giving an overall insight into how the rate of reaction is changing over time, these graphs are able to give information on the rate of a reaction at a given moment within the reaction. To do this you need to draw a tangent on your graph at the point you want to know the rate of reaction at. This tangent can then be used to calculate the gradient.



## Maxwell-Boltzmann distribution curves

The movement of molecules in a gas, liquid or solution is not uniform. Some molecules are moving very slowly with very low energy whilst others are moving very quickly with high energy. The most common speed is at close to the average speed and with average energy.

The spread of molecular energies in a gas sample is called the Maxwell-Boltzmann distribution. The graph shows the distribution of molecular energies as follows:



The Maxwell-Boltzmann distribution is marked with a line which represents the activation energy for a reaction. The shaded area on the graph shows the amount of molecules which have enough energy to overcome the activation energy.

The graph itself shows some features of the Maxwell-Boltzmann distribution:

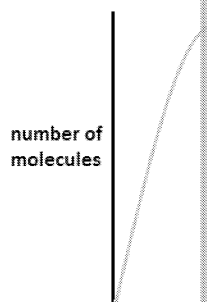
- The curve always starts at the origin (0,0). This is because there will be no molecules with zero energy.
- The curve will never meet the x-axis. This is because there is no maximum energy.
- The area under the curve represents the total number of molecules in the sample.

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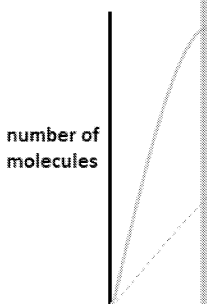
## The Maxwell-Boltzmann distribution and catalysts

You have already seen that a catalyst increases the rate of reaction by providing an alternative route with a lower activation energy. In the presence of a catalyst the number of molecules with energy equal to or exceeding the activation energy will increase and the probability of a successful collision will increase.



## The Maxwell-Boltzmann distribution and temperature

As temperature is increased the average amount of energy of the molecules in the reaction increases. This causes the distribution of energies on the Maxwell-Boltzmann distribution to shift. There will still be some molecules with low energy values, but fewer molecules will be higher in energy than at a previous lower temperature. The curve on the graph shifts to the right, the peak representing the average energy will move to the right-hand side, signifying the increase in average energy, but will also become slightly lower – the area under the curve must be the same as this represents the number of molecules in the reaction.



The amount of molecules with energy that is now equal to or exceeding the activation energy has increased, resulting in an increased rate of reaction.

## The Maxwell-Boltzmann distribution and concentration

Although an increase in concentration causes an increase in rate of reaction, the Maxwell-Boltzmann distribution remains unaffected. This is due to the fact that the energy of the molecules and activation energy remains unaltered by the change in concentration.

### Test your knowledge

1. What does the area under the curve on a Maxwell-Boltzmann distribution represent?
2. Use a Maxwell-Boltzmann distribution to explain why an increase in temperature results in an increase in rate of reaction.

## Rate equations

The rate equation for a chemical reaction is a way of expressing the mathematical relationship between the rate and the concentration of the reactants involved. It will take the form:

$$\text{Rate of reaction} = k [A]^m [B]^n$$

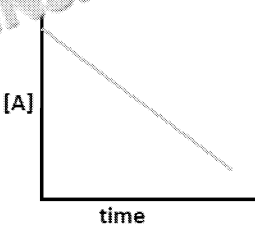
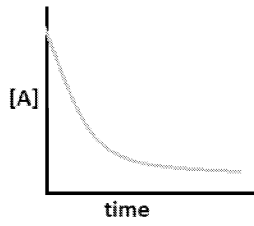
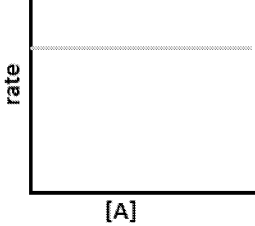
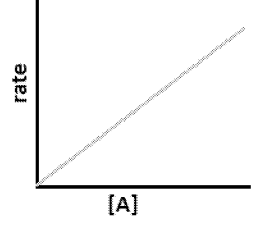
$k$  represents the rate constant, a constant which links the concentration of the reactants to the rate of reaction.  $[A]$  /  $[B]$  represents the concentration of the individual reactants.  $m$  /  $n$  represents the order of each individual reactant.

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## Order of reaction

Changing the concentration of a reactant in a reaction will have an effect on the rate. The order of reaction for a reactant is the measure of to what extent the reactant affects the rate of reaction and is the power to which the concentration will be raised to in the rate equation. Common orders are zero and first order. The overall order of the reaction is the sum of all the individual orders.

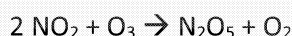
Order of reaction	Zero order	First order
<b>Effect of concentration change on rate</b>	If changing the concentration of a reactant has no effect on the rate of reaction then we would say the order for that reactant is zero.	If changing the concentration results in an identical change in rate then we say the order for that reactant is first order, e.g. doubling the concentration results in doubling the rate
<b>Mathematical relationship</b>	$\text{Rate} \propto [\text{A}]^0$	$\text{Rate} \propto [\text{A}]^1$
<b>Concentration vs time graph</b>		
<b>Rate vs concentration graph</b>		

## Orders from experimental data

The order for each reactant can only be determined experimentally and not from the balanced equation. The reaction must be set up and then the initial rate measured and recorded as quickly as possible. This is then repeated, modifying the concentration of one of the reactants and the new rate measured.

### Example:

The reaction between nitrogen dioxide and ozone takes place as follows:



A series of reactions were carried out with various concentrations of reactants and the initial rates were obtained.

Experiment no.	$[\text{NO}_2] / \text{mol dm}^{-3}$	$[\text{O}_3] / \text{mol dm}^{-3}$
1	$1.0 \times 10^{-3}$	$2.5 \times 10^{-3}$
2	$1.0 \times 10^{-3}$	$5.0 \times 10^{-3}$
3	$2.0 \times 10^{-3}$	$5.0 \times 10^{-3}$

### Looking at experiments 1 and 2:

The concentration of  $\text{O}_3$  is doubled and this results in a doubling of rate.  $\text{O}_3$  is first order.

### Looking at experiments 2 and 3:

The concentration of  $\text{NO}_2$  is doubled and this results in a doubling of rate.  $\text{NO}_2$  is first order.

The rate equation is  $\text{rate} = k [\text{NO}_2] [\text{O}_3]$

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**Test your knowledge**

Reaction number	$[\text{CH}_3\text{COCH}_3] / \text{mol dm}^{-3}$	$[\text{I}_2] / \text{mol dm}^{-3}$	$[\text{H}^+] / \text{mol dm}^{-3}$
1	2	1.26	0.248
2	4	1.26	0.248
3	2	2.52	0.248
4	2	5.04	0.496

- What is the order of reaction with respect to each reagent?
- Write the rate equation for this reaction.

**Determining the rate constant**

As previously discussed, the rate constant can be considered as an exchange rate that can be converted into rate. It is possible to calculate the rate constant for a reaction if you know the rate and the orders of reaction with respect to each reactant.

Using the reaction between nitrogen dioxide and ozone and the data given in experiment 1, the rate constant would be calculated as follows:

**Step 1:** rearrange the rate equation to make the rate constant,  $k$ , the subject:

$$\text{rate} = k [\text{NO}_2] [\text{O}_3] \rightarrow k = \frac{\text{rate}}{[\text{NO}_2] [\text{O}_3]}$$

**Step 2:** substitute in the data from the table for experiment 1 and solve:

$$k = \frac{\text{rate}}{[\text{NO}_2] [\text{O}_3]} = \frac{3.2 \times 10^{-8}}{1 \times 10^{-3} \times 2.5 \times 10^{-3}} = 1.28 \times 10^{-2} \text{ s}^{-1}$$

This value for the rate constant would have been the same regardless of the data set used for the calculation. The rate constant is not affected by concentration, only by temperature.

**Test your knowledge**

Reaction number	$[\text{CH}_3\text{COCH}_3] / \text{mol dm}^{-3}$	$[\text{I}_2] / \text{mol dm}^{-3}$	$[\text{H}^+] / \text{mol dm}^{-3}$
1	2	1.26	0.248
2	4	1.26	0.248
3	2	2.52	0.248
4	2	5.04	0.496

- Use the data above to determine the rate constant for this set of data.

**Determining units for the rate constant**

The units of the rate constant depend on the overall order of the reaction itself and are determined by the units of the rate and the concentrations of the reactants. Each new rate constant calculated will have its own units.

Units for the rate constant can be calculated by:

- Rearrange the rate equation to make  $k$  the subject
- Substitute in the required units;  $\text{mol dm}^{-3} \text{ s}^{-1}$  for rate and  $\text{mol dm}^{-3}$  for concentration
- Cancel out any necessary units and determine the overall units for  $k$

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**For a zero order reaction:**

$$\text{Rate} = k[A]^0 \rightarrow k = \text{rate}$$

$$k = \text{mol dm}^{-3} \text{ s}^{-1} \quad \text{units: mol dm}^{-3} \text{ s}^{-1}$$

**For a first order reaction:**

$$\text{Rate} = k[A]^1 \rightarrow k = \frac{\text{rate}}{[A]^1}$$

$$k = \frac{\text{mol dm}^{-3} \text{ s}^{-1}}{\text{mol dm}^{-3}} \quad \text{units: s}^{-1}$$

**For a second order reaction:**

$$\text{Rate} = k[A]^2 \rightarrow k = \frac{\text{rate}}{[A]^2}$$

$$k = \frac{\text{mol dm}^{-3} \text{ s}^{-1}}{\text{mol dm}^{-3} \text{ mol dm}^{-3}} \quad \text{units: mol}^{-1} \text{ dm}^3 \text{ s}^{-1}$$

**Test your**

What would  
following ra

1. rate =
2. rate =
3. rate =
4. rate =

?

**Recall questions: Chemical kinetics**

- 1 a) The following data is obtained when 50 cm<sup>3</sup> of 0.10 mol dm<sup>-3</sup> hydrochloric acid reacts with calcium carbonate chips at 20 °C:  $\text{CaCO}_{3(s)} + 2\text{HCl}_{(aq)} \rightarrow \text{CaCl}_{2(aq)} + \text{CO}_{2(g)}$

Time (s)	0	10	20	30	40	50
Volume of CO <sub>2</sub> (cm <sup>3</sup> )	0	30	45	54	59	60

Plot a graph to show this data and include a line of best fit. (3 marks)

- b) Sketch and label lines for similar reactions done under the conditions
- i) 50 cm<sup>3</sup> of 0.10 mol dm<sup>-3</sup> hydrochloric acid reacts with small calcium carbonate chips at 40 °C (1 mark)
  - ii) 50 cm<sup>3</sup> of 0.10 mol dm<sup>-3</sup> hydrochloric acid reacts with calcium carbonate chips at 20 °C (1 mark)
  - iii) 25 cm<sup>3</sup> of 0.10 mol dm<sup>-3</sup> hydrochloric acid reacts with small calcium carbonate chips at 20 °C (2 marks)
- c) Explain the reasons behind the new graph curves you have drawn in part b) (3 marks)
- 2 a) Sketch the Maxwell-Boltzmann distribution for a sample of particles in a gas at 20 °C. Ensure you correctly label both axes. (4 marks)
- b) On the same axis sketch a new distribution to show the same gas sample at 40 °C. (2 marks)
- c) Use a Maxwell-Boltzmann distribution to help explain how a catalyst changes the rate of a reaction. (3 marks)
- 3 Sodium reacts with chlorine to form sodium chloride.  $2\text{Na} + \text{Cl}_2 \rightarrow 2\text{NaCl}$
- A series of experiments was carried out to determine the rate equation for the reaction.

Experiment Number	[Na] (mol dm <sup>-3</sup> )	[Cl <sub>2</sub> ] (mol dm <sup>-3</sup> )	Initial rate (mol dm <sup>-3</sup> s <sup>-1</sup> )
1	0.2	0.3	
2	0.2	0.15	
3	0.1	0.6	
4	0.3	0.15	
5	0.1	0.3	

- a) Determine and explain the order with respect to
- i) Na (2 marks)
  - ii) Cl<sub>2</sub> (2 marks)
- b) State the rate equation. (1 mark)
- c) Determine the value of the rate constant. (3 marks)
- d) Determine the units of the rate constant. (2 marks)

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## D1.3 Chemical energetics



### Key points covered

- Use of enthalpy profile diagrams to explain exothermic and endothermic reactions
- Use of the terms standard conditions, enthalpy change of combustion, of formation and of reaction
- Use of Hess cycle to calculate enthalpy changes indirectly

## Enthalpy change

Enthalpy,  $H$ , can be considered as the amount of heat energy stored inside a **chemical system**. It is also sometimes thought of as the energy stored within the bonds of a chemical.

In a chemical reaction it is usually the case that the reactants and the products will have different enthalpies. It is not possible to directly measure enthalpy, but you can measure enthalpy changes done experimentally by monitoring the energy transfer between the **system** and the surroundings. The difference in these enthalpies is the enthalpy change. An enthalpy change can be either positive or negative depending on whether the products have more or less enthalpy than the reactants.

If enthalpy change is positive, then heat energy has moved from the environment into the system. A reaction is described as endothermic.

If enthalpy change is negative, then heat energy has moved from the **system** into the surroundings. A reaction is described as exothermic.

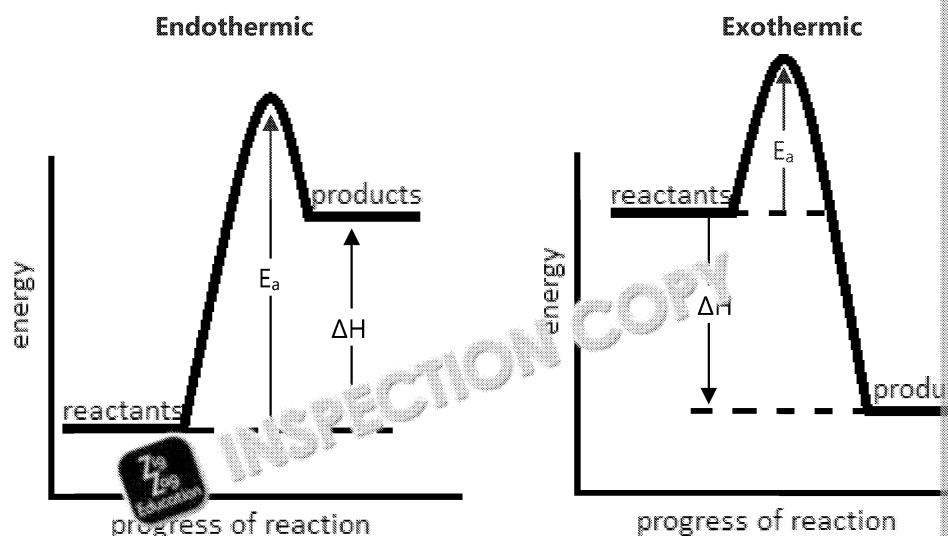
Type of enthalpy change	Endothermic	Exothermic
Effect on environment	Surroundings lose energy and the external temperature decreases	Surroundings gain energy and the external temperature increases
Energy level diagram		
Examples	Photosynthesis, sports injury packs	Combustion of fuels

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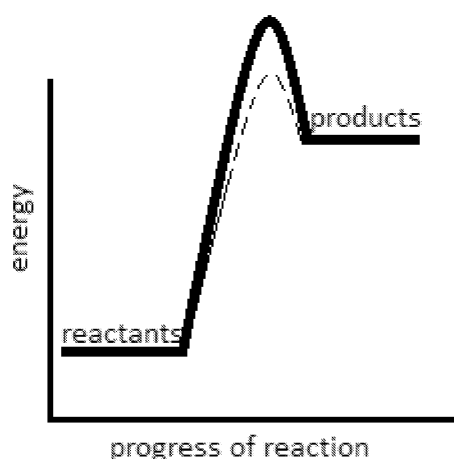


## Reaction profile diagrams

These are graphs which show the changes in energy throughout the progress of a reaction. They are able to determine the activation energy, enthalpy change and nature of the reaction.



As previously covered, catalysts increase the rate of reaction by providing an alternative pathway with a lower activation energy. This too can be shown on a reaction profile diagram as seen below.



The thinner, dotted line shows the energy changes for this reaction once a catalyst change is the same, but the activation energy peak has been lowered.

## Standard enthalpy changes

The enthalpy for a reaction will change slightly based on the conditions under which it is carried out. In order to allow for consistency, most enthalpy changes are quoted as the values obtained under **standard conditions**. When data has been calculated using standard conditions is being given, it will be accompanied by a standard sign,  $\ominus$ .

The conditions stated as standard conditions have been chosen as they are close to laboratory conditions. They are as follows:

- Standard temperature: 298 K (25 °C)
- Standard pressure: 1 atm
- Standard concentration: 1 mol dm<sup>-3</sup>
- Standard state: the physical state you would find a substance in at the conditions given

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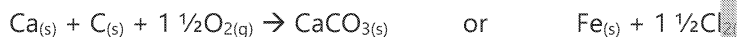


## Standard enthalpy change of formation

This is the enthalpy change when one mole of a substance is formed from its constituent elements in their standard states, with all substances in their standard states,  $\Delta_f H^\ominus$ .

According to this definition, the enthalpy of formation for any element must be 0 kJ mol<sup>-1</sup>.

Balanced equations that show enthalpy of formation reactions for compounds will be written to ensure that only one mole of compound is formed as per the definition above.



## Enthalpy change of combustion

This is the enthalpy change when one mole of substance is completely burned in oxygen under standard conditions,  $\Delta_c H^\ominus$ .

When any substance reacts in oxygen, the products formed are known as oxides.

As with enthalpy of formation equations, balanced equations that show enthalpy of combustion sometimes use fractional coefficients to ensure it is only one mole of fuel being burned. For example:



## Enthalpy change of reaction

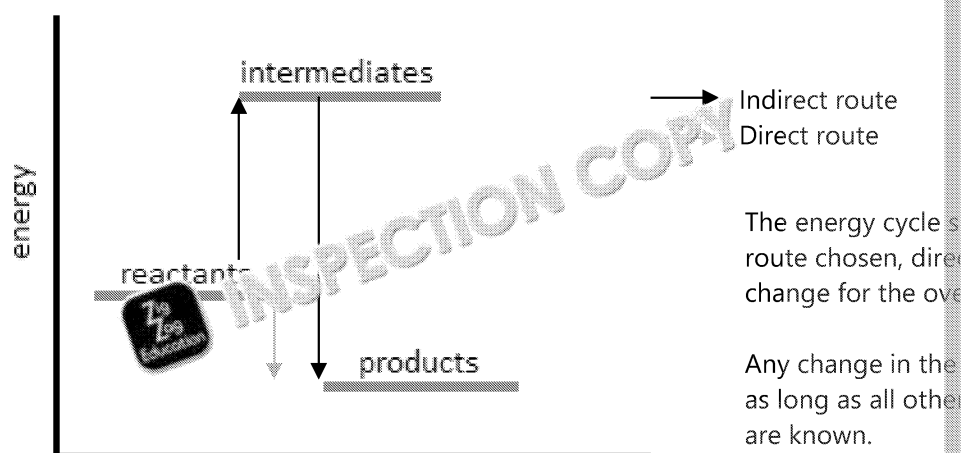
This is the enthalpy change when a chemical reaction occurs in the molar quantities specified in the equation under standard conditions,  $\Delta_r H^\ominus$ .

Enthalpy of reaction always refers to the specific reaction stated in the equation. Therefore, if the reaction changes, the enthalpy value will too. For example:



## Hess's law

In some cases enthalpy changes can be determined directly from experimental data. However, in some cases that the enthalpy change cannot be determined experimentally and an energy cycle must be used. Hess's law is based on the conservation of energy and states that the overall enthalpy change for a reaction is independent of the route taken, as long as the start and end points are the same. This is known as Hess's law of constant heat summation.



