

A Level Chemistry OCR

YOUR NOTES



2. Foundations in Chemistry

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 - 2.5.1 The Shapes of Simple Molecules & Ions
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2.1 Atoms & Reactions

2.1.1 Atomic Structure & Isotopes

Subatomic Structure of Atoms & Ions

- All matter is composed of **atoms**, which are the smallest parts of an element that can take place in **chemical reactions**
- Atoms are mostly made up of **empty space**
- The mass of an atom is **concentrated** in the nucleus, because the nucleus contains the heaviest subatomic particles (the neutral neutrons and positive protons)
 - The mass of the electron is negligible

Relative mass & charge of subatomic particles table

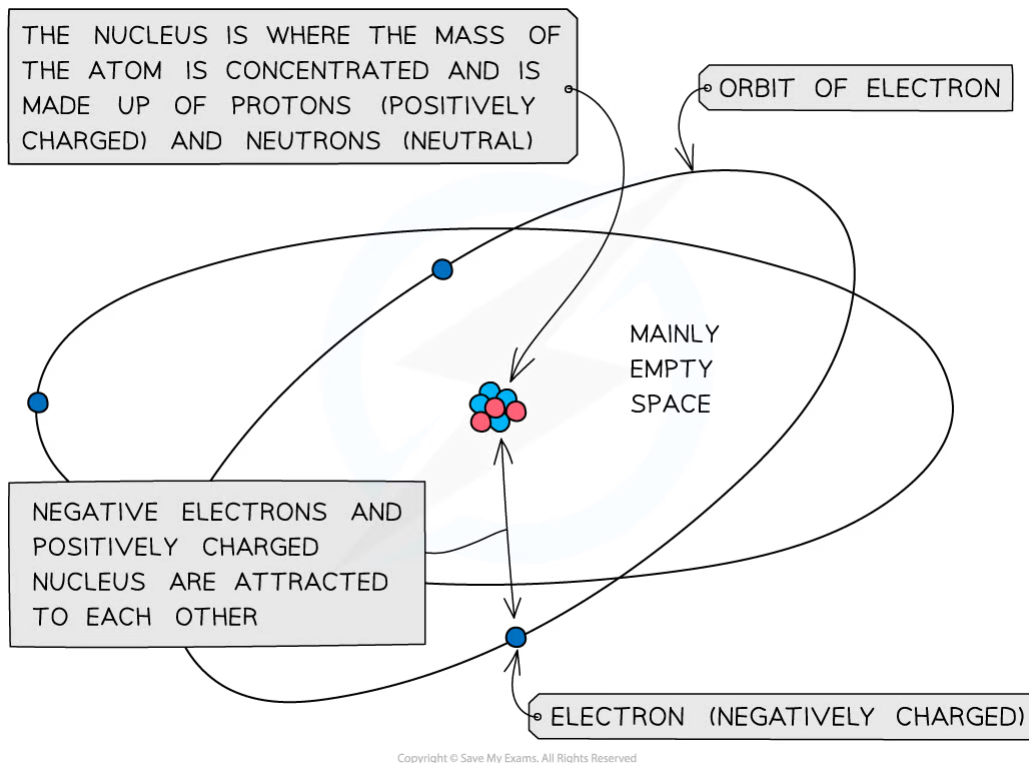
| Subatomic Particle | Relative Charge | Relative Mass |
|--------------------|-----------------|------------------|
| Proton | +1 | 1 |
| Neutron | 0 | 1 |
| Electron | -1 | $\frac{1}{1836}$ |

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- The nucleus is also **positively charged** due to the protons
- **Negatively charged** electrons orbit the nucleus of the atom, contributing very little to its overall mass, but creating a 'cloud' of negative charge
- The **electrostatic attraction** between the **positive nucleus** and **negatively charged electrons** orbiting around it is what holds an atom together

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The mass of the atom is concentrated in the positively charged nucleus which is attracted to the negatively charged electrons orbiting around it

- ♦ An atom is **neutral** and has no overall charge
- ♦ Ions on the other hand are formed when atoms either **gain** or **lose** electrons, causing them to become **charged**
- ♦ The number of **subatomic particles** in atoms and ions can be determined given their atomic (proton) number, mass (nucleon) number and charge

Protons

- ♦ The atomic number of an atom and ion determines which element it is
- ♦ Therefore, all atoms and ions of the **same element** have the same number of protons (atomic number) in the nucleus
 - E.g. lithium has an atomic number of 3 (three protons) whereas beryllium has atomic number of 4 (4 protons)
- ♦ The number of protons equals the **atomic (proton) number**
- ♦ The number of protons of an **unknown** element can be calculated by using its mass number and number of neutrons:

$$\text{Mass number} = \text{number of protons} + \text{number of neutrons}$$

$$\text{Number of protons} = \text{mass number} - \text{number of neutrons}$$



? Worked Example

Determine the number of protons of the following ions and atoms:

1. Mg^{2+} ion
2. Carbon atom
3. An unknown atom of element X with mass number 63 and 34 neutrons

Answers

Answer 1: The atomic number of a magnesium atom is 12 indicating that the number of protons in the magnesium element is 12

- Therefore the number of protons in a **Mg^{2+} ion** is also 12

Answer 2: The atomic number of a carbon atom is 6 indicating that a **carbon atom** has 6 protons in its nucleus

Answer 3: Use the formula to calculate the number of protons

$$\text{Number of protons} = \text{mass number} - \text{number of neutrons}$$

$$\text{Number of protons} = 63 - 34$$

$$\text{Number of protons} = 29$$

- **Element X** is therefore copper

Electrons

- An atom is **neutral** and therefore has the **same** number of **protons** and **electrons**
- Ions have a different number of electrons to their atomic number depending on their charge
 - A positively charged ion, or **cation**, has **lost** electrons and therefore has **fewer** electrons than protons
 - A negatively charged ion, or **anion**, has **gained** electrons and therefore has **more** electrons than protons

? Worked Example

Determine the number of electrons of the following ions and atoms:

1. Mg^{2+} ion
2. Carbon atom
3. An unknown atom of element X with mass number 63 and 34 neutrons

Answers

Answer 1: The atomic number of a magnesium atom is 12 suggesting that the number of protons in the **neutral** magnesium **atom** is 12

- However, the 2+ charge in Mg^{2+} ion suggests it has **lost** two electrons



- It only has 10 electrons left now

Answer 2: The atomic number of a carbon atom is 6 suggesting that the **neutral carbon atom** has 6 electrons orbiting around the nucleus

Answer 3: The number of protons of element **X** can be calculated by:

$$\text{Number of protons} = \text{mass number} - \text{number of neutrons}$$

$$\text{Number of protons} = 63 - 34$$

$$\text{Number of protons} = 29$$

- The **neutral atom** of element **X** therefore also has 29 electrons

Neutrons

- ♦ The **mass** and **atomic numbers** can be used to find the number of **neutrons** in **ions** and **atoms**:

$$\text{Number of neutrons} = \text{mass number (A)} - \text{number of protons (Z)}$$



Worked Example

Determine the number of neutrons of the following ions and atoms:

1. Mg^{2+} ion
2. Carbon atom
3. An unknown atom of element X with mass number 63 and 29 protons

Answers

Answer 1: The atomic number of a magnesium atom is 12 and its mass number is 24

$$\text{Number of neutrons} = \text{mass number (A)} - \text{number of protons (Z)}$$

$$\text{Number of neutrons} = 24 - 12$$

$$\text{Number of neutrons} = 12$$

- The Mg^{2+} ion has 12 neutrons in its nucleus

Answer 2: The atomic number of a carbon atom is 6 and its mass number is 12

$$\text{Number of neutrons} = \text{mass number (A)} - \text{number of protons (Z)}$$

$$\text{Number of neutrons} = 12 - 6$$

$$\text{Number of neutrons} = 6$$

- The **carbon atom** has 6 neutrons in its nucleus



Answer 3: The atomic number of an element X atom is 29 and its mass number is 63

Number of neutrons = mass number (A) - number of protons (Z)

Number of neutrons = 63 - 29

Number of neutrons = 34

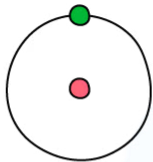

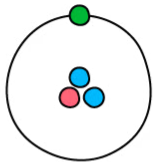
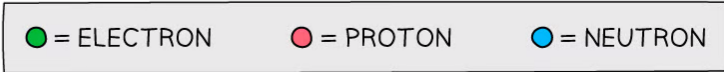
- The **neutral atom** of element X has 34 neutrons in its nucleus

Subatomic Structure of Isotopes

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- Isotopes are atoms of the **same element** that contain the same number of **protons** and electrons but a different number of **neutrons**
- The symbol for an isotope is the **chemical symbol** (or **word**) followed by a **dash** and then the **mass number**
 - E.g. carbon-12 and carbon-14 are isotopes of carbon containing 6 and 8 neutrons respectively

| | PROTIUM | DEUTERIUM | TRITIUM |
|-----------------|--|---|--|
| |  |  |  |
| PROTONS | 1 | 1 | 1 |
| NEUTRONS | 0 | 1 | 2 |
| ISOTOPIC SYMBOL | ${}^1_1\text{H}$ | ${}^2_1\text{H}$ | ${}^3_1\text{H}$ |
| |  | | |

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The atomic structure and symbols of the three isotopes of hydrogen

- Isotopes have the **same chemical properties** but **different physical properties**

Chemical properties

- Isotopes of the same element display the **same chemical characteristics**
- This is because they have the same number of electrons in their **outer shells**
- Electrons take part in **chemical reactions** and therefore determine the **chemistry** of an atom

Physical properties

- The only difference between isotopes is the number of **neutrons**
- Since these are neutral subatomic particles, they only add **mass** to the atom
- As a result of this, isotopes have different **physical properties** such as small differences in their **mass** and **density**

Relative Mass

- The relative mass of an atom uses the carbon-12 isotope as the international standard
- One atom of carbon-12 has an accepted mass of $1.992646538 \times 10^{-26}$ kg
- It is not realistic to work with this value so the mass of a carbon-12 atom is fixed as exactly 12 atomic mass units / 12u
- The standard mass for atomic mass is 1u
 - Therefore, the standard mass for comparison is the mass of $\frac{1}{12}$ of a carbon-12 atom

Relative isotopic mass

- Relative isotopic mass is defined as the mass of an isotope relative to $\frac{1}{12}$ of a carbon-12 atom
- For A Level Chemistry it is common to work with mass values rounded to one decimal place, for example:
- The accurate relative isotopic mass of nitrogen is 14.00307401 but this is rounded to 14.0
- The accurate relative isotopic mass of oxygen is 15.99491464 but this is rounded to 16.0

Relative atomic mass

- Most elements on the Periodic Table represent a mixture of different isotopes, which is shown as their relative atomic mass (A_r)
- The relative atomic mass is the weighted mean / average mass of an atom relative to $\frac{1}{12}$ of the mass of a carbon-12 atom

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2.1.2 Atomic Structure & Mass Spectrometry

Isotopes & Relative Atomic Mass

- **Isotopes** are different atoms of the **same element** that contain the same number of **protons** and electrons but a different number of **neutrons**.
 - Isotopes can also be described as atoms of the same **elements** but with different mass numbers
- Therefore, the mass of an element is given as **relative atomic mass (A_r)** by using the average mass of the isotopes
- The relative atomic mass of an element can be calculated by using the **relative abundance** values by using the following equation:
 - $$\frac{(\text{relative abundance}_{\text{isotope 1}} \times \text{mass}_{\text{isotope 1}}) + (\text{relative abundance}_{\text{isotope 2}} \times \text{mass}_{\text{isotope 2}}) \text{ etc}}{100}$$
 - The relative abundance of an isotope is either given or can be read off the mass spectrum



Worked Example

Calculating relative atomic mass of oxygen

A sample of oxygen contains the following isotopes:

| Isotope | Percentage abundance |
|-----------------|----------------------|
| ^{16}O | 99.76 |
| ^{17}O | 0.04 |
| ^{18}O | 0.20 |

What is the relative atomic mass of oxygen in this sample, to 2dp?

- A. 16.00
- B. 17.18
- C. 16.09
- D. 17.00

Answer

The correct answer option is A

- $A_r = \frac{(99.76 \times 16) + (0.04 \times 17) + (0.20 \times 18)}{100}$
- $A_r = 16.0044$
- $A_r = 16.00$

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Mr from Mass Spectra

- The percentage abundance of the isotopes in an element can be found by the use of a **mass spectrometer**
- The basic processes of mass spectrometry are:
 - The sample is **vapourised**
 - The sample is **ionised** to form positive ions
 - The ions are **accelerated**
 - Heavy ions move slower / are less **deflected**
 - The ions are **detected** as a mass-to-charge ratio, written as m/z
 - Each ion produces a signal, so the larger the signal, the greater the abundance
- The mass spectra produced can be used to calculate the relative atomic mass of an element and its isotopes

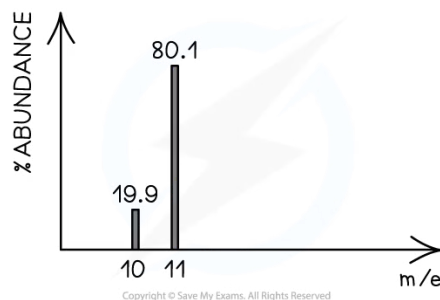
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Worked Example

Calculating relative atomic mass of boron

Calculate the relative atomic mass of boron using its mass spectrum, to 2dp:



Answer

- $A_r = \frac{(19.9 \times 10) + (80.1 \times 11)}{100}$
- $A_r = 10.801$
- $A_r = 10.80$

Relative molecular and formula mass

- These are essentially the same ideas
 - **Relative molecular mass** is applied to chemicals that have a fixed formula in terms of the number of atoms involved, e.g. ethanol, C_2H_5OH , contains two carbon atoms, six hydrogen atoms and one oxygen
 - **Relative formula mass** is applied to chemicals that use an empirical formula to represent them, e.g. calcium chloride, $CaCl_2$, is an ionic lattice containing a ratio of 1 calcium ion : 2 chloride ions throughout the structure

- These terms are often mis-used, with relative molecular mass being applied to any compound regardless of its composition
- The relative molecular and formula mass are both calculated by adding up the relative atomic masses of all the component atoms

? Worked Example

Calculate:

1. The relative molecular mass of ethanol, C_2H_5OH
2. The relative formula mass of calcium chloride, $CaCl_2$

(A_r values: C = 12.0, H = 1.0, O = 16.0, Ca = 40.1, Cl = 35.5)

Answers

Answer 1: $(2 \times C) + (5 \times H) + O + H = (2 \times 12.0) + (5 \times 1.0) + 16.0 + 1.0 = 46.0$

Answer 2: $Ca + (2 \times Cl) = 40.1 + (2 \times 35.5) = 111.1$

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2.1.3 Compounds, Formulae & Equations

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Chemical Formulae

- ♦ **Ionic compounds** are formed from a **metal** and a **non-metal** bonded together
- ♦ Ionic compounds are electrically neutral; the positive charges equal the negative charges

Charges on positive ions

- ♦ All metals form **positive** ions
 - There are also some non-metal positive ions, such as ammonium, NH_4^+ , and hydrogen, H^+
- ♦ The **metals** in Group 1, Group 2 and Group 3 (13) have a charge of 1+ and 2+ and 3+ respectively
- ♦ The charge on the ions of the **transition elements can vary** which is why **Roman numerals** are often used to indicate their charge
- ♦ **Roman numerals** are used in some compounds formed from transition elements to show the **charge** (or **oxidation state**) of metal ions
 - E.g. in copper(II) oxide, the copper ion has a charge of 2+ whereas in copper(I) nitrate, the copper has a charge of 1+

Non-metal ions

- ♦ The **non-metals** in group 15 to 17 have a negative charge and have the suffix '**ide**'
 - E.g. nitride, chloride, bromide, iodide
- ♦ Elements in group 17 gain 1 electron so have a 1- charge, eg. Br^-
- ♦ Elements in group 16 gain 2 electrons so have a 2- charge, eg. O^{2-}
- ♦ Elements in group 15 gain 3 electrons so have a 3- charge, eg. N^{3-}
- ♦ There are also **polyatomic** negative ions, which are negative ions made up of more than one type of atom

| GROUP | | | | | | | | 18 |
|---------------|------------------|------------------------|------------------|----|----|-----------------|---------------|------|
| 1 | 2 | H^+ | 13 | 14 | 15 | 16 | 17 | NONE |
| Li^+ | Be^{2+} | | | | | O^{2-} | F^- | NONE |
| Na^+ | Mg^{2+} | | Al^{3+} | | | S^{2-} | Cl^- | NONE |
| K^+ | Ca^{2+} | TRANSITION ELEMENTS | Ga^{3+} | | | | Br^- | NONE |
| Rb^+ | Sr^{2+} | | | | | | I^- | NONE |

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The charges of simple ions depend on their position in the Periodic Table

Formulae of Ionic Compounds Table

| Ion | Formula and Charge |
|--------------------|--------------------|
| Silver (I) | Ag^+ |
| Ammonium | NH_4^+ |
| Zinc(II) | Zn^{2+} |
| Hydroxide | OH^- |
| Nitrate | NO_3^- |
| Sulfate | SO_4^{2-} |
| Carbonate | CO_3^{2-} |
| Hydrogen carbonate | HCO_3^- |
| Phosphate | PO_4^{3-} |

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Worked Example

Formulae

Determine the formulae of the following ionic compounds

1. Magnesium chloride
2. Iron(III) oxide
3. Aluminium nitrate

Answer

Answer 1: Magnesium chloride

- Magnesium is in Group 2 so has a charge of 2+
- Chlorine is in group 17 so has a charge of 1-
- Magnesium needs two chloride ions for each magnesium ion to be balanced so the formula is **MgCl₂**

Answer 2: Iron (III) oxide

- The Roman numeral states that iron has a charge of 3+
- Oxygen is in group 16 so has a charge of 2-

- The charges need to be equal so 2 iron ions to 3 oxide ions will balance electrically, so the formula is Fe_2O_3

Answer 3: Aluminum nitrate

- Aluminium is in group 13 so has a charge of 3+
- Nitrate is a **polyatomic ion** and has a charge of 1-
- The **polyatomic ion** needs to be placed in a bracket if more than 1 is needed
- The formula of aluminium nitrate is $\text{Al}(\text{NO}_3)_3$



Exam Tip

Remember: **Polyatomic ions** are ions that contain more than one type of element, such as OH^-

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Balancing Chemical Equations

- A **symbol** equation is a shorthand way of describing a chemical reaction using **chemical symbols** to show the number and type of each atom in the reactants and products
- A **word** equation is a longer way of describing a chemical reaction using only **words** to show the reactants and products

Balancing equations

- During chemical reactions, atoms cannot be **created** or **destroyed**
- The number of each atom on each side of the reaction must therefore be the **same**
 - E.g. the reaction needs to be **balanced**
- When balancing equations remember:
 - Not to change any of the formulae
 - To put the numbers used to balance the equation **in front** of the formulae
 - To balance **firstly** the carbon, then the hydrogen and **finally** the oxygen in **combustion reactions** of organic compounds
- When balancing equations follow the following the steps:
 - Write the formulae of the reactants and products
 - Count the numbers of atoms in each reactant and product
 - Balance the atoms one at a time until all the atoms are balanced
 - Use appropriate state symbols in the equation
- The **physical state** of reactants and products in a chemical reaction is specified by using **state symbols**
 - **(s)** solid
 - **(l)** liquid
 - **(g)** gas
 - **(aq)** aqueous

Ionic equations

- In aqueous solutions ionic compounds **dissociate** into their ions
- Many chemical reactions in aqueous solutions involve ionic compounds, however only some of the ions in solution take part in the reactions
- The ions that do **not** take part in the reaction are called **spectator ions**
- An **ionic equation** shows **only** the ions or other particles taking part in a reaction, and not the spectator ions



Worked Example

Balance the following equation:

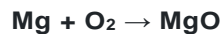


Answer:

Step 1: Write out the symbol equation showing reactants and products

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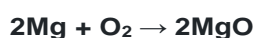


Step 2: Count the numbers of atoms in each reactant and product

| | Mg | O |
|-----------|----|---|
| Reactants | 1 | 2 |
| Products | 1 | 1 |

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Step 3: Balance the atoms one at a time until all the atoms are balanced



This is now showing that 2 moles of magnesium react with 1 mole of oxygen to form 2 moles of magnesium oxide

Step 4: Use appropriate **state symbols** in the fully balanced equation



Worked Example

1. Balance the following equation



2. Write down the ionic equation for the above reaction

Answer 1:

Step 1: To balance the equation, write out the symbol equation showing reactants and products

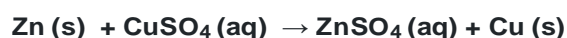


Step 2: Count the numbers of atoms in each reactant and product. The equation is already balanced

| | Zn | Cu | S | O |
|-----------|----|----|---|---|
| Reactants | 1 | 1 | 1 | 4 |
| Products | 1 | 1 | 1 | 4 |

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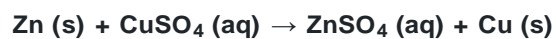
Step 3: Use appropriate **state symbols** in the equation



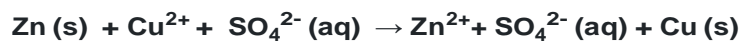


Answer 2:

Step 1: The full chemical equation for the reaction is



Step 2: Break down reactants into their respective ions



Step 3: Cancel the spectator ions on both sides to give the ionic equation



2.2 Amount of Substance

2.2.1 Amount of Substance

The Mole & the Avogadro Constant

- **Amount of substance** is the name given when counting the number of particles in a substance
 - Amount of substance is often seen in calculations using the letter / symbol n
 - The units for amount of substance are moles / mol
- Amount of substance links to the **Avogadro constant**, N_A , which is the number of particles equivalent to the relative atomic, molecular or formula mass of a substance
 - The Avogadro constant applies to atoms, molecules, ions and electrons
 - The value of N_A is **$6.02 \times 10^{23} \text{ g mol}^{-1}$**
- The mass of a substance with this number of particles is called a **mole** (mol)
 - This can be called the **molar mass**
 - This is the mass of substance that contains the same number of fundamental units as exactly 12.00 g of carbon-12
- The amount / number of moles of a substance, n , the mass of the substance, m , and the molar mass, M , are linked by the equation:

$$n = \frac{\text{mass, } m}{\text{Molar mass, } M}$$

- The molar gas volume is the volume occupied by one mole of any gas, at room temperature and pressure
 - The molar volume is equal to 24 dm^3
- One mole of any element is equal to the relative atomic mass of the element, in grams
 - For example, if you had one mole of carbon in your hand, you would be holding 6.02×10^{23} atoms of carbon which have a mass of 12.0 g
 - If you were holding one mole of water, you would be holding 6.02×10^{23} molecules of water which have a mass of 18.0 g (2 hydrogen + 1 oxygen = $(2 \times 1.0) + 16.0 = 18.0 \text{ g}$)

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Worked Example

Molar mass and molar gas volume

1. Calculate the molar mass of:

- a. Carbon dioxide, CO_2
 - b. Magnesium nitrate, $\text{Mg}(\text{NO}_3)_2$
- (A_r data: C = 12.0, O = 16.0, Mg = 24.3, N = 14.0)

2. Calculate the number of moles of each gas:

- a. 36.0 dm^3 of carbon monoxide, CO
- b. 9.6 dm^3 of chlorine, Cl_2

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Answers

Answer 1:

The molar mass is the mass of one mole of any substance

- a. Carbon dioxide, $\text{CO}_2 = 12.0 + (16.0 \times 2) = 44.0 \text{ g}$
- b. Magnesium nitrate, $\text{Mg}(\text{NO}_3)_2 = 24.3 + (14.0 \times 2) + (16.0 \times 3 \times 2) = 148.3 \text{ g}$

Answer 2:

One mole of any gas occupies 24.0 dm^3

- a. 36.0 dm^3 is 1.5 times the molar gas volume of 24.0 dm^3 , therefore, there are 1.5 moles of carbon monoxide, CO
- b. 9.6 dm^3 is 0.4 times the molar gas volume of 24.0 dm^3 , therefore, there are 0.4 moles of chlorine, Cl_2

2.2.2 Determining Formulae

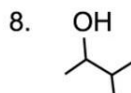
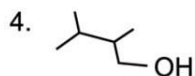
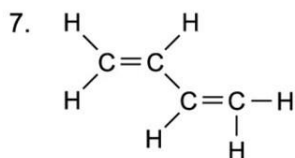
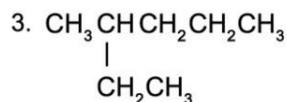
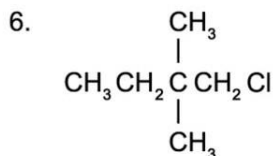
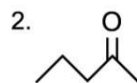
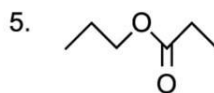
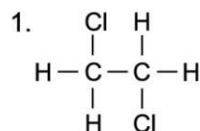
Defining Empirical & Molecular Formulae

- The **molecular formula** shows the number and type of each atom in a molecule
 - E.g. the molecular formula of ethanoic acid is $C_2H_4O_2$
- The **empirical formula** shows the simplest whole number ratio of the elements present in one molecule of the compound
 - E.g. the empirical formula of ethanoic acid is CH_2O



Worked Example

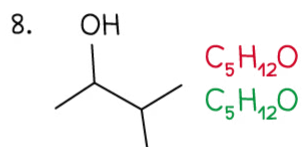
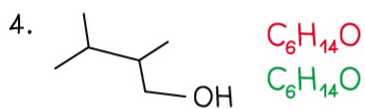
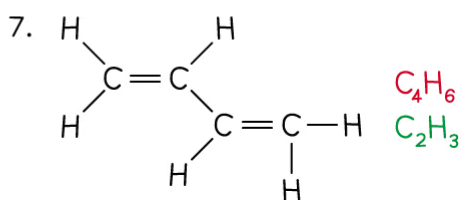
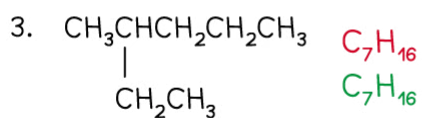
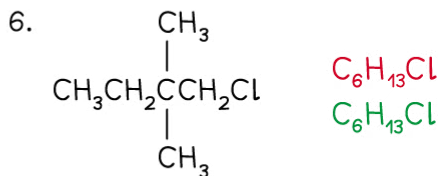
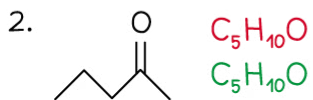
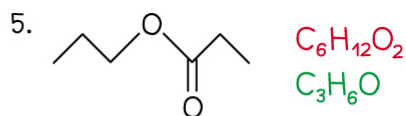
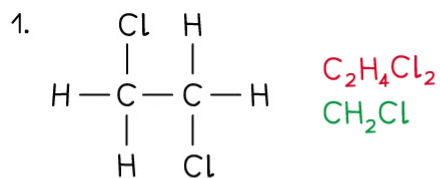
Deducing molecular & empirical formulae Deduce the molecular and empirical formula of the following compounds:



YOUR NOTES



Answer



MOLECULAR FORMULA
EMPERICAL FORMULA

YOUR NOTES



Calculating Empirical & Molecular Formulae

YOUR NOTES



Empirical formula

- **Empirical formula** is the **simplest whole number ratio** of the elements present in one molecule or formula unit of the compound
- It is calculated from knowledge of the ratio of masses of each element in the compound
- The empirical formula can be found by determining the **mass** of each element present in a sample of the compound
- It can also be deduced from data that gives the **percentage compositions by mass** of the elements in a compound



Worked Example

Empirical formula from mass

Determine the empirical formula of a compound that contains 10 g of hydrogen and 80 g of oxygen.

| | Hydrogen | Oxygen |
|---|--------------------------------|--------------------------------|
| Note the mass of each element | 10 g | 80 g |
| Divide the masses by atomic masses | $= \frac{10}{1.0}$ = 10 mol | $= \frac{80}{16}$ = 5.0 mol |
| Divide by the lowest figure to obtain the ratio | $= \frac{10}{5.0}$ = 2.0 | $= \frac{5.0}{5.0}$ = 1.0 |
| Empirical formula | H ₂ O | |

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- The above example shows how to calculate empirical formula from the mass of each element present in the compound
- The example below shows how to calculate the empirical formula from percentage composition



Worked Example

Empirical formula from %

Determine the empirical formula of a compound that contains 85.7% carbon and 14.3% hydrogen.



| | Carbon | Hydrogen |
|---|--|---|
| Note the % by mass of each element | 85.7 | 14.3 |
| Divide the % by atomic masses | $= \frac{85.7}{12.0}$ $= 7.142 \text{ mol}$ | $= \frac{14.3}{1.00}$ $= 14.3 \text{ mol}$ |
| Divide by the lowest figure to obtain the ratio | $= \frac{7.142}{7.142}$ $= 1.00$ | $= \frac{14.3}{7.142}$ $= 2.00$ |
| Empirical formula | CH ₂ | |

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Molecular formula

- The **molecular formula** gives the exact numbers of atoms of each element present in the formula of the compound
- The molecular formula can be found by dividing the **relative molecular mass** of the **molecular formula** by the **relative formula mass** of the **empirical formula**
- **Multiply** the number of each element present in the empirical formula by this number to find the molecular formula



Worked Example

Calculating molecular formula

The empirical formula of X is C₄H₁₀S and the relative molecular mass of X is 180.2

What is the molecular formula of X?