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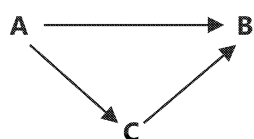




## Hess's law using combustion data

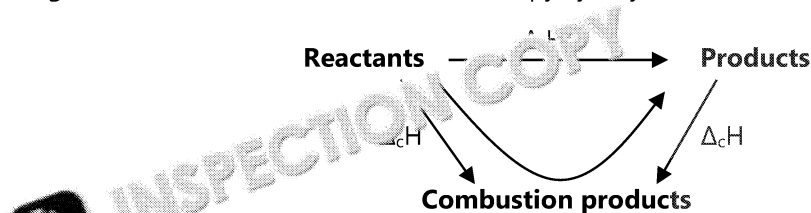
If you are provided with standard enthalpy change of combustion values you can use them to calculate the standard enthalpy change for a given reaction.

Hess's law states that the enthalpy change is independent of the route taken.



For example, the energy change in going from A → B

When you are given combustion data to use, the enthalpy cycle you would draw to

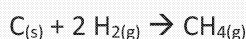


Using this cycle you can see that  $\Delta_r H$  of the direct route is equivalent to  $\Delta_c H$  of the

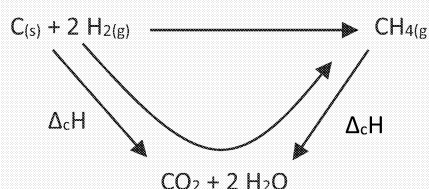
$$\Delta_r H = [\sum \Delta_c H \text{ of the reactants}] - [\sum \Delta_c H \text{ of the products}]$$

### Example:

Calculate the enthalpy change for the reaction shown using the standard enthalpy



	$C_{(s)}$	$H_{2(g)}$	$CH_{4(g)}$
$\Delta_c H / \text{kJ mol}^{-1}$	-393	-286	-890



$$\begin{aligned} \Delta_r H &= [\sum \Delta_c H \text{ of the reactants}] - [\sum \Delta_c H \text{ of the products}] \\ \Delta_r H &= [\Delta_c H C + 2(\Delta_c H H_2)] - [\Delta_c H CH_4] \\ \Delta_r H &= [-393 + 2(-286)] - [-890] \\ \Delta_r H &= [-393 + -572] - [-890] \\ \Delta_r H &= -965 - -890 \\ \Delta_r H &= -75 \text{ kJ mol}^{-1} \end{aligned}$$

### Test your knowledge

- Calculate the enthalpy for the reaction shown below using the given standard enthalpies of formation:  $2C + 3H_2 + \frac{1}{2}O_2 \rightarrow C_2H_5OH$   $\Delta_f H^\circ(C) = -393$ ,  $\Delta_f H^\circ(H_2) = -286$ ,  $\Delta_f H^\circ(C_2H_5OH) = -286$
- Calculate the enthalpy of formation of methane,  $CH_4(g)$ , using the enthalpies of combustion:  $\Delta_c H^\circ(C) = -393$ ,  $\Delta_c H^\circ(H_2) = -286$ ,  $\Delta_c H^\circ(CH_4) = -890$

**HINT** Start by writing the equation that shows the enthalpy of formation



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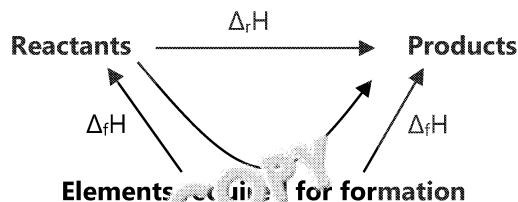


## Hess's law using formation data

If you are provided with standard enthalpy change of formation values you can use them to calculate the enthalpy change for a given reaction.

Hess's law states that the enthalpy change is independent of the route taken.

When you are given formation data to use, the enthalpy cycle you would draw takes the form:

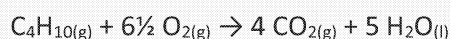


Using this cycle you can see that  $\Delta_r H$  of the direct route is equivalent to  $-\Delta_f H$  of the indirect route. This can be written mathematically as:

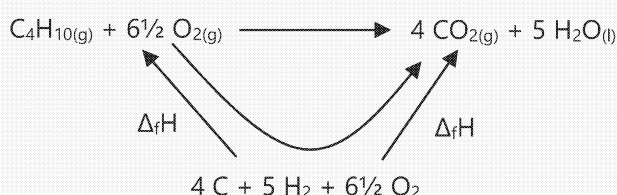
$$\Delta_r H = [\sum \Delta_f H \text{ of the products}] - [\sum \Delta_f H \text{ of the reactants}]$$

### Example:

Calculate the enthalpy change for the reaction shown using the standard enthalpy change of formation values.



	$\text{C}_4\text{H}_{10(g)}$	$\text{CO}_{2(g)}$	
$\Delta_f H / \text{kJ mol}^{-1}$	-125	-393	



$$\begin{aligned} \Delta_r H &= [\sum \Delta_f H \text{ of the products}] - [\sum \Delta_f H \text{ of the reactants}] \\ \Delta_r H &= [4(\Delta_f H \text{ CO}_2) + 5(\Delta_f H \text{ H}_2\text{O})] - [\Delta_f H \text{ C}_4\text{H}_{10}] \\ \Delta_r H &= [4(-393) + 5(-286)] - [-125] \\ \Delta_r H &= [-1572 + -1430] - [-125] \\ \Delta_r H &= -3002 - (-125) \\ \Delta_r H &= -2877 \text{ kJ mol}^{-1} \end{aligned}$$

### Test your knowledge

- Calculate the enthalpy change for the reactions shown below using the given standard enthalpy change of formation values.
- a)  $\text{CH}_4 + 2 \text{O}_2 \rightarrow \text{CO}_2 + 2 \text{H}_2\text{O}$   $\Delta_f H: \text{CH}_4 = -75, \text{CO}_2 = -393, \text{H}_2\text{O} = -286 \text{ kJ mol}^{-1}$
- b)  $3 \text{Fe} + 4 \text{H}_2\text{O} \rightarrow 4 \text{H}_2 + \text{Fe}_3\text{O}_4$   $\Delta_f H: \text{H}_2\text{O} = -286, \text{Fe}_3\text{O}_4 = -1117 \text{ kJ mol}^{-1}$

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### Recap questions: Chemical Energetics

- Draw an energy level diagram for this reaction:  
 $\text{C}_2\text{H}_4 + 3 \text{O}_2 \rightarrow 2 \text{CO}_2 + 2 \text{H}_2\text{O}$   $\Delta H = -890 \text{ kJ mol}^{-1}$  (3 marks)
  - Draw a labelled arrow on your energy diagram to show the overall enthalpy change.
  - Draw a labelled arrow on your energy diagram to show the activation energy.
- Write an equation that represents the enthalpy of combustion for ethanol.
  - Write an equation that represents the enthalpy of formation for sodium hydroxide.
- Calculate the enthalpy of combustion of propane,  $\text{C}_3\text{H}_{8(g)}$ , given the following standard enthalpy change of formation values:  
 $\Delta_f H \text{ C}_3\text{H}_{8(g)} = -104 \text{ kJ mol}^{-1}$   $\Delta_f H \text{ CO}_{2(g)} = -394 \text{ kJ mol}^{-1}$   $\Delta_f H \text{ H}_2\text{O}_{(l)} = -286 \text{ kJ mol}^{-1}$
  - Calculate the enthalpy of formation of propan-1-ol,  $\text{C}_3\text{H}_7\text{OH}_{(l)}$ , given the following standard enthalpy change of formation values:  
 $\Delta_f H \text{ C}_3\text{H}_7\text{OH}_{(l)} = -2010 \text{ kJ mol}^{-1}$   $\Delta_f H \text{ C}_{(s)} = -394 \text{ kJ mol}^{-1}$   $\Delta_f H \text{ H}_{2(g)} = 0$



## D1.4 Chemical equilibrium



### Key points covered

- Definition and features of dynamic equilibrium
- Use of Le Chatelier's principle to predict the effect of changes to the position of equilibrium
- Calculation of equilibrium concentrations of substances

### Dynamic equilibrium

When a reversible reaction is occurring in a **closed system** you will reach a point where the rate of the forward reaction is equal to the rate of the backward reaction.

Under these conditions on a large scale there appears to be no change to the overall composition of the mixture. This is known as dynamic equilibrium. The concentrations will change at the beginning of the reaction, but only until equilibrium is reached.

Do not confuse this idea with the idea of concentrations of all substances being equal – all equivalent to each other. The reactants may be dominant or there could be a large amount of product. The relative amounts of reactants and products in a reaction can be described by the position of equilibrium. If equilibrium lies to the left then the reactants are dominant, whereas if it lies to the right, there are more amounts of product if equilibrium lies to the right.

**Le Chatelier's principle** – if a change is made to a system at equilibrium the position of equilibrium will shift to counteract the effect of this change.

### Le Chatelier's principle

Le Chatelier's principle can be used to predict how changes in the conditions of a reaction will impact and change the position of equilibrium. Factors that can be considered using Le Chatelier's principle are concentration, pressure and temperature.

### Concentration

Equilibrium will shift to counteract the effect of changing concentration in the following ways:

Change in concentration	Effect on equilibrium
Increase in concentration of a reagent	Equilibrium will shift (left or right) to favour the reaction where the reagent is used up
Decrease in concentration of a reagent	Equilibrium will shift (left or right) to favour the reaction where the reagent is produced

**Example:**  $\text{N}_2(\text{g}) + 3 \text{H}_2(\text{g}) \rightleftharpoons 2 \text{NH}_3(\text{g})$

If the concentration of hydrogen is increased, equilibrium will shift to the right, favouring the forward reaction, to use up the hydrogen and counteract the increase in concentration.

If the concentration of ammonia is decreased, equilibrium will shift to the right, favouring the forward reaction, to produce more ammonia and counteract the decrease in concentration.

### Test your knowledge

Chromate ions ( $\text{CrO}_4^{2-}$ ) are yellow in colour. Dichromate ions ( $\text{Cr}_2\text{O}_7^{2-}$ ) are orange in colour. The following reaction takes place:  $\text{CrO}_4^{2-} + 2\text{H}^+ \rightleftharpoons \text{Cr}_2\text{O}_7^{2-} + \text{H}_2\text{O}$  and is allowed to reach equilibrium.

- If acid is added to an equilibrium mixture, will it become more yellow or more orange? Explain your answer.
- If alkali is added to an equilibrium mixture, will it become more yellow or more orange? Explain your answer.

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## Pressure

When considering the effect of pressure on a system at equilibrium, you are only concerned with the number of gas molecules. Equilibrium will shift in the following ways:

Change in pressure	Effect on equilibrium
Increase in pressure	Equilibrium will shift (left or right) to favour the smaller amount of gas molecules are produced
Decrease in pressure	Equilibrium will shift (left or right) to favour the larger amount of gas molecules are produced

**Example:**  $\text{N}_{2(g)} + 3 \text{H}_{2(g)} \rightleftharpoons 2 \text{NH}_{3(g)}$

If the pressure is increased, equilibrium will shift to the right, favouring the forward reaction, to produce the smaller amount of gas molecules and reduce the pressure.

If the pressure is decreased, equilibrium will shift to the left, favouring the backward reaction, to produce a greater amount of gas molecules and increase the pressure.

### Test your knowledge

- Sulfur trioxide is made by the reaction  $2 \text{SO}_{2(g)} + \text{O}_{2(g)} \rightleftharpoons 2 \text{SO}_{3(g)}$  which is exothermic. Explain what happens to the equilibrium position of sulfur trioxide if the pressure is increased.
- Iodine trichloride breaks down into monochloride and chlorine  $\text{ICl}_{3(g)} \rightleftharpoons \text{ICl}_{(g)} + \text{Cl}_{2(g)}$ . This reaction is endothermic. Explain what happens to the equilibrium position of chlorine if the pressure is increased.

## Temperature

Equilibrium will shift to counteract the effect of changing temperature in the following ways:

Change in temperature	Effect on equilibrium
Increase in temperature	Equilibrium will shift (left or right) to favour the reaction which is <b>endothermic</b>
Decrease in temperature	Equilibrium will shift (left or right) to favour the reaction which is <b>exothermic</b>

**Example:**  $\text{N}_{2(g)} + 3 \text{H}_{2(g)} \rightleftharpoons 2 \text{NH}_{3(g)}$   
exo  
endo

If the temperature is increased, equilibrium will shift to the left, favouring the backward reaction, which is endothermic.

If the temperature is decreased, equilibrium will shift to the right, favouring the forward reaction, which is exothermic.

### Test your knowledge

- Sulfur trioxide is made by the reaction  $2 \text{SO}_{2(g)} + \text{O}_{2(g)} \rightleftharpoons 2 \text{SO}_{3(g)}$  which is exothermic. Explain what happens to the equilibrium position of sulfur trioxide if the temperature is increased.
- Iodine trichloride breaks down into monochloride and chlorine  $\text{ICl}_{3(g)} \rightleftharpoons \text{ICl}_{(g)} + \text{Cl}_{2(g)}$ . This reaction is endothermic. Explain what happens to the equilibrium position of chlorine if the temperature is increased.

## Catalysts

Catalysts have no effect on the position of equilibrium. A catalyst is a substance which speeds up a reaction. Catalysts increase the rate of the forward reaction and backward reaction. Although they cause equilibrium to be reached more quickly, the position of equilibrium remains the same.

## The equilibrium constant

The exact position of equilibrium can be determined using the equilibrium constant. The equilibrium constant also gives a quick insight into the composition of the equilibrium mixture.

- An equilibrium constant  $>1$  indicates that the mixture contains a higher proportion of products.
- An equilibrium constant of 1 indicates that the mixture contains a 50 : 50 mix of products and reactants.
- An equilibrium constant  $<1$  indicates that the mixture contains a higher proportion of reactants.

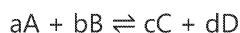
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## The equilibrium constant, $K_c$

The equilibrium constant can be linked to the concentration of each substance in an equilibrium expression.

For a given reaction



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

[ ] = concentration of named substance at equilibrium

a, b, c, d = moles of named substance according to the balanced chemical equation

### Example:

Write the equilibrium expression for the following reaction.  $N_{2(g)} + O_{2(g)} \rightleftharpoons 2NO_{(g)}$

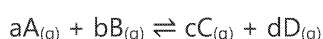
$$K_c = \frac{[C]^c [D]^d}{[A]^a [B]^b} \quad K_c = \frac{[NO_{(g)}]^2}{[N_{2(g)}] [O_{2(g)}]}$$

The equilibrium expression will only contain substances that can have a change in concentration. Solids and liquids are excluded from the expression.

## The equilibrium expression, $K_p$

When working with gases it can be very difficult to measure their concentration and instead we use their pressures. As the square brackets present in the  $K_c$  equilibrium expression, the equilibrium expression when referring to pressures will take a slightly different form.

For a given equation



$$K_p = \frac{p(C)^c p(D)^d}{p(A)^a p(B)^b}$$

$p$  = the equilibrium partial pressure of the named substance

As only gases are affected by pressure, all other states of matter are ignored when constructing  $K_p$  expressions.

## Calculations using $K_c$

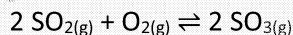
If you know the equilibrium concentrations of each substance in the reaction it is simply a case of substituting these into the equilibrium expression and then solving for  $K_c$ . As with rate constants, the units for  $K_c$  have to be determined in each individual case, using the indices laws.

### Test your knowledge

1. Write the  $K_c$  equilibrium expression for the following reactions:
  - a)  $CH_{4(g)} + H_2O_{(g)} \rightleftharpoons CO_{(g)} + 3H_{2(g)}$
  - b)  $2NO_{2(g)} \rightleftharpoons N_2O_{4(g)}$
2. Write the  $K_p$  equilibrium expression for the following reactions:
  - a)  $PCl_{5(g)} \rightleftharpoons PCl_{3(g)} + Cl_{2(g)}$
  - b)  $2O_{3(g)} \rightleftharpoons 3O_{2(g)}$

### Example:

Calculate  $K_c$  for the following reaction. Analysis of the mixture at equilibrium shows  $SO_2 = 0.058$ ,  $O_2 = 0.343$  and  $SO_3 = 0.230$  mol dm<sup>-3</sup>.



**Step 1:** write the  $K_c$  expression

$$K_c = \frac{[SO_3]^2}{[SO_2]^2 [O_2]}$$

**Step 2:** substitute in equilibrium concentrations and solve

$$K_c = \frac{0.230^2}{0.058^2 \times 0.343} = \frac{0.0529}{0.00115} = 46$$

**Step 3:** determine the units for  $K_c$

$$K_c = \frac{(\text{mol dm}^{-3})^2}{(\text{mol dm}^{-3})^2 \text{ mol dm}^{-3}} = \text{mol}^{-1} \text{ dm}^3$$

$$K_c = 46 \text{ mol}^{-1} \text{ dm}^3$$

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Sometimes, rather than an equilibrium concentration, the information you are given may refer to an amount of moles at equilibrium. In this case, before substituting your values in, you would need to determine the concentration using the equation: concentration = moles ÷ volume (dm<sup>3</sup>)

It is also possible to determine the concentration of a substance at equilibrium if you are provided with the value for the equilibrium constant. In this scenario, you would begin by rearranging the K<sub>c</sub> expression to make the concentration of the unknown the subject.

### Test your knowledge

When PCl<sub>5</sub> is heated, it dissociates into PCl<sub>3</sub> and Cl<sub>2</sub>. In a closed system the following equilibrium is established:

Analysis of the mixture shows that it contains 0.05 mol dm<sup>-3</sup> PCl<sub>3</sub> and 0.5 mol dm<sup>-3</sup> Cl<sub>2</sub>. Determine the value of K<sub>c</sub>.

#### Example:

In the following reaction:  $\text{H}_{2(g)} + \text{I}_{2(g)} \rightleftharpoons 2 \text{HI}_{(g)}$  K<sub>c</sub> = 54.1  
It was found, when analysed, that the equilibrium mixture of H<sub>2</sub> had a concentration of 4.80 mol dm<sup>-3</sup> and HI a concentration of 3.53 mol dm<sup>-3</sup>. Use this data to determine what the concentration of I<sub>2</sub> must have been.

**Step 1:** write down the K<sub>c</sub> expression

$$K_c = \frac{[\text{HI}]^2}{[\text{H}_2][\text{I}_2]}$$

**Step 2:** rearrange to make [I<sub>2</sub>] the subject

$$[\text{I}_2] = \frac{[\text{HI}]^2}{[\text{H}_2] K_c}$$

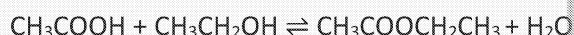
**Step 3:** substitute in known values and solve

$$[\text{I}_2] = \frac{3.53^2}{4.80 \times 54.1} = \frac{12.46}{259.68} = 0.048 \text{ mol dm}^{-3}$$

The final type of K<sub>c</sub> calculation, and the most challenging, is when you are supplied with initial concentrations and asked to determine equilibrium concentrations. In this situation you would need to use the 'RICE' table (shown below) is the easiest way to do this.

#### Example:

The reaction below was set up and allowed to reach equilibrium. 2 moles of CH<sub>3</sub>COOH was used. The mixture was analysed at equilibrium and it was found that 0.845 moles of CH<sub>3</sub>COOCH<sub>2</sub>CH<sub>3</sub> had been formed. Determine the K<sub>c</sub> value.



	CH <sub>3</sub> COOH	CH <sub>3</sub> CH <sub>2</sub> OH	CH <sub>3</sub> COOCH <sub>2</sub> CH <sub>3</sub>
<b>Ratio using the balanced equation</b>	1	1	1
<b>Initial number of moles</b>	2	1	0
<b>Change in concentration</b>	-0.845 The ratio from the equation shows that the change in moles will be the same, but will decrease as it is a reactant	-0.845 The ratio from the equation shows that the change in moles will be the same, but will decrease as it is a reactant	+0.845
<b>Equilibrium number of moles</b>	2 - 0.845 = 1.155	1 - 0.845 = 0.155	0.845

The equilibrium number of moles can now be used in the usual way.

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**Test your knowledge**

When 4 moles of  $\text{PCl}_5$  is heated in a  $3 \text{ dm}^3$  closed system the following reaction occurs



Analysis of the equilibrium mixture showed it to contain 2.4 moles of  $\text{Cl}_2$ . Use this information to determine the value of  $K_c$  and its units.

**Calculations involving  $K_p$** 

When working with  $K_p$ , instead of concentration you are required to substitute into the reaction the **partial pressures** of the gases involved. This requires you to know the **mole fraction** of each gas.

Due to the fact that as long as the temperature and pressure is the same, the same volume of two different gases will contain the same number of moles, you can determine the mole fraction of a named gas using the following equation:

$$\text{mole fraction of gas X} = \frac{\text{number of moles of gas X}}{\text{total number of moles of gas in the mixture}}$$

The sum of all mole fractions in a mixture of gases must equal 1.

**Example:**

Earth's atmosphere is made up of 78 % nitrogen, 21 % oxygen and 1 % other gas. Calculate the mole fraction of each gas present in the atmosphere.

$$\text{N}_2 = \frac{\text{number of moles of gas X}}{\text{total number of moles of gas in the mixture}} = \frac{78}{100} = 0.78$$

$$\text{O}_2 = \frac{\text{number of moles of gas X}}{\text{total number of moles of gas in the mixture}} = \frac{21}{100} = 0.21$$

$$\text{others} = \frac{\text{number of moles of gas X}}{\text{total number of moles of gas in the mixture}} = \frac{1}{100} = 0.01$$

$$\text{Sum of mole fractions} = 0.78 + 0.21 + 0.01 = 1.00$$

Once the mole fraction has been determined, the partial pressure of each gas can be determined using the following equation:

$$\text{partial pressure of gas X} = \text{mole fraction of gas X} \times \text{total pressure}$$

The sum of all partial pressures in a mixture of gases must equal the same as the overall pressure.

**Example:**

If a sample of Earth's atmosphere was placed under a pressure of 175 kPa, determine the partial pressure of each gas present.

$$\text{N}_2 = \text{mole fraction of gas X} \times \text{total pressure of the system} = 0.78 \times 175 = 136.5 \text{ kPa}$$

$$\text{O}_2 = \text{mole fraction of gas X} \times \text{total pressure of the system} = 0.21 \times 175 = 36.75 \text{ kPa}$$

$$\text{others} = \text{mole fraction of gas X} \times \text{total pressure of the system} = 0.01 \times 175 = 1.75 \text{ kPa}$$

$$\text{Sum of partial pressures} = 136.5 + 36.75 + 1.75 = 175$$

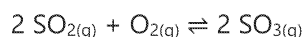
These partial pressures could then be substituted into the  $K_p$  equilibrium expression to determine the value of  $K_p$ .

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## Test your knowledge

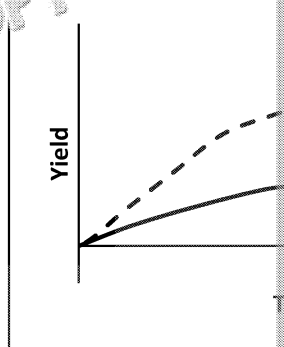


5 moles of  $\text{SO}_2$  are combined with 4 moles of  $\text{O}_2$  and allowed to reach equilibrium. The mixture showed that there was 1.5 moles of  $\text{SO}_3$ . The total pressure in the system is 100 kPa. Calculate the value of  $K_p$  and its units.

**HINT:** Begin by determining the number of moles of each substance at equilibrium. Then use these values to determine the mole fraction and partial pressure.

## Interpretation of yield graphs

Graphs showing the yield of reactions produced under different conditions can be interpreted to give information about the reaction itself. For example, in the graph shown here you can see that the higher the temperature, the higher the yield.



From this you are able to infer that the reaction must be endothermic in the forward direction. This is due to higher temperatures causing equilibrium to shift to the right and yield increasing.

Finally, this graph also shows that the lower the pressure the higher the yield. Graphs of this type are used to ensure all possible information has been obtained from them.



## Recap questions: Chemical equilibrium

- What is meant by the following terms?
  - Dynamic equilibrium (1 mark)
  - Closed system (1 mark)
- Explain how the following changes affect the position of equilibrium:
  - Increasing temperature (2 marks)
  - Decreasing pressure (2 marks)
  - Adding a catalyst (2 marks)
- Hydrogen can be made via the following process:  $\text{CO}_{(g)} + \text{H}_2\text{O}_{(g)} \rightleftharpoons \text{CO}_{2(g)} + \text{H}_{2(g)}$ 
  - If the temperature of this equilibrium was decreased, what would happen and why? (2 marks)
  - If the pressure of this equilibrium was increased, what would happen to the yield and why? (2 marks)
- For the equations given below, write the  $K_c$  equilibrium constant expression:
  - $2\text{SO}_3 \rightleftharpoons 2\text{SO}_2 + \text{O}_2$  (2 marks)
  - $\text{PCl}_3 + \text{Cl}_2 \rightleftharpoons \text{PCl}_5$  (2 marks)
- 1.9 moles of hydrogen was reacted with 1.9 moles of iodine and then left to reach equilibrium. When the mixture was analysed it was found to contain 3 moles of hydrogen iodide. Calculate the value of  $K_c$  for this reaction.
  - Write the  $K_c$  expression for this reaction. (1 mark)
  - Determine the equilibrium concentration of each chemical. (2 marks)
  - Calculate the value for  $K_c$  and give its units. (3 marks)
- For the equations given below write the  $K_p$  equilibrium constant expression (assume all pressures are measured in Pa).
  - $\text{CO}_{(g)} + 3 \text{H}_{2(g)} \rightleftharpoons \text{CH}_{4(g)} + \text{H}_2\text{O}_{(g)}$  (2 marks)
  - $2 \text{O}_{3(g)} \rightleftharpoons 3 \text{O}_{2(g)}$  (2 marks)
- An equilibrium is set up between three gases, A, B and C, as follows:  $2 \text{A}_{(g)} + \text{B}_{(g)} \rightleftharpoons 3 \text{C}_{(g)}$ . At equilibrium there are 2.0 moles of A, 2.5 moles of B and 1.5 moles of C. The total pressure is 100 kPa. Calculate the value of  $K_p$ . (12 marks)

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## D1.5 Applications of chemical kinetics, equilibrium in industry



### Key points covered

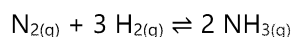
- Use of the idea of chemical compromise when determining ideal conditions for chemical processes.

Two important chemical industries which produce chemicals on a large scale are the Haber process and the contact process. As the aim of these industries is to produce the highest amount of product possible, it is important they carefully select the conditions they operate under carefully.

### The Haber process

The Haber process provides the synthesis of ammonia, a highly valuable chemical used in fertilisers, pharmaceuticals and explosives.

Ammonia is produced via a reversible reaction, combining nitrogen with hydrogen.



### Temperature

Due to Le Chatelier's principle, in order to produce the maximum yield of ammonia the reaction should be carried out at as low a temperature as possible. This is due to the forward reaction being exothermic. A low temperature results in equilibrium shifting to the right-hand side, favouring the forward reaction.

However, low temperature would result in a very low rate of reaction, due to the particles having less energy and therefore very unlikely to be involved in a successful collision.

Therefore a compromise temperature of 450 °C is used to ensure a suitable yield of ammonia at a reasonable rate.

### Pressure

Due to Le Chatelier's principle, in order to produce the maximum yield of ammonia the reaction should be carried out at as high a pressure as possible. This is due to the forward reaction producing fewer gas molecules and therefore a high pressure results in equilibrium shifting to the right-hand side.

However, high pressures are very expensive and dangerous to create and maintain.

Therefore a compromise pressure of 200 atm is used to ensure a suitable yield of ammonia at a reasonable rate and with good profits.

### Catalyst

In order to increase overall rate of reaction an iron catalyst is added.

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### Recap Question: Applications of chemical kinetics, energetics and equilibrium

- The contact process is used to synthesise sulfuric acid via the following reaction. It is exothermic in the forward direction.
  - Describe and explain the conditions required to ensure the highest yield of sulfuric acid.
  - 'Due to a high  $K_p$  value, a pressure of only 1 atm is used.' Explain this statement. (3 marks)
  - Why is a compromise temperature of 450 °C used? (1 mark)
  - The contact process uses vanadium(V) oxide as a catalyst.
    - Explain what this does to the position of equilibrium. (1 mark)
    - Explain what this does to rate. (2 marks)

## D1.6 Applications of green chemistry



### Key points covered

- Use of atom economy when determining reaction routes
- Discussion of ideas on how chemical industries are as green as possible

### Sustainable chemistry

The chemical industry is having to readjust its working practices to become more **sustainable**. We cannot continue to operate in a manner where resources are being used up quicker than they can be replenished, and it is important to ensure we preserve resources and the environment for future generations.

There are five main ways industry can consider when trying to adopt more greener processes:

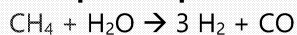
1. **Minimise waste by using high atom economy reactions.** Greener processes in chemical industry aim to operate via reactions that have a high **atom economy**.
2. **Use as few chemicals as possible and don't use hazardous chemicals.** Dangerous chemicals in chemical processes are switched out for less risky alternatives. Products also need to be considered and should also be designed to be as harmless as possible.
3. **Use renewable resources (i.e. from plants) whenever possible.** This allows materials to be replaced and results in a more sustainable process.
4. **Use alternative energy resources such as solar energy, rather than non-renewable fossil fuels.** Fossil fuel consumption is beneficial in two main ways: it cuts down on the production of greenhouse gas emissions and preserves a valuable resource for future generations.
5. **Ensure that any waste products are non-toxic and either recyclable or biodegradable.** Products will be broken down by natural processes and this minimises the amount of waste requiring further treatment after their production. Recycling any unwanted products will reduce the need for raw materials.

### Calculating atom economy

**Atom economy** is calculated using the following equation:

$$\% \text{ atom economy} = \frac{\text{mass of desired products}}{\text{total mass of products}} \times 100$$

#### Example: the production of hydrogen by reacting methane with steam:



$$16 \text{ g mol}^{-1} + 18 \text{ g mol}^{-1} \rightarrow 6 \text{ g mol}^{-1} + 28 \text{ g mol}^{-1}$$

Total mass of hydrogen produced =  $3 \times 2 \text{ g mol}^{-1} = 6 \text{ g}$

Total mass of all products produced =  $6 \text{ g}$  (hydrogen) +  $28 \text{ g}$  (carbon monoxide)

$6 \text{ g}$  out of the  $34 \text{ g}$  of products produced is useful.

$$\% \text{ atom economy} = \frac{\text{mass of desired products}}{\text{total mass of products}} \times 100 = \frac{6}{34} \times 100 = 17.6 \%$$

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### Test your knowledge

1. Calculate the atom economy when producing sodium through the electrolysis of sodium chloride.  
 $2 \text{NaCl} \rightarrow 2 \text{Na} + \text{Cl}_2$
2. Calculate the atom economy when making oxygen from hydrogen peroxide.  
 $2 \text{H}_2\text{O}_2 \rightarrow 2 \text{H}_2\text{O} + \text{O}_2$

## Catalysts

The use of catalysts results in a faster reaction at lower temperatures and pressures, economic benefits, in terms of lower energy costs, and environmental benefits, in terms of lower emissions due to lower consumption of fossil fuels.

Use of a catalyst can result in new routes being developed. These routes could include economies and therefore less waste is produced.

Enzymes are ideal to use as catalysts. They produce very specific products and due to their nature, they operate around room temperature and low pressures, which again are all valuable features of greener procedures.

?

### Recap questions: Applications of green chemistry

- 1 Explain how a catalyst can save money whilst reducing the environmental impact of a process. (4 marks)
- 2 Ethanol can be produced via two alternative processes:

**Process 1: Fermentation of glucose to produce ethanol:**  $\text{C}_6\text{H}_{12}\text{O}_6(\text{g}) \rightarrow \text{C}_2\text{H}_5\text{OH}(\text{g}) + 2\text{CO}_2(\text{g})$

Sugar or starch is dissolved in water and yeast is added. The mixture is then kept at a temperature between 25 °C and 35 °C with the absence of oxygen for a few days.

**Process 2: Hydration of ethane:**  $\text{C}_2\text{H}_4(\text{g}) + \text{H}_2\text{O}(\text{g}) \rightarrow \text{C}_2\text{H}_5\text{OH}(\text{g})$

A mixture of ethene and steam is passed over a hot catalyst of phosphoric acid at a temperature of approximately 300 °C. The pressure used is 60 atm.

- a) What is the atom economy of process 1? Give your answer to 3 s.f. (3 marks)
- b) Give **two** advantages of using process 1 over process 2. (2 marks)
- c) Give **two** disadvantages of using process 1 over process 2. (3 marks)

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# E: Organic chemistry

## E1.1 Key terms



### Key points covered

- Use of the terms saturated and unsaturated when describing hydrocarbons
- Defining key terms used in organic chemistry
- Giving general formulae for homologous series

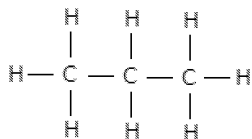
## Organic chemistry

Organic chemistry is the study of carbon-based compounds. Carbon is a unique element that forms stable bonds with other atoms, allowing for a vast diversity of molecules. These molecules range from simple ones like methane ( $\text{CH}_4$ ), to complex structures like DNA, which carries your genetic information.

Carbon's ability to form four bonds makes it incredibly versatile. It can bond with other carbon atoms to form chains and rings, leading to an almost infinite variety of structures. This versatility is the foundation of organic chemistry.

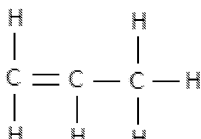
## Hydrocarbons

Hydrocarbons are organic compounds composed exclusively of hydrogen and carbon atoms. They form the simplest type of organic molecule and are the fundamental structures upon which more complex organic compounds are built. Hydrocarbons can be categorised into different types based on the types of bonds between the carbon atoms: alkanes, which have single bonds (**saturated** hydrocarbons); alkenes, which have at least one double bond; and alkynes, which have at least one triple bond.



**Propane**

Saturated alkane



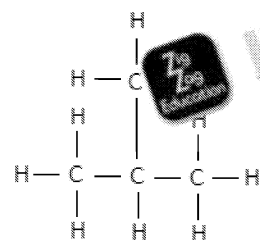
**Propene**

Unsaturated alkene

Hydrocarbons can be organised into different structures: straight chain, branched, and cyclic. Each type has unique characteristics based on the arrangement of carbon atoms within the molecule.

## Straight chain hydrocarbons

These hydrocarbons consist of carbon atoms connected in a single, continuous chain. Each carbon atom, except for the ones at the ends, is bonded to two other carbon atoms, with hydrogen atoms filling the remaining available bonds. An example of a straight chain hydrocarbon is hexane ( $\text{C}_6\text{H}_{14}$ ), where six carbon atoms form a linear sequence.



## Branched chain hydrocarbons

In these hydrocarbons, the carbon chain has one or more branches. A branch is a carbon atom or group of atoms attached to the main continuous chain. This branching affects the physical and chemical properties of the molecule. For example, methylpropane ( $\text{C}_4\text{H}_{10}$ ) is a branched chain hydrocarbon where three carbon atoms form the main chain and one carbon atom branches off from the second carbon of the main chain.

## Cyclic hydrocarbons

These hydrocarbons have carbon atoms arranged in a ring or circle, with each carbon atom bonded to two other carbon atoms to form a closed loop. A common cyclic hydrocarbon is cyclohexane ( $\text{C}_6\text{H}_{12}$ ), which forms a six-membered ring.

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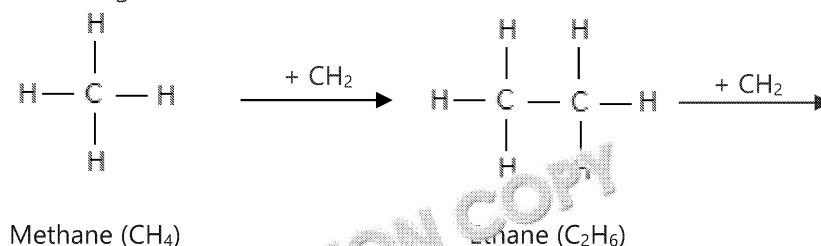
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## Homologous series

A homologous series is a group of organic compounds that have the same **functional group** and differ from each other by a  $-\text{CH}_2$  unit. This consistent difference results in predictable patterns in properties such as boiling point, melting point, and solubility.

The simplest homologous series is the alkanes.



## Functional groups

As well as hydrogen, carbon has the ability to bond to other elements such as oxygen.

**Functional groups** are specific groups of atoms within molecules that have characteristic chemical properties. They are the main deciding factor in the chemical behaviour of organic compounds. The study of functional groups is important in organic chemistry because they allow chemists to predict the reactions that compounds can undergo. By identifying the functional groups in a molecule, you can infer the molecule's reactivity, solubility, and other key properties.

Some common functional groups include:

<p><i>Alkane group</i> (<math>-\text{C}-\text{C}-</math>): alkanes are the simplest type of hydrocarbons, consisting of only single bonds between carbon atoms</p>	<p><i>Alkene group</i> (<math>\text{C}=\text{C}</math>): found in alkenes, these molecules are more reactive than alkanes</p>
$  \begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \\   \quad   \quad   \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{H} \\   \quad   \quad   \\ \text{H} \quad \text{H} \quad \text{H} \end{array}  $	$  \begin{array}{c} \text{H} \\   \\ \text{C}=\text{C} \\   \\ \text{H} \end{array}  $
<p>Alkane (<math>\text{C}_n\text{H}_{2n+2}</math>) Propane</p>	<p>Alkene (<math>\text{C}_n\text{H}_{2n}</math>) Ethene</p>
<p><i>Halogenoalkanes</i> (<math>-\text{X}</math>, where X is a <b>halogen</b>): halogenoalkanes contain a halogen atom (such as fluorine, chlorine, bromine, or iodine) bonded to a carbon chain</p>	<p><i>Hydroxyl group</i> (<math>-\text{OH}</math>): found in alcohols, it makes molecules polar and soluble in water</p>
$  \begin{array}{c} \text{H} \quad \text{H} \quad \text{H} \\   \quad   \quad   \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{Cl} \\   \quad   \quad   \\ \text{H} \quad \text{H} \quad \text{H} \end{array}  $	$  \begin{array}{c} \text{H} \\   \\ \text{H}-\text{C}-\text{OH} \\   \\ \text{H} \end{array}  $
<p>Halogenoalkane (<math>\text{C}_n\text{H}_{2n+1}\text{X}</math>) Chloropropane</p>	<p>Alcohol (<math>\text{C}_n\text{H}_{2n+1}\text{OH}</math>) Propan-1-ol</p>

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Each new homologous series has its own general formula. In organic chemistry, a general formula describes the structure of an entire family of compounds using a simple, algebraic representation. The number of carbon (C) and hydrogen (H) atoms are in each molecule, and sometimes includes oxygen (O). This helps us understand and predict the structure and properties of different compounds.

**For example:**

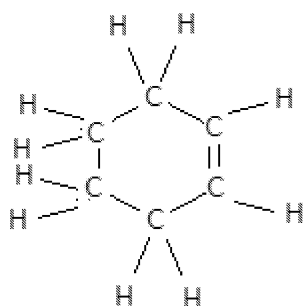
- Alkanes: alkanes are the simplest type of hydrocarbons, and their general formula is  $C_nH_{2n+2}$ . So, if  $n=3$ , the formula is  $C_3H_8$ , which is propane.
- Alkenes: alkenes have at least one double bond between carbon atoms, and their general formula is  $C_nH_{2n}$ . For example, if  $n=2$ , the formula is  $C_2H_4$ , which is ethene.