(A_r data: C = 12.0, H = 1.0, S = 32.1)

Answer

Step 1: Calculate relative mass of the empirical formula

- Relative empirical mass = (C × 4) + (H × 10) + (S × 1)
- Relative empirical mass = (12.0 × 4) + (1.0 × 10) + (32.1 × 1)
- Relative empirical mass = 90.1

Step 2: Divide relative molecular mass of X by relative empirical mass

- Ratio between M_r of X and the M_r of the empirical formula = 180.2 / 90.1
- Ratio between M_r of X and the M_r of the empirical formula = 2

Step 3: Multiply each number of elements by 2

- (C₄ × 2) + (H₁₀ × 2) + (S × 2)
- (C₈) + (H₂₀) + (S₂)



- Molecular formula of X is $C_8H_{20}S_2$

YOUR NOTES

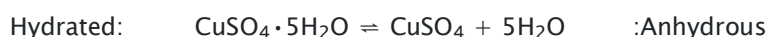


Hydrated salts & Water of Crystallisation

YOUR NOTES



- **Water of crystallisation** is when some compounds can form **crystals** which have **water** as part of their structure
- A compound that contains water of crystallisation is called a **hydrated compound**
- The water of crystallisation is separated from the main formula by a **dot** when writing the chemical formula of hydrated compounds
 - E.g. hydrated copper(II) sulfate is $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$
- A compound which doesn't contain water of crystallisation is called an **anhydrous compound**
 - E.g. anhydrous copper(II) sulfate is CuSO_4
- A compound can be hydrated to **different degrees**
 - E.g. cobalt(II) chloride can be hydrated by **six** or **two** water molecules
 - $\text{CoCl}_2 \cdot 6\text{H}_2\text{O}$ or $\text{CoCl}_2 \cdot 2\text{H}_2\text{O}$
- The conversion of anhydrous compounds to hydrated compounds is reversible by heating the hydrated salt:



- The degree of hydration can be calculated from experimental results:
 - The mass of the hydrated salt must be measured before heating
 - The salt is then heated until it reaches a constant mass
 - The two mass values can be used to calculate the number of moles of water in the hydrated salt – known as the water of crystallisation



Worked Example

Calculating water of crystallisation

10.0 g of hydrated copper sulfate are heated to a constant mass of 5.59 g. Calculate the formula of the original hydrated copper sulfate.

(M_r data: $\text{CuSO}_4 = 159.6$, $\text{H}_2\text{O} = 18.0$)

Answer

| | | |
|---|---|-----------------------------|
| List the components | CuSO_4 | H_2O |
| Note the mass of each component | 5.59 g | $10 - 5.59 = 4.41$ g |
| Divide the component mass by the components M_r | $\frac{5.59}{159.6} = 0.035$ | $\frac{4.41}{18.0} = 0.245$ |
| Divide by the lowest figure to obtain the ratio | $\frac{0.035}{0.035} = 1$ | $\frac{0.245}{0.035} = 7$ |
| Hydrated salt formula | $\text{CuSO}_4 \cdot 7\text{H}_2\text{O}$ | |

YOUR NOTES



Exam Tip

A water of crystallisation calculation can be completed in a similar fashion to an empirical formula calculation

- Instead of elements, you start with the salt and water
- Instead of dividing by atomic masses, you divide by molecular / formula masses
- The rest of the calculation works the same way as the empirical formula calculation

2.2.3 Reaction Calculations

Mass Calculations

- The number of moles of a substance can be found by using the following equation:

$$\text{number of moles (mol)} = \frac{\text{mass of a substance (g)}}{\text{molar mass (g mol}^{-1}\text{)}}$$

- It is important to be clear about the type of particle you are referring to when dealing with moles
 - E.g. one mole of CaF_2 contains one mole of CaF_2 formula units, but one mole of Ca^{2+} and two moles of F^- ions

Reacting masses

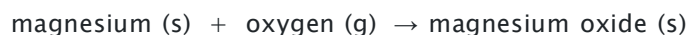
- The masses of reactants are useful to determine how much of the reactants **exactly** react with each other to prevent waste
- To calculate the reacting masses, the balanced chemical equation is required
- This equation shows the ratio of moles of all the reactants and products, also called the **stoichiometry**, of the equation
- To find the mass of products formed in a reaction the following pieces of information are needed:
 - The mass of the reactants
 - The molar mass of the reactants
 - The balanced equation



Worked Example

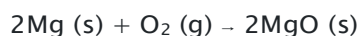
Mass calculation using moles

Calculate the mass of magnesium oxide that can be made by completely burning 6 g of magnesium in oxygen.



Answer

Step 1: The balanced symbol equation is:



Step 2: The relative formula masses are:

$$\text{Mg} = 24.3, \text{O}_2 = 32.0, \text{MgO} = 40.3$$

Step 3: Calculate the moles of magnesium used in the reaction:

$$\text{number of moles} = \frac{6.0 \text{ g}}{24.3 \text{ g mol}^{-1}} = 0.25 \text{ moles}$$

YOUR NOTES





Step 4: Find the ratio of magnesium to magnesium oxide using the balanced chemical equation

| | Magnesium | Magnesium Oxide |
|---------------|-----------|-----------------|
| Mol | 2 | 2 |
| Ratio | 1 | 1 |
| Change in mol | -0.25 | +0.25 |

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Therefore, 0.25 mol of MgO is formed

Step 5: Find the mass of magnesium oxide

$$\begin{aligned} \text{Mass} &= \text{mol} \times M_r \\ \text{Mass} &= 0.25 \text{ mol} \times 40 \text{ g mol}^{-1} \\ \text{Mass} &= 10 \text{ g} \end{aligned}$$

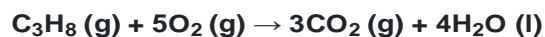
Therefore, the mass of magnesium oxide produced is 10 g

Stoichiometric relationships

- The stoichiometry of a reaction can be found if the **exact amounts** of reactants and products formed are known
- The **amounts** can be found by using the following equation:

$$\text{number of moles (mol)} = \frac{\text{mass of a substance (g)}}{\text{molar mass (g mol}^{-1}\text{)}}$$

- The gas volumes can be used to deduce the **stoichiometry** of a reaction
 - E.g. in the **combustion** of 50 cm³ of propane reacting with 250 cm³ of oxygen, 150 cm³ of carbon dioxide is formed suggesting that the ratio of propane : oxygen : carbon dioxide is 1 : 5 : 3



Volume Calculations

YOUR NOTES



- The **concentration** of a solution is the amount of **solute** dissolved in a **solvent** to make 1 dm³ of **solution**
 - The solute is the substance that dissolves in a solvent to form a solution
 - The solvent is often water

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

- A **concentrated** solution is a solution that has a **high** concentration of solute
- A **dilute** solution is a solution with a **low** concentration of solute
- When carrying out calculations involving concentrations in mol dm⁻³ the following points need to be considered:
 - Change mass in grams to **moles**
 - Change cm³ to dm³
- To calculate the **mass** of a substance present in solution of known **concentration and volume**:
 - Rearrange the concentration equation

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

- Multiply the moles of solute by its molar mass

$$\text{mass of solute (g)} = \text{number of moles (mol)} \times \text{molar mass (g mol}^{-1}\text{)}$$



Worked Example

Calculating volume from concentration

Calculate the volume of hydrochloric acid of concentration 1.0 mol dm⁻³ that is required to react completely with 2.5 g of calcium carbonate

Answer

Step 1: Write the balanced symbol equation



Step 2: Calculate the amount, in moles, of calcium carbonate that reacts

$$\text{number of moles (CaCO}_3\text{)} = \frac{2.5 \text{ g}}{100 \text{ g mol}^{-1}} = 0.025 \text{ mol}$$

Step 3: Calculate the moles of hydrochloric acid required using the reaction's stoichiometry

1 mol of CaCO₃ requires 2 mol of HCl

So 0.025 mol of CaCO₃ requires 0.05 mol of HCl



Step 4: Calculate the volume of HCl required

$$\text{volume of HCl (dm}^3\text{)} = \frac{\text{amount (mol)}}{\text{concentration (mol dm}^{-3}\text{)}} = \frac{0.05 \text{ mol}}{1.0 \text{ mol dm}^{-3}} = 0.05 \text{ dm}^3$$

Volume of hydrochloric acid = 0.05 dm³



Worked Example

Neutralisation calculation

25.0 cm³ of 0.050 mol dm⁻³ sodium carbonate was completely neutralised by 20.0 cm³ of dilute hydrochloric acid. Calculate the concentration in mol dm⁻³ of the hydrochloric acid.

Answer

Step 1: Write the balanced symbol equation



Step 2: Calculate the amount, in moles, of sodium carbonate reacted by rearranging the equation for amount of substance (mol) and dividing the volume by 1000 to convert cm³ to dm³

$$\text{amount (Na}_2\text{CO}_3\text{)} = 0.025 \text{ dm}^3 \times 0.050 \text{ mol dm}^{-3} = 0.00125 \text{ mol}$$

Step 3: Calculate the moles of hydrochloric acid required using the reaction's stoichiometry

1 mol of Na₂CO₃ reacts with 2 mol of HCl, so the molar ratio is 1 : 2

Therefore 0.00125 moles of Na₂CO₃ react with 0.00250 moles of HCl

Step 4: Calculate the concentration, in mol dm⁻³, of hydrochloric acid

$$\text{concentration of HCl (mol dm}^{-3}\text{)} = \frac{\text{amount (mol)}}{\text{volume (dm}^3\text{)}} = \frac{0.00250}{0.0200} = 0.125 \text{ mol dm}^{-3}$$

Volumes of gases

- ♦ **Avogadro** suggested that 'equal volumes of gases contain the same number of molecules' (also called **Avogadro's hypothesis**)
- ♦ At room temperature (20 degrees Celsius) and pressure (1 atm) **one mole** of any gas has a volume of 24.0 dm³
- ♦ This **molar gas volume** of 24.0 dm³ mol⁻¹ can be used to find:
 - The volume of a given mass or number of moles of gas:

$$\text{volume of gas (dm}^3\text{)} = \text{amount of gas (mol)} \times 24 \text{ dm}^3 \text{ mol}^{-1}$$

- ♦ The mass or number of moles of a given volume of gas:

$$\text{amount of gas (mol)} = \frac{\text{volume of gas (dm}^3\text{)}}{24.0 \text{ (dm}^3 \text{ mol}^{-1}\text{)}}$$

YOUR NOTES



Worked Example

Calculation volume of gas using excess & limiting reagents

Calculate the volume the following gases occupy:

1. Hydrogen (3 mol)
2. Carbon dioxide (0.25 mol)
3. Oxygen (5.4 mol)
4. Ammonia (0.02 mol)

Calculate the moles in the following volumes of gases:

1. Methane (225.6 dm³)
2. Carbon monoxide (7.2 dm³)
3. Sulfur dioxide (960 dm³)

Answer



| Gas | Amount of Gas (mol) | Volume of Gas (dm ³) |
|-----------------|--------------------------|----------------------------------|
| Hydrogen | 3.0 | $3 \times 24 = 72$ |
| Carbon dioxide | 0.25 | $0.25 \times 24 = 6.0$ |
| Oxygen | 5.4 | $5.4 \times 24 = 129.6$ |
| Ammonia | 0.02 | $0.02 \times 24 = 0.48$ |
| Methane | $\frac{225.6}{24} = 9.4$ | 225.6 |
| Carbon monoxide | $\frac{7.2}{24} = 0.30$ | 7.2 |
| Sulfur dioxide | $\frac{960}{24} = 40$ | 960 |

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YOUR NOTES



2.2.4 The Ideal Gas Equation

Ideal Gas Equation & Calculations

YOUR NOTES



Kinetic theory of gases

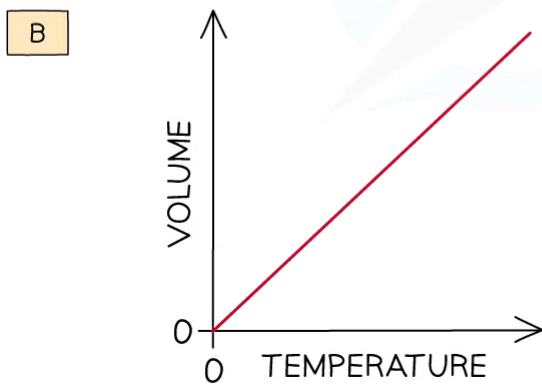
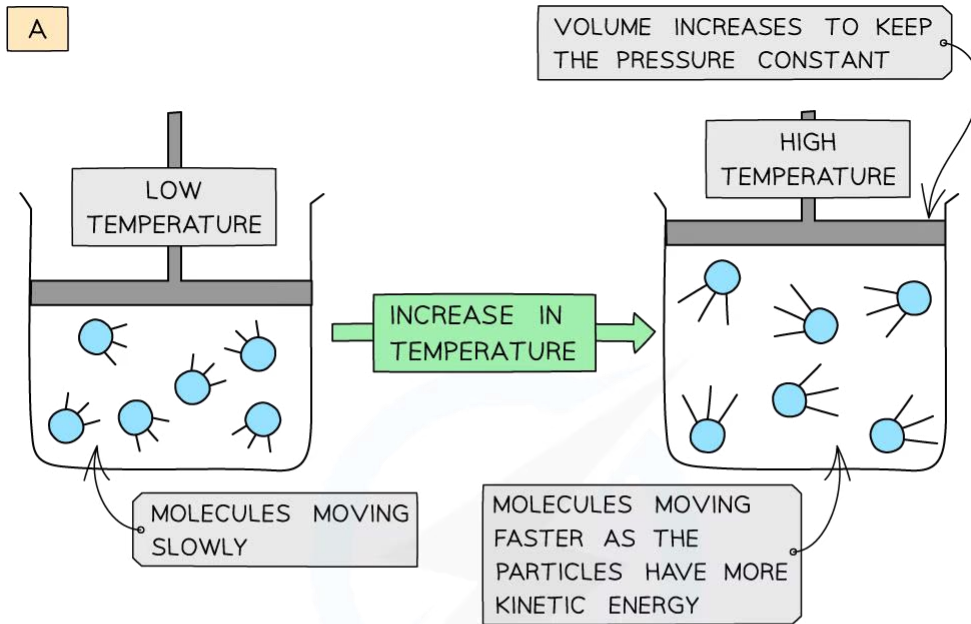
- **The kinetic theory of gases** states that molecules in gases are constantly moving
- The theory makes the following assumptions:
 - That gas molecules are moving very fast and randomly
 - That molecules hardly have any volume
 - That gas molecules do not attract or repel each other (**no intermolecular forces**)
 - No kinetic energy is lost when the gas molecules collide with each other (**elastic collisions**)
 - The temperature of the gas is related to the average kinetic energy of the molecules
- Gases that follow the kinetic theory of gases are called **ideal gases**
- However, in reality gases do not fit this description exactly **but** may come very close and are called **real gases**

Ideal gases

- The volume that an ideal gas occupies depends on:
 - Its pressure
 - Its temperature
- When a gas is **heated** (at constant pressure) the particles gain more **kinetic energy** and undergo more **frequent collisions** with the container wall
- To keep the **pressure constant**, the molecules must get further apart and therefore the **volume increases**
- The **volume** is therefore **directly proportional** to the **temperature** (at constant pressure)



YOUR NOTES
↓



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The volume of a gas increases upon heating to keep a constant pressure (a); volume is directly proportional to the temperature (b)

Limitations of the ideal gas law

- At very **low temperatures** and **high pressures** real gases do not obey the kinetic theory as under these conditions:
 - Molecules are close to each other
 - There are instantaneous dipole- induced dipole or permanent dipole- permanent dipole forces between the molecules
 - These attractive forces pull the molecules away from the container wall
 - The volume of the molecules is not negligible
- Real gases therefore do not obey the following kinetic theory **assumptions** at low temperatures and high pressures:
 - There is zero attraction between molecules (due to attractive forces, the **pressure is lower** than expected for an ideal gas)

- The volume of the gas molecules can be ignored (**volume** of the gas is **smaller** than expected for an ideal gas)

Ideal gas equation

- The **ideal gas equation** shows the relationship between pressure, volume, temperature and number of moles of gas of an ideal gas:

$$PV = nRT$$

P = pressure (pascals, Pa)

V = volume (m³)

n = number of moles of gas (mol)

R = gas constant (8.31 J K⁻¹ mol⁻¹)

T = temperature (kelvin, K)



Worked Example

Calculating the volume of a gas

Calculate the volume occupied by 0.781 mol of oxygen at a pressure of 220 kPa and a temperature of 21 °C

Answer

Step 1: Rearrange the ideal gas equation to find volume of gas

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

Step 2: Calculate the volume the oxygen gas occupies

$$p = 220 \text{ kPa} = 220\,000 \text{ Pa}$$

$$n = 0.781 \text{ mol}$$

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

$$T = 21 \text{ }^\circ\text{C} = 294 \text{ K}$$

$$V = \frac{0.781 \text{ mol} \times 8.31 \text{ J K}^{-1} \text{ mol}^{-1} \times 294 \text{ K}}{220\,000 \text{ Pa}} = 0.00867 \text{ m}^3 = 8.67 \text{ dm}^3$$

YOUR NOTES





Worked Example

Calculating the molar mass of a gas

A flask of volume 1000 cm³ contains 6.39 g of a gas. The pressure in the flask was 300 kPa and the temperature was 23 °C. Calculate the relative molecular mass of the gas.

Answer

Step 1: Rearrange the ideal gas equation to find the number of moles of gas

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

Step 2: Calculate the number of moles of gas

$$p = 300 \text{ kPa} = 300\,000 \text{ Pa}$$

$$V = 1000 \text{ cm}^3 = 1 \text{ dm}^3 = 0.001 \text{ m}^3$$

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

$$T = 23 \text{ °C} = 296 \text{ K}$$

$$n = \frac{300000 \text{ Pa} \times 0.001 \text{ m}^3}{8.31 \text{ J K}^{-1} \text{ mol}^{-1} \times 296 \text{ K}} = 0.12 \text{ mol}$$

Step 3: Calculate the molar mass using the number of moles of gas

$$n = \frac{\text{mass}}{\text{molar mass}}$$

$$\text{Molar mass} = \frac{6.39 \text{ g}}{0.12 \text{ mol}} = 53.25 \text{ g mol}^{-1}$$



Exam Tip

To calculate the temperature in Kelvin, add 273 to the Celsius temperature – e.g. 100 °C is 373 Kelvin

You must be able to rearrange the ideal gas equation to work out all parts of it

The units are incredibly important in this equation – make sure you know what units you should use, and do the necessary conversions when doing your calculations!



Percentage Yield Calculations

Percentage yield

- In a lot of reactions, not all reactants react to form products which can be due to several factors:
 - Other reactions take place simultaneously
 - The reaction does not go to **completion**
 - Products are **lost** during separation and purification
- The **percentage yield** shows how much of a particular product you get from the reactants compared to the maximum theoretical amount that you can get:

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

- The **actual yield** is the number of moles or mass of product obtained **experimentally**
- The **theoretical yield** is the number of moles or mass obtained by a reacting mass calculation



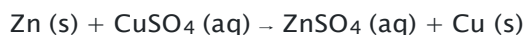
Worked Example

In an experiment to displace copper from copper(II) sulfate, 6.5 g of zinc was added to an excess of copper(II) sulfate solution. The resulting copper was filtered off, washed and dried. The mass of copper obtained was 4.8 g.

Calculate the percentage yield of copper.

Answer:

Step 1: The balanced symbol equation is:



Step 2: Calculate the amount of zinc reacted in moles

$$\text{number of moles} = \frac{6.5 \text{ g}}{65.4 \text{ g mol}^{-1}} = 0.10 \text{ mol}$$

Step 3: Calculate the maximum amount of copper that could be formed from the molar ratio:

Since the ratio of Zn(s) to Cu(s) is 1:1 a maximum of 0.10 moles can be produced



Step 4: Calculate the maximum mass of copper that could be formed (theoretical yield)

$$\begin{aligned}\text{mass} &= \text{mol} \times M \\ \text{mass} &= 0.10 \text{ mol} \times 63.55 \text{ g mol}^{-1} \\ \text{mass} &= 6.4 \text{ g (2 sig figs)}\end{aligned}$$

Step 5: Calculate the percentage yield of copper

$$\text{percentage yield} = \frac{4.8 \text{ g}}{6.4 \text{ g}} \times 100 = 75\%$$

Atom Economy Calculations

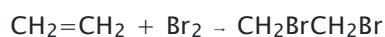
YOUR NOTES



- The atom economy of a reaction shows how many of the atoms used in the reaction become the desired product
 - The rest of the atoms or mass is wasted
- It is found directly from the balanced equation by calculating the M_r of the desired product

$$\text{Atom economy} = \frac{\text{molecular mass of desired product}}{\text{sum of molecular masses of ALL reactants}} \times 100$$

- In addition reactions, the atom economy will always be 100% because all of the atoms are used to make the desired product
 - Whenever there is only one product, the atom economy will always be 100%
 - For example, in the reaction between ethene and bromine:



- The atom economy could also be calculated using mass, instead of M_r
 - In this case, you would divide the mass of the desired product formed by the total mass of all reactants, and then multiply by 100
- Questions about atom economy often asked in qualitative or quantitative terms



Worked Example

Qualitative atom economy

Ethanol can be produced by various reactions, such as:



Explain which reaction has a higher atom economy.

Answer

Hydration of ethene has a higher atom economy (of 100%) because all of the reactants are converted into products, whereas the substitution of bromoethane produces NaBr as a waste product



Worked Example

Quantitative atom economy

The blast furnace uses carbon monoxide to reduce iron(III) oxide to iron.



Calculate the atom economy for this reaction, assuming that iron is the desired product.

(A_r / M_r data: $\text{Fe}_2\text{O}_3 = 159.6$, $\text{CO} = 28.0$, $\text{Fe} = 55.8$, $\text{CO}_2 = 44.0$)

Answer

Step 1: Write the equation:

$$\text{Atom economy} = \frac{\text{molecular mass of desired product}}{\text{sum of molecular masses of ALL reactants}} \times 100$$

Step 2: Substitute values and evaluate:

$$\text{Atom economy} = \frac{2 \times 55.8}{159.6 + (3 \times 28.0)} \times 100 = 45.8\%$$



Exam Tip

Careful: Sometimes a question may ask you to show your working when calculating atom economy. In this case, even if it is an addition reaction and it is obvious that the atom economy is 100%, you will still need to show your working.

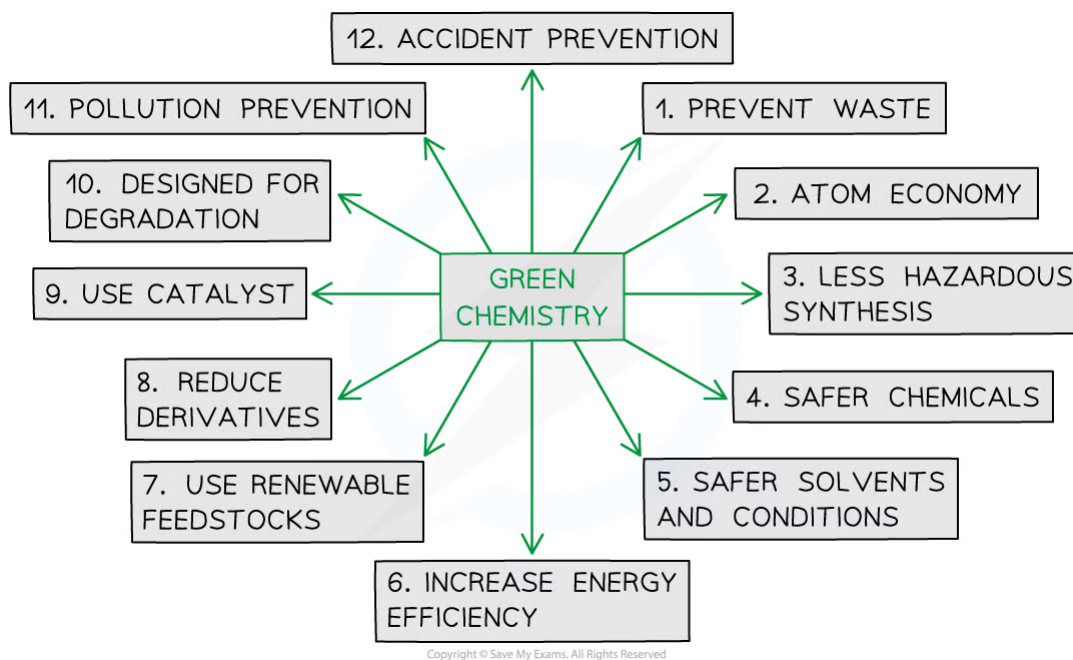
Benefits of High Atom Economy

- Chemists use percentage yield as one possible measure of how efficient a reaction is
 - A high percentage yield suggests that a process is effective at converting reactants into products
- The estimated percentage yield for a single run of the Haber Process is around 15%
 - This is a compromise due to the cost and safety of the required conditions against the overall rate of ammonia production
 - Any unreacted materials are also recycled so it is estimated that the percentage conversion of all reactants to products is around 97%
- Whilst a high percentage yield can be good for profits, it does not account for any waste products
 - A reaction can have a high percentage yield but low atom economy which essentially means that more waste products are produced
- Atom economy is a measure of the percentage of reactants that become useful products and is calculated by:

$$\text{Percentage atom economy} = \frac{\text{mass of desired product}}{\text{total mass of ALL reactants}} \times 100$$

Atom Economy and Green Chemistry

- Chemists will often have several choices of reaching a target molecule and those choices need to take into the principles of **Green Chemistry**



The twelve principles of green chemistry

- By choosing a reaction pathway that has fewer steps, you can prevent waste and reduce energy demands which is better for the environment
 - This also reduces production costs

YOUR NOTES



- One of the key ideas behind Green Chemistry is to find reaction pathways with high percentage yield and high atom economy
- By analysing the atom economy of each step, you can select reactions that give a higher atom economy and / or select other reactions to reduce the number of steps involved in a reaction pathway
 - For example, the synthesis of ibuprofen that was patented by Boots in the 1960's was a six-step synthesis
 - Even if each step has an atom economy of 90%, a six-step synthesis would have an overall atom economy of 53%
 - The modern production of ibuprofen is a three-step synthesis, which with the same assumptions as before, gives an overall atom economy of 73%
- Higher atom economy means that there is less waste produced
 - This can be considered environmentally friendly even though it may not influence the reaction conditions
 - It also means that reactions are more sustainable and often use less natural / finite resource

YOUR NOTES



2.3 Acid–base & Redox Reactions

2.3.1 Acids

Acids, Bases & Dissociation

Strong acids dissociating

- Strong acids will **fully** dissociate in solution
- For example, when hydrogen chloride (HCl) is dissolved in water 100% of the product will be ions.
 - $\text{HCl (aq)} \rightarrow \text{H}^+ \text{(aq)} + \text{Cl}^- \text{(aq)}$
 - In this case hydrogen ions are released, $\text{H}^+ \text{(aq)}$
 - The same applies with strong bases

Strong bases dissociating

- Strong bases will **fully** dissociate in solution
 - $\text{NaOH (aq)} \rightarrow \text{Na}^+ \text{(aq)} + \text{OH}^- \text{(aq)}$
 - In this case hydroxide ions are released, $\text{OH}^- \text{(aq)}$

Weak acids dissociating

- Weak acids only **partially** dissociate in solution, only a small percentage of the products will be ions
- In an equilibrium reaction, the products are formed at the same rate as the reactants are used
- This means that at equilibrium, both reactants and products are present in the solution
- For example, ethanoic acid (CH_3COOH) is a weak acid that partially dissociates in solution
 - $\text{CH}_3\text{COOH (aq)} \rightleftharpoons \text{CH}_3\text{COO}^- \text{(aq)} + \text{H}^+ \text{(aq)}$
 - The same applies with weak bases

Weak bases dissociating

- Weak bases only **partially** dissociate in solution, only a small percentage of the products will be ions
- An equilibrium is established containing reactants and products
- For example, ethylamine ($\text{CH}_3\text{CH}_2\text{NH}_2$) is a weak base and will partially dissociate in solution and produce hydroxide ions
 - $\text{CH}_3\text{CH}_2\text{NH}_2 \text{(aq)} + \text{H}_2\text{O (l)} \rightleftharpoons \text{CH}_3\text{CH}_2\text{NH}_3^+ \text{(aq)} + \text{OH}^- \text{(aq)}$

Examples of acids and bases

YOUR NOTES





| Strong Acids | Weak Acids | Strong Bases | Weak Bases |
|--------------------------------|------------------------------------|---------------------|---|
| HCl | HCOOH | NaOH | NH ₃ |
| H ₂ SO ₄ | CH ₃ COOH | KOH | CH ₃ NH ₂ |
| HNO ₃ | C ₆ H ₅ COOH | Ba(OH) ₂ | CH ₃ CH ₂ NH ₂ |

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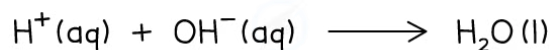
Neutralisation

- A neutralisation reaction is one in which an acid (pH < 7) and a base/alkali (pH > 7) react together to form water (pH = 7) and a salt



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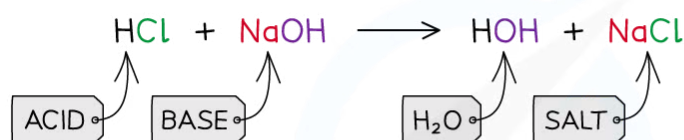
- The proton of the acid reacts with the hydroxide of the base to form water



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- The spectator ions which are not involved in the formation of water, form the salt

MAIN NEUTRALISATION REACTION:



THE TWO INDIVIDUAL REACTIONS TAKING PLACE ARE:



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The diagram shows a neutralisation reaction of HCl and NaOH and the two individual reactions that take place to form the water and salt

- The name of the salt produced can be predicted from the acid that has reacted

Acid Reacted & Salt Table

| Acid Reacted | Salt produced |
|-------------------|---------------|
| Hydrochloric Acid | A Chloride |
| Nitric Acid | A Nitrate |
| Sulfuric Acid | A Sulfate |

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Metals and acids

- The typical reaction of a metal and an acid can be summarized as



acid + metal → salt + hydrogen

- For example:



hydrochloric acid + zinc → zinc chloride + hydrogen

- Clearly, the extent of reaction depends on the **reactivity** of the metal and the **strength** of the acid
- Very reactive metals would react dangerously with acids and these reactions are not usually carried out
- Metals low in **reactivity** do not react at all, for instance copper does not react with dilute acids
- **Stronger acids** will react **more vigorously** with metals than weak acids. What signs of reaction would be expected to be different between the two?
 - Faster reaction, seen as
 - more effervescence
 - the metal dissolves faster
 - more exothermic

Metals and oxides

- The reaction of an acid with a metal oxide forms two products:

acid + metal oxide → salt + water

- For example:



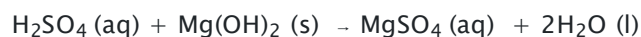
hydrochloric acid + calcium oxide → calcium chloride + water

Metals and hydroxides

- The reaction with a metal hydroxide and an acid follows the same pattern as an oxide:

acid + metal hydroxide → salt + water

- For example



sulfuric acid + magnesium hydroxide → magnesium sulfate + water

Metals and carbonates

- The reaction between a metal carbonate and an acid produces three products:

acid + metal carbonate → salt + water + carbon dioxide

- For example:



nitric acid + copper carbonate → copper nitrate + water + carbon dioxide

2.3.2 Acid-base Titrations

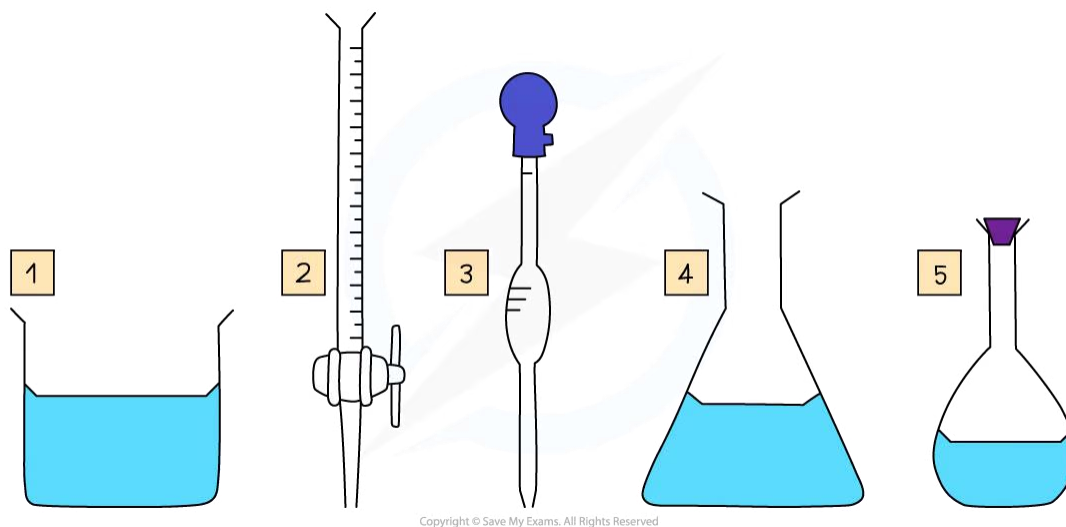
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Acid-base Titrations

Volumetric Analysis

- Volumetric analysis is a process that uses the volume and concentration of one chemical reactant (**standard solution**) to determine the concentration of another unknown solution
- The technique most commonly used is a **titration**
- The volumes are measured using two precise pieces of equipment, a **volumetric** or **graduated pipette** and a **burette**
- Before the titration can be done, the standard solution must be prepared
- Specific apparatus must be used both when preparing the standard solution and when completing the titration, to ensure that volumes are measured precisely

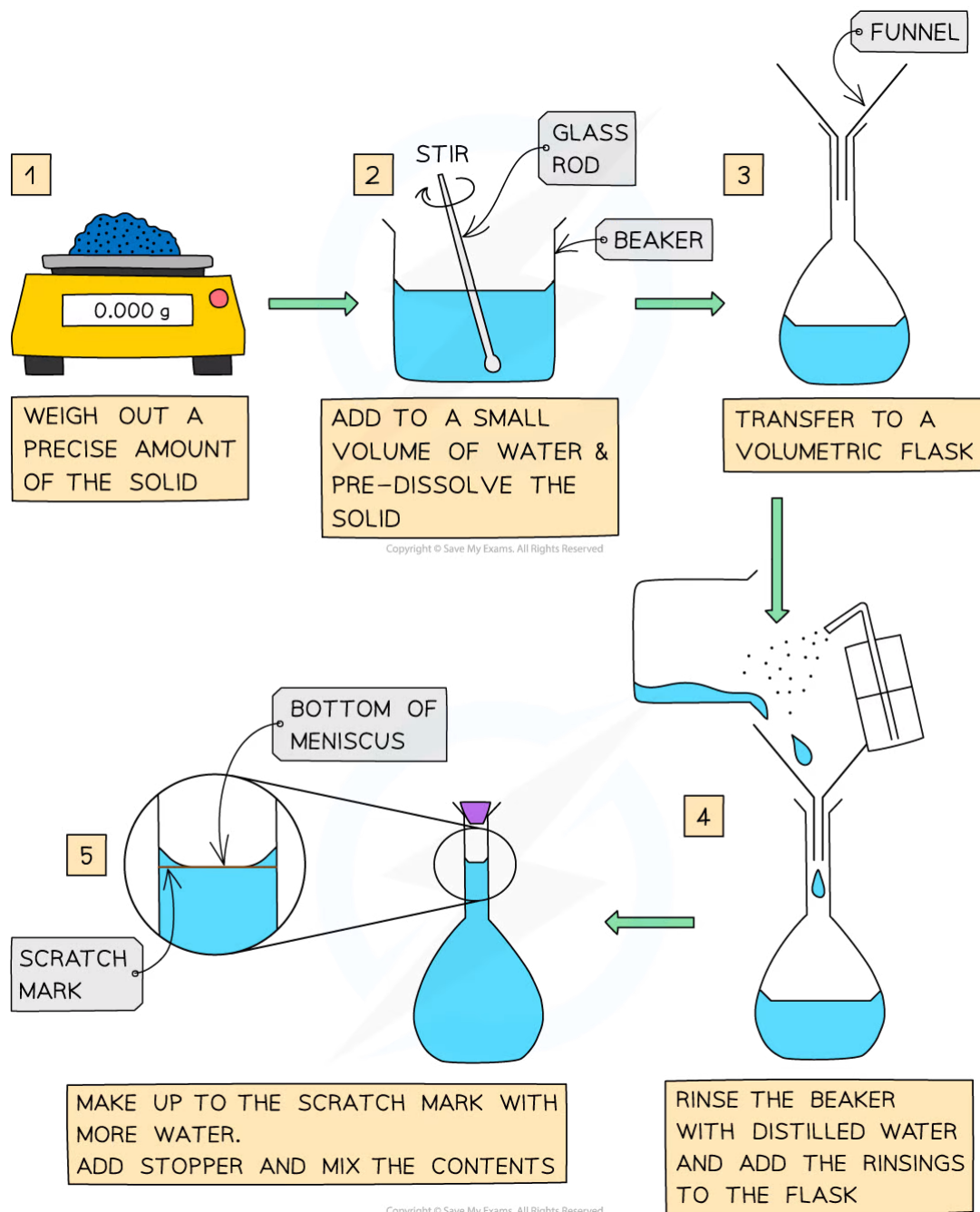


Some key pieces of apparatus used to prepare a volumetric solution and perform a simple titration

1. Beaker
2. Burette
3. Volumetric Pipette
4. Conical Flask
5. Volumetric Flask

Making a Standard Solution

- Chemists routinely prepare solutions needed for analysis, whose concentrations are known precisely
- These solutions are termed **volumetric solutions** or **standard solutions**
- They are made as accurately and precisely as possible using three decimal place balances and volumetric flasks to reduce the impact of measurement uncertainties
- The steps are:



Volumes & concentrations of solutions

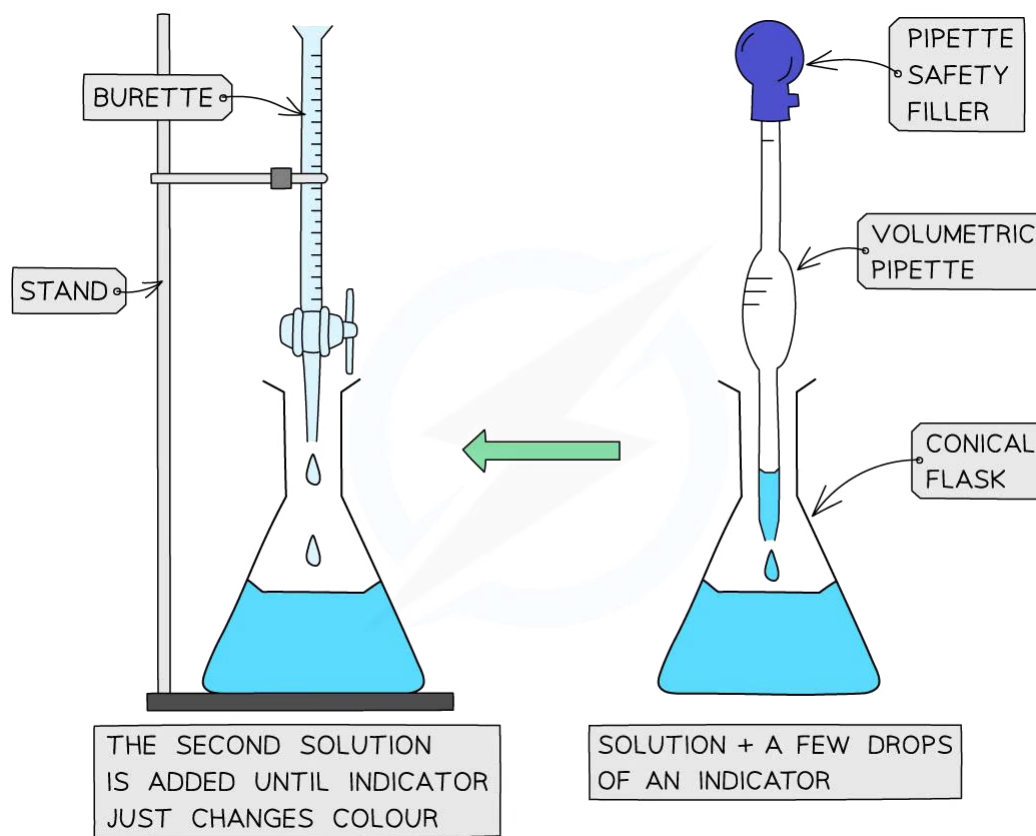
- ♦ The **concentration** of a solution is the amount of **solute** dissolved in a **solvent** to make 1 dm³ of **solution**
 - The solute is the substance that dissolves in a solvent to form a solution
 - The solvent is often water
- ♦ A **concentrated** solution is a solution that has a **high** concentration of solute
- ♦ A **dilute** solution is a solution with a **low** concentration of solute
- ♦ Concentration is usually expressed in one of three ways:

- moles per unit volume
- mass per unit volume
- parts per million

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↓

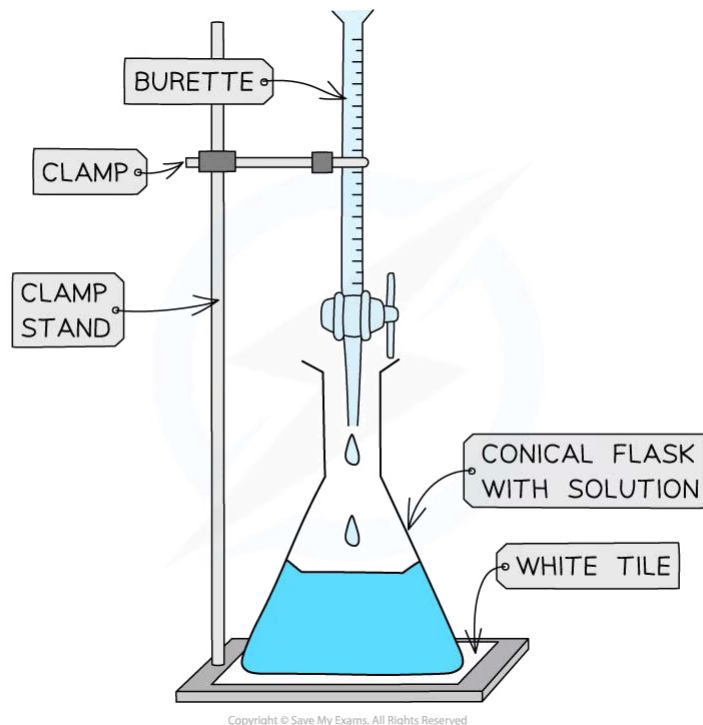
Performing the Titration

- The key piece of equipment used in the titration is the burette
- **Burettes** are usually marked to a precision of 0.10 cm^3
 - Since they are analogue instruments, the uncertainty is recorded to **half** the smallest marking, in other words to $\pm 0.05 \text{ cm}^3$
- The **end point** or **equivalence point** occurs when the two solutions have reacted completely and is shown with the use of an **indicator**



The steps in a titration

- A white tile is placed under the conical flask while the titration is performed, to make it easier to see the colour change



The steps in a titration

- The steps in a titration are:
 - Measuring a known volume (usually 20 or 25 cm³) of one of the solutions with a volumetric pipette and placing it into a conical flask
 - The other solution is placed in the burette
 - To start with, the burette will usually be filled to 0.00 cm³
 - A few drops of the indicator are added to the solution in the conical flask
 - The tap on the burette is carefully opened and the solution added, portion by portion, to the conical flask until the indicator starts to change colour
 - As you start getting near to the end point, the flow of the burette should be slowed right down so that the solution is added dropwise
 - You should be able to close the tap on the burette after one drop has caused the colour change
 - Multiple runs are carried out until **concordant** results are obtained
 - Concordant results are within 0.1 cm³ of each other

Recording and processing titration results

- Both the initial and final burette readings should be recorded and shown to a precision of ± 0.05 cm³, the same as the uncertainty

YOUR NOTES



ALL RESULTS ARE RECORDED TO 2 DECIMAL PLACES INCLUDING ZERO READINGS

| | Rough | Run 1 | Run 2 | Run 3 |
|---------------------------------------|-------|---------|---------|-------|
| Initial burette reading ± 0.05 ml | 0.00 | 23.15 | 0.20 | 23.00 |
| Final burette reading ± 0.05 ml | 23.75 | 45.95 | 23.00 | 46.10 |
| Volume delivered ± 0.10 ml | 23.75 | 22.80 ✓ | 22.80 ✓ | 23.10 |

THE FINAL DIGIT IS 0 OR 5

DOUBLE THE UNCERTAINTY

THE ROUGH RESULT IS USUALLY FAR OVER THE END-POINT

THIS RESULT IS DISCARDED AS IT IS TOO HIGH

✓ = CONCORDANT RESULTS
USED TO CALCULATE THE AVERAGE

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A typical layout and set of titration results

- ♦ The volume delivered (titre) is calculated and recorded to an uncertainty of ± 0.10 cm³
 - The uncertainty is doubled, because two burette readings are made to obtain the titre ($V_{\text{final}} - V_{\text{initial}}$), following the rules for propagation of uncertainties
- ♦ **Concordant** results are then averaged, and non-concordant results are discarded
- ♦ The appropriate calculations are then done

Percentage Uncertainties

- ♦ Percentage uncertainties are a way to compare the significance of an absolute uncertainty on a measurement
- ♦ This is not to be confused with percentage error, which is a comparison of a result to a literature value
- ♦ The formula for calculating percentage uncertainty is as follows:

$$\text{percentage uncertainty} = \frac{\text{uncertainty}}{\text{measured value}} \times 100\%$$

Adding or subtracting measurements

- ♦ When you are adding or subtracting two measurements then you add together the **absolute** measurement uncertainties
- ♦ For example,
 - Using a balance to measure the initial and final mass of a container

- Using a thermometer for the measurement of the temperature at the start and the end
- Using a burette to find the initial reading and final reading
- In all these examples you have to read the instrument **twice** to obtain the quantity
- If each time you read the instrument the measurement is 'out' by the stated uncertainty, then your final quantity is potentially 'out' by twice the uncertainty

YOUR NOTES



Acid–base Titration Calculations

YOUR NOTES



Volumes & concentrations of solutions

- The **concentration** of a solution is the amount of **solute** dissolved in a **solvent** to make 1 dm³ of **solution**
 - The solute is the substance that dissolves in a solvent to form a solution
 - The solvent is often water

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

- A **concentrated** solution is a solution that has a **high** concentration of solute
- A **dilute** solution is a solution with a **low** concentration of solute
- When carrying out calculations involve concentrations in mol dm⁻³ the following points need to be considered:
 - Change mass in grams to **moles**
 - Change cm³ to dm³
- To calculate the **mass** of a substance present in solution of known **concentration and volume**:
 - Rearrange the concentration equation

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

- Multiply the moles of solute by its molar mass

$$\text{mass of solute (g)} = \text{number of moles (mol)} \times \text{molar mass (g mol}^{-1}\text{)}$$



Worked Example

Neutralisation calculation

25.0 cm³ of 0.050 mol dm⁻³ sodium carbonate was completely neutralised by 20.00 cm³ of dilute hydrochloric acid. Calculate the concentration in mol dm⁻³ of the hydrochloric acid.

Answer

Step 1: Write the balanced symbol equation



Step 2: Calculate the amount, in moles, of sodium carbonate reacted by rearranging the equation for amount of substance (mol) and dividing the volume by 1000 to convert cm³ to dm³

$$\text{amount (Na}_2\text{CO}_3\text{)} = 0.025 \text{ dm}^3 \times 0.050 \text{ mol dm}^{-3} = 0.00125 \text{ mol}$$

Step 3: Calculate the moles of hydrochloric acid required using the reaction's stoichiometry

1 mol of Na_2CO_3 reacts with 2 mol of HCl, so the molar ratio is 1 : 2

Therefore 0.00125 moles of Na_2CO_3 react with 0.00250 moles of HCl

Step 4: Calculate the concentration, in mol dm^{-3} , of hydrochloric acid

$$\text{concentration (HCl) (mol dm}^{-3}\text{)} = \frac{\text{amount (mol)}}{\text{volume (dm}^3\text{)}}$$

$$\text{concentration (HCl) (mol dm}^{-3}\text{)} = \frac{0.00250}{0.0200}$$

$$\text{concentration (HCl) (mol dm}^{-3}\text{)} = 0.125 \text{ mol dm}^{-3}$$

YOUR NOTES





Oxidation Number

Oxidation Number Rules

- A few simple rules help guide you through the process of determining the oxidation number of any element
- Remember, you are determining the oxidation state of a *single* atom

Oxidation Numbers

- The **oxidation state** of an atom is the charge that would exist on an individual atom if the bonding were completely ionic
- It is like the electronic 'status' of an element
- **Oxidation numbers** are used to
 - Tell if oxidation or reduction has taken place
 - Work out what has been oxidised and/or reduced
 - Construct half equations and balance redox equations

Oxidation Numbers of Simple Ions

| | | |
|----------------|----------------------------|--|
| Atoms | Na in Na = 0 | neutral already, no need to add any electrons |
| Cations | Na in Na ⁺ = +1 | need to add 1 electron to make Na ⁺ neutral |
| Anions | Cl in Cl ⁻ = -1 | need to take 1 electron away to make Cl ⁻ neutral |

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Oxidation Rules Table



| Rule | Example |
|--|--|
| 1. The oxidation state of any uncombined element is zero | H ₂ Zn O ₂ |
| 2. Many atoms or ions have fixed oxidation state in compounds | Group 1 elements are always +1 Group 2 elements are always +2 Fluorine is always -1 Hydrogen is +1 (except for in metal hydrides like NaH, where it is -1) Oxygen is -2 (except in peroxides, where it is -1 and in F ₂ O where it is +2) |
| 3. The oxidation state of an element in a mono-atomic ion is always same as the charge | Zn ²⁺ oxidation state = +2 Fe ³⁺ oxidation state = +3 Cl ⁻ oxidation state = -1 |
| 4. The sum of the oxidation state in a compound is zero | NaCl oxidation state of Na = +1 oxidation state of Cl = -1 sum oxidation state = 0 |
| 5. The sum of oxidation state in ion is equal to the charge on the ion | SO ₄ ²⁻ oxidation state of S = +6 oxidation state of 4 O atoms = 4 × (-2) sum oxidation state = -2 |
| 6. In either a compound or an ion, the more electronegative element is given the oxidation state | F ₂ O oxidation state of both F atoms = 2 × (-1) oxidation state of O = +2 |

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Molecules or Compounds

- In molecules or compounds, the sum of the oxidation number on the atoms is zero

Oxidation Number in Molecules or Compounds



| | | |
|------------------|---------------------------|---|
| Elements | H in H ₂ = 0 | Both are the same and must add up to zero |
| Compounds | C in CO ₂ = +4 | 1 × (+4) and 2 × (-2) = 0 |
| | O in CO ₂ = -2 | |

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- Because CO₂ is a neutral molecule, the sum of the oxidation number must be zero
- For this, one element must have a positive oxidation number and the other must be negative

How do you determine which is the positive one?