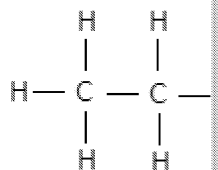
**Recap questions: Key terms**

- Define the term 'homologous series'. (1 mark)
- $CH_2OH$ ,  $C_2H_4OH$ ,  $C_3H_7OH$  are all members of the same homologous series. (2 marks)
  - What is the functional group present in this group of compounds. (1 mark)
  - Use the general formula to predict the molecular formula of the fifth member of the series. (1 mark)
- Classify the following molecules as being:
  - Saturated or unsaturated (4 marks)
  - Straight chain, branched or cyclic (4 marks)

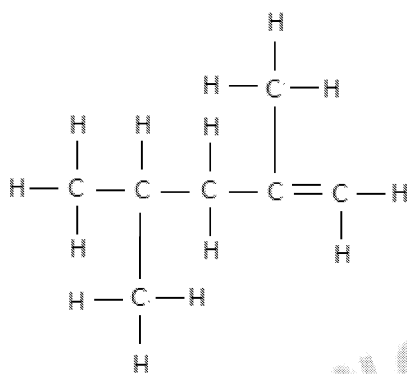
i)



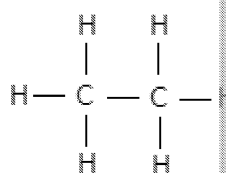
ii)



iii)



iv)



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## E1.2 Structure representations



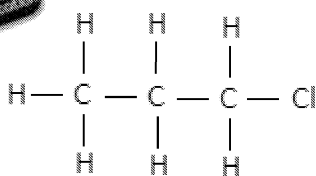
### Key points covered

- Use of structural, skeletal and 3D diagrams of organic compounds

A variety of chemical formula types can be used in organic chemistry to show the structure of a substance. The molecular formula of a substance will tell you the type and number of atoms found in it, but it does not tell you about how these atoms have been bonded and arranged. The purpose of the structural formula is to help inform you of the location of these atoms within the molecule and the shape of the molecule.

### Full displayed structural formula

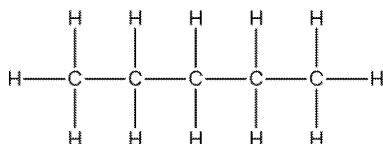
A displayed formula gives the most information about the structure of an organic compound. It shows the position and the bonds it has. For example, 1-chloropropane has the molecular formula  $C_3H_7Cl$ . Its displayed formula can be seen below. Ethanol has the chemical formula  $C_2H_5OH$ . Its displayed formula can be seen below.



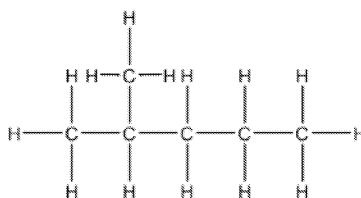
1-chloropropane

### Condensed structural formula

In diagrams showing the condensed structural formula, less detail is shown. Every bond is missing and instead you see the groups that have been bonded together. Below are the condensed structural formulae for a selection of organic compounds and their corresponding full displayed structural formulae.



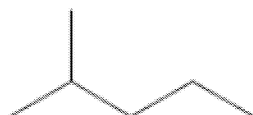
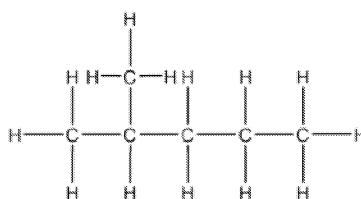
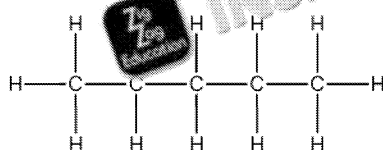
$CH_3CH_2CH_2CH_2CH_3$



$CH_3CH(CH_3)CH_2CH_2CH_3$

### Skeletal formula

Skeletal formula is a simplified diagram of organic molecules which show only the carbon skeleton. Single covalent bonds between carbon atoms are represented by lines. There are no labels for hydrogen atoms. Any bonds to hydrogen atoms are also shown as lines.

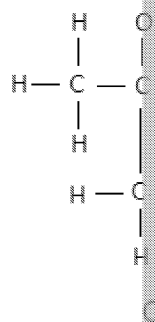
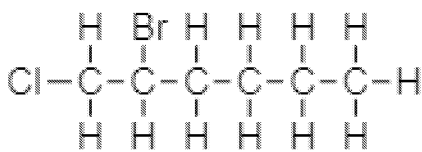


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Any functional groups present in the molecule must also be shown in the skeletal formula.



### 3D diagrams of organic molecules

#### Reminder

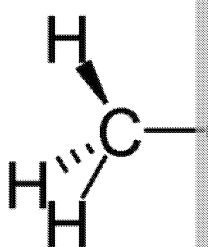
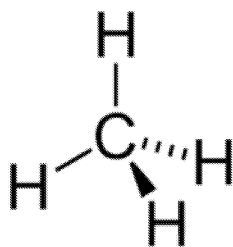
It can be hard to represent a three-dimensional shape on a two-dimensional sheet. A series of wedges has been created to help chemists portray and visualise molecular shapes.

A solid line represents a bond that lies in the same plane as the paper.

A dotted wedge represents a bond that goes into the plane of the paper.

A solid wedge represents a bond that comes out of the plane of the paper.

Hydrocarbons adopt different shapes based on the number of bonds around the carbon atom. The geometry to be adopted is tetrahedral, with bond angles of  $109^\circ$ .



However, in alkenes, the double bond between two carbon atoms causes a trigonal planar geometry with bond angles of  $120^\circ$ .

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#### Recap questions: Condensed and skeletal representations

- 1
  - a) Draw out the full displayed structural formulae for the two hydrocarbons with the molecular formula  $\text{C}_4\text{H}_{10}$ . (2 marks)
  - b) Write out the condensed structural formulae for the two molecules. (2 marks)
- 2 Draw the skeletal formula for the hydrocarbon with the molecular formula  $\text{C}_5\text{H}_{12}$  where the second carbon has a methyl group attached. (2 marks)
- 3 Draw the skeletal formula for the alcohol that is cyclic and contains five carbon atoms. (2 marks)
- 4 Draw the full displayed structural formula for the halogenoalkane which has the molecular formula  $\text{C}_4\text{H}_9\text{Br}$  where the halogen is not on the end of the chain. (2 marks)





## E1.3 Naming alkanes, alkenes, halogenoalkanes



### Key points covered

- Use of IUPAC naming conventions to name key organic homologous series

### IUPAC nomenclature

Due to carbon's ability to form up to four bonds per atom, in straight chain or cyclic form, there are over 19 million known organic compounds in existence, many of which may contain functional groups. In order to ensure consistency and a common language when giving each of these compounds a name, a system has been drawn up and should be adhered to. The International Union of Pure and Applied Chemistry (IUPAC) is the recognised authority with regard to chemical names, and they have devised a method by which every possible organic compound has a name from which you are able to draw an unambiguous structure.

### Carbon chain length

All names in organic chemistry are based primarily on the main alkane found in the molecule. Once the number of carbons in the longest chain, the appropriate stem can be selected.

Number of carbons	1	2	3	4
Stem to be used	Meth-	Eth-	Prop-	But-

### Functional groups

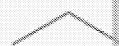
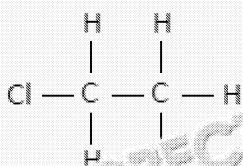
Once the stem of the name has been identified, any functional groups in the molecule must be identified. This is done in the form of either a prefix or suffix, as shown below.

Functional group	Nomenclature	Prefix/suffix
Alkane	-ane	Suffix
Alkene	-ene	Suffix
Halogenoalkane	Fluoro(alkane) Chloro(alkane) Bromo(alkane) Iodo(alkane)	Prefix
Alcohol	-anol	Suffix

#### Example:

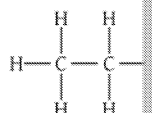
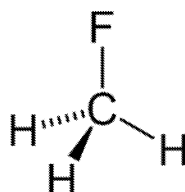
This molecule has two carbons in its longest chain (eth-). It also has the halogenoalkane functional group. Therefore its name is chloroethane.

This molecule has six carbons in its longest chain (hex-). It also has the alcohol functional group. Therefore its name is hexanol.



### Test your knowledge

Name the following organic compounds:



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## Branched alkanes

Any side chains within the alkane backbone can be identified by adding the suffix. These side chains are known as alkyl groups.

### Example:

This is butanol with an ethyl group as a side chain. It would be called ethylbutanol	This is fluoropropane with a methyl side chain. It would be called methylfluoropropane

If there are multiple side chains on your molecule they should be named in alphabetical order. Identical side chains are prefixed with di- (for two) or tri- (for three) would be added in front.

### Example:

This is propane with two methyl group side chains. It would be called dimethylpropane.	This is hexanol with a methyl side chain. It would be called methylhexanol.

## Locants

Side chains and functional groups should have their position indicated by giving the carbon number they are found on. Carbons should always be numbered starting from the end that will give the lowest number to the functional group or side chain, even if this feels like you are working backwards.

Any adjacent numbers should be separated using a comma, and numbers should be separated from letters by a hyphen.

### Example:

This is pentane with the bromine located on carbon 2. Its name is 2-bromopentane.	This is hexane with the methyl and ethyl side chains. The carbon number 2 (numbered from the end closest to the lowest number).
This would be called 3-ethyl-2-methylhexane.	This is 2,2-dimethylpropane.

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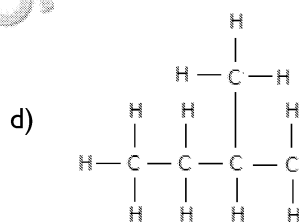
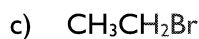
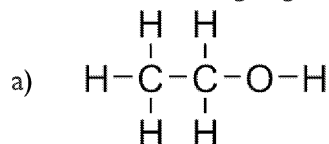
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## Recap questions: Naming alkanes, alkenes, halogenoalkanes and

1 Draw the following organic molecules. (4 marks)

- 3-methylhexane
- Pentan-3-ol
- Trichlorofluoromethane
- Pent-1-ene

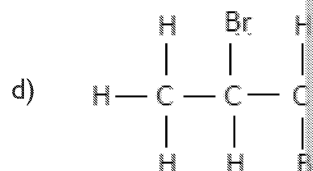
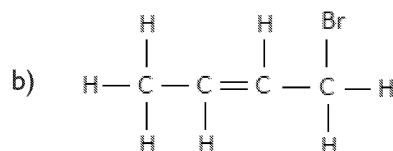
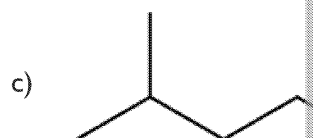
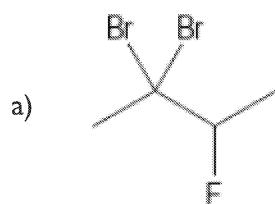
2 Name the following organic molecules. (4 marks)



3 Draw the following organic molecules. (4 marks)

- 2,3-dimethylpentane
- 2,3-dimethylpent-3-ene
- 3-bromo-3-fluoro-2-methylhexane
- 2-methylpropan-2-ol

4 Name the following organic molecules. (4 marks)



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## E1.4 Isomerism



### Key points covered

- Defining types of isomerism present in organic compounds
- Identifying isomers in organic compounds

### Isomerism

In organic chemistry there can be many molecules with the same molecular formula but which are arranged differently from molecule to molecule. Compounds with the same molecular formula but different arrangements of atoms are called **isomers**.

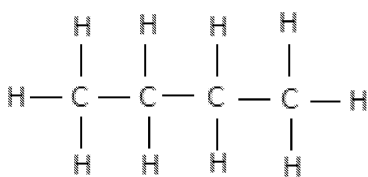
There is a variety of types of isomerism. In this applied science course the focus is on structural and stereoisomerism.

### Structural isomerism

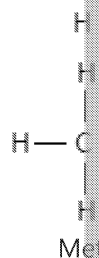
Structural isomers are defined as being compounds with the same molecular formula but different structural arrangements.

#### Branched alkanes

Structural isomerism is exhibited repeatedly in the alkane homologous series. If you are given the formula  $C_4H_{10}$  there are two possible structures that can be drawn:



Butane

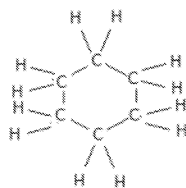


Methylpropane

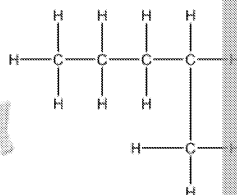
### Test your knowledge

Justify if each pair of molecules are isomers of each other.

a)



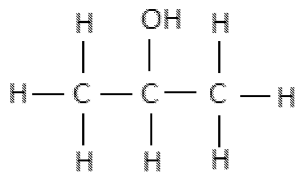
b)



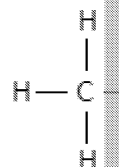
and

### Positioning of the functional group

In functional groups containing compounds, such as alkenes, halogenoalkanes and alcohols, the functional group can be placed at different positions along the carbon chain. The molecular formula is the same for all isomers. The following two structures are examples:



Propan-2-ol



Propan-1-ol

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## Stereoisomerism

Stereoisomers are defined as being compounds with the same molecular formula but different arrangements of atoms in space. This differs from the previously discussed structural isomers as the connectivity of the atoms is identical in both isomers, it is simply the orientation of the atoms in respect of each other that differs.

### Test your knowledge

How many isomers of the molecular formula  $C_4H_8$  can be written in full displayed form? Name them all?

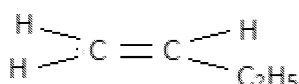
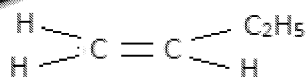
## Stereoisomerism in alkenes

The double bond in an alkene is formed from one  $\sigma$  bond and one  $\pi$  bond. The  $\pi$  bond position and restricts any rotation around that bond. This causes any atoms bonded in fixed positions relative to each other.

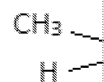
## E/Z isomerism

In order to display E/Z isomerism a molecule must satisfy two criteria:

1. It must contain a  $C=C$  double bond.
2. Different groups must be bonded to each carbon in the double bond.

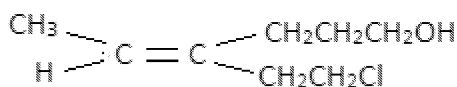


But-1-ene does not show E/Z isomerism as the two groups bonded to the left-hand carbon in the double bond are identical. This means both versions of the alkene are identical.



But-2-ene does show E/Z isomerism as different groups are attached to each carbon; a hydrogen atom and a methyl group.

If these criteria are met then two isomers of the alkene will be formed: the E isomer and the Z isomer. To determine the correct name the priority of the bonded groups has to be determined. This is decided based upon its atomic number; the higher the atomic number, the higher the priority. If the groups bonded to the carbons are initially identical you need to find the first point of difference to determine the priority from this point.



The groups attached to the right-hand carbon are initially identical. However, after the first point of difference, the top group has a third  $CH_2$  bonded, the atom at the end of this chain is an oxygen, and the bottom group has a Cl attached, with an atomic number of 17. The bottom group is the higher priority.

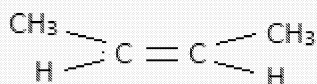
- If the groups with the highest priority are on the same side of the double bond, the compound is the Z isomer.

highest priority  
lowest priority

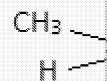
- If the groups with the highest priority are on opposite sides of the double bond, the compound is the E isomer.

highest priority  
lowest priority

### Example:



The methyl group on each carbon is the higher priority group and these are located on the same side of the double bond. This is Z-but-2-ene.



The methyl group on each carbon is the higher priority group and these are located on opposite sides of the double bond. This is E-but-2-ene.

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## Cis/trans isomerism

This is a very specific type of E/Z isomerism. For a compound to show cis/trans isomerism it would need to meet the same two requirements as for E/Z isomerism (it must contain a C=C, different groups bonded to each carbon in the double bond). However, additionally, to satisfy the criteria for cis/trans isomerism one of the bonded groups on each of the double bond must be the same.

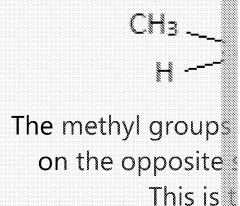
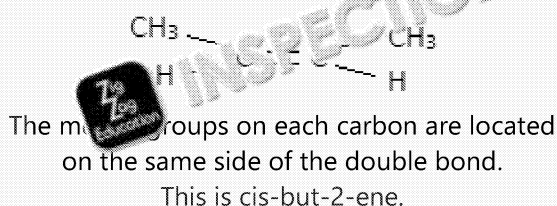
### Test your knowledge

Would pent-1-ene show cis/trans isomerism?  
What about pent-2-ene?  
Do you have any stereoisomers for pent-2-ene?  
What about these two compounds?


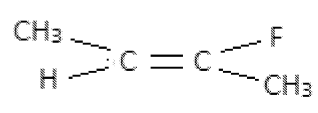
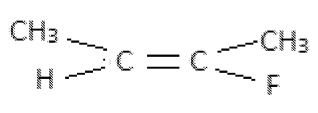
When these criteria are met, then

- the Z isomer will be known as the **cis** isomer
- the E isomer will be known as the **trans** isomer

### Example:



### Recap questions: Isomerism

- Define the terms
  - structural isomers (1 mark)
  - stereoisomers (1 mark)
- Identify which type of isomerism is present in the pairs of isomers shown below.
  -  (1 mark)
  -  and  (1 mark)
- Draw and name all isomers with the chemical formula C<sub>6</sub>H<sub>14</sub>. (10 marks)
- Draw the following alkenes and decide if they will show stereoisomerism.
  - 2-methylpent-2-ene (2 marks)
  - hex-3-ene (2 marks)
  - 2,3-dichlorobut-2-ene (2 marks)
- Draw the stereoisomers of hex-2-ene and correctly name each one. (4 marks)
- State which type of isomerism, if any, the following molecules could display.
  - C<sub>4</sub>H<sub>10</sub>
  - C<sub>4</sub>H<sub>8</sub>
  - C<sub>4</sub>H<sub>10</sub>

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## E1.5 Sigma and pi molecular orbitals



### Key points covered

- Describing the formation of sigma molecular orbitals
- Describing the formation of pi molecular orbitals

### Bonding in carbon

Carbon has four valence shell electrons, which means it has the ability to form four covalent bonds with other atoms in order to obtain a full and stable outer shell. As discussed previously, the electrons in an atom exist in orbitals; for carbon, the outer shell electrons are found in the 2s and 2p orbitals ( $1s^2 2s^2 2p^2$ ). To form a covalent bond these orbitals must overlap to form a combined orbital called the molecular orbital. Depending on the form this overlap takes, two types of covalent bonds can be formed:  $\sigma$  (sigma) or  $\pi$  (pi) bonds.

#### $\sigma$ (sigma) bonds

$\sigma$  bonds can be formed from either s or p orbitals and involve the end-to-end overlap. The diagram below shows end-to-end overlap between two s orbitals, an s orbital and a p orbital, and two p orbitals.



The shared electron density that occurs as a result of this overlap is shared between two nuclei.  $\sigma$  bonds are the strongest type of covalent bond and are often common in organic molecules.

#### $\pi$ (pi) bonds

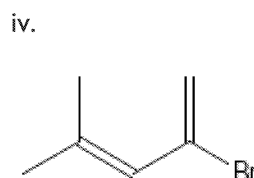
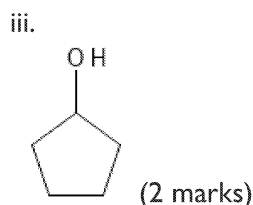
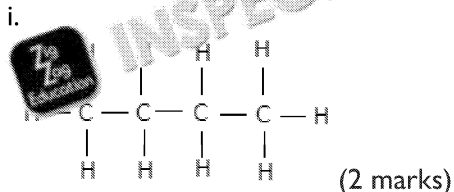
$\pi$  bonds are formed by p orbitals and involve the sideways overlap of two that are adjacent. The diagram (right) shows the overlap between the two lobes of neighbouring p orbitals, which lie above and below the plane of the nuclei.