- The more electronegative species will have the negative value
- Electronegativity increases across a period and decreases down a group
- O is further to the right than C in the periodic table so it has the negative value

How do you determine the value of an element's oxidation number?

- From its position in the periodic table and/or
- The other element(s) present in the formula
- The oxidation states of all other atoms in their compounds can vary
- By following the oxidation number rules, the oxidation state of any atom in a compound or ion can be deduced
- The position of an element in the periodic table can act as a guide to the oxidation number

Oxidation Numbers & the Periodic Table

| | |
|-------------------|--|
| Metals | ◦ Have positive values in compounds |
| | ◦ Value is usually that of the Group Number Al is +3 |
| | ◦ Where there are several possibilities the values go no higher than the Group No. |
| | Sn can be +2 or +4, Mn can be +2, +4, +6, +7 |
| Non-metals | ◦ Mostly negative based on their usual ion |
| | Cl usually -1 |
| | ◦ Can have values up to their Group No. |
| | Cl +1 +3 +5 or +7 |

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- Test your understanding on the following examples:



Worked Example

Deducing oxidation numbers

Give the oxidation number of the elements in **bold** in these compounds or ions:



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Answers

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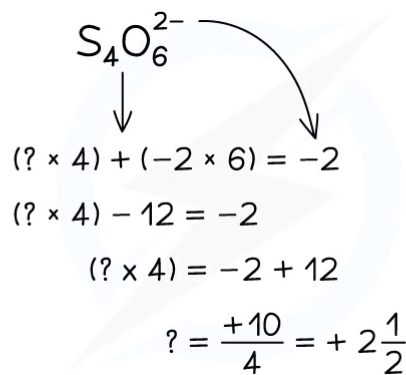


| Example | Explanation |
|----------------|--|
| a. P_2O_5 | ox. no. 5 O atoms = $5 \times (-2)$ = -10 Overall charge compound = 0 ox. no. of 2 P atoms = $+10$ ox. no. of P = $+5$ |
| b. SO_4^{2-} | ox. no. 4 O atoms = $4 \times (-2)$ = -8 Overall charge compound = -2 ox. no. of S = $+6$ |
| c. H_2S | ox. no. 2 H atoms = $2 \times (+1)$ = $+2$ Overall charge compound = 0 ox. no. of S = -2 |
| d. Al_2Cl_6 | ox. no. 6 Cl atoms = $Cl \times (-1)$ = -6 Overall charge compound = 0 ox. no. of 2 Al atoms = $+6$ ox. no. of Al = $+3$ |
| e. NH_3 | ox. no. 3 H atoms = $3 \times (+1)$ = $+3$ Overall charge compound = 0 ox. no. of N = -3 |
| f. ClO_2^- | ox. no. 2 O atoms = $2 \times (-2)$ = -4 Overall charge compound = -1 ox. no. of Cl = $+3$ |

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Are oxidation numbers always whole numbers?

- The answer is yes and no
- When you try and work out the oxidation numbers of sulfur in the tetrathionate ion $S_4O_6^{2-}$ you get an interesting result!



The oxidation number of sulfur in $\text{S}_4\text{O}_6^{2-}$ is a fraction

- The fact that the oxidation number comes out to +2.5 does not mean it is possible to get half an oxidation number
- This is only a mathematical consequence of four sulfur atoms sharing +10 oxidation number
- Single atoms can only have an integer oxidation number, because you cannot have half an electron!

Roman numerals

- Roman numerals are used to show the oxidation states of **transition metals** which can have more than one oxidation state
- Iron can be both +2 and +3 so Roman numerals are used to distinguish between them
 - Fe^{2+} in FeO is written as **iron(II) oxide**
 - Fe^{3+} in Fe_2O_3 is written as **iron(III) oxide**

YOUR NOTES



Redox Reactions & Equations

- Metals can react with acid to form a salt and hydrogen



- During this reaction, there are changes in oxidation number
 - This means that the reaction can be classified as a redox reaction



Worked Example

Explain why each of the following reactions is a redox reaction:

1. Zinc + hydrochloric acid – zinc chloride + hydrogen
2. Magnesium + sulfuric acid – magnesium sulfate + hydrogen

Answer 1

Step 1: Write the balanced symbol equation



Step 2: Deduce the changes in oxidation number

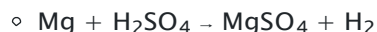
- Zinc – starts at 0, changes to +2
- Hydrogen – starts at +1, changes to 0
- Chlorine – remains at -1 throughout

Step 3: Explain which species is reduced / oxidised

- Zinc is oxidised as its oxidation number increases from 0 to +2
- Hydrogen is reduced as its oxidation number decreases from +1 to 0

Answer 2

Step 1: Write the balanced symbol equation



Step 2: Deduce the changes in oxidation number

- Magnesium – starts at 0, changes to +2
- Hydrogen – starts at +1, changes to 0
- Sulfate ion – remains at -2 throughout

Step 3: Explain which species is reduced / oxidised

- Magnesium is oxidised as its oxidation number increases from 0 to +2
- Hydrogen is reduced as its oxidation number decreases from +1 to 0

YOUR NOTES





Exam Tip

Remember that oxidation number increases in oxidation reactions and decreases in reductions reactions

If you are asked to explain why a reaction is a redox reaction, you should always talk about one of the following:

- Gain / loss of oxygen
- Gain / loss of hydrogen
- Gain / loss of electrons
- Changes in oxidation numbers

Simply saying that it a reaction is a redox reaction because "*reduction and oxidation happen at the same time*" is describing, **not** explaining

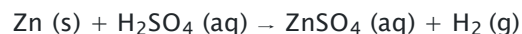
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Interpreting Redox

We can identify the oxidation and reducing agents in a reaction by using the oxidation state.

- For example



- If we look at zinc, Zn, in the reaction above we can see that it increases from 0 to +2 in zinc sulfate, ZnSO₄
- An increase in oxidation number indicates oxidation has occurred
- Therefore zinc is the reducing agent
- If we look at sulfuric acid, H₂SO₄, the oxidation state of hydrogen has decreased from +1 to 0 in H₂
- A decrease in oxidation number indicates reduction has occurred
- Therefore sulfuric acid is the oxidising agent



Worked Example

Identify the oxidising agent and reducing agent in the following reaction:



Answer

Step 1: Deduce the oxidation numbers of nitrogen and chlorine in the equation (hydrogen = +1, oxygen = -2, sodium = +1)

N in NH₃ is -3

Cl in NaClO is +1

N in N₂H₄ is -2

Cl in NaCl is -1

Step 2

Identify which species has been oxidised and which has been reduced by looking at the oxidation numbers

Nitrogen is increasing in oxidation number, therefore has been oxidised

Chlorine is decreasing in oxidation number, therefore has been reduced

Step 3

Identify the oxidising and reducing agent

NH₃ is the reducing agent (it has been oxidised itself)

NaClO is the oxidising agent (it has been reduced itself)

Remember, the whole species is the reducing agent, not just the element (e.g. NH₃ is the reducing agent, not N on its own)

YOUR NOTES



2.4 Electrons, Bonding & Structure

2.4.1 Electron Structure

Electrons & Orbitals

Shells

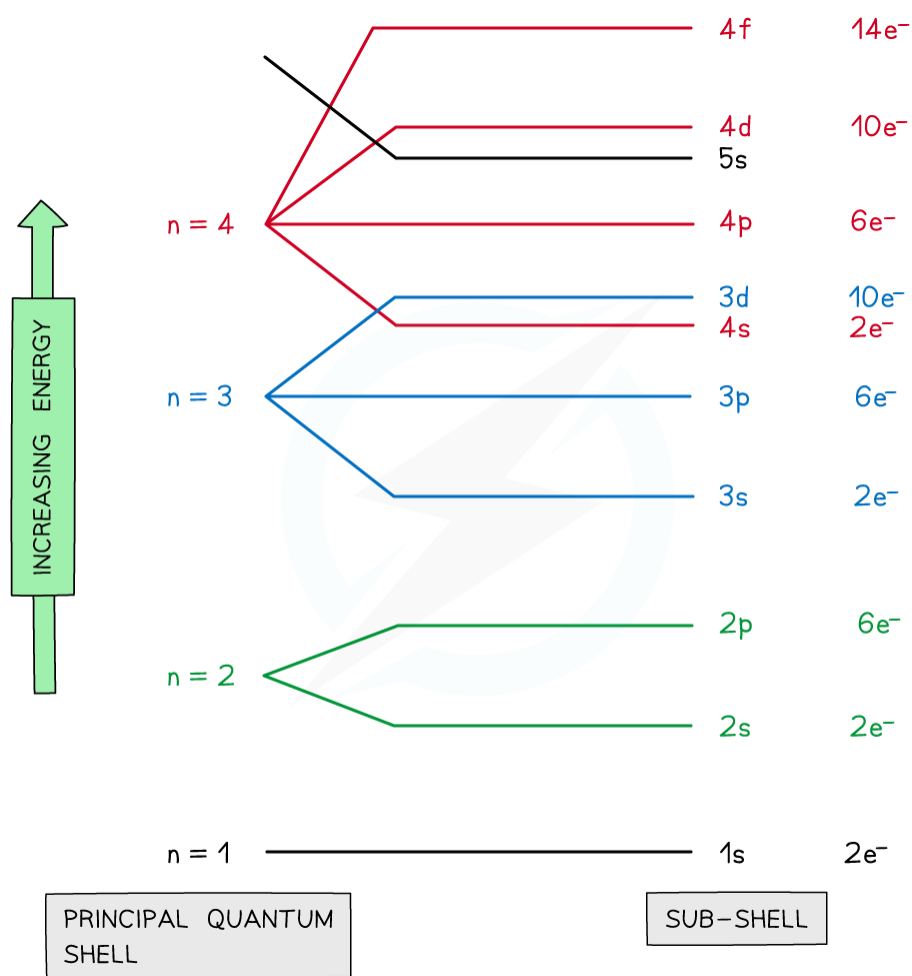
- The arrangement of electrons in an atom is called the **electron configuration**
- Electrons are arranged around the nucleus in **principal energy levels** or **principal quantum shells**
- **Principal quantum numbers** (n) are used to number the energy levels or quantum shells
 - The **lower** the principal quantum number, the closer the shell is to the nucleus
 - So, the first shell which is the closest to the nucleus is $n = 1$
 - The **higher** the principal quantum number, the greater the energy of the shell and the further away from the nucleus
- Each principal quantum number has a **fixed** number of electrons it can hold, as follows:
 - $n = 1$: up to 2 electrons
 - $n = 2$: up to 8 electrons
 - $n = 3$: up to 18 electrons
 - $n = 4$: up to 32 electrons

Subshells

- The principal quantum shells are split into **subshells** which are given the letters **s**, **p** and **d**
 - Elements with more than 57 electrons also have an **f** shell
 - The energy of the electrons in the subshells increases in the order $s < p < d$
- The order of subshells appear to overlap for the higher principal quantum shells as seen in the diagram below:

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Electrons are arranged in principal quantum shells, which are numbered by principal quantum numbers

Orbitals

- ♦ Subshells contain one or more **atomic orbitals**
- ♦ Orbitals exist at **specific** energy levels and electrons can only be found at these specific levels, **not** in between them
 - Each atomic orbital can be occupied by a maximum of two electrons
- ♦ This means that the number of orbitals in each subshell is as follows:
 - **s** : one orbital (1 × 2 = total of 2 electrons)
 - **p** : three orbitals (3 × 2 = total of 6 electrons)
 - **d** : five orbitals (5 × 2 = total of 10 electrons)
 - **f** : seven orbitals (7 × 2 = total of 14 electrons)
- ♦ The orbitals have specific 3-D shapes

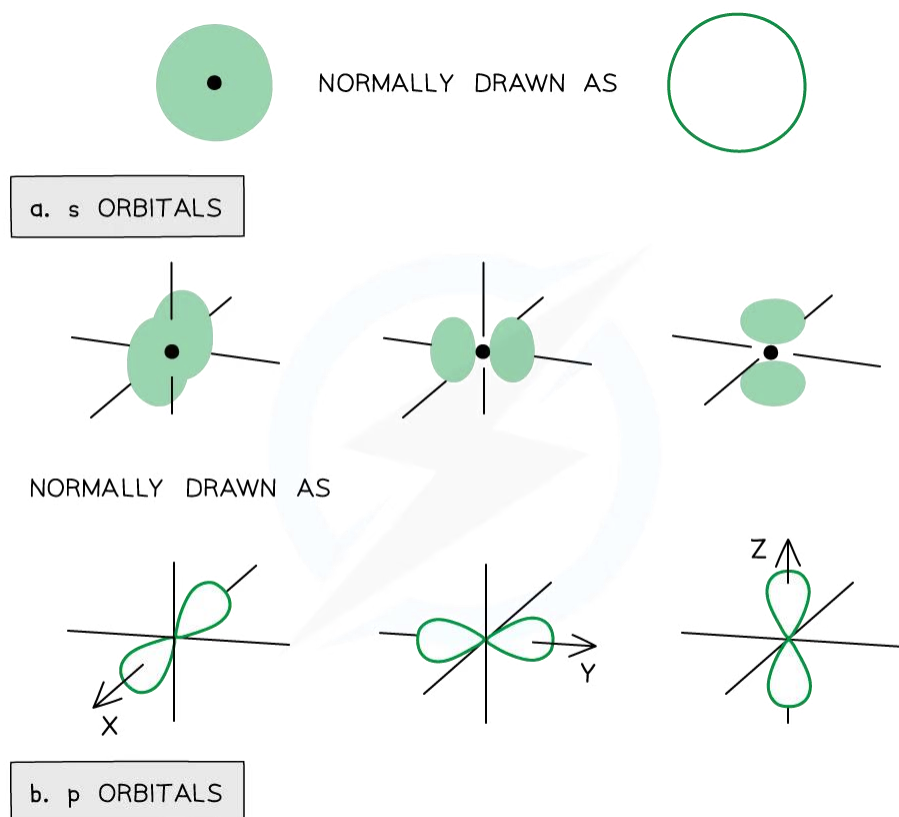
s orbital shape

- ♦ The s orbitals are **spherical** in shape

- The **size** of the s orbitals increases with increasing shell number
 - E.g. the s orbital of the **third** quantum shell ($n = 3$) is bigger than the s orbital of the **first** quantum shell ($n = 1$)

p orbital shape

- The p orbitals have a **dumbbell shape**
- Every shell has three p orbitals except for the first one ($n = 1$)
- The p orbitals occupy the x, y and z axes and point at right angles to each other, so are oriented **perpendicular** to one another
- The lobes of the p orbitals become **larger** and **longer** with increasing shell number



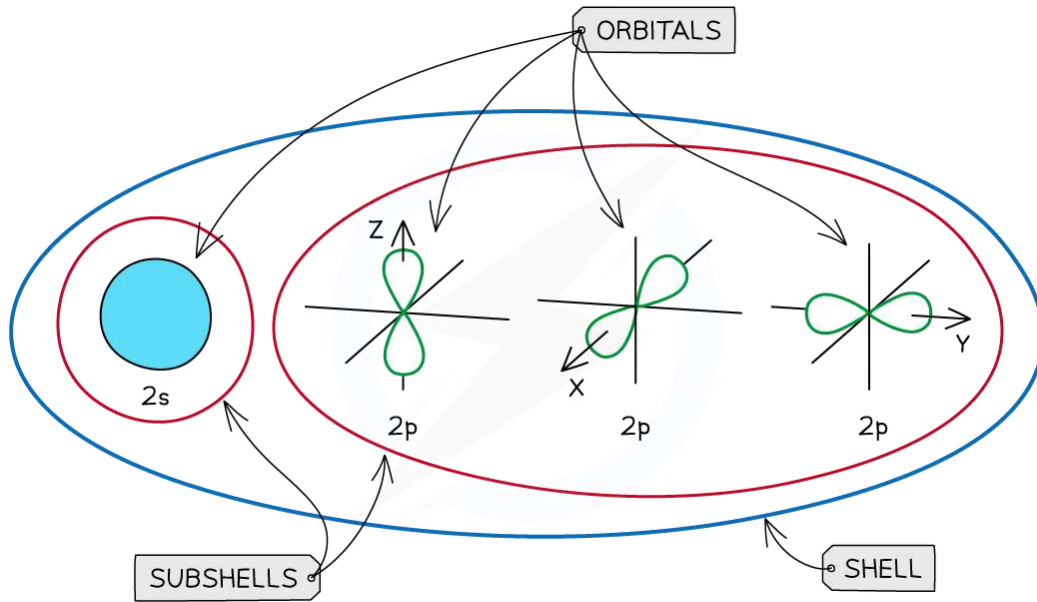
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Representation of orbitals (the dot represents the nucleus of the atom) showing spherical s orbitals (a), p orbitals containing 'lobes' along the x, y and z axis

- Note that the shape of the d orbitals is **not** required

YOUR NOTES





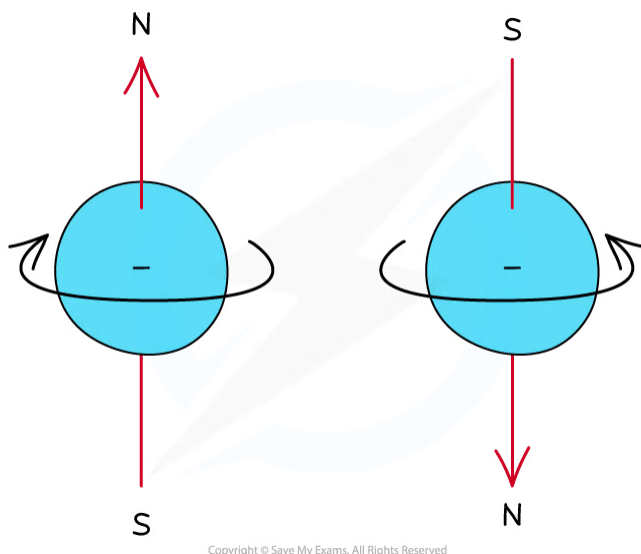
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An overview of the shells, subshells and orbitals in an atom

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↓

Filling Orbitals

- Electrons can be imagined as small **spinning charges** which rotate around their own axis in either a **clockwise** or **anticlockwise direction**
 - The spin of the electron is represented by its direction
 - The spin creates a tiny magnetic field with N-S pole pointing up or down



Electrons can spin either in a clockwise or anticlockwise direction around their own axis

- Electrons with the same **spin** repel each other which is also called **spin-pair repulsion**
 - Therefore, electrons will occupy separate orbitals in the same subshell first to minimise this repulsion and have their **spin** in the same direction
 - They will then pair up, with a second electron being added to the first p orbital, with its spin in the **opposite** direction
- This is known as **Hund's Rule**
 - E.g. if there are three electrons in a **p subshell**, one electron will go into each p_x , p_y and p_z orbital



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Electron configuration: three electrons in a p subshell

- The principal quantum number indicates the energy level of a particular shell but also indicates the energy of the electrons in that shell

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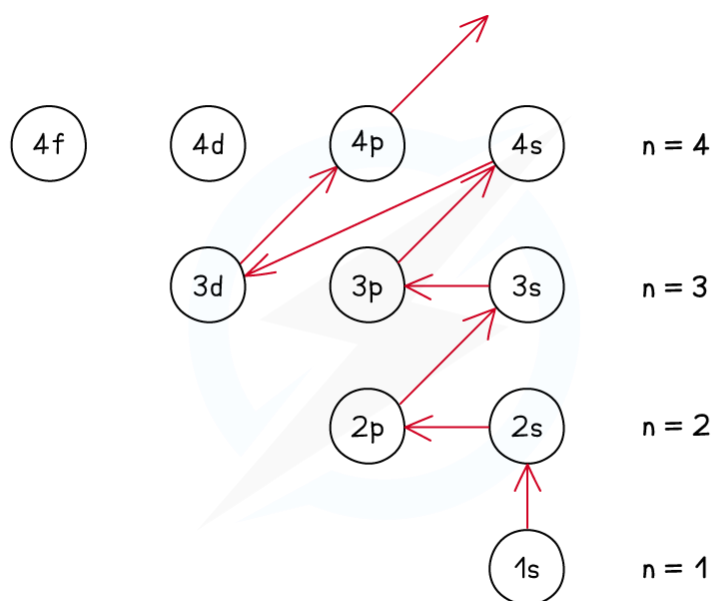




- A 2p electron is in the second shell and therefore has an energy corresponding to $n = 2$
- ♦ Even though there is repulsion between negatively charged electrons, they occupy the same region of space in orbitals
- ♦ An orbital can only hold two electrons and they must have opposite spin – this is known as the **Pauli Exclusion Principle**
- ♦ This is because the energy required to jump to a higher empty orbital is **greater** than the inter-electron repulsion
- ♦ For this reason, they pair up and occupy the lower energy levels first

Ground state

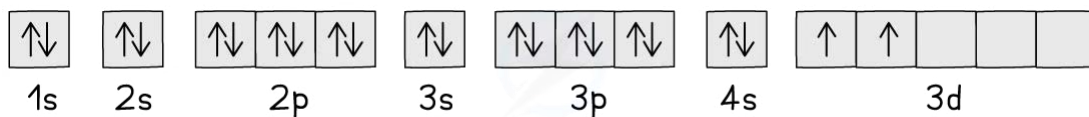
- ♦ The **ground state** is the **most stable electronic configuration** of an atom which has the **lowest amount of energy**
- ♦ This is achieved by filling the subshells of energy with the lowest energy first (1s)
- ♦ The order of the subshells in terms of increasing energy does **not** follow a regular pattern at $n = 3$ and higher



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The ground state of an atom is achieved by filling the lowest energy subshells first

- ♦ The **electron configuration** can also be represented using the **orbital spin diagrams**
- ♦ Each box represents an **atomic orbital**
- ♦ The boxes are arranged in order of **increasing** energy from lower to higher (i.e. starting from closest to the nucleus)
- ♦ The electrons are represented by opposite arrows to show the **spin** of the electrons
 - E.g. the box notation for titanium is shown below



The electrons in titanium are arranged in their orbitals as shown. Electrons occupy the lowest energy levels first before filling those with higher energy

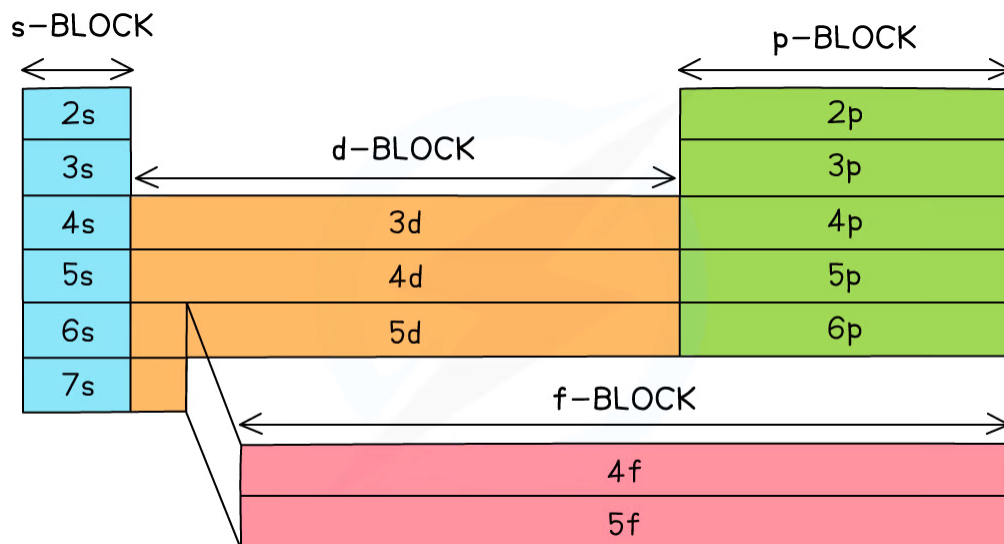
YOUR NOTES
↓

Electron Configuration of Atoms & Ions

YOUR NOTES



- Writing out the **electronic configuration** tells us how the electrons in an atom or ion are arranged in their shells, subshells and orbitals
- This can be done using the **full** electron configuration or the **shorthand** version
 - The **full** electron configuration describes the arrangement of all electrons from the 1s subshell up
 - The **shorthand** electron configuration includes using the symbol of the nearest preceding **noble gas** to account for however many electrons are in that noble gas, followed by the rest of the electron configuration
- **Ions** are formed when atoms **lose** or **gain** electrons
 - Negative ions are formed by **adding** electrons to the outer subshell
 - Positive ions are formed by **removing** electrons from the outer subshell
 - The transition metals **fill** the 4s subshell before the 3d subshell, but they also **lose** electrons from the 4s first rather than from the 3d subshell
- The Periodic Table is split up into four main blocks depending on their electronic configuration:
 - s block elements (valence electron(s) in s orbital)
 - p block elements (valence electron(s) in p orbital)
 - d block elements (valence electron(s) in d orbital)
 - f block elements (valence electron(s) in f orbital)



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The elements can be divided into four blocks according to their outer shell electron configuration

Exceptions to the Aufbau Principle

- Chromium and copper have the following electron configurations:
 - Cr is $[\text{Ar}] 3d^5 4s^1$ **not** $[\text{Ar}] 3d^4 4s^2$
 - Cu is $[\text{Ar}] 3d^{10} 4s^1$ **not** $[\text{Ar}] 3d^9 4s^2$

- This is because the $[\text{Ar}] 3d^5 4s^1$ and $[\text{Ar}] 3d^{10} 4s^1$ configurations are **energetically favourable**
- By promoting an electron from 4s to 3d, these atoms achieve a half full or full d-subshell, respectively

YOUR NOTES



? Worked Example

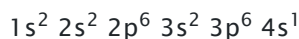
Write down the full and shorthand electron configuration of the following elements:

1. Potassium
2. Calcium
3. Gallium
4. Ca^{2+}

Answer:

Answer 1:

- Potassium has 19 electrons so the **full electronic configuration** is:

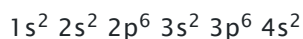


- The 4s orbital is lower in energy than the 3d subshell and is therefore filled first
- The nearest preceding noble gas to potassium is **argon** which accounts for 18 electrons so the **shorthand electron configuration** is:



Answer 2:

- Calcium has 20 electrons so the **full electronic configuration** is:



- The 4s orbital is lower in energy than the 3d subshell and is therefore filled first
- The **shorthand** version is $[\text{Ar}] 4s^2$ since argon is the nearest preceding noble gas to calcium which accounts for 18 electrons

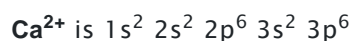
Answer 3:

- Gallium has 31 electrons so the **full electronic configuration** is:



Answer 4:

- If you ionise calcium and remove two of its outer electrons, the electronic configuration of the Ca^{2+} ion is identical to that of argon:



Ar is also $1s^2 2s^2 2p^6 3s^2 3p^6$



Exam Tip

Orbital spin diagrams can be drawn horizontally or vertically, going up or down the page – there is no hard and fast rule about this. The important thing is that you label the boxes and have the right number of electrons shown. The arrows you use for electrons can be full or half-headed arrows, but they must be in opposite directions in the same box.