One  $\pi$  bond is represented as two clouds of electron density. This means that a double covalent bond is made up of one  $\sigma$  bond and one  $\pi$  bond.



### Recap questions: Sigma and pi molecular orbitals

- Draw the molecular orbital that results when an s orbital is involved in a p orbital. (1 mark)
  - Name the type of covalent bond that is formed. (1 mark)
- Draw the molecular orbital formed in a pi bond. (1 mark)
  - Which orbitals must overlap to form a pi bond? (1 mark)
- How does a sigma bond differ from a pi bond? (2 marks)
- Identify how many...
  - sigma bonds
  - pi bonds
 ... are in each of these compounds.



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## E1.6 Changes in boiling point



### Key points covered

- Explaining differences in boiling point due to chain length
- Explaining differences in boiling point due to chain branching

Alkanes are obtained from crude oil via the process of fractional distillation. Oil ref is a mixture of hydrocarbons as each alkane has a different boiling point. In order to separate them you need to break the intermolecular forces that hold the molecules together. This is done through London forces; the stronger the London forces, the higher the boiling point.

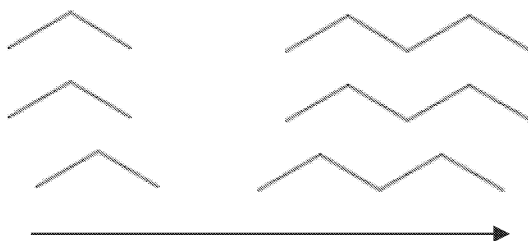
### Boiling point and chain length

As the length of the hydrocarbon chain increases, boiling point increases as shown.

Alkane	methane	ethane	propane	butane	pentane	hexane
Boiling point / °C	-162	-89	-42	-1	36	69

The longer the chain, the larger the surface area of the molecule. This results in more contact occurring between the molecules and therefore greater London forces which would increase the boiling point.

Shorter chain length  
Less surface area contact  
Weaker London forces



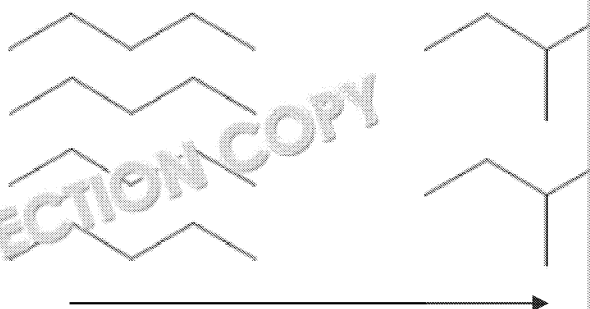
### Boiling point and chain branching

As the level of branching in the hydrocarbon chain increases, boiling point decreases.

Alkane	butane	2-methylpropane
Boiling point / °C	36	28

The branches on the alkane chains prevent the molecules from approaching each other closely. They also reduce the surface area of the alkane and this results in less surface contact. Fewer contact factors result in weaker London forces which require less energy to break.

Less branching  
More surface area contact  
Stronger London forces



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### Recap questions: Changes in boiling point

1 Rank the following alkanes in order of boiling point, from highest to lowest.



2 Explain the reason behind your order in question 1. (4 marks)



## E1.7 Reactions of organic compounds



### Key points covered

- Describe the reaction conditions required for a range of organic conversions
- Predict the products of a range of organic conversions

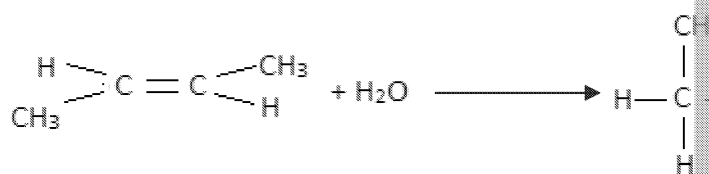
Organic compounds can undergo a variety of reactions due to the varying properties of different functional groups. Understanding these reactions is vital for knowing how different molecules are formed. This knowledge is fundamental in areas such as pharmaceuticals, materials science, and environmental science.

Organic reactions are the backbone of organic chemistry, enabling the synthesis of a wide range of compounds. These reactions can be grouped into several types, each with its own characteristic mechanisms.

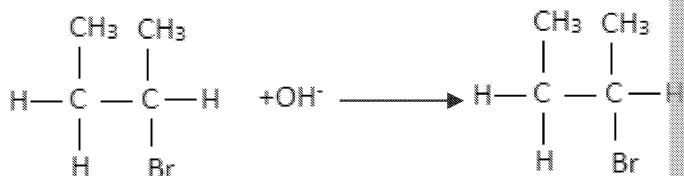
### Types of organic reactions

Organic reactions are typically categorised based on the changes occurring in the molecules. The main categories include:

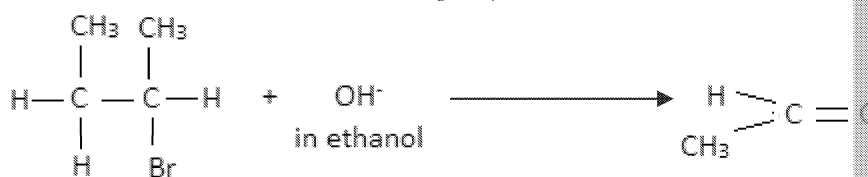
**Addition reactions:** where two reactants combine to form one product.



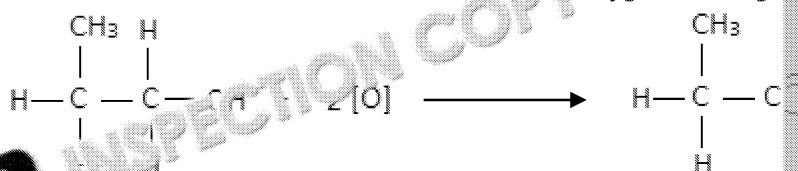
**Substitution reactions:** involving the replacement of an atom or group in a molecule.



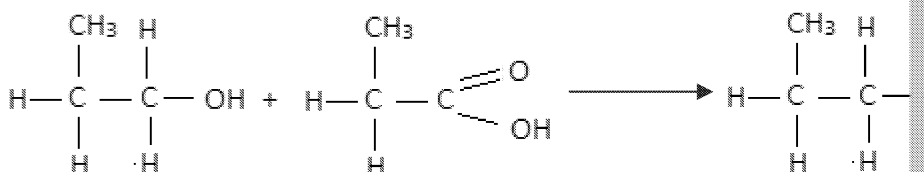
**Elimination reactions:** where atoms or small groups of atoms are removed from a molecule.



**Oxidation reactions:** where a molecule loses electrons or gains oxygen, altering its structure.



**Condensation reactions:** where two molecules combine to form a larger molecule and a small molecule like water.



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## Addition reactions

Addition reactions are common in unsaturated compounds such as alkenes. Due to the presence of a double bond in alkenes there is a high area of electron density that is very susceptible to attack by electrophilic species. In an addition reaction the carbon-carbon double bond is broken and each carbon forms a new single bond. There is a variety of addition reactions that alkenes can undergo.

### Hydrogenation

Hydrogenation is the addition of hydrogen ( $H_2$ ) to a double bond, converting alkenes to alkanes. This reaction requires a catalyst, such as platinum (Pt) or nickel (Ni) and heat, 423 K. Ethene will react with hydrogen in the presence of a catalyst at 423 K to form ethane.

### Halogenation

Halogenation involves the addition of halogens ( $Cl_2$ ,  $Br_2$ ) to alkenes to form dihalogenoalkanes. This reaction takes place at room temperature and requires no special conditions. Ethene will react with bromine to form 1,2-dibromoethane.

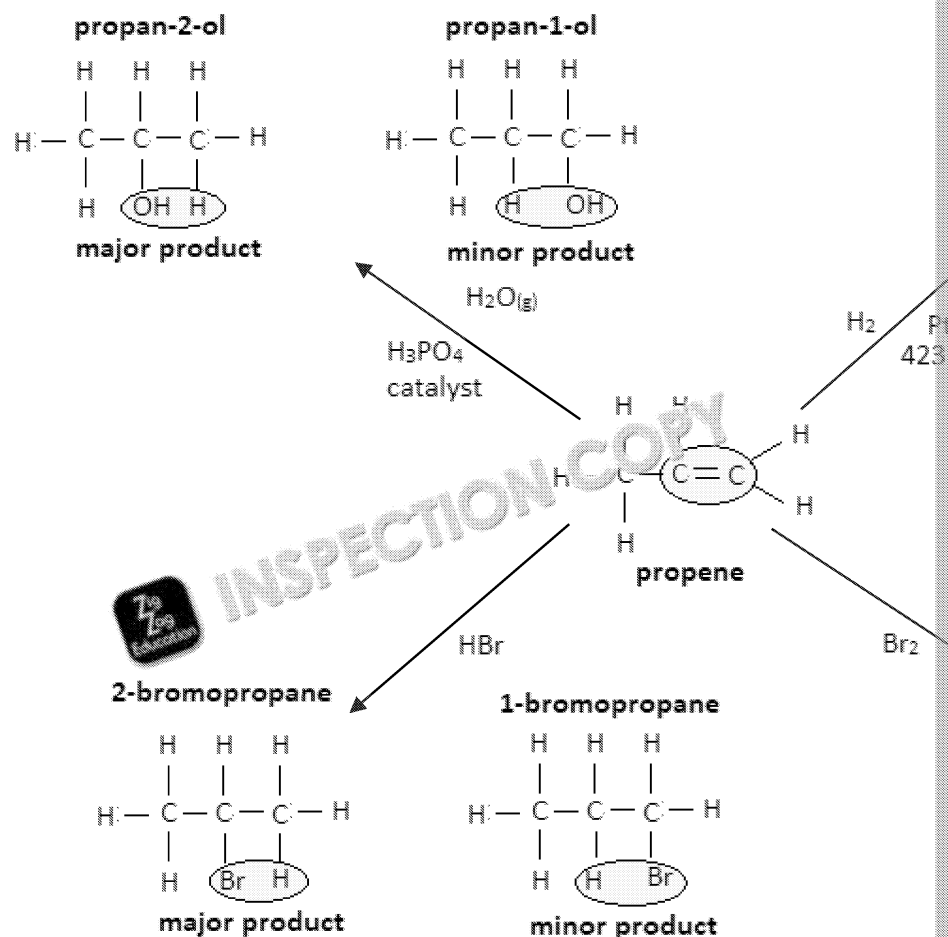
### Reaction with hydrogen halides

The addition of hydrogen halides (HCl, HBr) to alkenes produces halogenoalkanes. When the alkene is unsymmetrical, there are two possible products that can be formed. This is determined by Markovnikov's rule. The dominant product is that where the hydrogen atom from the halide adds to the carbon with the greater number of hydrogen atoms, and the halogen attaches to the carbon with fewer hydrogen atoms (see diagram below). Ethene reacts with hydrogen bromide to form bromoethane.

### Hydration

Hydration involves the addition of water, in the form of steam ( $H_2O$ ), to alkenes to produce alcohols. This reaction requires a catalyst in the form of phosphoric acid ( $H_3PO_4$ ). This reaction also takes place on unsymmetrical alkenes. Ethene reacts with water in the presence of a catalyst to form ethanol.

Each of these reaction types is represented visually in the diagram below, using propene as an example.



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### Test your knowledge

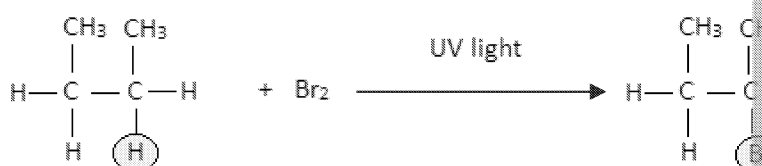
1. Draw the full structural formulae of three different alkenes which would be expected to react with hydrogen at 423 K in the presence of a Pt catalyst.
2. Draw the two structural isomers formed when pent-2-ene reacts with HBr.
3. Explain why there are two products formed when pent-1-ene reacts with H<sub>2</sub> and H<sub>3</sub>PO<sub>4</sub> catalyst. Which product will be the major product? Why?

## Substitution reactions

Substitution reactions are a key type of reaction in organic chemistry. In a substitution reaction, one or more atoms in a molecule is replaced by another atom or group. Substitution reactions are often referred to as a chemical 'swap' where one part of a molecule is exchanged for another. For example, if a bromine atom is attached to a molecule, we might replace the bromine with a different group, like a hydroxyl group. This changes the molecule into a new compound with different properties. These reactions cover a wide variety of organic compounds and are commonly used in both laboratory and industrial settings.

### Substitution reactions of alkanes to form halogenoalkanes

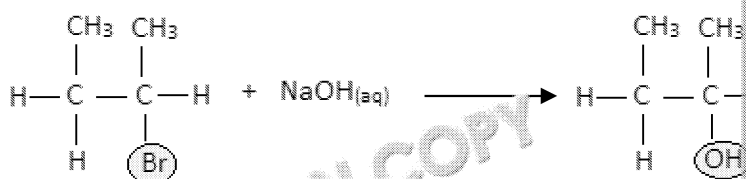
Due to their low reactivity, in order to make an alkane react a large amount of energy is needed. This energy is given to the reaction in the form of UV light. UV light will break the bond between two halogen atoms to break and form a **radical** which is then able to attack the alkane. It is then able to proceed to substitute itself for one of the hydrogen atoms in the alkane chain. This reaction is uncontrollable; you are unable to control where or how many substitutions occur.



### Substitution reactions of halogenoalkanes to form alcohols

**Nucleophile** – a molecule or atom that is attracted to positive charge. Usually a species with a negative charge or lone pair of electrons.

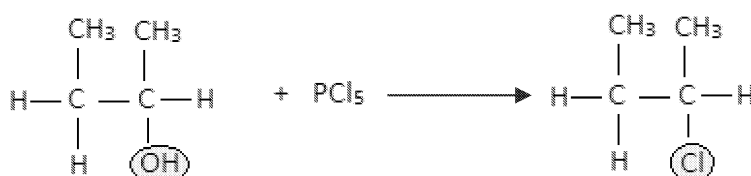
Halogenoalkanes are far more reactive than alkanes. The presence of a halogen causing an uneven distribution of charge. The carbon atom that is bonded to the halogen having a  $\delta+$  charge. **nucleophiles**. The reaction of a nucleophile with a halogenoalkane results in the formation of an alcohol where the halogen is replaced by a hydroxyl group.



### Substitution reactions of alcohols to form halogenoalkanes

The conversion of an alcohol to a halogenoalkane, known as halogenation, requires a halogen. The halogen you intend to substitute for the hydroxyl group.

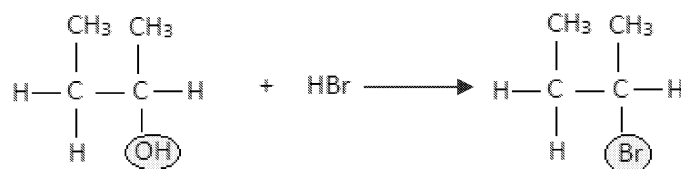
In order to chlorinate the ring you can add phosphorus(V) chloride, PCl<sub>5</sub>. This causes a vigorous reaction which gives off hot, steamy fumes of HCl. Due to the vigorous nature of the reaction, it is often carried out in a fume cupboard.



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Bromination of an alcohol simply requires the addition of HBr.



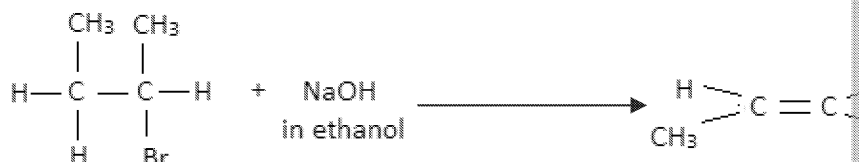
### Test your knowledge

1. Write the equation to show the reaction between propan-2-ol and  $\text{PCl}_5$ .
2. Why is UV light required for the substitution reactions of alkanes?
3. What conditions would be needed to convert 2-chlorobutane into butan-2-ol?
4. What addition inorganic product is formed when an alcohol reacts with HBr?

## Elimination reactions

### Elimination reactions of halogenoalkanes to form alkenes

In this reaction, a small molecule, HX (where X is the halogen present), is removed from a halogenoalkane to form a C=C double bond. This is achieved by heating the halogenoalkane with **ethanolic** sodium hydroxide. The reaction conditions are very important; if aqueous sodium hydroxide is used then substitution, as described above, would occur.



## Oxidation reactions

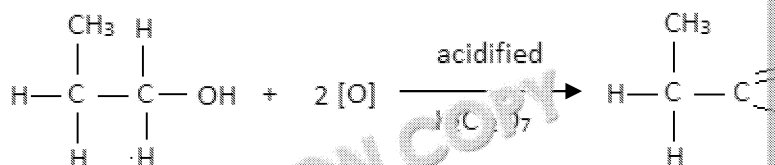
### Oxidation of primary alcohols to carboxylic acids

In organic chemistry, oxidation reactions are processes where a molecule gains oxygen or loses hydrogen. The oxidation of primary alcohols to carboxylic acids is an

**Carboxylic acid** – a molecule containing the  $-\text{COOH}$  functional group

**Aldehyde** – a molecule containing the  $-\text{CHO}$  functional group

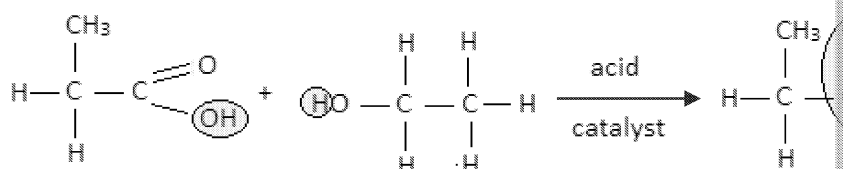
important reaction in organic chemistry. Using **oxidising agents** like potassium dichromate in acidic conditions, primary alcohols can be fully oxidised, passing through an **aldehyde** stage. The oxidation is carried out using acidified potassium dichromate, where the oxidising agent changes colour from orange to green.



## Condensation reactions

### Condensation reactions to form esters

Esterification is a key reaction in organic chemistry that produces esters from alcohols and carboxylic acids. The reaction is catalysed by an acid, such as sulfuric acid, and requires heating. Esters are everyday products such as fragrances and flavourings.



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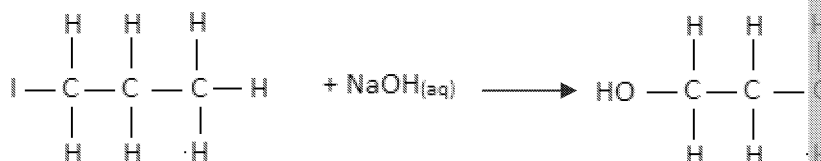




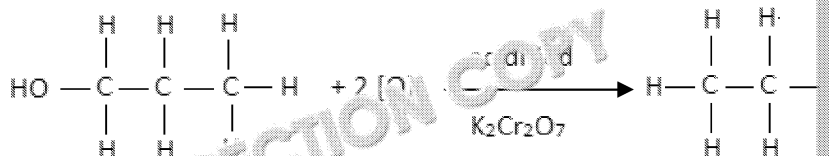
## Recap questions: Reactions of organic compounds

- 1 Classify the following conversions as either: addition, substitution, elimination

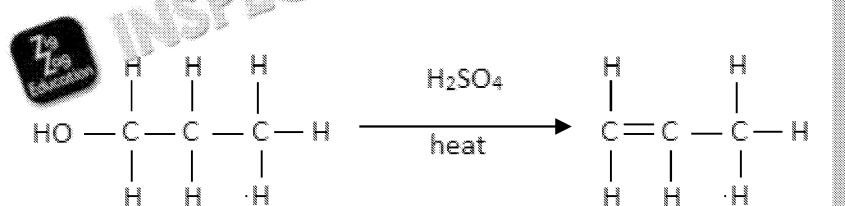
a)



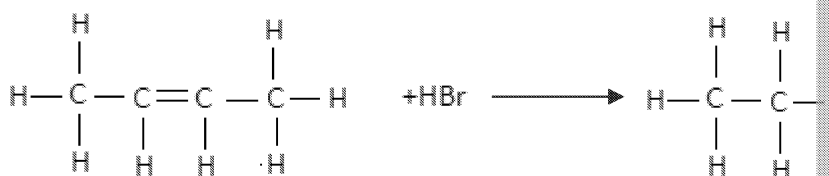
b)



c)



d)

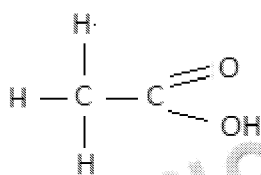


- 2 State the reactants and conditions needed for the following conversions.