YOUR NOTES



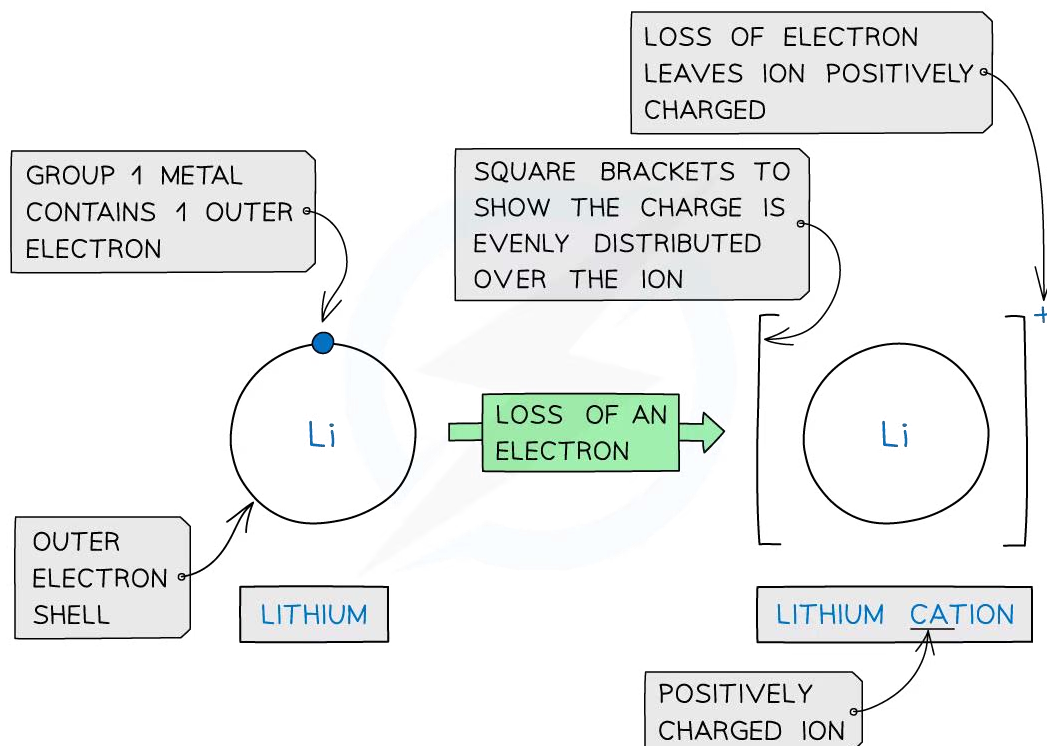
2.4.2 Ionic Bonding & Structure

YOUR NOTES



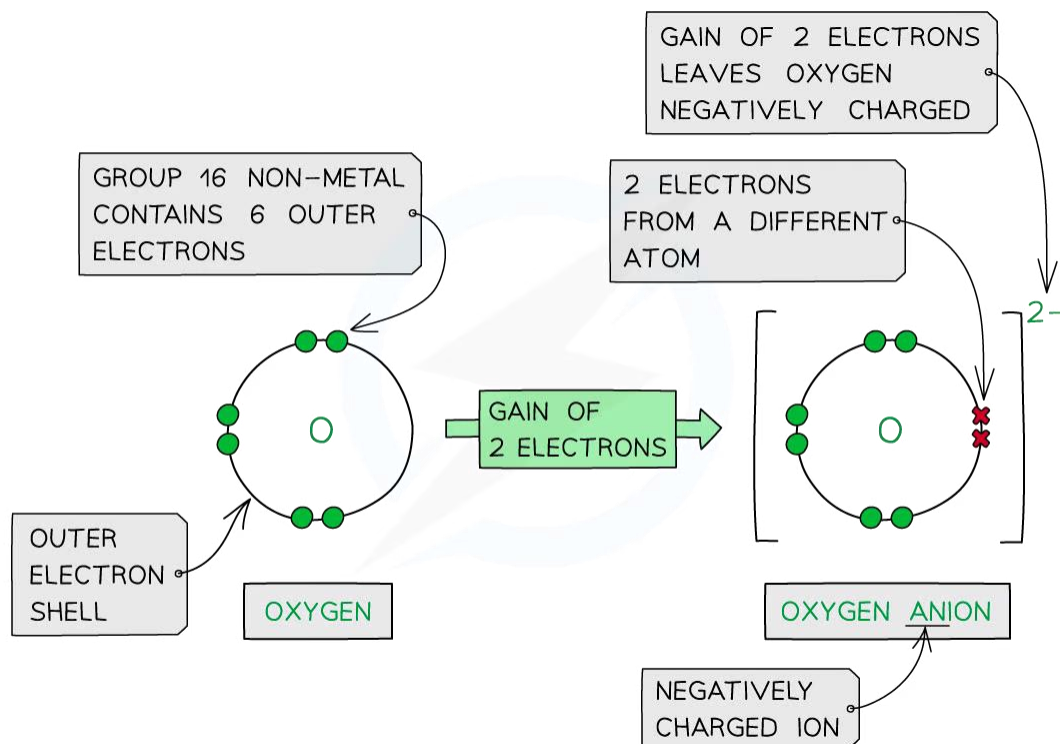
Ionic Bonding & Structure

- As a general rule, **metals** are on the **left** of the periodic table and **nonmetals** are on the **right-hand** side
- **Ionic bonding** involves the **transfer** of electrons from a **metallic** element to a **non-metallic** element
- Transferring electrons usually leaves the metal and the non-metal with a **full outer shell**
- Metals **lose** electrons from their valence shell forming **positively charged cations**
- Non-metal atoms **gain** electrons forming **negatively charged anions**
- Once the atoms become ions, their electronic configurations are the same as a noble gas
 - A potassium ion (K^+) has the same electronic configuration as argon: $[2,8,8]^+$
 - A chloride ion (Cl^-) also has the same electronic configuration as argon: $[2,8,8]^-$



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Forming cations by the removal of electrons from metals

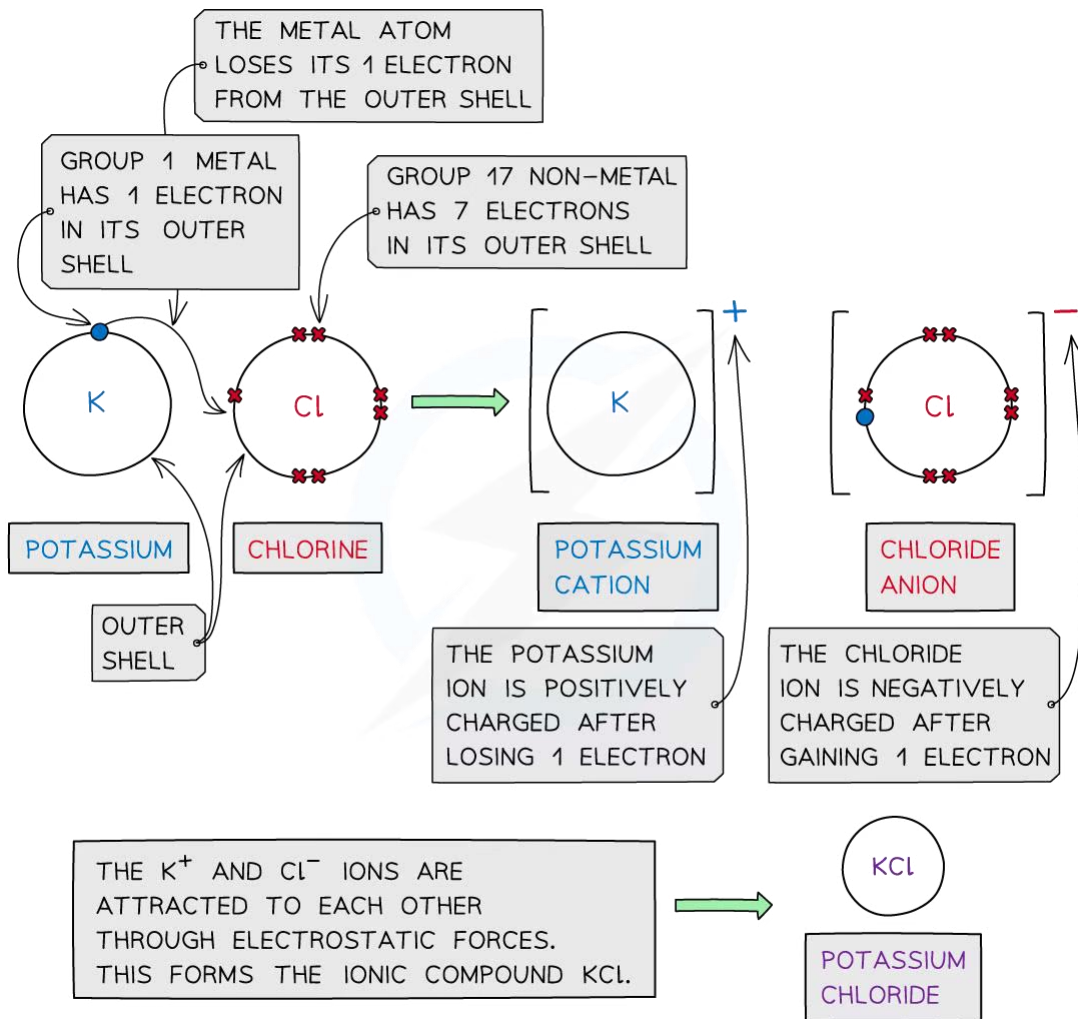


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Forming anions by the addition of electrons to nonmetals

- **Cations** and **anions** are oppositely charged and therefore attracted to each other
- **Electrostatic attractions** are formed between the oppositely charged ions to form **ionic compounds**
- The **ionic bond** is the **electrostatic attraction** formed **between the oppositely charged ions**, which occurs in all directions (this called **non-directional bonding**)
- This form of attraction is **very strong** and requires a **lot of energy** to overcome
 - This causes high melting points in ionic compounds

YOUR NOTES
↓



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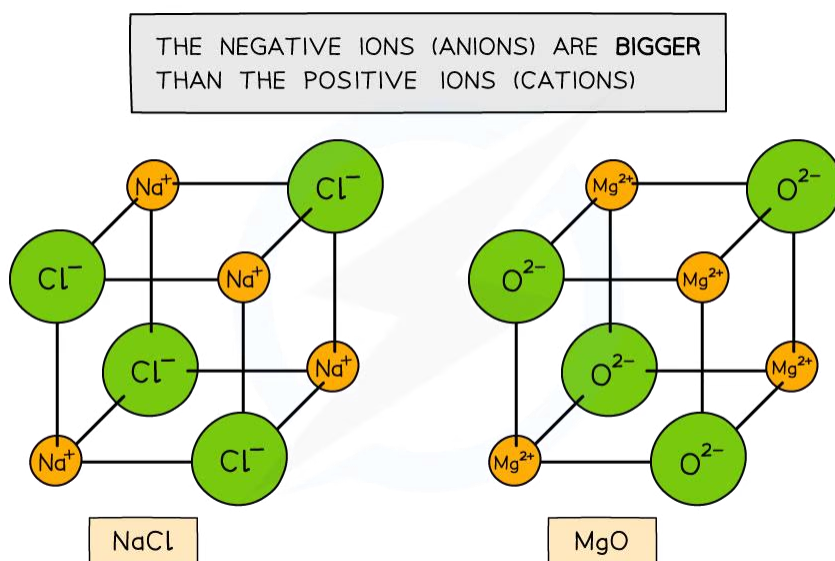
Cations and anions bond together using strong electrostatic forces, which require a lot of energy to overcome

Giant Ionic Lattices

- Most ionic, metallic and covalent solids are **crystalline lattices**
- The ions, atoms or molecules are arranged in a **regular and repeating arrangement**

Giant ionic lattices

- An **ionic bond** is an electrostatic force of attraction between a positively charged metal (**cation**) ion and a negatively charged non-metal (**anion**) ion
 - The metal becomes positively charged as it transfers electrons to the non-metal which then becomes negatively charged
 - When an ionic compound is formed, the attraction between the ions happens in all directions
- Ionic compounds are arranged in giant **ionic lattices** (also called **giant ionic structures**)
- The type of lattice formed depends on the sizes of the **positive** and **negative** ions which are arranged in an **alternating** fashion
 - The ionic lattice of MgO and NaCl are **cubic**

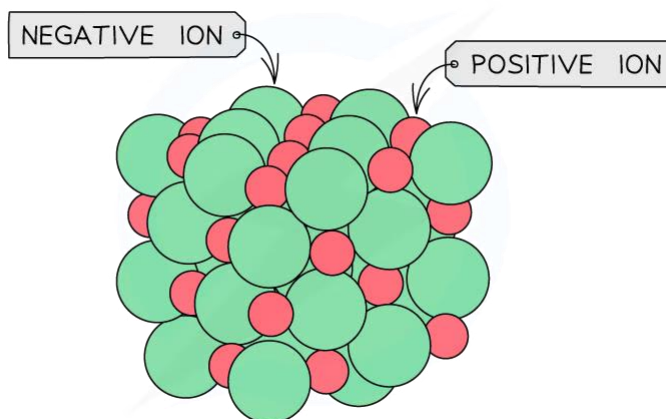


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Ionic lattices of the ionic compounds NaCl and MgO

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General ionic lattice which shows the actual packing of the ions

YOUR NOTES



Physical Properties of Ionic Compounds

- ♦ The giant ionic lattice and ionic bonding can be used to explain many of the physical properties of ionic compounds

Melting and boiling point

- ♦ Most ionic compounds are solids at room temperature
- ♦ This is because there isn't enough energy to overcome the strong electrostatic forces of attraction between the oppositely charged ions that make up the lattice
- ♦ Therefore, high temperatures are required to make an ionic compound melt or boil
- ♦ Melting (and boiling) points are also higher for lattices that contain ions with a greater ionic charge
 - For example, the melting point of sodium oxide, Na_2O , is 1405 K while the melting point of calcium oxide, CaO , is 2845 K
 - This is due to a stronger attraction between the ions – the size of the ions is not a factor here as the Na^+ and Ca^{2+} ions are a similar size

Solubility

- ♦ Many ionic compounds will dissolve in **polar** solvents, e.g. water
- ♦ Solubility is dependent on two main factors:
 1. Breaking down the ionic lattice
 2. The polar molecules attracting and surrounding the ions
- ♦ Polar molecules, such as water, can break down or disrupt the ionic lattice and surround each ion in solution
- ♦ The δ^+ end of the polar molecule can surround the negative anion
- ♦ The δ^- end of the polar molecule can surround the positive cation
- ♦ The solubility of an ionic compound depends on the relative strength of the electrostatic forces of attraction within the ionic lattice and the attractions between the ions and the polar molecule
- ♦ In general, the greater the ionic charge the less soluble an ionic compound is
 - For example, 356.9 g of sodium chloride, NaCl , will dissolve in one dm^3 of water while only 74.4 g of calcium chloride will dissolve in one dm^3 of water
 - This is a general rule though and there are many exceptions

Electrical conductivity

- ♦ Ionic compounds do not conduct electricity when solid
 - This is because the ions are in fixed positions within the solid lattice so there are no mobile charge carriers
- ♦ Ionic compounds can conduct electricity when they are molten or aqueous
 - This is because the ions are no longer in fixed positions as the lattice has broken down, therefore, the ions are free to act as mobile charge carriers

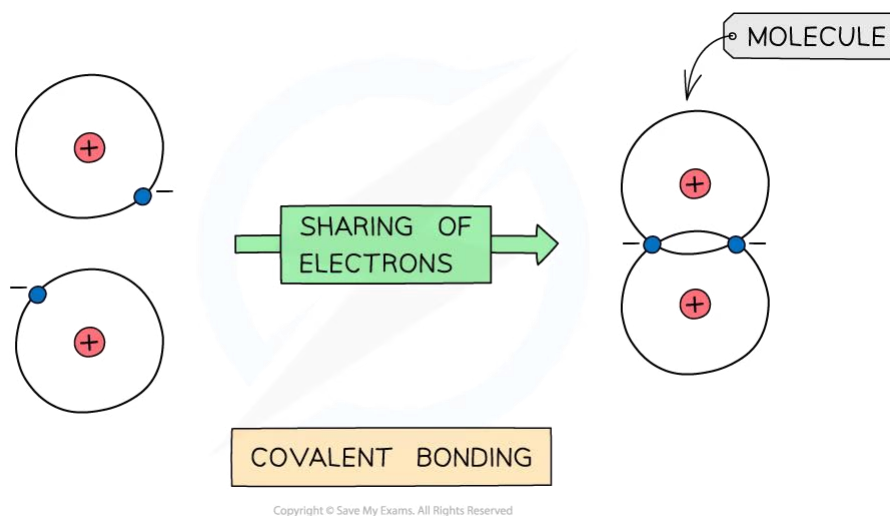
YOUR NOTES



2.4.3 Covalent Bonding & Structure

Covalent Bonds & Strength

- **Covalent** bonding occurs between two **non-metals**
- A covalent bond involves the **electrostatic attraction** between nuclei of two atoms and the bonding electrons of their outer shells
- **No electrons** are **transferred** but only **shared** in this type of bonding



The positive nucleus of each atom has an attraction for the bonding electrons shared in the covalent bond

- **Non-metals** are able to **share** pairs of electrons to form different types of covalent bonds
- Sharing electrons in the covalent bond allows each of the 2 atoms to achieve an electron configuration similar to a noble gas
 - This makes each atom more stable

Covalent Bonds & Shared Electrons Table

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| Type of covalent bond | Number of electrons shared |
|-----------------------|----------------------------|
| Single (C – C) | 2 |
| Double (C = C) | 4 |
| Triple (C ≡ C) | 6 |

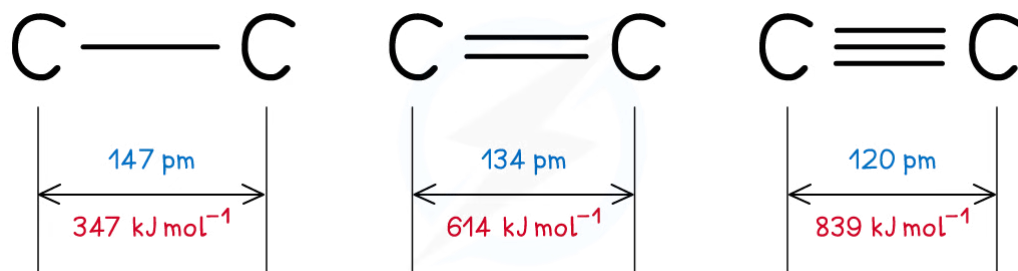
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Bond energy

- The **bond energy** is the energy required to **break** one mole of a particular covalent bond in the gaseous states
 - Bond energy has units of kJ mol^{-1}
- The **larger** the bond energy, the **stronger** the covalent bond is
- **Average bond enthalpy** is also used as a measurement of the strength of a covalent bond
 - The average bond enthalpy term is the average amount of energy needed to break a specific type of bond, measured over a wide variety of different molecules

Bond length

- The **bond length** is the **internuclear distance of two covalently bonded atoms**
 - It is the distance from the nucleus of one atom to another atom which forms the covalent bond
- The **greater** the forces of attraction between electrons and nuclei, the more the atoms are pulled closer to each other
- This **decreases** the **bond length** of a molecule and **increases** the **strength** of the covalent bond
- **Triple bonds** are the **shortest** and **strongest** covalent bonds due to the large electron density between the nuclei of the two atoms
- This increase the forces of attraction between the electrons and nuclei of the atoms
- As a result of this, the atoms are pulled closer together causing a shorter bond length
- The increased forces of attraction also means that the covalent bond is **stronger**



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Triple bonds are the shortest covalent bonds and therefore the strongest ones



Exam Tip

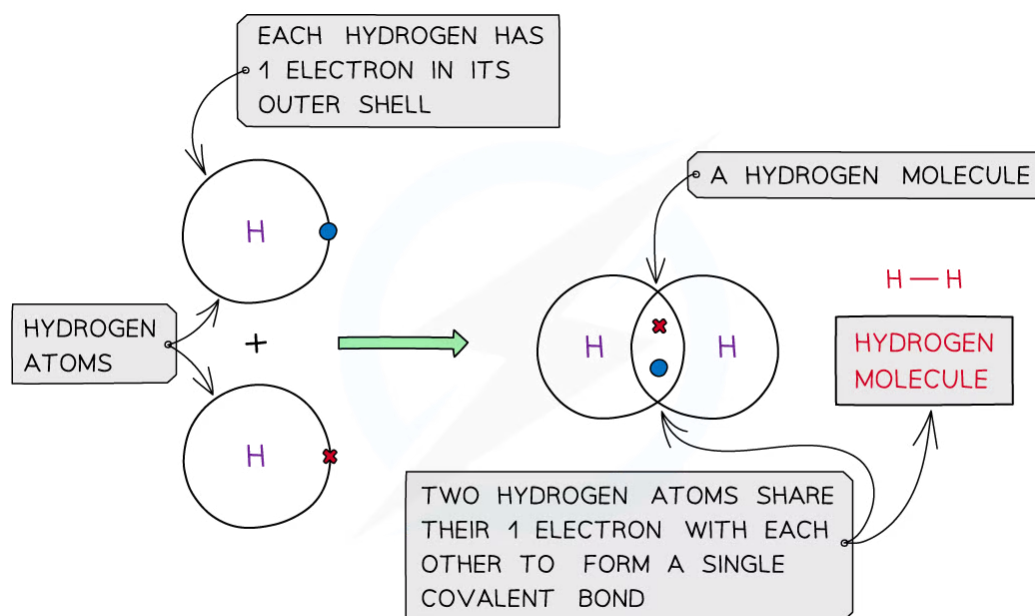
The values for bond length and bond enthalpy are often different depending on which source they are taken from

Dot & cross diagrams

- **Dot and cross diagrams** are used to represent covalent bonding
- They show just the **outer shell** of the atoms involved
- To differentiate between the two atoms involved, **dots** for electrons of one atom and **crosses** for electrons of the other atom are used
- Electrons are shown in **pairs** on dot-and-cross diagrams

Single covalent bonding

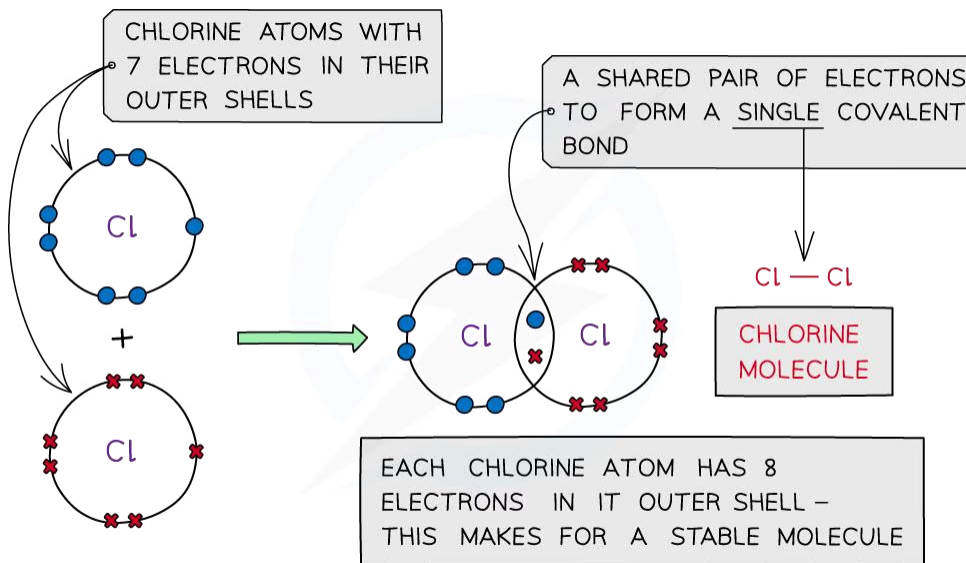
Hydrogen, H₂



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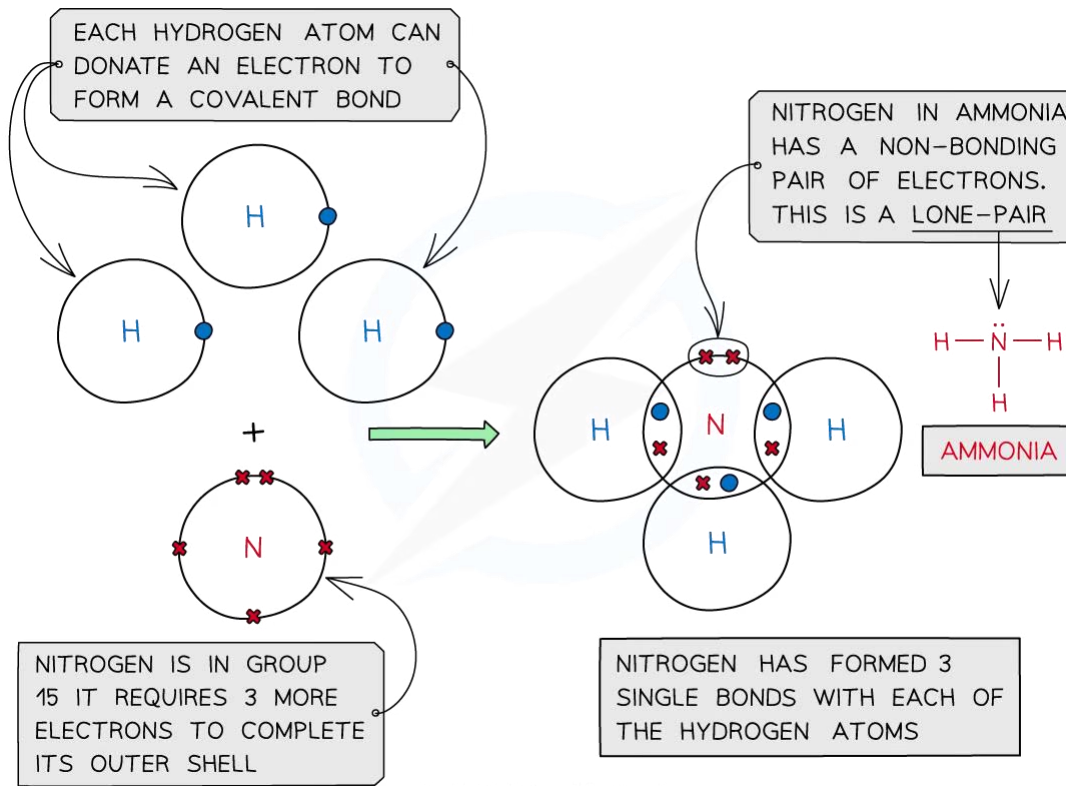
Covalent bonding in hydrogen