- pent-2-ene to pentan-1-ol (2 marks)
- 2-chlorobutane to butan-2-ol (2 marks)
- ethanol to ethene (2 marks)
- but-1-ene to butane (3 marks)
- propane to 2-chloropropane (2 marks)

- 3 Predict the structure of the **major** organic product formed in the following

- a) butan-1-ol heated with acidified potassium dichromate (1 mark)



- propan-2-ol and  $\text{K}_2\text{Cr}_2\text{O}_7$  heated with sulfuric acid (1 mark)
- ethene and hydrogen at  $423^\circ\text{C}$  with a nickel catalyst (1 mark)
- pent-1-ene and steam with  $\text{H}_3\text{PO}_4$  (1 mark)

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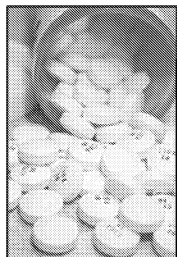
# E1.8 Reactions of commercial importance

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## Key points covered

- Predict the products formed from a range of important organic conversions
- Write equations to industrial conversions



Organic chemicals have a wide range of uses, but are particularly desired in the medical, agricultural and material industries.

**Polymers** are used in the synthesis of modern materials such as plastic and rubber. Short chain hydrocarbons, such as methane and ethane, are vital for use as fuels in heating and cooking. Many different organic substances are the starting material for drug synthesis in the pharmaceutical industry.

## Combustion

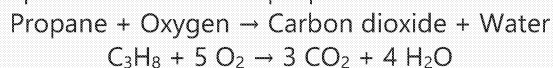
Combustion is a chemical process that occurs when a substance, typically a fuel, reacts with oxygen, releasing energy in the form of heat and light. This exothermic reaction is vital to many technologies, from everyday heating and cooking to industrial energy production and transport.

There are two main types of combustion that can occur: complete and incomplete.

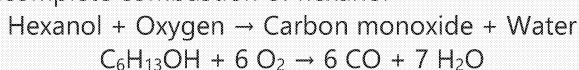
- Complete combustion:** occurs when there is enough oxygen (excess) for the fuel to react completely, producing carbon dioxide and water.
- Incomplete combustion:** happens when there is insufficient oxygen, leading to the production of **carbon monoxide** alongside water.

### Example:

Complete combustion of propane



Incomplete combustion of hexanol



### Test your knowledge

Write out the balanced equations for:

- complete combustion of propane
- complete combustion of hexanol
- incomplete combustion of propane
- incomplete combustion of hexanol

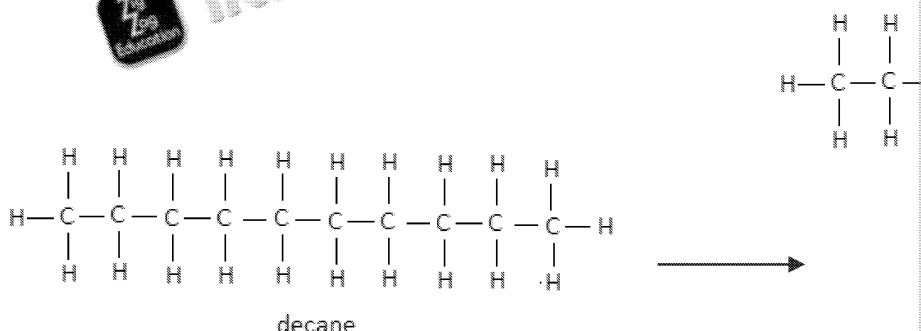
## Cracking

**Volatility** – the ability of a substance to evaporate at standard temperatures

**Viscosity** – a measure of a substance's resistance to flow

Short chain hydrocarbons are more useful and valuable than long chain equivalents. This is due to their higher flammability, lower **viscosity** making them ideal substances for transport. The composition of crude oil favours long chain alkanes, so cracking is needed to convert these alkanes into shorter chain hydrocarbons.

Thermal decomposition is used in order to address this supply and demand issue. It breaks down long chain alkanes and converts them into more useful, short chain alkanes and alkenes.



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Cracking can occur in one of two ways:

- **Thermal cracking:** this requires very high temperatures of approximately 1000 °C alongside high pressures of approximately 70 atm.
- **Catalytic cracking:** this reaction operates at lower temperatures and pressures but requires a catalyst such as aluminium oxide.

### Test your knowledge

Complete the balanced equation for the following:

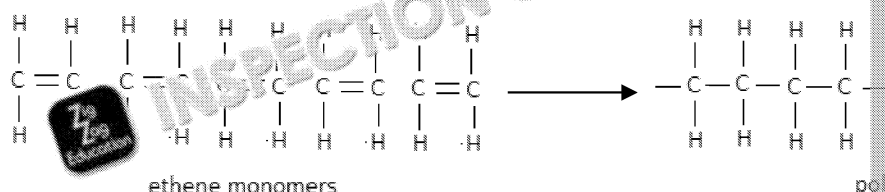
- $C_8H_{18} \rightarrow C_2H_6 + \dots$
- $\dots \rightarrow C_6H_6$
- $C_{16}H_{34} \rightarrow \dots$
- $C_{20}H_{42} \rightarrow C_4H_{10} + \dots$

## Addition polymerisation

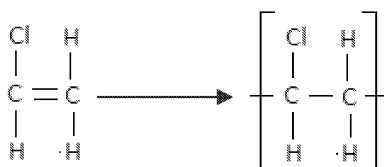
**Monomer** – a molecule that can react with similar molecules to form a long, repeating chain

Addition polymerisation is a type of polymerisation in which monomers join together without the loss of any small molecules to form a polymer.

This process involves the opening of a double bond in the monomer to form a single bond, linking together in a chain. The monomers involved in addition polymerisation are:



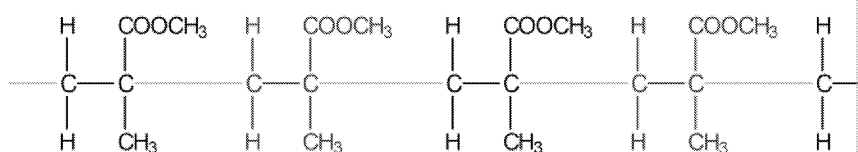
As well as showing the structural formula of the polymer, you can also show the repeating unit. This is simply the monomer, with its double bond broken ready to join with a second monomer.



Polymers are also known as plastics. Addition polymerisation is extremely important as it is able to produce a wide variety of plastics, based on the monomers that began their formation. Plastics are essential in everyday life, such as polyethene, used in packaging (like plastic bags), and polystyrene, used for products like disposable cutlery and household products.

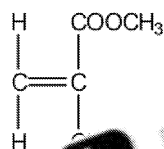
### Test your knowledge

- Acrylic is a polymer with the following structure:



Draw the monomer that forms acrylic.

- The monomer used to form superglue has the following structure:



Draw the polymer chain formed from this monomer. The chain

## Condensation polymerisation

Condensation polymerisation is an alternative method of polymerisation that involves monomers joining together to form large molecules called polymers. During this process, water (H<sub>2</sub>O) or methanol (CH<sub>3</sub>OH) are released as by-products. This is different from addition polymerisation where monomers simply add together without releasing any by-products.

Condensation polymerisation is important because it helps produce many useful materials, such as polyesters which are used in making plastic bottles, food packaging, and polyamides (e.g. Nylon): used in making textiles, ropes, and fishing nets because of their strength.

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## Formation of polyesters

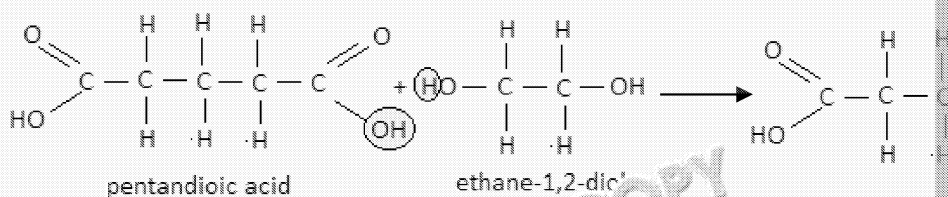
A polyester is formed when a **dicarboxylic acid** reacts with a **diol**. There is a loss of water and the two monomers are then bonded together by an ester link.

**Dicarboxylic acid** –

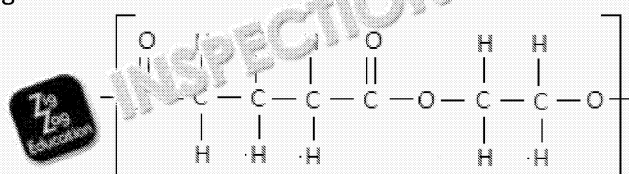
-COOH functional group

**Diol** – an organic molecule with two hydroxyl groups at either end of the carbon chain

**Example:**



Repeating unit =

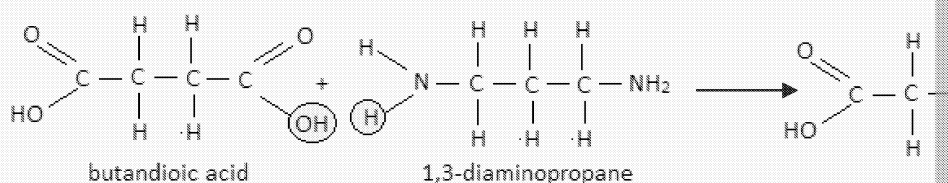


## Formation of polyamides

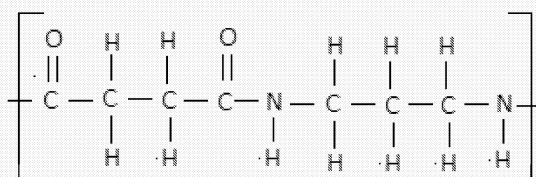
A polyamide is formed when a dicarboxylic acid reacts with a **diamine**. There is a loss of water and the two monomers are then bonded together by an amide link.

**Diamine** – an organic molecule with two amino groups at either end of the carbon chain

**Example:**



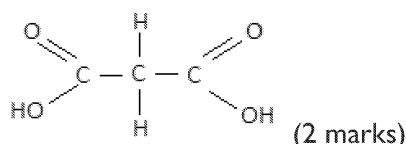
Repeating unit =



?

**Recap questions: Reactions of carboxylic acids – importance**

- 1 a) Write the balanced chemical equation for the reaction of propan-2-ol with oxygen. (2 marks)
- b) How would the products formed would be different if there was a limited amount of oxygen? (2 marks)
- 2 Explain why there is a need for cracking alkanes. (3 marks)
- 3 One of the products produced in cracking can be used in a further commercial process. Identify the functional group present in this product and then describe the subsequent reaction. (3 marks)
- 4 Draw the products formed as a result of the reaction between butan-1,4-diol with ethanedioic acid. (2 marks)



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## E1.9 Combustion, CFCs, polymers and alcohol

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### Key points covered

- Description of the benefits provided by a variety of organic reactions and chemicals
- Description of the environmental and health problems caused by organic reactions and chemicals

Organic reactions are key for many industries, helping to make progress in medicine and protecting the environment. They allow us to create complex medicines, improve crops and pesticides, and develop new materials like plastics and biofuels. Organic chemistry is used in biotechnology, perfumes, flavours, dyes, and new medical treatments. However, some organic reactions cause problems for the environment and our health. Using certain solvents can pollute the environment. Many organic reactions produce hazardous waste that needs careful disposal to avoid environmental damage. Some processes use a lot of energy, leading to high carbon emissions, and toxic chemicals like cyanides can be dangerous to both people and nature. Some organic compounds are non-biodegradable, meaning they don't break down easily and can build up in the environment, causing pollution. To address these issues, scientists are working to develop greener, more sustainable chemical processes.

	Benefits	Problems
<b>Combustion</b>	Provides large amounts of energy quickly, reliably and relatively cheaply.	Production of carbon dioxide, a greenhouse gas. Production of carbon monoxide from incomplete combustion. Consumption of fossil fuels, a non-renewable resource.
<b>Halogenoalkanes (CFCs)</b>	Non-flammable and non-toxic so good for use as refrigerants and propellants.	Collect in the upper atmosphere, where they can absorb UV radiation, leading to skin cancer and cataracts.
<b>Polymers (plastics)</b>	The wide range of monomers means that a wide variety of polymers can be made with different properties.	Consumption of fossil fuels, a non-renewable resource. Polymers are non-biodegradable and can persist in the environment for hundreds of years.
<b>Alcohol</b>	Used as an alternative fuel in cars which can be considered carbon-neutral and therefore cleaner burning.	Consumption of fossil fuels, a non-renewable resource. Use of large areas of land for growing crops for food and bioethanol production.

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### Recap questions: Combustion, CFCs, polymers and alcohol

- 1 What are some industries that benefit from organic reactions, and how do they benefit?
- 2 What are some environmental and health problems caused by organic reactions?
- 3 List **three** benefits and **three** problems associated with the combustion of fossil fuels.
- 4 Why are halogenoalkanes (CFCs) useful, and what environmental issue do they cause?
- 5 State **one** benefit and **two** problems associated with the use of polymers.

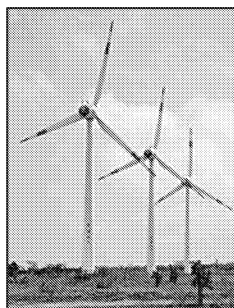


## E1.10 Solutions to environmental problems



### Key points covered

- Discussion of ways to overcome environmental problems caused by a variety of organic compounds



### Combustion

As one of the major uses of combustion is in energy generation, one way to overcome the environmental impact is to invest and research in renewable energy resources such as solar, wind and hydroelectricity. These can produce large amounts of energy, whilst conserving a vital finite resource.

### CFCs

CFCs were initially developed due to their low toxicity and flammability. However, upon reaching the upper atmosphere they break down, releasing chlorine radicals which break down the ozone layer. Alternatives have been developed, such as HFCs (hydrofluorocarbons). These are of equally low flammability and have low toxicity, however, they lack chlorine atoms within them and so will not cause ozone depletion.

### Polymers

Recycling polymers helps reduce landfill waste. Recycling also conserves resources from crude oil products. However, recycling is labour-intensive because polymers are often identified by recycling symbols and numbers on the product. Mixed polymers can be difficult, complicating recycling. For example, PVC contains toxic chlorine, which can be released during recycling.

Some polymers derived from crude oil or natural gas are difficult to recycle. They contain significant energy in their chains and can be incinerated to generate power, similar to coal-fired power stations. However, burning releases carbon dioxide, contributing to global warming, and other toxic by-products like hydrogen chloride from PVC.

Bioplastics are made from renewable resources such as plant starch, cellulose, plant oils, and proteins. They provide a sustainable alternative to traditional polymers, which are derived from finite resources like crude oil. Bioplastics can be decomposed by microorganisms, resulting in by-products like carbon dioxide, water, and other organic compounds. Polyamides, which can be broken down by hydrolysis reactions, are biodegradable, unlike polyalkenes, which do not easily degrade.

Photodegradable polymers have bonds that weaken when exposed to light, leading to degradation. However, oil-based, but additives that absorb light can be included to encourage degradation.

### Alcohol

The production of alcohol can be made more sustainable by ensuring sustainable farming practices to obtain the crops used for alcohol production. Practices such as organic farming and crop rotation can help to minimise the environmental impact of this process.



### Revision questions: Solutions to environmental problems

- 1 What are **three** renewable energy resources that can be used to produce electricity? (3 marks)
- 2 Why were CFCs initially developed, and what environmental harm do they cause?
- 3 How do HFCs differ from CFCs in terms of environmental impact? (3 marks)
- 4 What are the benefits and challenges of recycling polymers? (5 marks)
- 5 How can the production of alcohol be made more sustainable? (3 marks)

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# Answers for Recap Questions

## A: Atomic and electronic structure

### Features of the periodic table

- Similarities: same number of protons, 16 (1) same number of electrons, 16 (1)  
Differences: different number of neutrons:  $^{32}\text{S}$ , 16;  $^{33}\text{S}$ , 17;  $^{34}\text{S}$ , 18;  $^{36}\text{S}$ , 20 (1)
- $[14.0 + (1.0 \times 4)] \times 2 + [12.0 + (16.0 \times 3)]$  (1)  
= 96 (1)
  - $\text{HSO}_4 = 32.0 + (16.0 \times 4) = 96$  (1)  
 $267.2 - 96 = 171.2$  (1)  
RAM of group 1 element = 85.6 = Rubidium Rb (1)
  - $\text{O}_2 = 32.0$ ;  $74 - 32 = 42$  (1)  
 $42 \div 12 = 3.5$  which means 3 or 4. These will have a mass of 36 so the value is 32 + 36 = 68 which is a value 1.5 away from the  $M_r$  so therefore 6 hydrogen (1)
- RAM =  $[(39 \times 0.9316) + (41 \times 0.07) + (41 \times 6.73)]$  (1)  
 $1000 \div 25.6 = 39.14$  (1)
  - 1 mark for each correct row in the table:

Isotope	Protons	Neutrons
$^{40}\text{K}$	19	21
$^{41}\text{K}^+$	19	22

- Chlorine-35 is the most abundant isotope (1 mark) as the relative atomic mass is closest to 35 (1)

### Electronic structure

- 2 (1)
  - 3 (1)
  - 10 (1)
  - 2 (1)
  - 18 (1)

1s	2s	2p	3s	4p	3d
$\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$	$\uparrow\downarrow$	$\uparrow\downarrow$ $\uparrow\downarrow$ $\uparrow\downarrow$	$\uparrow$ $\uparrow$ $\uparrow$ $\uparrow$ $\uparrow$

Correct number of electrons (1)

Correct filling order (1)

Correct spin (1)

- The highest subshell is the 3p subshell (1)

It contains 4 electrons (1)

The  $3p_x$ ,  $3p_y$  and  $3p_z$  are first singly filled (1)

The final electron is then placed in a 3p orbital with opposite spin to the electron already in the orbital (1)

### Ionisation energy

- $\text{O}_{(g)} \rightarrow \text{O}^+_{(g)} + \text{e}^-$  (1)  
 $\text{O}^+_{(g)} \rightarrow \text{O}^{2+}_{(g)} + \text{e}^-$  (1)  
 The nuclear attraction on the remaining electrons is higher (1) and more energy is required (1)
- Aluminium (1); there is a large increase between the third and fourth ionisation energy (1) as the fourth electron must be being taken from a new shell, closer to the nucleus (1)
- Because the outer electron is being taken from the 2p subshell (1) which is higher in energy than the 3s subshell where  $\text{Mg}^{2+}$  electron is removed from (1)
  - Because the outer electron is being taken from a fully occupied orbital (1) and the next electron is already in the orbital (1)

## B: Bonding and structure

### Types of bonding

- The bonding is ionic bonding (1); a strong electrostatic attraction (1) between  $\text{Al}^{3+}$  and  $\text{O}^{2-}$  ions (1)
- Each metal atom delocalises (1) its outer shell electrons (1)
- There is a shared pair of electrons between each hydrogen and the oxygen atom (1) forming a covalent bond (1)
- Both substances have a giant covalent structure (1). In diamond, each carbon atom is bonded to four other carbon atoms (1). In graphite, each carbon atom makes three single covalent bonds and the fourth electron is delocalised (1)

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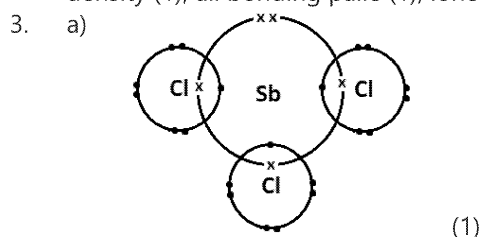
## Physical properties of substances

1. X – simple covalent bonding (1); it has a very low melting point due to weak intermolecular forces (1); it cannot conduct electricity due to a lack of charged particles (1)  
Y – giant ionic lattice (1); high melting point due to strong electrostatic attractions (1); it can only conduct when liquid as ions are immobile when in solid form (1)  
Z – giant metallic lattice (1); high melting point due to strong electrostatic attractions (1); it can conduct electricity in any form as electrons (in sea of delocalised electrons) can move (1); it can carry the charge through the substance (1)
2. Both substances contain metallic bonding (1); when melted you need to overcome the electrostatic attractions between the sea of electrons and the positive metal ions (1); as magnesium ions have a 2+ charge of sodium (1) the electrostatic attraction is stronger and more energy is needed to overcome it (1)
3. Ionic bonding (1); strong electrostatic forces of attraction between oppositely charged ions (1); at 25 °C it is solid and unable to conduct electricity (1); at 3000 °C the substance has melted (1); now the ions are free to move and carry the charge, so electricity is conducted (1)

## Molecular shape

1.
 

	Bond angle / ° (1 mark each)	Shape (1 mark each)
a) <chem>CCl4</chem>	109.5	Tetrahedral
b) <chem>CO2</chem>	180	Linear
c) <chem>PF3</chem>	107	Pyramidal
d) <chem>H2O</chem>	104.5	Non-linear
e) <chem>SF6</chem>	90	Octahedral
2. NH3 has 4 areas of electron density (1); 3 bonding pairs and 1 lone pair (1); where the lone pair is located (1); all bonding pairs (1); lone pairs repel more than bonding pairs (1)



- b) Pyramidal (1)  
c) 107° (1)  
d) It has 3 bonding pairs and 1 lone pair (1); electron pairs repel each other as much as possible (1)

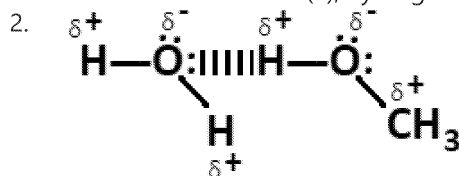
## Electronegativity and polarity

1.
 

1 mark for correct shape, then 1 mark for correct dipole on each C-Cl bond
2. It is polar as there is an uneven distribution of charge (1)

## Intermolecular forces

1. Each substance has simple covalent bonding and this means the boiling point depends on the strength of the intermolecular forces (1). Fluorine has the lowest boiling point as it only contains London dispersion forces (1); these are the weakest intermolecular force (1); chloromethane has permanent dipole-dipole intermolecular forces (1); hydrogen fluoride contains the strongest intermolecular forces (1); hydrogen bonding (1)



1 mark for all dipoles and lone pairs correctly shown, 1 mark for correct hydrogen bonding (1)

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## Hydrogen bonding and properties of water

1. Water has a smaller density when solid than when liquid (1). Hydrogen bonds between molecules further apart than normal when solid (1), meaning less mass per unit volume (1).
2. When water boils, hydrogen bonding must be overcome (1); this is the strongest type of intermolecular force (1) requires lots of energy (1); there are 2 hydrogen bonds formed per water molecule (1).
3. High surface tension allows objects such as insects to walk on water (1); the water molecules are able to form hydrogen bonds to fewer molecules than internal molecules (1) as the forces that exist are extremely strong (1).

## C: Periodicity

### Properties of period 3 elements

1. Argon (1); across the period there are more protons (1) but the outer electrons are further from the nucleus (1) so the stronger nuclear pull pulling the electrons closer to the nucleus (1).
2. All melting points will be high as strong metallic bonding (1)  $\text{Al} > \text{Mg} > \text{Na}$  (1) as the number of delocalised electrons increases (1) and the attractions get stronger (1) due to the higher charge on metal ions (1) and more delocalised electrons (1).
3. Melting point is observed as  $\text{chlorine} < \text{phosphorus} < \text{sulfur}$  (1); these elements exist as simple molecular substances (1) with weak London forces (1) as the number of electrons increases and therefore strength of London forces increases (1).

### Oxidation numbers, oxidation and reduction

1. a)  $\text{Na} +1$ ,  $\text{C} +4$ ,  $\text{O} -2$  (1)  
b)  $\text{Cr} +3$ ,  $\text{O} -2$  (1)  
c)  $\text{Cr} +6$ ,  $\text{O} -2$  (1)  
d)  $\text{Mn} +6$ ,  $\text{O} -2$  (1)  
e)  $\text{Mn} +7$ ,  $\text{O} -2$  (1)
2. a) Oxidised:  $\text{N}$ ,  $-3 \rightarrow 0$  (1)  
Reduced:  $\text{Cu}$ ,  $+2 \rightarrow 0$  (1)  
b) Oxidised:  $\text{Cl}$ ,  $-1 \rightarrow 0$  (1)  
Reduced:  $\text{Mn}$ ,  $+4 \rightarrow +2$  (1)  
c) Oxidised:  $\text{Mg}$ ,  $0 \rightarrow +2$  (1)  
Reduced:  $\text{H}$ ,  $+1 \rightarrow 0$  (1)
3. a)  $\text{Na} \rightarrow \text{Na}^+ + \text{e}^-$  (1) oxidation (1)  
b)  $\text{Pb}^{4+} + 2\text{e}^- \rightarrow \text{Pb}^{2+}$  (1) reduction (1)  
c)  $\text{H}_2 \rightarrow 2\text{H}^+ + 2\text{e}^-$  (1) oxidation (1)  
d)  $2\text{Br}^- \rightarrow \text{Br}_2 + 2\text{e}^-$  (1) oxidation (1)  
e)  $2\text{Hg}^{2+} + 2\text{e}^- \rightarrow \text{Hg}_2^{2+}$  (1) reduction (1)
4. a)  $5\text{Ce}^{3+} + \text{MnO}_4^- + 8\text{H}^+ \rightarrow \text{Mn}^{2+} + 4\text{H}_2\text{O} + 5\text{Ce}^{4+}$  (1 mark for correct species, 1 for correct balancing)  
b)  $2\text{MnO}_4^- + 6\text{H}^+ + 5\text{H}_2\text{O}_2 \rightarrow 2\text{Mn}^{2+} + 8\text{H}_2\text{O} + 5\text{O}_2$  (1 mark for correct species, 1 for correct balancing)  
c)  $2\text{FeO}_4^{2-} + 16\text{H}^+ + 3\text{C}_2\text{O}_4^{2-} \rightarrow 2\text{Fe}^{3+} + 8\text{H}_2\text{O} + 6\text{CO}_2$  (1 mark for correct species, 1 for correct balancing)

### Reaction of period 3 elements

1. a) Yellow flame (1) giving white smoke (1)  
b)  $\text{P}_4 + 5\text{O}_2 \rightarrow \text{P}_4\text{O}_{10}$ ; correct formula for phosphorus(V) oxide (1) Correctly balanced (1)
2. a) Sodium hydroxide (1) and hydrogen (1);  $2\text{Na} + 2\text{H}_2\text{O} \rightarrow 2\text{NaOH} + \text{H}_2$  (1)  
b) A coating of protective aluminium oxide is present (1) the water must be warmed (1)
3.  $\text{NaCl}$  (1)  $\text{Na} = +1$  (1);  $\text{Al}_2\text{Cl}_6$  (1)  $\text{Al} = +3$  (1);  $\text{SiCl}_4$  (1)  $\text{Si} = +4$  (1);  $\text{PCl}_5$  (1)  $\text{P} = +5$  (1)

### Physical properties of period 3 oxides and chlorides

1. Magnesium oxide has strong ionic bonding (than sodium oxide) (1) due to the high charge on the magnesium ions (1) compared to sodium ions (1).
2.  $\text{P}_4\text{O}_{10}$  is a simple molecular (1) with weak induced dipole-dipole forces OR little energy is required to overcome the induced dipole-dipole forces (1).
3. Magnesium chloride can conduct when molten or dissolved (1) as the ions are free to move (1) phosphorus chloride can never conduct (1) as it has no free ions or electrons (1).

### Acid-base behaviour of period 3 oxides and hydroxides

1. a) The pH generally decreases / becomes more acidic (1 mark)  
b) The oxides of aluminium and silicon (1)
2. a) The pH is 9–11 inc. (1) due to the formation of  $\text{Mg}(\text{OH})_2$  (1)  
b) pH 2–3 (1) due to the formation of  $\text{H}_2\text{SO}_3$  (1)
3.  $\text{Al}(\text{OH})_3(\text{s}) + 3\text{HCl}(\text{aq}) \rightarrow \text{AlCl}_3(\text{s}) + 3\text{H}_2\text{O}(\text{l})$ ; correct formula for all species (1); correct balancing (1)  
 $\text{Al}(\text{OH})_3(\text{s}) + \text{NaOH}(\text{aq}) \rightarrow \text{NaAl}(\text{OH})_4(\text{aq})$ ; correct formula for all species (1); correct balancing (1)

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## Reaction of water and period 3 chlorides

1. pH decreases / acidity increases (1)
2. A white precipitate is formed (1); white fumes given off (1);  $\text{SiCl}_{4(l)} + 2\text{H}_2\text{O}_{(l)} \rightarrow \text{SiO}_2$  (1)
3. Hydrochloric acid (1); phosphoric acid (1)

## Predicting physical and chemical properties

1. a) Carbon; group 4 so therefore has a giant covalent structure (1)  
b) Beryllium; has a giant metallic structure (1)  
c) Beryllium; stronger electrostatic attractions as higher number of delocalised electrons (1)
2. fluorine > sulfur > phosphorus > boron (1)
3. Neon (1); ionisation energy is the amount of energy needed to remove an electron from the outermost shell so requires the most energy (1); all period 2 atoms have the same number of shells so atomic radius remains similar for all (1)
4. True (1); there are more protons in the oxygen nucleus (1), but the extra electron is in the same shell as the previous electrons (1); the nucleus has a stronger attraction to the oxygen electrons (1)

## Uses of period 3 elements and compounds

1.  $\text{Al}(\text{OH})_3 + 3\text{HCl} \rightarrow \text{AlCl}_3 + 3\text{H}_2\text{O}$  (1); the acid is neutralised to salt and water (1)
2. High melting point; large numbers of strong covalent bonds to overcome (1)  
Strength of covalent structure is very strong (1)

## D: Physical chemistry

### Moles

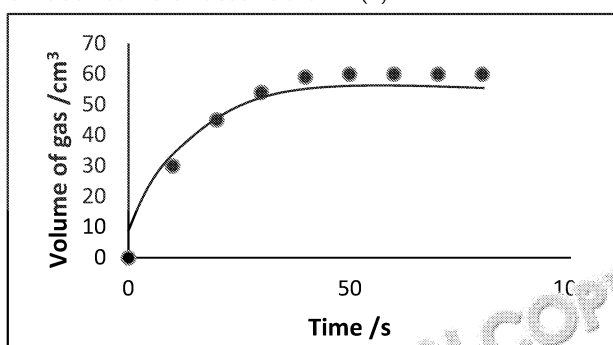
1. a)  $\text{Mg} + 2\text{HNO}_3 \rightarrow \text{Mg}(\text{NO}_3)_2 + \text{H}_2$  (1)  
b)  $\text{CuCl}_2 + 2\text{NaOH} \rightarrow \text{Cu}(\text{OH})_2 + 2\text{NaCl}$  (1)  
c)  $4\text{Na} + \text{O}_2 \rightarrow 2\text{Na}_2\text{O}$  (1)  
d)  $\text{Ca} + 2\text{HCl} \rightarrow \text{CaCl}_2 + \text{H}_2$  (1)
2. a)  $72 \div 24 = 2.96$  (1)  
b) 50.3 (1)  
c) 0.5 (1)  
d) 0.107 (1)
3. a) Moles of  $\text{Fe}_2\text{O}_3 = 32\,000 \div 159.6 = 200.5$  mol (1)  
1 mole of  $\text{Fe}_2\text{O}_3$  forms 2 moles of Fe  $\therefore$  moles of Fe =  $2 \times 200.5 = 401.0$  mol (1)  
Mass of Fe = moles  $\times M_r = 401.0 \times 55.8 = 22\,400$  g (3 s.f.) (1)  
b) Moles of  $\text{NH}_3 = 102 \div 17 = 6.00$  mol (1)  
4 moles of  $\text{NH}_3$  reacts with 3 moles of  $\text{O}_2$   $\therefore$  moles of  $\text{O}_2 = 6.00 \times \frac{3}{4} = 4.50$  mol (1)  
Mass of  $\text{O}_2 = \text{moles} \times M_r = 4.50 \times 32.0 = 144$  g (3 s.f.) (1)
4. a) Moles of  $\text{Al}_2\text{O}_3 = 1000 \div 102 = 9.8$  mol (1)  
2 moles of  $\text{Al}_2\text{O}_3$  produces 4 moles of Al  $\therefore$  moles of Al =  $9.8 \times 2 = 19.61$  mol (1)  
Mass of Al = moles  $\times M_r = 19.61 \times 27 = 529$  g (3 s.f.) (1)  
b) Percentage yield =  $(500 \div 529) \times 100 = 94.5\%$  (1)
5. a) Moles of iron =  $3.53 \div 56 = 0.063$  (1)  
Mass of chlorine =  $10.24 - 3.53 = 6.71$  g (1)  
Moles of chlorine =  $6.71 \div 35.5 = 0.189$  (1)  
Ratio = 1 Fe : 3 Cl (1)  
Formula =  $\text{FeCl}_3$  (1)  
b) Moles of carbon =  $33.3 \div 12 = 2.78$  (1)  
Moles of hydrogen =  $6.7 \div 1 = 6.7$  (1)  
Moles of oxygen =  $53.5 \div 16 = 3.34$  (1)  
Ratio = C : H : O = 1 : 2.4 : 1.2 (1)  
Empirical formula =  $\text{CH}_2\text{O}$  (1)  
 $M_r$  of empirical formula unit = 30 (1)  
Molecular formula =  $\text{C}_6\text{H}_{12}\text{O}_6$  (1)
6. a) Ratio: 1  $\text{C}_4\text{H}_8$  : 6  $\text{O}_2$  (1)  
 $6 \times 100 = 600$  cm<sup>3</sup>  $\text{O}_2$  needed (1)  
b) Ratio: 1  $\text{C}_4\text{H}_8$  : 6  $\text{O}_2$  (1)  
6 dm<sup>3</sup> of  $\text{O}_2$  is used up (1)  
4 dm<sup>3</sup> of  $\text{O}_2$  is left over (1)

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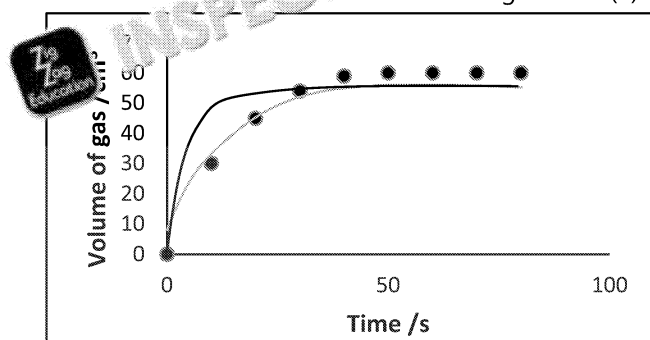


## Chemical kinetics

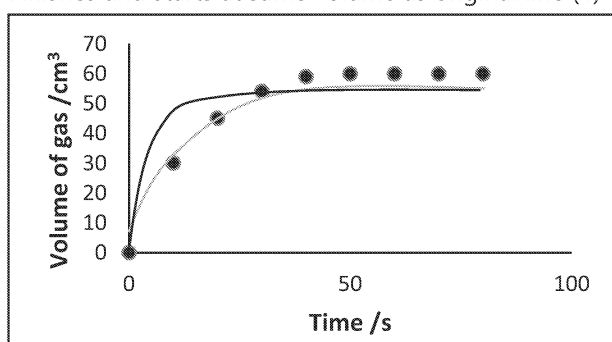
1. a) Labels on axes with units (1)  
Points correctly plotted (1)  
Smooth curve of best fit drawn (1)



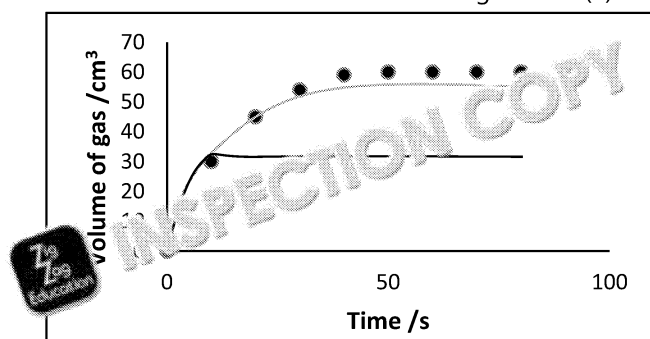
- b) i) Curves with a steeper gradient (1)  
Finishes and starts at same volume as original line (1)



- ii. Curves with a steeper gradient (1)  
Finishes and starts at same volume as original line (1)



- iii. Curves with the same gradient (1)  
Finishes at a volume 50 % less than original line (1)

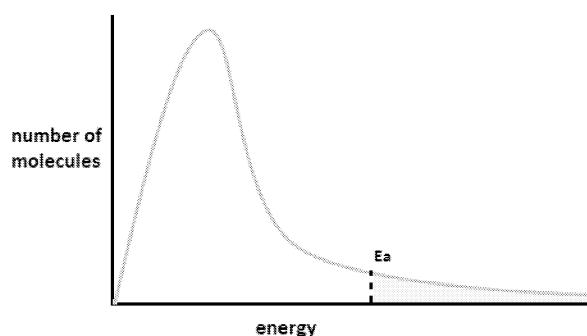


- c) The higher temperature increases rate (1) because the particles have more kinetic energy (1). The powder has a larger surface area and so faster rate (1) meaning collisions will occur more frequently (1). The smaller number of particles present (1) means there is also a lower amount of gas produced (1).