Chlorine, Cl₂



Covalent bonding in chlorine

Ammonia, NH₃

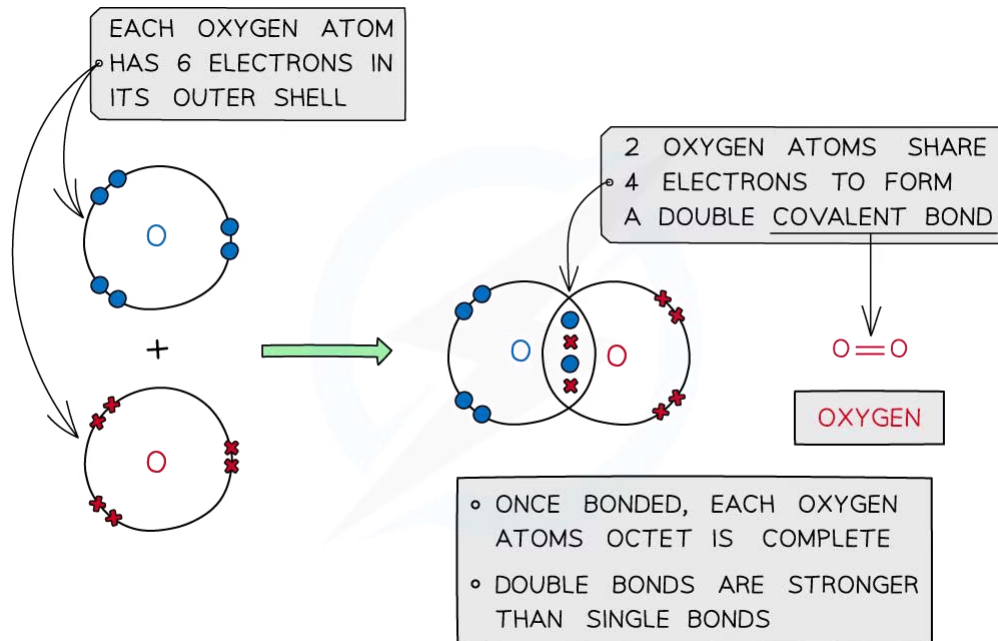


Covalent bonding in ammonia

Double covalent bonding

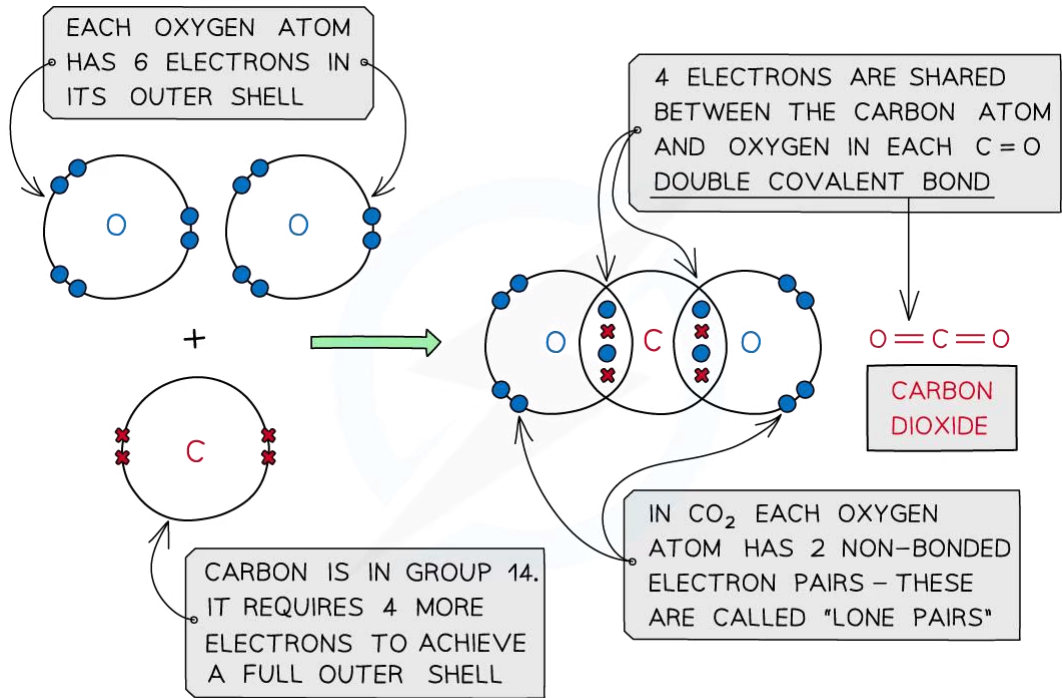
YOUR NOTES
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Oxygen, O₂



Covalent bonding in oxygen

Carbon dioxide, CO₂



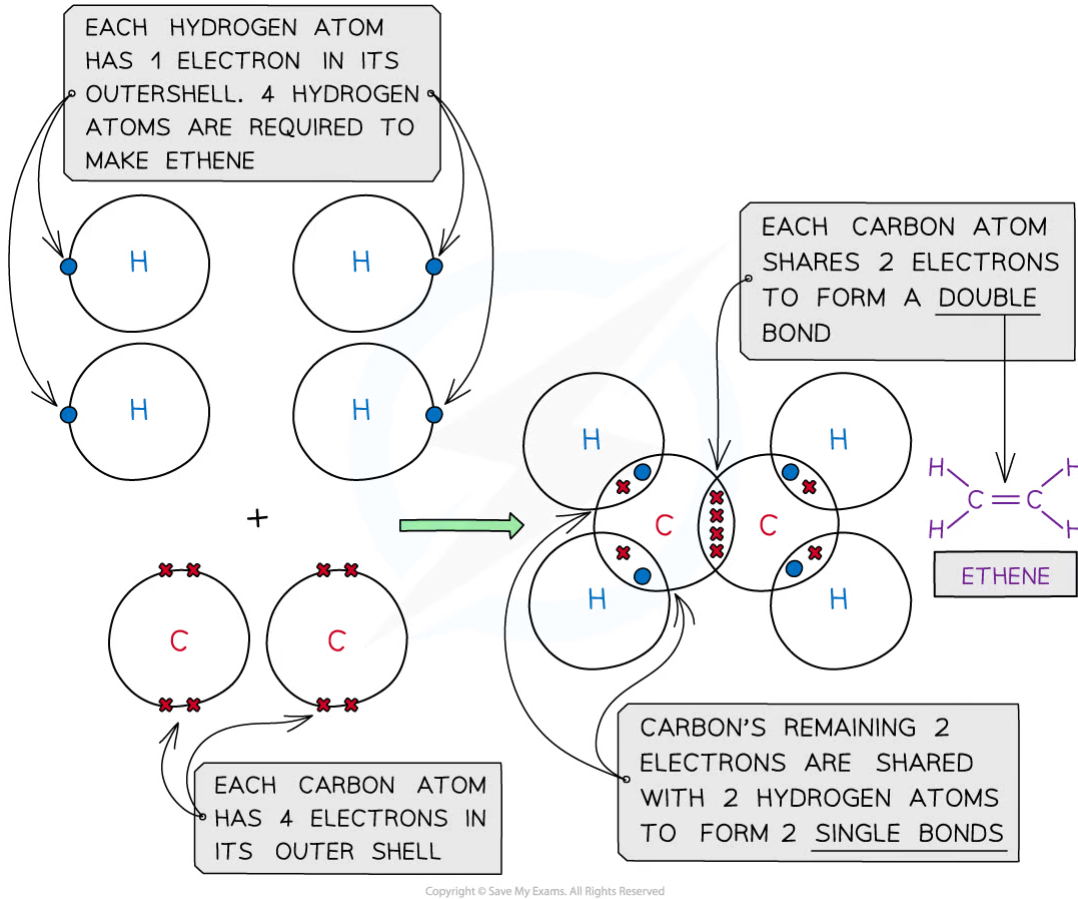
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Covalent bonding in carbon dioxide

Ethene, C₂H₄

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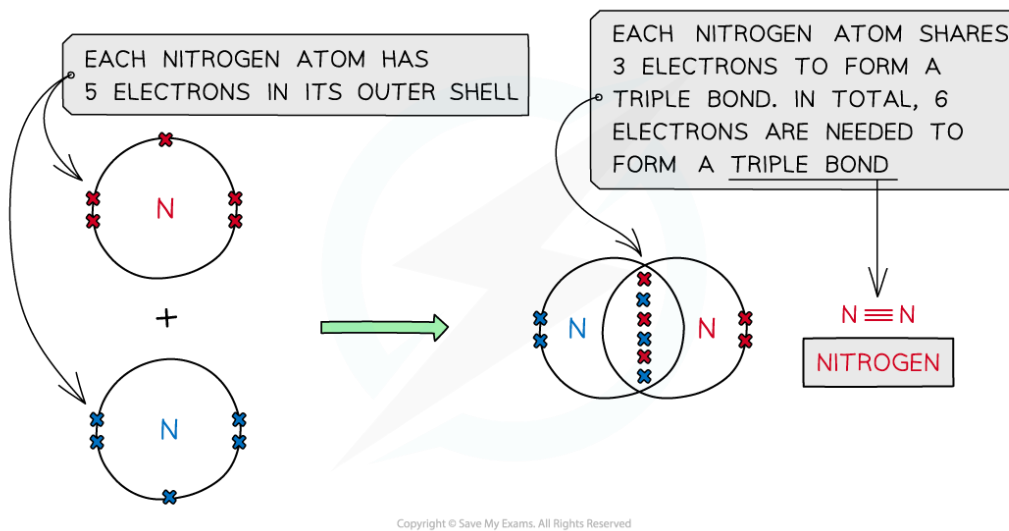




Covalent bonding in ethene

Triple covalent bonding

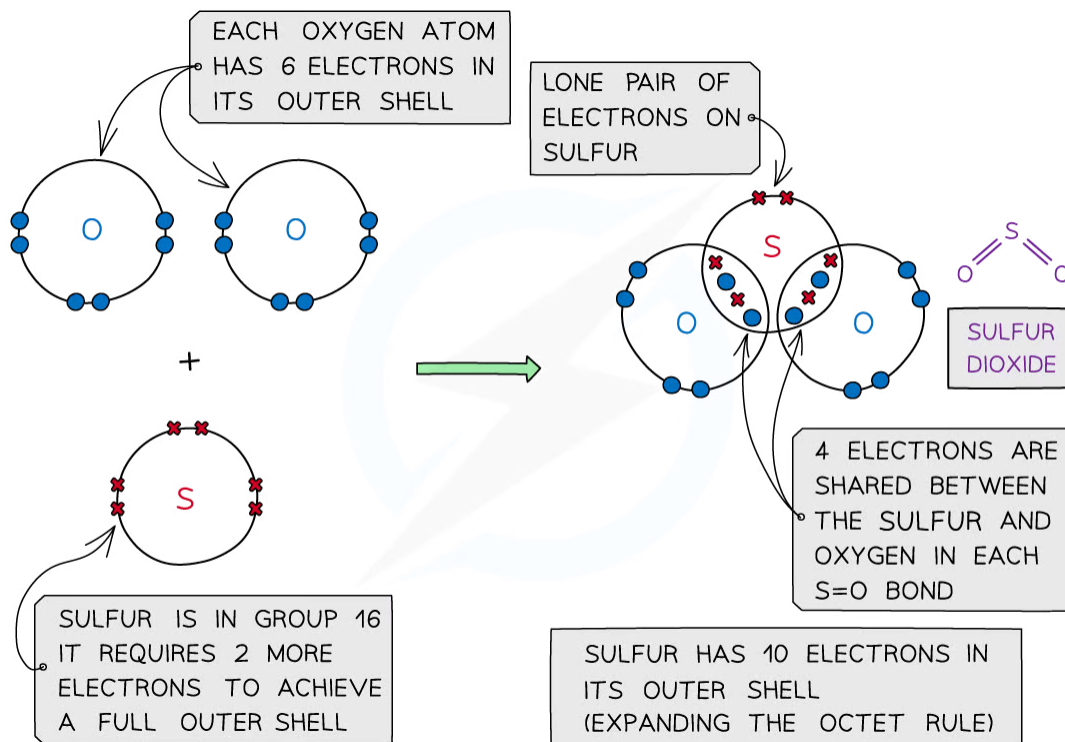
Nitrogen, N₂



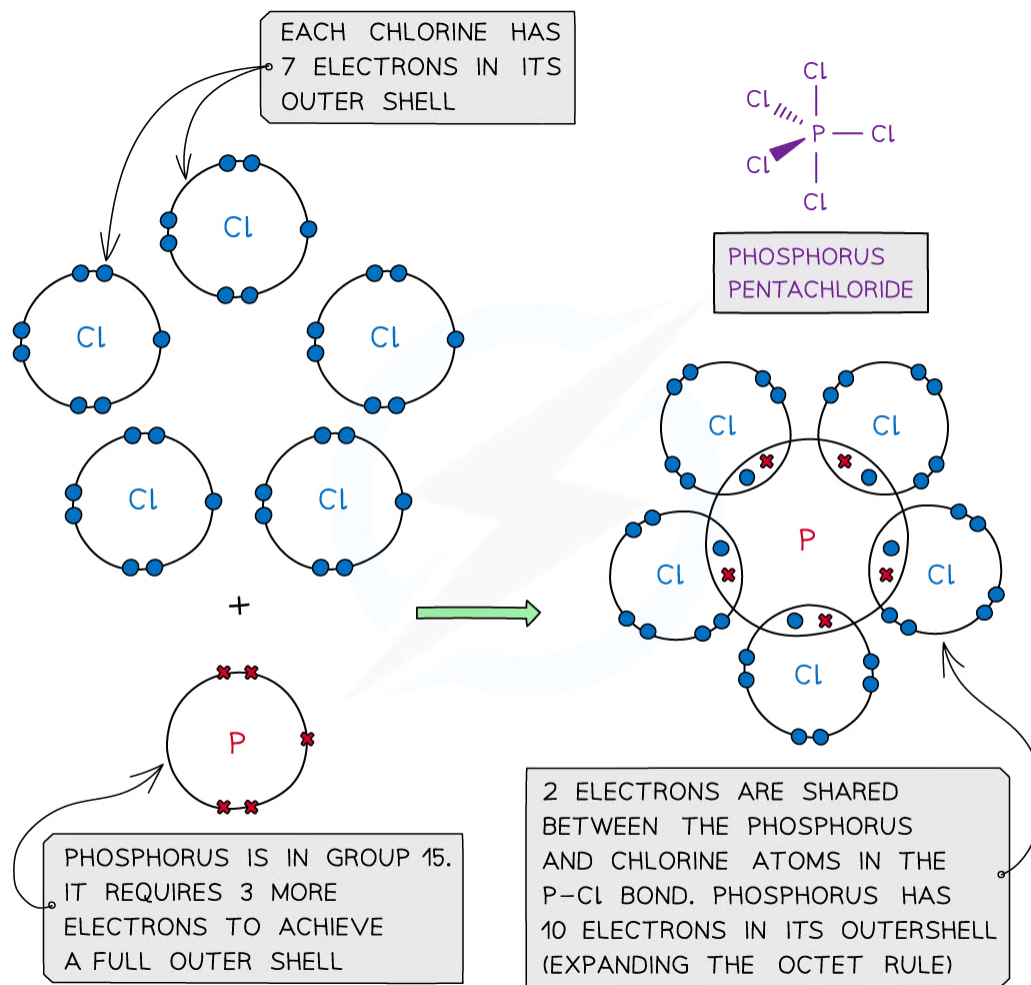
Covalent bonding in nitrogen

- In some instances, the central atom of a covalently bonded molecule can accommodate **more** or **less** than 8 electrons in its outer shell
- Being able to accommodate **more** than 8 electrons in the outer shell is known as '**expanding the octet rule**'
- Some examples of this occurring can be seen with period 3 elements

YOUR NOTES

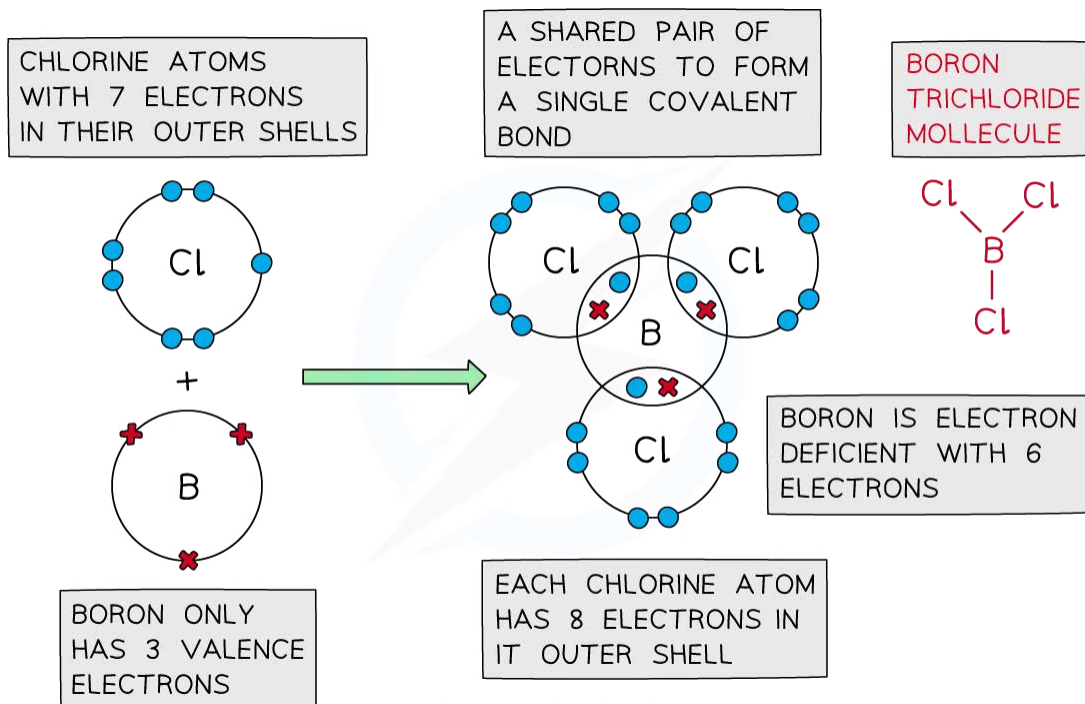


Sulfur dioxide, SO_2 – dot and cross diagram



Phosphorus pentachloride, PCl_5 – dot and cross diagram

- Accommodating **less** than 8 electrons in the outer shell means that the central atom is **'electron deficient'**



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Boron trichloride, BCl_3 - dot and cross diagram



Exam Tip

Covalent bonding takes place between nonmetal atoms. Remember to use the periodic table to decide how many electrons are in the outer shell of a nonmetal atom.

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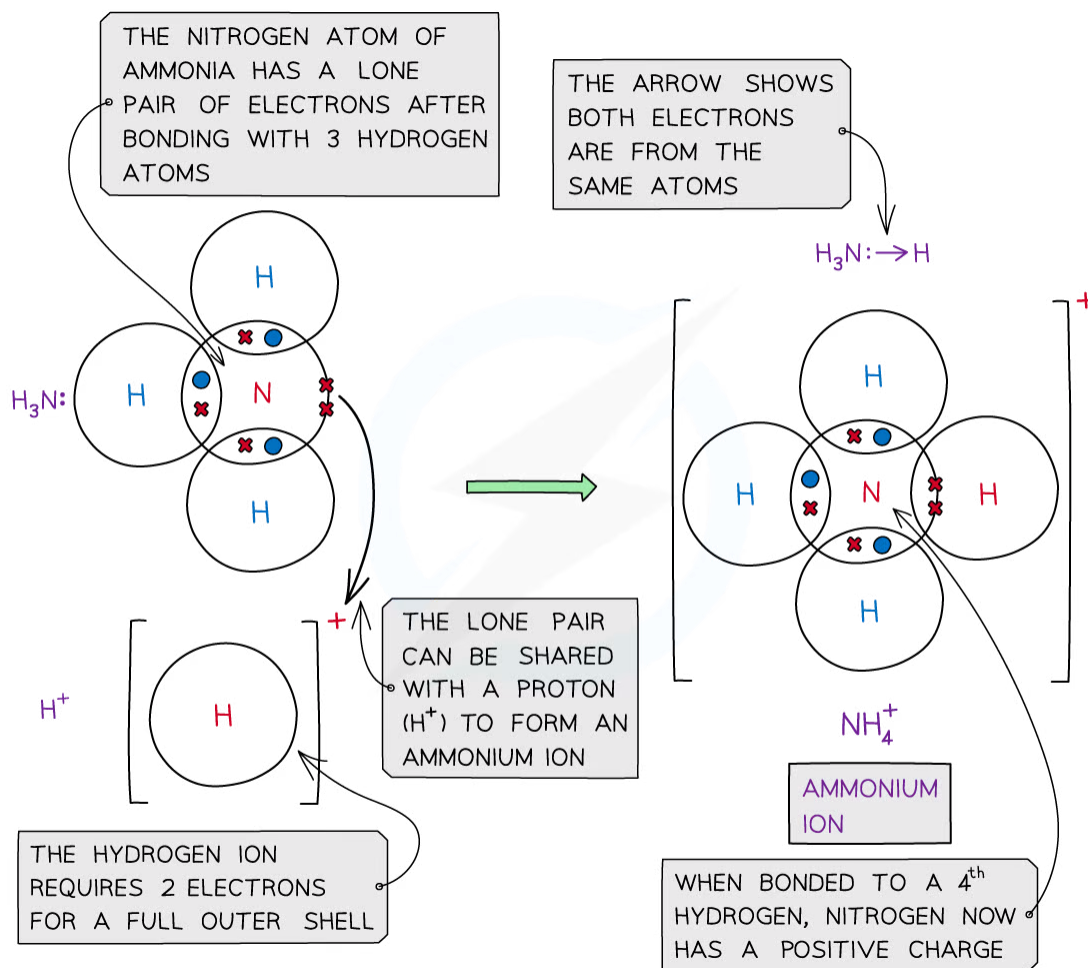


Dative Covalent / Coordinate Bonding

YOUR NOTES



- In **simple covalent bonds**, the two atoms involved share electrons
- Some molecules have a **lone pair** of electrons that can be donated to form a bond with an **electron-deficient** atom
 - An electron-deficient atom is an atom that has an **unfilled outer orbital**
- So **both electrons** are from the **same atom**
- This type of bonding is called **dative covalent bonding** or **coordinate bonding**
- An example with a dative bond is in an **ammonium ion**
 - The hydrogen ion, H^+ is **electron-deficient** and has space for two electrons in its shell
 - The nitrogen atom in ammonia has a lone pair of electrons which it can donate to the hydrogen ion to form a dative covalent bond



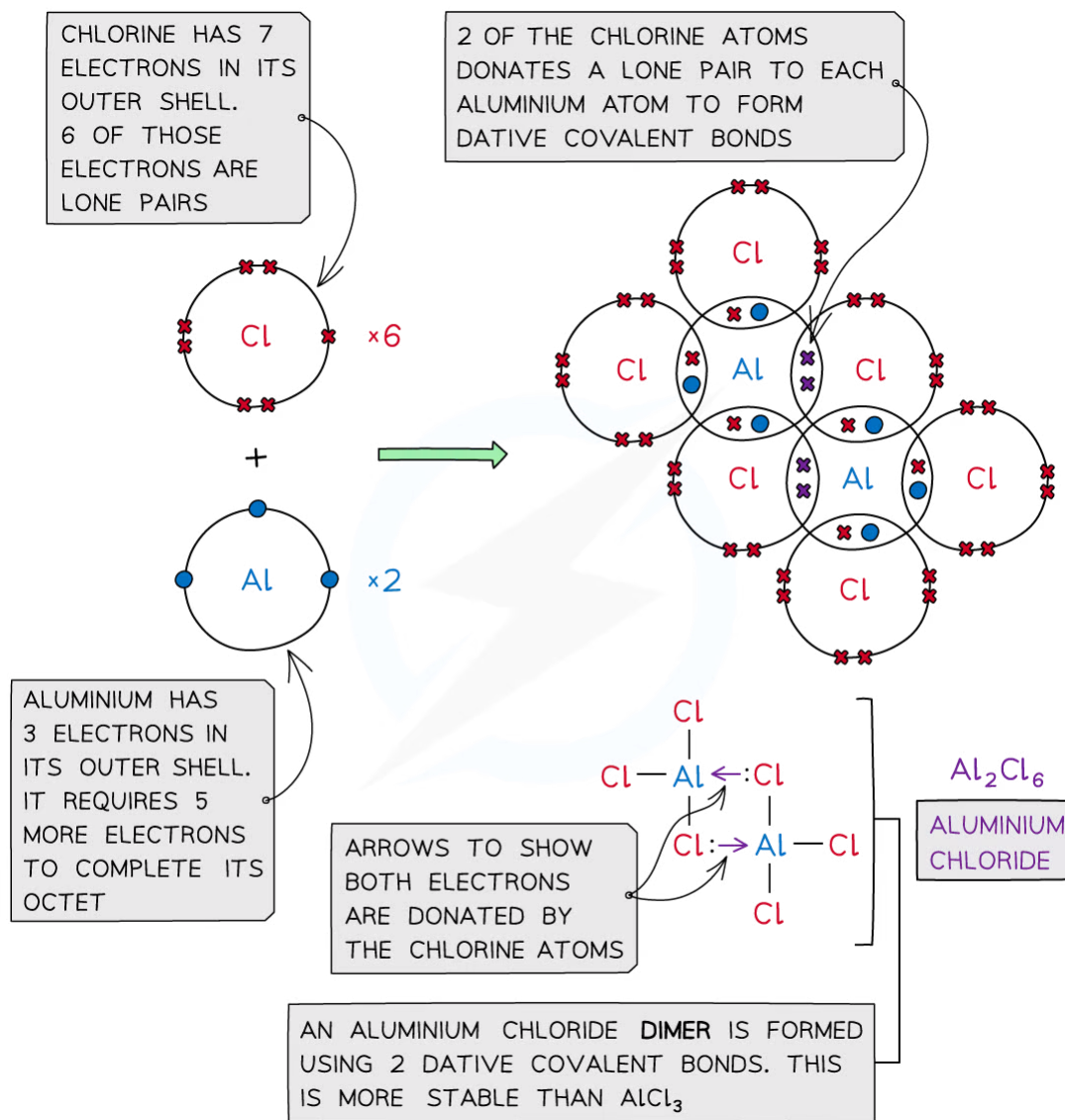
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Ammonia (NH_3) can donate a lone pair to an electron-deficient proton (H^+) to form a charged ammonium ion (NH_4^+)

- **Aluminium chloride** is also formed using dative covalent bonding



- ♦ At **high temperatures** aluminium chloride can exist as a **monomer** (AlCl_3)
 - The molecule is electron-deficient and needs two electrons to complete the aluminium atom's outer shell
- ♦ At **lower temperatures** the two molecules of AlCl_3 join together to form a dimer (Al_2Cl_6)
 - The molecules combine because lone pairs of electrons on two of the chlorine atoms form **two coordinate bonds** with the aluminium atoms



Aluminium chloride is also formed with a dative covalent bond in which two of the chlorine atoms donate their lone pairs to each of the aluminium atoms to form a dimer



Exam Tip

In dative covalent bonding, both electrons in the covalent bond are shared by one atom. A dative covalent bond is drawn using an arrow from the donated pair of electrons to the electron-deficient atom.