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2. a)



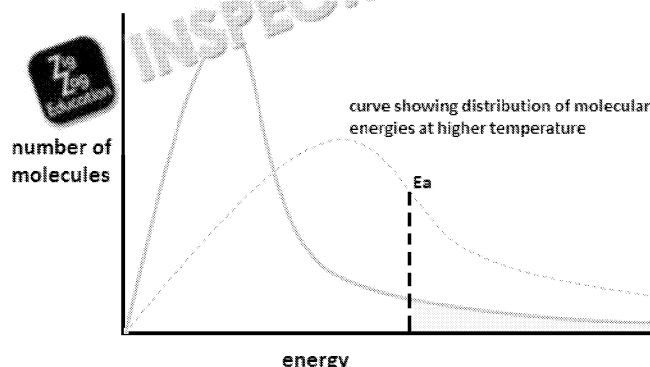
y-axis labelled correctly (1)

x-axis labelled correctly (1)

Line correct shape (1)

Line starting at 0,0 and never crossing the x-axis (1)

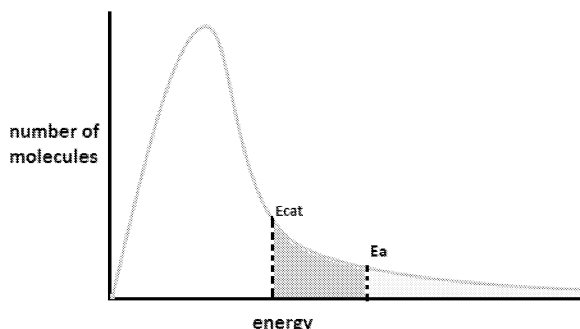
b)



Peak of curve shifted to the right (1)

Peak of curve at a lower height than previously (1)

c)



Curve showing  $E_a$  for catalysed and uncatalysed reaction (1)

Explanation stating that a catalyst lowers activation energy by providing an alternative pathway (1)

3. a) i) Na: order = 0 (1) in reactions 1 and 5 the concentration of Na is halved  
 ii)  $\text{Cl}_2$ : order = 2 (1) in reactions 1 and 3 the concentration of  $\text{Cl}_2$  is doubled

b)  $\text{rate} = k [\text{Cl}_2]^2$  (1)

c)  $k = \frac{\text{rate}}{[\text{Cl}_2]^2}$  (1)

Answer states substitution using any row of data (1)

$k = \frac{0.0007777777}{0.0001} = 7.7777777$  (1)

d)  $k = \frac{\text{mol dm}^{-3} \text{s}^{-1}}{(\text{mol dm}^{-3})^2}$  (1)

$k = \text{mol}^{-1} \text{dm}^3 \text{s}^{-1}$  (1)

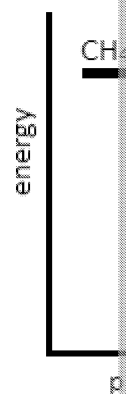
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## Chemical energetics

- Products lower than reactants (1)  
Both axes correctly labelled (1)  
Reactants and products labelled with chemicals (1)
  - See diagram (1)
  - See diagram (1)

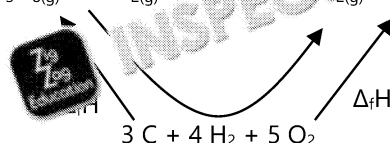


- $\text{C}_2\text{H}_5\text{OH}(\text{l}) + 3 \text{O}_{2(\text{g})} \rightarrow 2 \text{CO}_{2(\text{g})} + 3 \text{H}_2\text{O}(\text{g})$   
Species correct (1) balancing correct (1)

- $\text{Na}(\text{s}) + \frac{1}{2} \text{F}_{2(\text{g})} \rightarrow \text{NaF}(\text{s})$

Species correct (1) balancing correct (1)

- $\text{C}_3\text{H}_8(\text{g}) + 5 \text{O}_{2(\text{g})} \rightarrow 3 \text{CO}_{2(\text{g})} + 4 \text{H}_2\text{O}(\text{l})$



$\Delta_r H = [\Sigma \Delta_f H \text{ of the products}] - [\Sigma \Delta_f H \text{ of the reactants}]$

$\Delta_r H = [3(\Delta_f H \text{ CO}_2) + 4(\Delta_f H \text{ H}_2\text{O})] - [1(\Delta_f H \text{ C}_3\text{H}_8) + 5(\Delta_f H \text{ O}_2)]$

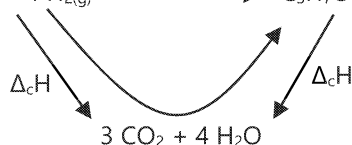
$\Delta_r H = [3(-394) + 4(-286)] - [1(-1182) + 5(0)]$

$\Delta_r H = [-1182 + -1144] - [-1182 + 0]$

$\Delta_r H = -2326 - -104$

$\Delta_r H = -2222 \text{ kJ mol}^{-1}$  (1)

- $3 \text{C}(\text{s}) + 4 \text{H}_{2(\text{g})} \rightarrow \text{C}_3\text{H}_7\text{OH}(\text{l})$



$\Delta_r H = [\Sigma \Delta_c H \text{ of the reactants}] - [\Sigma \Delta_c H \text{ of the products}]$

$\Delta_r H = [3(\Delta_c H \text{ C}) + 4(\Delta_c H \text{ H}_2)] - [\Delta_c H \text{ C}_3\text{H}_7\text{OH}]$

$\Delta_r H = [3(-394) + 4(-286)] - [-1182]$

$\Delta_r H = [-1182 + -1144] - [-1182]$

$\Delta_r H = -2326 - -2010$

$\Delta_r H = -316 \text{ kJ mol}^{-1}$  (1)

## Chemical equilibrium

- Dynamic equilibrium: when the forward reaction and backward reaction are proceeding at the same rate in a closed system (1)
  - Closed system: where nothing can enter or leave the reaction (1)
- Equilibrium will shift in the direction of the endothermic reaction (1) to oppose the change and increase temperature back down again (1)
  - Equilibrium will shift in the direction of the reaction that produces the most moles of gas to oppose the change and increase pressure (1)
  - No effect on the position of equilibrium (1); just causes it to reach equilibrium faster (1)
- Equilibrium would shift to the right (1) as this is the exothermic reaction (1)
  - Equilibrium would be unaffected (1) as there is the same number of gaseous molecules on both sides (1)
- $K_c = \frac{[\text{SO}_2]^2 [\text{O}_2]}{[\text{SO}_3]^2}$  (1) units =  $\frac{(\text{mol dm}^{-3})^3}{(\text{mol dm}^{-3})^2} = \text{mol dm}^{-3}$  (1)
  - $K_c = \frac{[\text{PCl}_5]}{[\text{Cl}_2][\text{PCl}_3]}$  (1) units =  $\frac{(\text{mol dm}^{-3})}{(\text{mol dm}^{-3})^2} = \text{mol}^{-1} \text{ dm}^3$  (1)
- $K_c = \frac{[\text{HI}]^2}{[\text{H}_2][\text{I}_2]}$  (1)
  - equilibrium moles of  $\text{H}_2 = 0.4$  (1), equilibrium moles of  $\text{I}_2 = 0.4$  (1)
  - $K_c = \frac{0.4^2}{0.4 \times 0.4} = 1.0$  (1) no units (1)
- $K_p = \frac{p(\text{CH}_4) p(\text{H}_2\text{O})}{p(\text{CO}) p(\text{H}_2)^3}$  (1) Units =  $\text{Pa}^{-2}$  (1)
  - $K_p = \frac{p(\text{O}_2)^3}{p(\text{O}_3)^2}$  (1) Units =  $\text{Pa}$  (1)
- equilibrium moles of A = 2 (1), equilibrium moles of B = 2.5 (1), equilibrium moles of C = 1.5 (1)  
Mole fraction of A =  $2/6$  (1), Mole fraction of B =  $2.5/6$  (1), Mole fraction of C =  $1.5/6$  (1)  
Partial pressure of A =  $166.7$  (1), partial pressure of B =  $208.3$  (1), partial pressure of C =  $166.7$  (1)  
 $K_p = \frac{p(\text{C})^2}{p(\text{A})^2 p(\text{B})}$  (1) Units =  $\text{kPa}^{-1}$  (1)

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**Applications of chemical kinetics, energetics and equilibrium**

- Low temperature (1); equilibrium will shift to the right-hand side to favour the products (1)  
High pressure (1); equilibrium will shift to the right-hand side to favour the side with fewer gas molecules (1)
  - A high  $K_p$  value means the position of equilibrium sits far to the side of the products (1) and is therefore safer (1) and less expensive (1).
  - To increase rate (1)
  - No effect on position of equilibrium (1)
    - Increases rate (1), provides an alternative route with a lower activation energy (1)

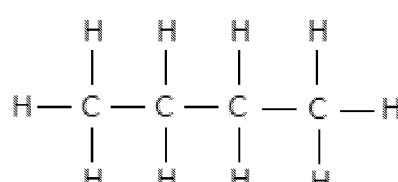
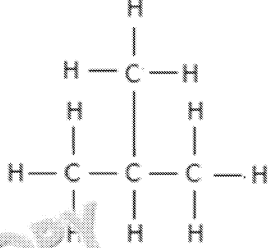
**Applications of green chemistry**

- Allows a reaction to occur at lower temperatures (1); this reduces the need to burn fossil fuels (1) and therefore reduces in lower fuel costs (1) and lower production of greenhouse gases (1)
- $\% \text{ atom economy} = (\text{M}_r \text{ useful products} \div \text{M}_r \text{ total products}) \times 100$   
 $\text{M}_r \text{ useful products} = 92$  (1)  
 $\text{M}_r \text{ total products} = 180$  (1)  
 $(92 \div 180) \times 100 = 51.1\%$  (1)
  - Uses a renewable feedstock (1); carried out at lower temperatures / lower fuel costs (1)
  - Avoids a very slow reaction (1); poor atom economy (1); production of carbon dioxide (1)

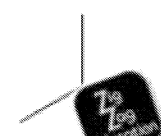
**E: Organic chemistry****Key terms**

- A compound made of only carbon and hydrogen atoms (1)
- A series of compounds with the same functional group (1) but differing by a  $\text{CH}_2$  group (1)
  - Alcohol (1)
  - General formula:  $\text{C}_n\text{H}_{2n+1}\text{OH}$  (1); fifth member =  $\text{C}_5\text{H}_{11}\text{OH}$  (1)
- Unsaturated (1)
    - Saturated (1)
    - Unsaturated (1)
    - Saturated (1)
  - Cyclic (1)
    - Branched (1)
    - Branched (1)
    - Straight chain (1)

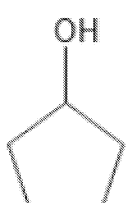
**Structure representations**

- 


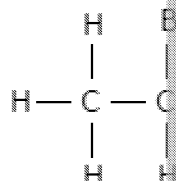
b)  $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$  (1);  $\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_3$  (1)

- 

Correct molecule (1); represented skeletally (1)

- 

Correct molecule (1); represented skeletally (1)

- 

Correct molecule (1); represented by full structural formula (1) Allow

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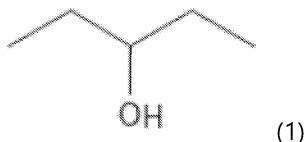
## Naming alkanes, alkenes, halogenoalkanes and alcohols

1. (Accept any type of structural representation as long as the molecule is correct)

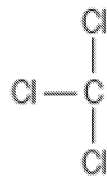
a)



b)



c)



d)



2. a) Ethanol (1)

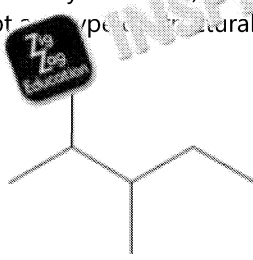
b) But-1-ene (1)

c) Bromoethane (1)

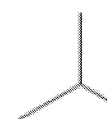
d) 2-methylbutane (1)

3. (Accept any type of structural representation as long as the molecule is correct)

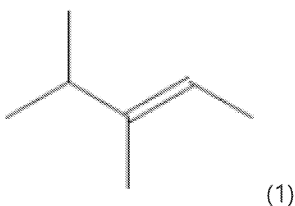
a)



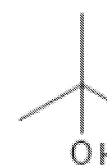
c)



b)



d)



4. a) 2,2-dibromo-3-fluorobutane (1)

b) 1-bromobut-2-ene (1)

c) 3-methylbutan-1-ol (1)

d) 2,3-dibromobutane (1)

## Isomerism

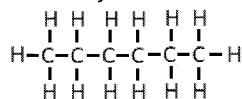
1. a) Compounds with the same molecular formula but different structural formulae

b) Compounds with the same structural formula but different arrangements of atoms

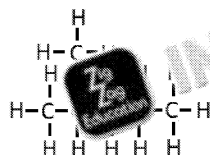
2. a) Structural isomerism (1)

b) Stereoisomerism (1)

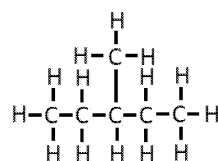
3. Allow any structural representation. (1) for each correct structure; (1) for each correct



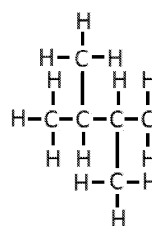
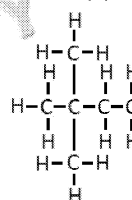
HEXANE



2-METHYLPENTANE



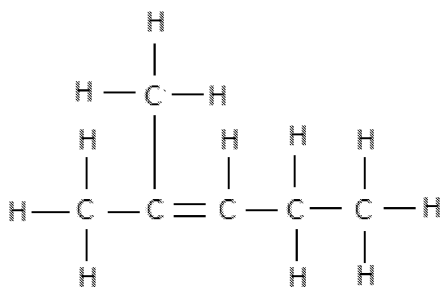
3-METHYLPENTANE



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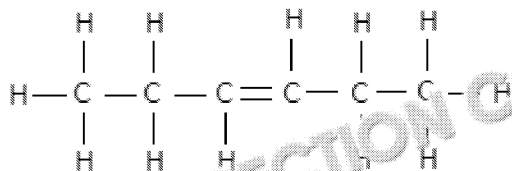


4. a)



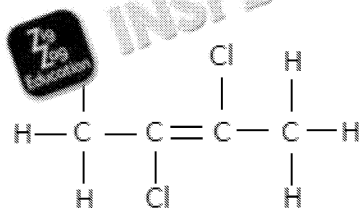
(1); No stereoisomerism (1)

b)



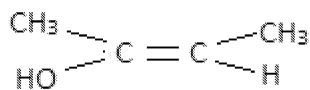
(1); Stereoisomerism (1)

c)

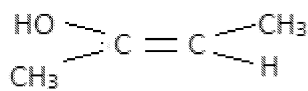


(1); Stereoisomerism (1)

5.



(1); E-but-2-en-2-ol or cis-but-2-en-2-ol (1)



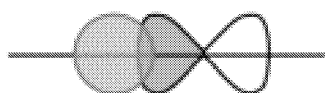
(1); Z-but-2-en-2-ol or trans-but-2-en-2-ol (1)

6.

- a) No isomerism (1)
- b) Stereoisomerism and structural isomerism (1)
- c) Structural isomerism (1)

## Sigma and pi molecular orbitals

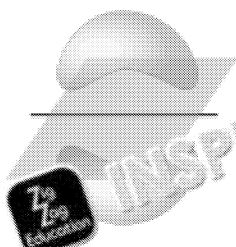
1. a)



(1)

b) Sigma bond (1)

2. a)



(1)

b) p orbitals (1)

3. Sigma bond has end-to-end overlap of orbitals whereas pi bond is sideways overlap. Sigma bond has shared electron density between the nuclei whereas pi bond has shared electron density above and below the plane of the nuclei (1)

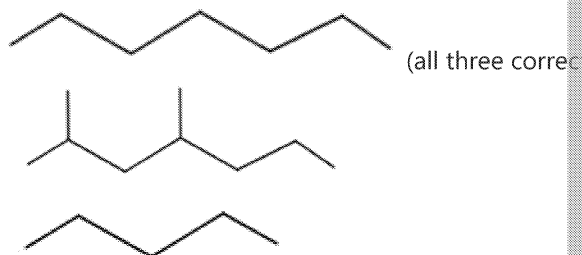
- 4. a) i. 13 (1) ii. 8 (1) iii. 16 (1) iv. 15 (1)
- b) i. 0 (1) ii. 1 (1) iii. 0 (1) iv. 2 (1)

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## Changes in boiling point

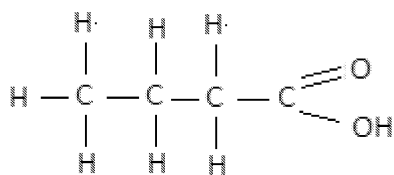
1. From highest to lowest:



2. The boiling point depends on the strength of the intermolecular/London forces (1). Higher the boiling point (1). Molecule b) has the longest chain and no branching (1) and London forces are great (1). Molecule a) has the shortest chain and therefore the weakest London forces (1).

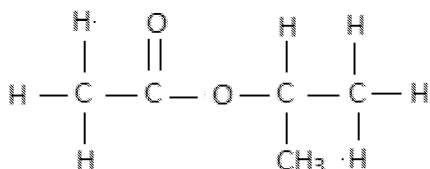
## Reactions of organic compounds

- Substitution (1)
  - Oxidation (1)
  - Elimination (1)
  - Addition (1)
- $\text{H}_2\text{O}_{(g)}$ /steam (1),  $\text{H}_3\text{PO}_4$  (1)
  - $\text{NaOH}$  (1), aqueous (1)
  - $\text{H}_2\text{SO}_4$  (1), heat (1)
  - $\text{H}_2$  (1), 423 K (1), Ni/Pt catalyst (1)
  - $\text{Cl}_2$  (1), UV light (1)
- 



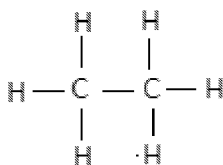
(1 mark for functional group)

b)



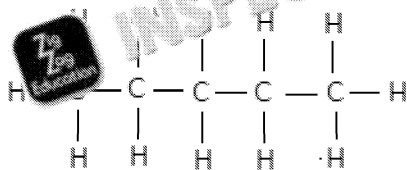
(1)

c)



(1)

d)



(1)

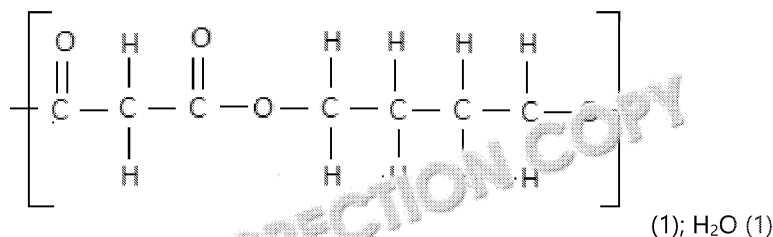
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## Reactions of commercial importance

- $\text{C}_3\text{H}_7\text{OH} + 4.5 \text{O}_2 \rightarrow 3 \text{CO}_2 + 4 \text{H}_2\text{O}$  (1 mark for correct products) (1 mark for correct balancing)
  - Incomplete combustion would occur (1); carbon monoxide / carbon (soot) would be produced (1); carbon dioxide (1)
- Short chain alkanes are more valuable/useful than long chains (1); the supply of short chain alkanes is limited (1); the demand (1); long chain alkanes are broken down to produce more – shorter chain alkanes (1)
- Alkene (1); undergoes addition polymerisation (1); the double bond breaks (1) and a new single bond forms (1); the chain length increases (1)
- A polymer containing the following repeating unit:



## Combustion of fuels, polymers and alcohol

- Any three from (1 mark each):  
Medicine, farming, materials, biotechnology, perfumes
- Any three from (1 mark each):  
Using certain solvents can pollute the air; Many organic reactions produce hazardous waste; High energy consumption leading to high carbon emissions; Use of toxic chemicals like heavy metals; Production of pollutants that don't break down easily
- Benefits: Provides large amounts of energy quickly (1), reliably (1), and relatively cheaply (1)  
Problems: Production of carbon dioxide, a greenhouse gas (1); Production of carbon monoxide (1); Consumption of non-renewable fossil fuels (1)
- Useful because they are non-flammable and non-toxic (1); Good for use as refrigerants (1)  
Problems: Environmental issue by destroying the ozone layer when they collect in the upper atmosphere (1)
- Benefits: Wide range of monomers allows a variety of polymers with different properties (1)  
Problems: Consumption of non-renewable fossil fuels (1); Non-biodegradable, leading to waste (1)

## Solutions to environmental problems

- Solar energy (1); Wind energy (1); Hydroelectric energy (1)
- Initially developed due to low toxicity and flammability (1); Cause environmental harm by releasing chlorine atoms into the upper atmosphere to form chlorine radicals (1); These chlorine radicals break down ozone (1)
- HFCs have low flammability and toxicity like CFCs (1); HFCs lack chlorine atoms (1); therefore they do not cause ozone depletion (1)
- Benefits: Reduces landfill waste (1); Conserves resources, especially crude oil products (1)  
Challenges: Labour-intensive due to the need for sorting by type (1); Mixed polymers are difficult to recycle (1); Toxic by-products, like hydrogen chloride from PVC, may be released (1)
- Using sustainable farming methods (1); Practices such as organic farming (1); Crop rotation (1)

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