YOUR NOTES

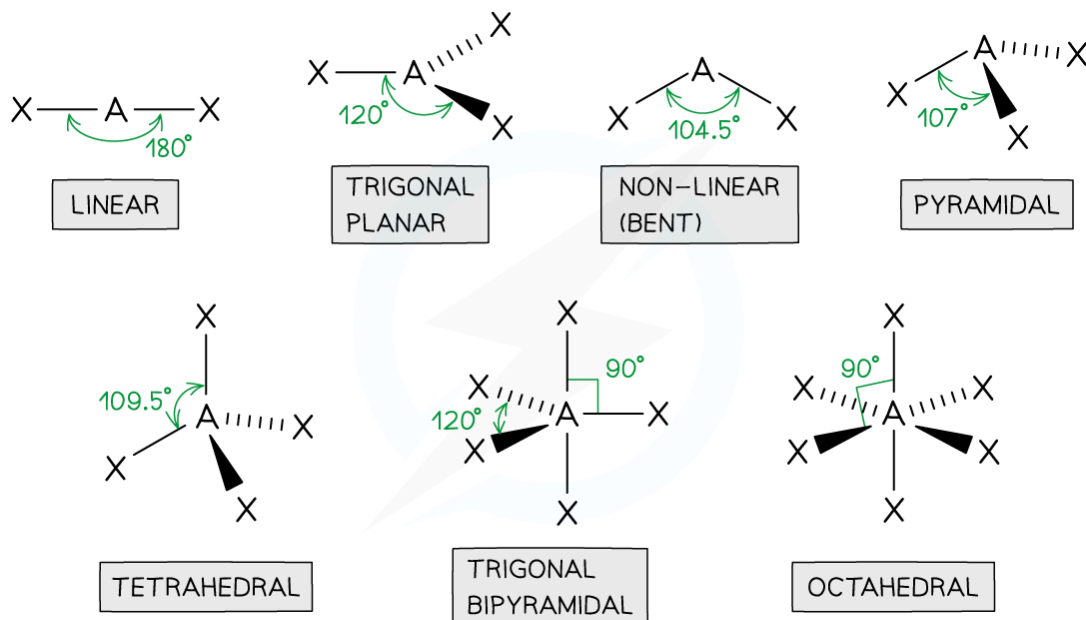


2.5 The Shapes of Simple Molecules & Ions

2.5.1 The Shapes of Simple Molecules & Ions

Shapes & Bond Angles

- Molecules can adapt the following shapes and bond angles:



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Molecules of different shapes can adapt with their corresponding bond angles

Examples

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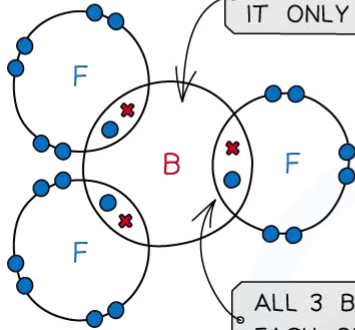
YOUR NOTES



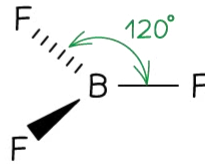
TRIGONAL PLANAR

BF_3 (120°)

BORON IS ELECTRON DEFICIENT AS IT ONLY HAS 6 ELECTRONS

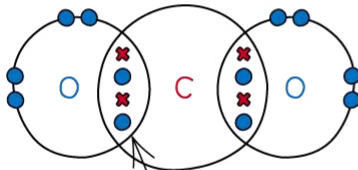


ALL 3 BONDING PAIR ELECTRONS REPEL EACH OTHER EQUALLY

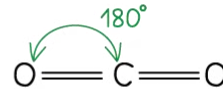


LINEAR

CO_2 (180°)



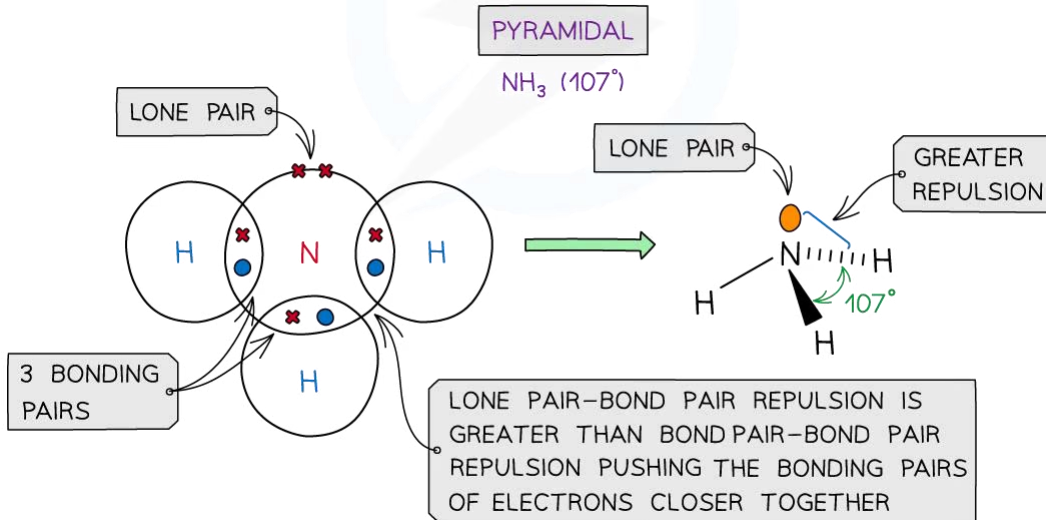
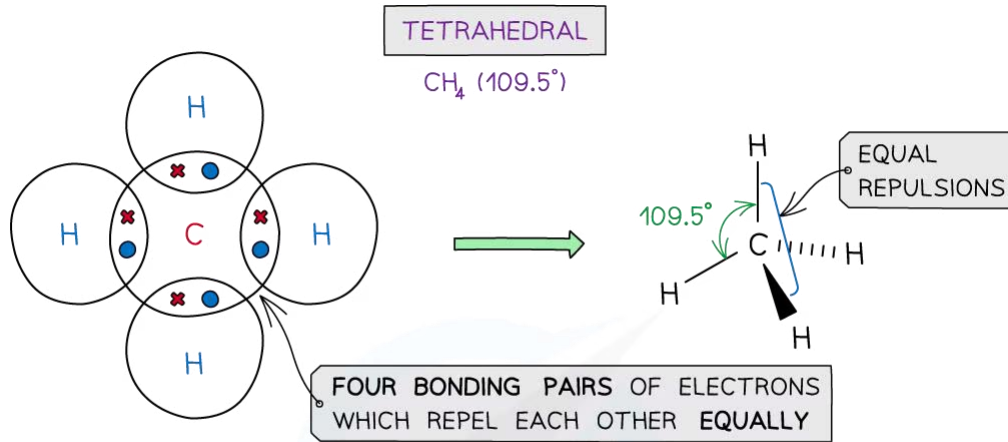
THESE 4 ELECTRONS IN THE $\text{C}=\text{O}$ BOND REPEL EACH OTHER IN A SIMILAR WAY TO TWO ELECTRONS IN A SINGLE BOND



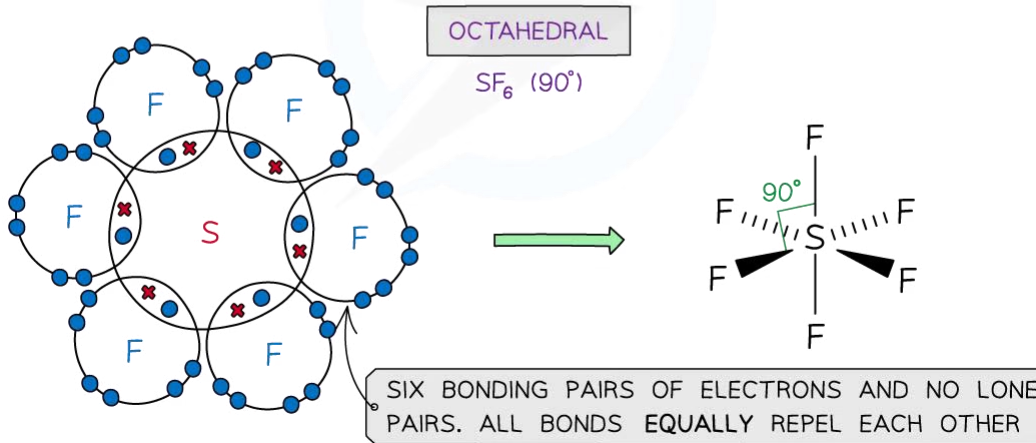
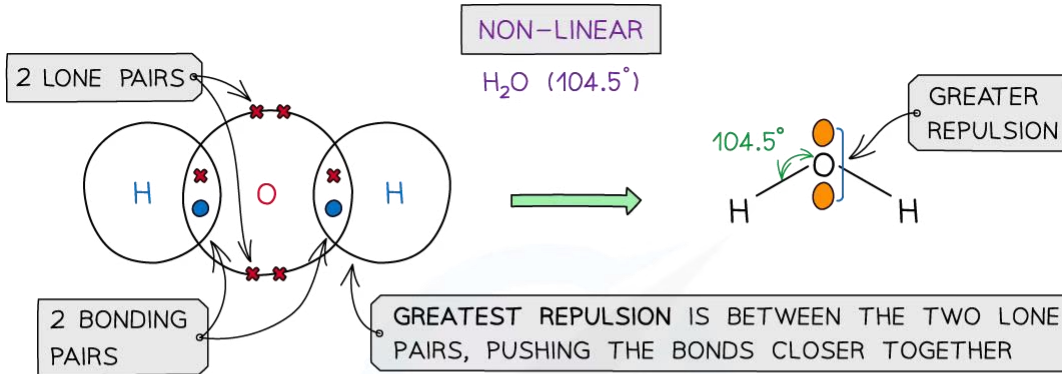
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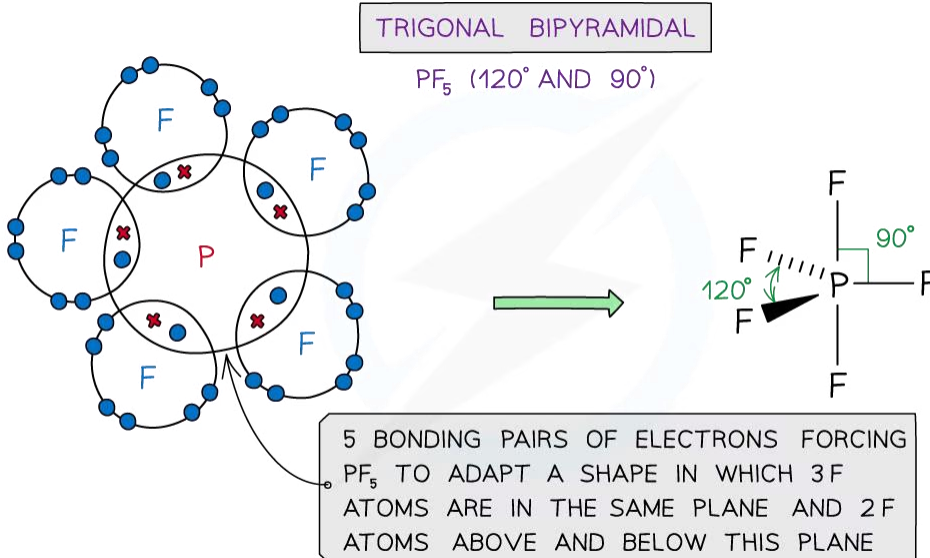
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Examples of molecules with different shapes and bond angles



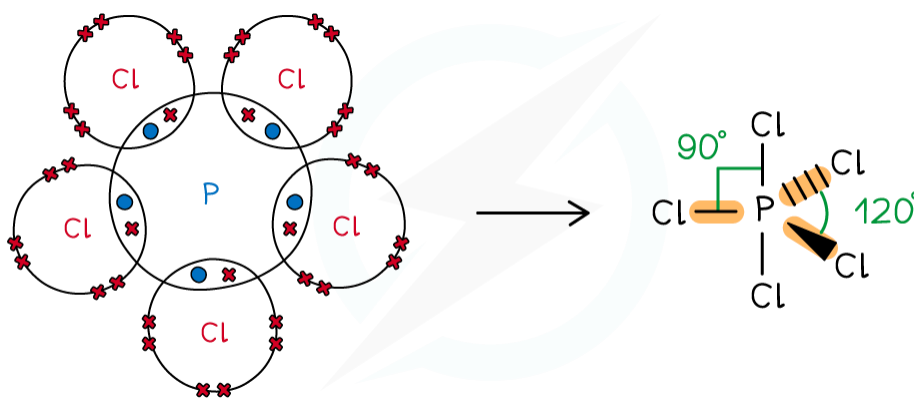
? Worked Example

Draw the shape of the following molecules:

1. Phosphorus(V) chloride
2. $\text{N}(\text{CH}_3)_3$
3. CCl_4

Answer 1:

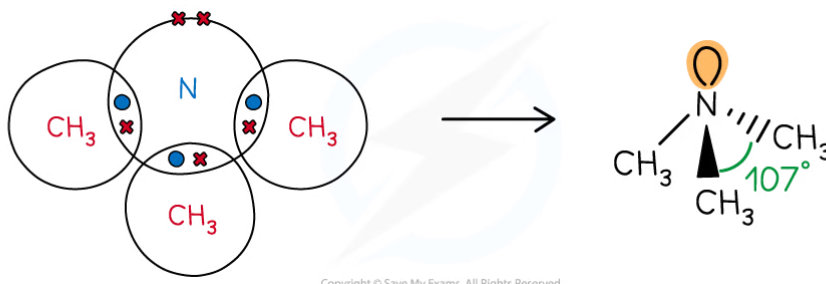
- Phosphorus is in group 15, so has 5 valence electrons; Cl is in group 17, so has 17 valence electrons
- All 5 electrons are used to form covalent bonds with Cl and there are no lone pairs
- This gives a **trigonal** (or **triangular**) **bipyramidal** shape:



Phosphorus pentachloride or phosphorus (V) chloride

Answer 2:

- Nitrogen is in group 15, so has 5 valence electrons; carbon is in group 14, so has 4 valence electrons, 3 of which are already used in the covalent bonds with hydrogen
- Three of the valence electrons in N are used to form bonding pairs, so there is one lone pair left
- $\text{N}(\text{CH}_3)_3$ has a **triangular pyramid** shape:

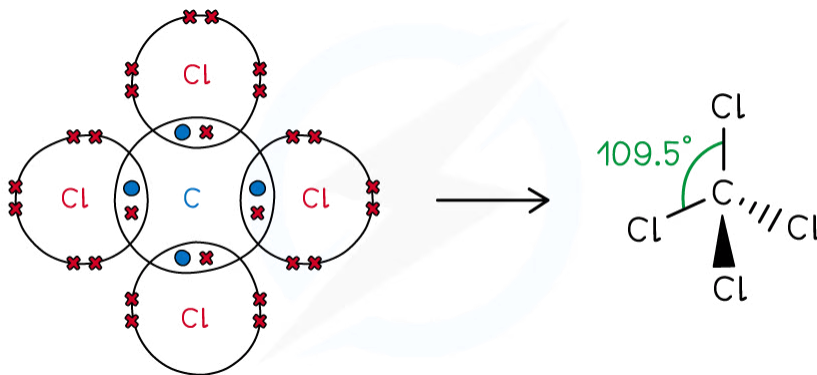


Trimethylamine



Answer 3:

- Carbon is in group 14, so has 4 valence electrons; chlorine is in group 17, so has 7 valence electrons
- All four valence electrons are used to bond with chlorine and there are no lone pairs
- The shape of CCl_4 is **tetrahedral**



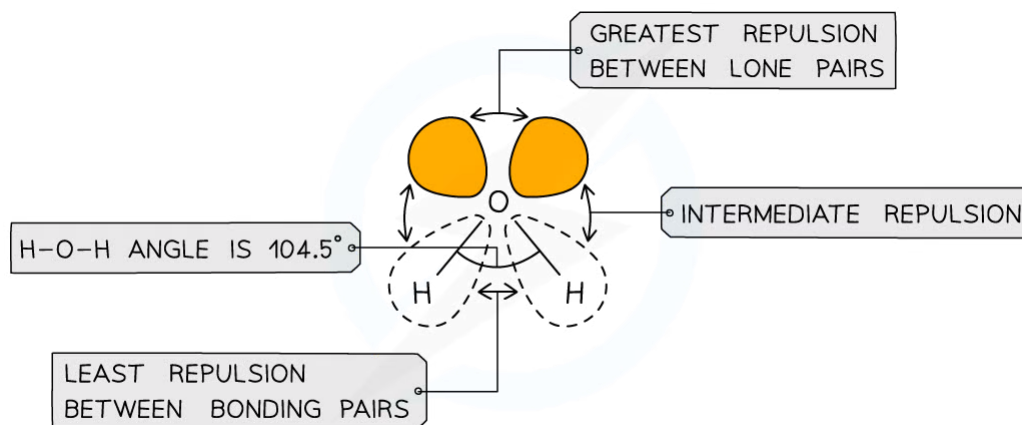
Tetrachloromethane

Electron Pair Repulsion

YOUR NOTES



- ♦ The **valence shell electron pair repulsion theory** (VSEPR) predicts the shape and bond angles of molecules
- ♦ Electrons are **negatively charged** and will repel other electrons when close to each other
- ♦ In a molecule, the **bonding pairs of electrons** will repel other electrons around the **central atom** forcing the molecule to adopt a shape in which these **repulsive forces** are minimised
- ♦ When determining the **shape** and **bond** angles of a molecule, the following VSEPR rules should be considered:
 - Valence shell electrons are those electrons that are found in the outer shell
 - Electron pairs repel each other as they have the same charge
 - Lone pair electrons repel each other more than bonded pairs
 - Repulsion between multiple and single bonds is treated the same as for repulsion between single bonds
 - Repulsion between pairs of double bonds are greater
 - The most stable shape is adopted to minimize the repulsion forces
- ♦ Different types of electron pairs have different repulsive forces
 - Lone pairs of electrons have a more concentrated electron charge cloud than bonding pairs of electrons
 - The cloud charges are wider and closer to the central atom's nucleus
 - The order of repulsion is therefore: lone pair - lone pair > lone pair - bond pair > bond pair - bond pair



Different types of electron pairs have different repulsive forces

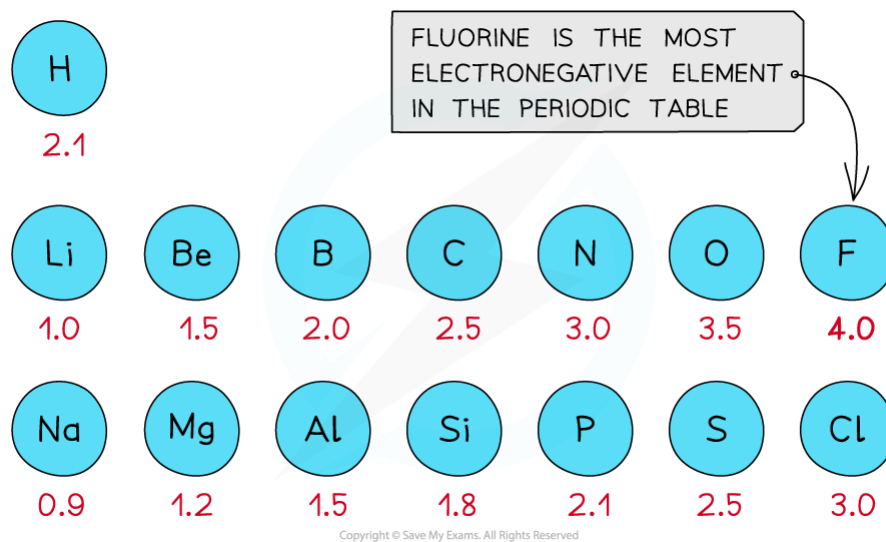
2.5.2 Electronegativity & Bond Polarity

YOUR NOTES



Electronegativity Trends

- Electronegativity is the power of an atom to attract the pair of electrons in a covalent bond towards itself
- The electron distribution in a covalent bond between elements with different electronegativities will be unsymmetrical
- This phenomenon arises from the ability of the positive nucleus to attract the negatively charged electrons, in the outer shells, towards itself
- The **Pauling scale** is used to assign a value of electronegativity for each atom



First three rows of the periodic table showing electronegativity values

- Fluorine is the most electronegative atom on the Periodic Table, with a value of 4.0 on the Pauling Scale
- It is best at attracting electrons towards itself when covalently bonded to another atom
- There are various factors which will affect the electronegativity of an element

Nuclear charge

- Attraction exists between the positively charged protons in the nucleus and negatively charged electrons found in the energy levels of an atom
- An **increase** in the number of **protons** leads to an **increase** in **nuclear attraction** for the electrons in the outer shells
- Therefore, an increased nuclear charge results in an increased electronegativity

Atomic radius

- The atomic radius is the distance between the nucleus and electrons in the outermost shell
- Electrons closer to the nucleus are more strongly attracted towards its positive nucleus

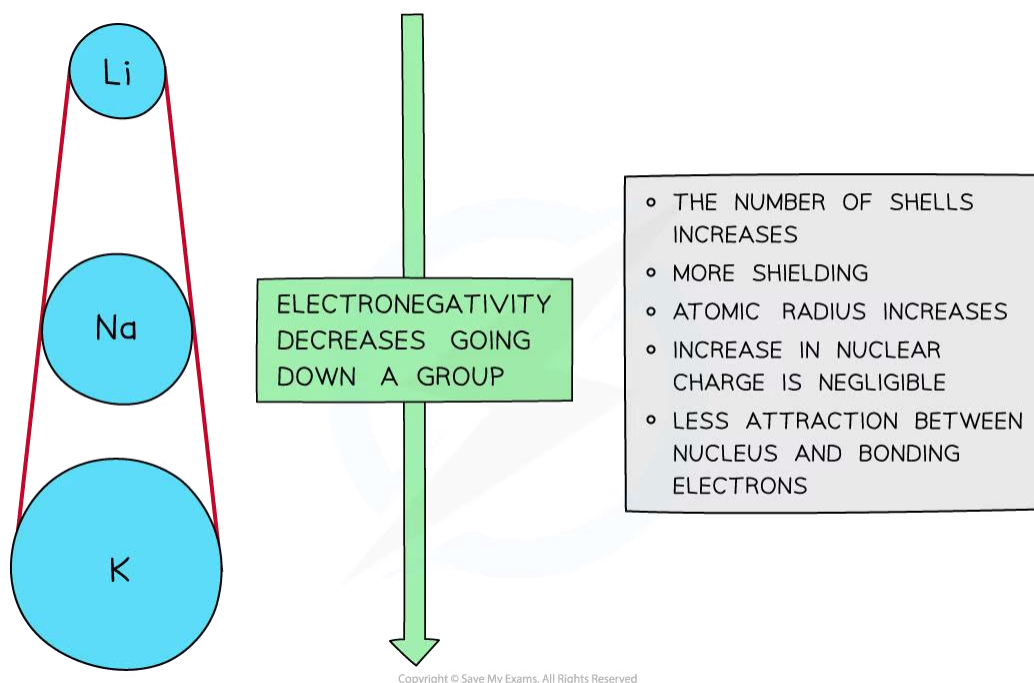
- Those electrons **further away** from the nucleus are **less strongly** attracted towards the **nucleus**
- Therefore, an increased atomic radius results in a decreased electronegativity

Shielding

- Filled energy levels can shield (mask) the effect of the nuclear charge causing the outer electrons to be **less attracted** to the nucleus
 - Sodium (period 3, group 1) has higher electronegativity than caesium (period 6, group 1) as it has fewer shells and therefore the outer electrons experience less shielding than in caesium
- Thus, an increased number of inner shells and subshells will result in a decreased electronegativity
- Electronegativity varies across periods and down the groups of the periodic table

Down a group

- There is a **decrease** in electronegativity going down the group
- The nuclear charge increases as more protons are being added to the nucleus
- However, each element has an extra filled electron shell, which increases shielding
- The addition of the extra shells increases the distance between the nucleus and the outer electrons resulting in larger atomic radii
- Overall, there is decrease in attraction between the nucleus and outer bonding electrons



Electronegativity decreases going down the groups of the periodic table

Across a period

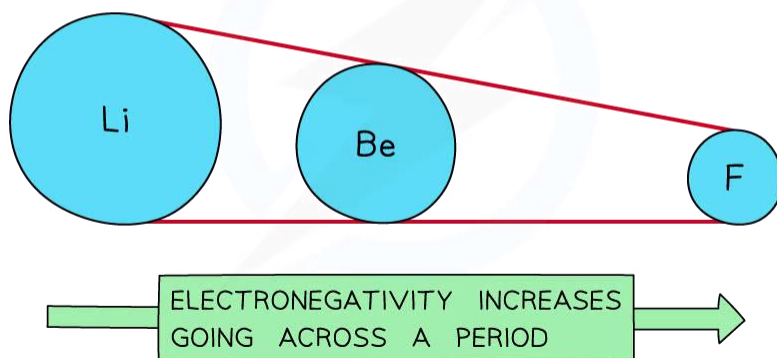
- Electronegativity **increases** across a period

YOUR NOTES



- The nuclear charge increases with the addition of protons to the nucleus
- Shielding remains relatively constant across the period as no new shells are being added to the atoms
- The nucleus has an increasingly strong attraction for the bonding pair of electrons of atoms across the period of the periodic table
- This results in smaller atomic radii

- NUCLEAR CHARGE INCREASES
- ATOMIC RADIUS DECREASES
- GREATER ATTRACTION BETWEEN NUCLEUS AND BONDING ELECTRONS



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Electronegativity increases going across the periods of the Periodic Table

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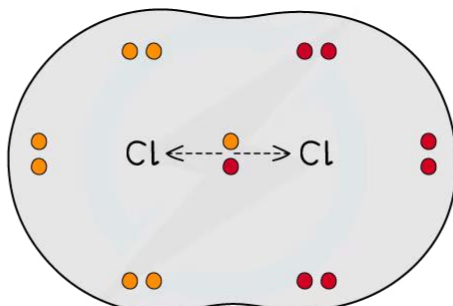




Bond Polarity

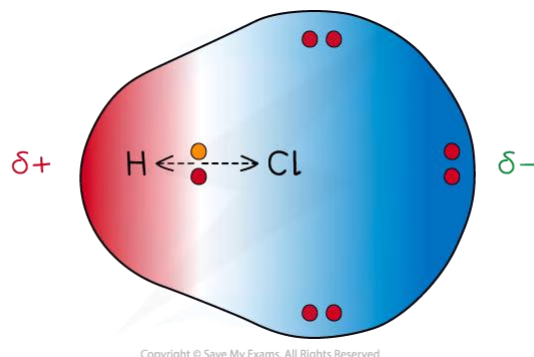
Polarity

- When two atoms in a covalent bond have the **same electronegativity** the covalent bond is **nonpolar**



The two chlorine atoms have the same electronegativities so the bonding electrons are shared equally between the two atoms

- When two atoms in a covalent bond have **different electronegativities** the covalent bond is **polar** and the electrons will be drawn towards the **more electronegative** atom
- As a result of this:
 - The negative charge centre and positive charge centre do not **coincide** with each other
 - This means that the **electron distribution** is **asymmetric**
 - The **less electronegative** atom gets a partial charge of $\delta+$ (**delta positive**)
 - The **more electronegative** atom gets a partial charge of $\delta-$ (**delta negative**)
- The greater the difference in **electronegativity** the more polar the bond becomes



Cl has a greater electronegativity than H causing the electrons to be more attracted towards the Cl atom which becomes delta negative and the H delta positive

Dipole moment

- The **dipole moment** is a measure of how **polar** a bond is
- The **direction** of the dipole moment is shown by the following sign in which the **arrow** points to the **partially negatively charged end** of the dipole:

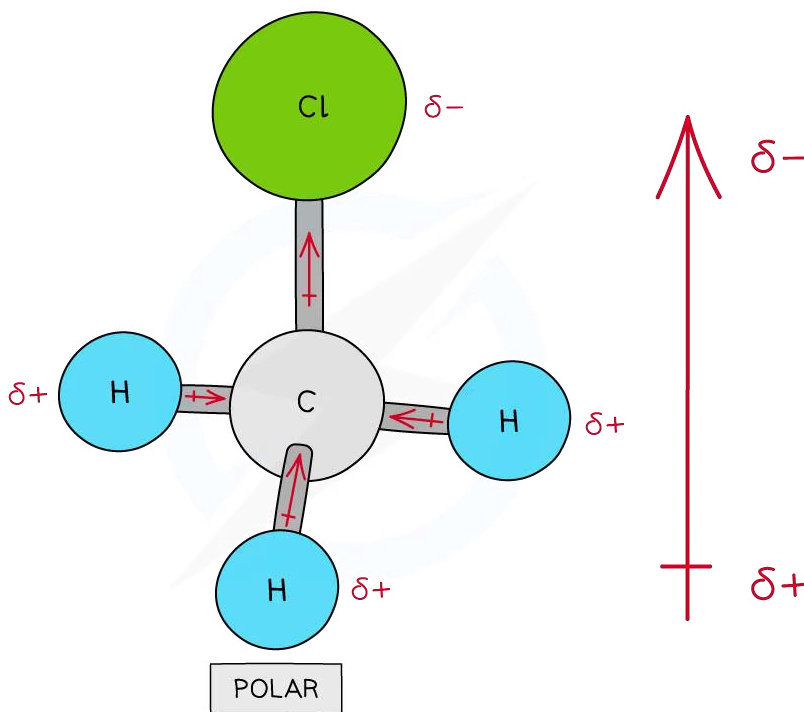


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The sign shows the direction of the dipole moment and the arrow points to the delta negative end of the dipole

Assigning polarity to molecules

- To determine whether a molecule with more than two different atoms is polar, the following things have to be taken into consideration:
 - The polarity of each bond
 - How the bonds are arranged in the molecule
- Some molecules have polar bonds but are overall not polar because the polar bonds in the molecule are arranged in such way that the individual dipole moments **cancel each other out**

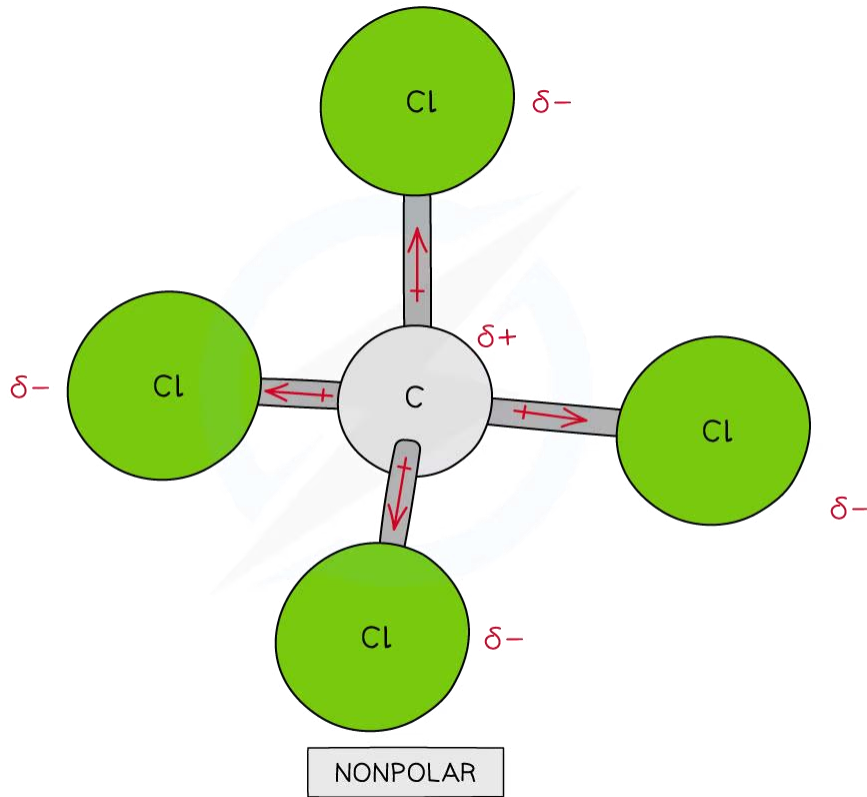


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There are four polar covalent bonds in CH_3Cl which do not cancel each other out causing CH_3Cl to be a polar molecule; the overall dipole is towards the electronegative chlorine atom



YOUR NOTES



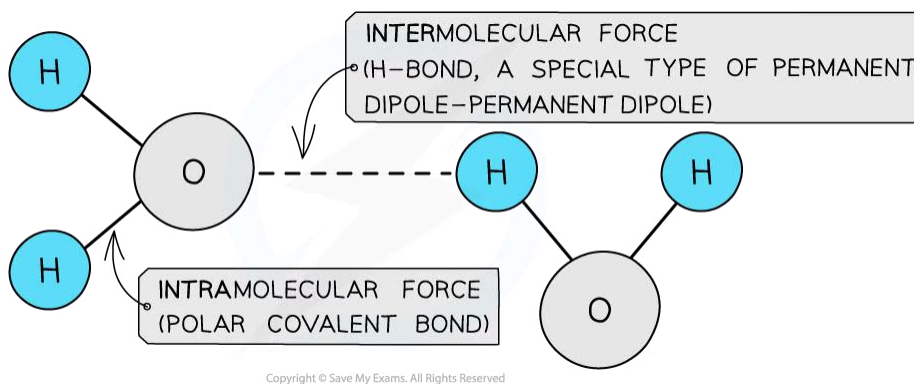
Though CCl_4 has four polar covalent bonds, the individual dipole moments cancel each other out causing CCl_4 to be a nonpolar molecule

2.5.3 Intermolecular Forces

Intermolecular Forces

Intramolecular forces

- **Intramolecular forces** are forces **within** a molecule and are usually covalent bonds
- **Covalent bonds** are formed when the outer electrons of two atoms are **shared**
- Single, double, triple and co-ordinate bonds are all types of intramolecular forces



Intermolecular forces

- Molecules also contain weaker **intermolecular forces** which are forces **between** the molecules
- There are three types of intermolecular forces:
 - **Induced dipole – dipole forces** are also called **London dispersion forces** or **van der Waals' forces**
 - **Permanent dipole – dipole forces** (also called van der Waals' forces) are the attractive forces between two neighbouring molecules with a permanent dipole
 - **Hydrogen Bonding** are a special type of **permanent dipole - permanent dipole** forces
 - **Intramolecular forces** are **stronger** than intermolecular forces
 - For example, a hydrogen bond is about one tenth the strength of a covalent bond

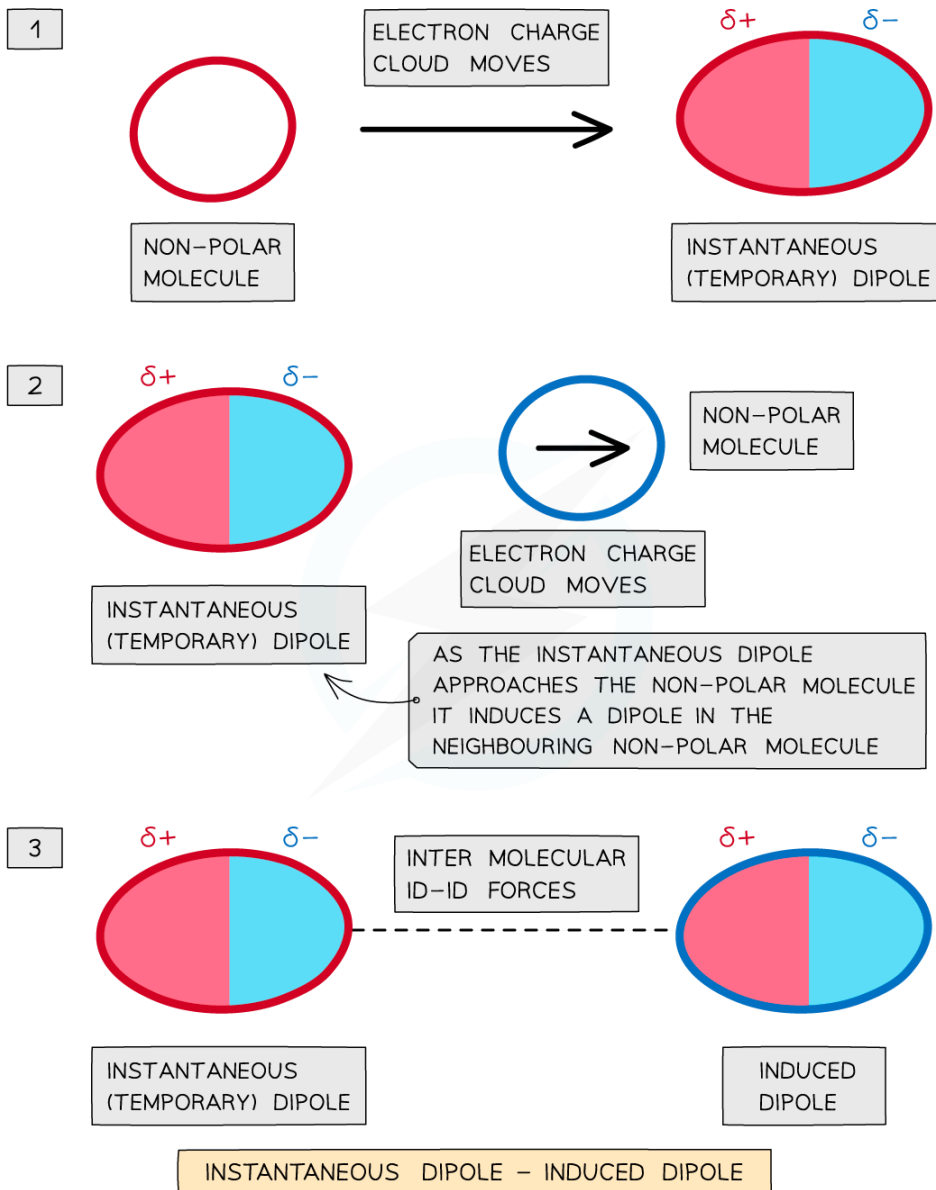
Induced dipole–dipole forces:

- **Induced dipole - dipole forces** exist between all atoms or molecules

YOUR NOTES



◦ They are also known as **van der Waals' forces** or **London dispersion forces**



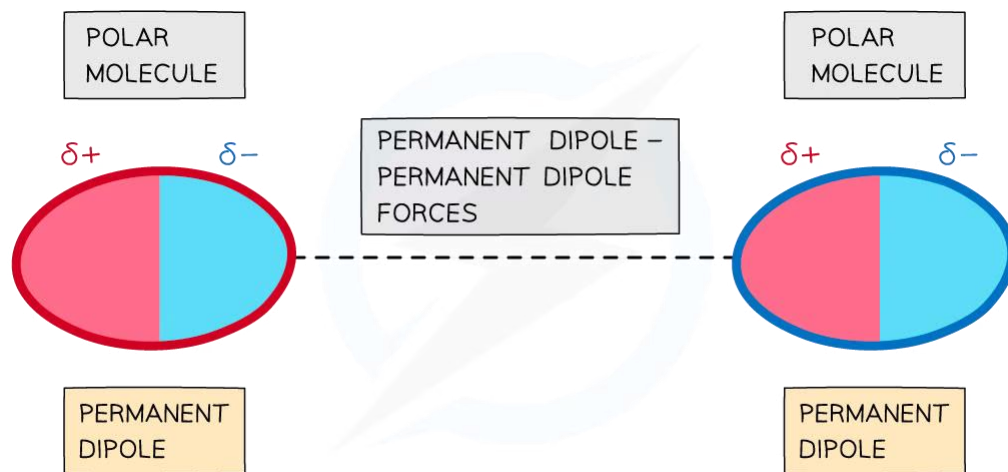
YOUR NOTES



- The electron charge cloud in non-polar molecules or atoms are constantly moving
- During this movement, the electron charge cloud can be more on one side of the atom or molecule than the other
- This causes a **temporary dipole** to arise
- This temporary dipole can **induce** a dipole on neighbouring molecules
- When this happens, the **$\delta+$ end of the dipole** in one molecule and the **$\delta-$ end of the dipole** in a neighbouring molecule are **attracted** towards each other
- Because the electron clouds are moving constantly, the dipoles are only temporary
- Therefore the greater the number of electrons the molecule has or the greater the relative molecular mass, the stronger the induced dipole-dipole forces
 - For example, pentane, C_5H_{12} has a higher boiling point than propane, C_3H_8

Permanent dipole – permanent dipole forces:

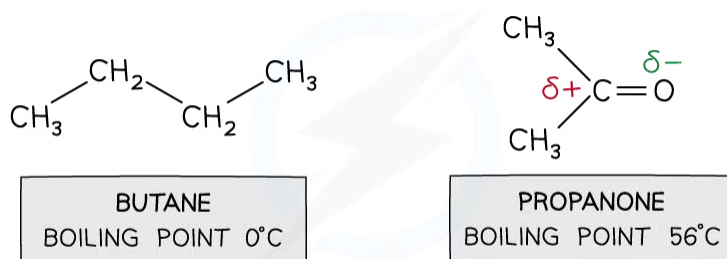
- **Polar molecules** have **permanent dipoles**
- The molecule will always have a **negatively** and **positively charged end**



- Forces between two molecules that have permanent dipoles are called **permanent dipole – dipole forces**
- The **$\delta+$ end of the dipole** in one molecule and the **$\delta-$ end of the dipole** in a neighbouring molecule are **attracted** towards each other

Relative strength

- For small molecules with **the same number of electrons**, permanent dipoles are **stronger** than induced dipoles
 - Butane and propanone have the same number of electrons
 - Butane is a nonpolar molecule and will have induced dipole forces
 - Propanone is a polar molecule and will have permanent dipole forces
 - Therefore, more energy is required to break the intermolecular forces between propanone molecules than between butane molecules
 - So, propanone has a higher boiling point than butane



Pd–pd forces are stronger than id–id forces in smaller molecules with an equal number of electrons

YOUR NOTES



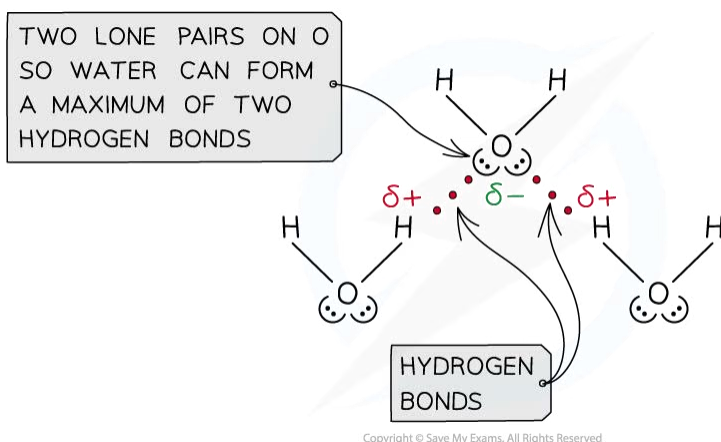
Hydrogen Bonding & Water

YOUR NOTES



Hydrogen bonding

- **Hydrogen bonding** is the **strongest** form of **intermolecular bonding**
 - Hydrogen bonding is a type of **permanent dipole – permanent dipole** bonding
- For hydrogen bonding to take place the following is needed:
 - A species which has an **O, N or F** (very **electronegative**) atom bonded to a hydrogen
- When hydrogen is covalently bonded to an O, N or F, the bond becomes highly polarised
- The H becomes so δ^+ charged that it can form a bond with the lone pair of an O, N or F atom in another molecule
- For example, in water
 - Water can form two hydrogen bonds, because the O has two lone pairs

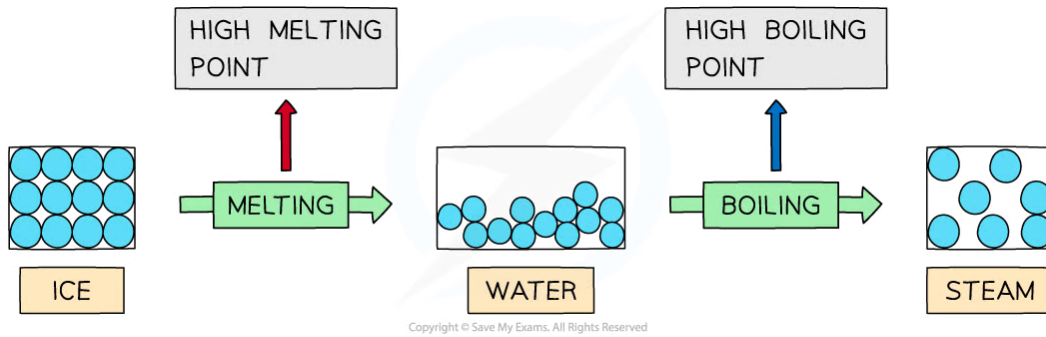


Properties of water

- Hydrogen bonding in water, causes it to have anomalous properties such as high melting and boiling points, high surface tension and anomalous density of ice compared to water

High melting & boiling points

- Water has high **melting** and **boiling points** which is caused by the **strong intermolecular forces** of hydrogen bonding between the molecules
- In **ice** (solid H₂O) and water (liquid H₂O) the molecules are tightly held together by hydrogen bonds
- A lot of energy is therefore required to break the water molecules apart and melt or boil them



Hydrogen bonds are strong intermolecular forces which are difficult to break causing water to have high melting and boiling points

YOUR NOTES
↓

Effects of Intermolecular Forces

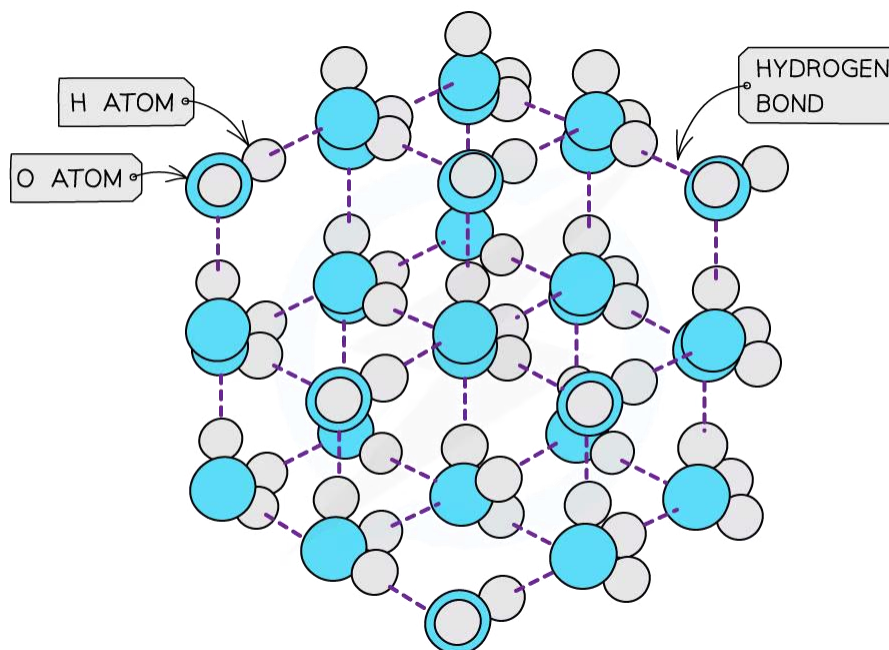
Properties of Molecular substances

YOUR NOTES



Ice

- **Solids** are **denser** than their **liquids** as the particles in solids are more **closely packed** together than in their liquid state
- In ice however, the water molecules are packed in a **3D hydrogen-bonded network** in a **rigid lattice**
- Each oxygen atom is surrounded by hydrogen atoms
- This way of packing the molecules in a solid and the relatively long **bond lengths** of the hydrogen bonds means that the water molecules are slightly further apart than in the liquid form
- Therefore, ice has a lower density than liquid water



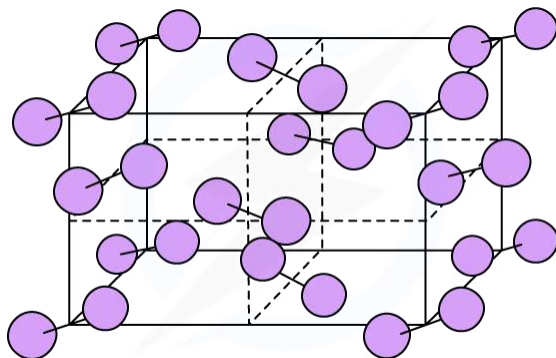
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The 'more open' structure of molecules in ice causes it to have a lower density than liquid water

Iodine

- The molecular lattice of iodine consists of a neat arrangement of molecules in the crystal lattice which is held together by the weak intermolecular forces
- Being a non-polar molecule, the weak intermolecular bonding is due to instantaneous dipole – induced dipole interactions (the weakest of the van der Waals' forces)

- Iodine tends to sublime at temperatures approaching 114 °C due to weak intermolecular force
 - A purple vapour is observed when iodine sublimes

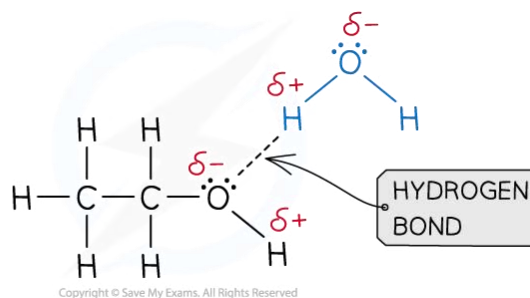


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Crystalline structure of Iodine

Solubility

- The general principle is that 'like dissolves like' so non-polar substances mostly dissolve in non-polar solvents, like hydrocarbons and they form dispersion forces between the solvent and the solute
- Polar covalent substances generally dissolve in polar solvents as a result of dipole-dipole interactions or the formation of hydrogen bonds between the solute and the solvent
- A good example of this is seen in organic molecules such as alcohols and water:



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Hydrogen bonds form between ethanol and water

- As covalent molecules become larger their solubility can decrease as the polar part of the molecule is only a smaller part of the overall structure
 - This effect is seen in alcohols for example where ethanol, C₂H₅OH, is readily soluble but hexanol, C₆H₁₃OH, is not
- Polar covalent substances are unable to dissolve well in non-polar solvents as their dipole-dipole attractions are unable to interact well with the solvent
- Giant covalent substances generally don't dissolve in any solvents as the energy needed to overcome the strong covalent bonds in the lattice structures is too great

Conductivity

YOUR NOTES





- As covalent substances do not contain any freely moving charged particles, they are unable to conduct electricity in either the solid or liquid state
- However, under certain conditions some polar covalent molecules can ionise and will conduct electricity
- Some giant covalent structures are capable of conducting electricity due to delocalised electrons

YOUR NOTES

**Comparing the Properties of Covalent Compounds Table**

| | Non-polar covalent substances | Polar covalent substances | Giant covalent substances | Ionic substances |
|----------------------------------|-------------------------------|---|----------------------------------|-----------------------------|
| Melting and boiling point | Low | Low | Very high | Very high |
| Volatility | Highest | High | Low | Low |
| Solubility in polar solvents | Insoluble | Some solubility depending on molecular size | Insoluble | Soluble |
| Solubility in non-polar solvents | Soluble | Some solubility depending on molecular size | None | Insoluble |
| Electrical conductivity | None | None | None – except graphite, graphene | Only when molten or aqueous |

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