Edexcel International AS Chemistry

Formulae & Equations

Contents

Your notes

Formulae – Definitions

Basic terms

- There are basic terms that you are expected to know from your previous studies
  - Atom
    - A single particle
    - The smallest part of an element that can participate in a chemical reaction
  - Element
    - An atom or group of atoms of only one type, which can be chemically joined or not
    - A substance that cannot be broken down into simpler substances
  - Ion
    - An atom that has become electrically charged
    - An atom (or group of atoms) that has gained or lost electrons to become a charged species
  - Molecule
    - Two or more atoms chemically joined together
  - Compound
    - A substance with two or more elements chemically joined together
  - Empirical formula
    - The smallest whole-number ratio of atoms (of each element) in a compound/molecule
  - Molecular formula
    - The actual number of atoms (of each element) in a compound/molecule

Mass – Definitions

- 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 $1/12$ of a carbon-12 atom

Relative isotopic mass

- Relative isotopic mass is defined as the mass of an isotope relative to $1/12$ 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 $1/12$ of the mass of a carbon-12 atom
- We have seen previously that the symbol for the relative atomic mass is A_r
- This is calculated from the **mass number** and **relative abundances** of all the **isotopes** of a particular element
- The symbol for the **relative formula mass** is $\boldsymbol{M_r}$ and it refers to the **total mass** of the substance
    - The term relative formula mass should be used for compounds with giant structures e.g. ionic compounds such as sodium chloride
    - If the substance is molecular you can use the term **relative molecular mass**
- To calculate the M_r of a substance, you have to add up the **relative atomic masses** of all the atoms present in the formula

Relative Formula Mass Calculations Table

Your notes

Substance	Atoms present	M_r
Hydrogen (H_2)	2 × H	(2 × 1) = 2
Water (H_2O)	(2 × H) + (1 × O)	(2 × 1) + 16 = 18
Potassium Carbonate (K_2CO_3)	(2 × K) + (1 × C) + (3 × O)	(2 × 39) + 12 + (3 × 16) = 138
Calcium Hydroxide ($Ca(OH)_2$)	(1 × Ca) + (2 × O) + (2 × H)	40 + (2 × 16) + (2 × 1) = 74
Ammonium Sulfate ($(NH_4)_2SO_4$)	(2 × N) + (8 × H) + (1 × S) + (4 × O)	(2 × 14) + (8 × 1) + 32 + (4 × 16) = 132

Examiner Tips and Tricks

It is expected that you will use relative atomic mass values from the Periodic Table

- This means that your values will be more accurate
- e.g. potassium carbonate = (2 x 39.1) + 12.0 + (3 x 16.0) = 138.2

If you are in any doubt whether to use relative molecular mass or relative formula mass, use the latter because it applies to all compounds whether they are ionic or covalent.

Your notes

Your notes

The Mole & Avogadro Calculations

- The **Avogadro constant** (N_A or L) is the number of particles equivalent to the relative **atomic mass** or **molecular mass** of a substance
  - The Avogadro constant applies to atoms, molecules, ions and electrons
- The value of N_A is **6.02×10^{23} 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 12.00g 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:

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

- One mole of any element is equal to the relative atomic mass of that element in grams
  - If you had one mole of carbon in your hand, that is 6.02×10^{23} atoms of carbon, you would have a mass of 12.00 g
  - One mole of water would have a mass of $(2 \times 1 + 16) = 18$ g

Worked Example

1. What is the molar mass of water?
2. How many moles are there in 100 g of water?
3. How many water molecules are there in 100g of water?

Answers

1. Molar mass of water, $H_2O = (2 \times 1.0) + 16.0 = 18.0$ g mol^{-1}
2. Moles $= \frac{mass}{molar\ mass} = \frac{100}{18.0} =$ 5.56 moles (to 3 s.f.)
3. Number of molecules = number of moles x Avogadro's constant = $5.56 \times (6.02 \times 10^{23}) = 3.35 \times 10^{24}$ molecules

Worked Example

What is the mass of the following:

1. Five hundred million atoms of platinum
2. (1.31×10^{22}) molecules of ethanol

Answer 1:

Number of moles $= \dfrac{\text{number of particles}}{\text{Avogadro's constant, } N_A} = \dfrac{500 \times 10^6}{6.02 \times 10^{23}} =$ 8.31 x 10^{-16} moles

Mass = moles x molar mass = (8.31×10^{-16}) x 195.1 = 1.62×10^{-13} g (lots of atoms, a tiny mass)

Answer 2:

Molar mass of ethanol, C_2H_5OH = (2 x 12.0) + (5 x 1.0) + 16.0 + 1.0 = 46.0 g mol^{-1}

Number of moles $= \dfrac{\text{number of particles}}{\text{Avogadro's constant, } N_A} = \dfrac{1.31 \times 10^{22}}{6.02 \times 10^{23}} =$ 0.0218 moles

Mass = moles x molar mass = 0.0218 x 46.0 = 1.00 g (an exceptionally large number of molecules in just 1 g)

Examiner Tips and Tricks

- When you are completing calculations using Avogadro's constant, you may end up with answers that seem very large or very small - don't automatically assume that they must be wrong
- Remember, Avogadro's constant is a VERY large number:
  - 6.02×10^{23} or 602 000 000 000 000 000 000 000
- So when you multiply or divide by Avogadro's constant, your answers will, naturally, become very large or very small

Your notes

Your notes

Writing & Balancing 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

Formulae for Ionic Compounds

- The formulae of simple ionic compounds can be calculated if you know the charge on the ions
- Below are some common ions and their charges:

Common Ions & Their Charges Table

ION	FORMULA AND CHARGE
IRON(II)	Fe^{2+}
COPPER(II)	Cu^{2+}
CHROMIUM(III)	Cr^{3+}
AMMONIUM	NH_4^+
HYDROXIDE	OH^-
NITRATE	NO_3^-
SULFATE	SO_4^{2-}
CARBONATE	CO_3^{2-}
HYDROGEN CARBONATE	HCO_3^-

- For ionic compounds you have to balance the charge of each part by multiplying each ion until the sum of the charges = 0
- Example: what is the formula of aluminium sulfate?
  - Write out the formulae of each ion, including their charges
  - Al^{3+} SO_4^{2-}
- Balance the charges by multiplying them out:

  Al^{3+} x **2** = +6 and SO_4^{2-} x **3** = -6; so +6 – 6 = 0
- So the formula is $Al_2(SO_4)_3$

Examiner Tips and Tricks

Another method that also works is to 'swap the numbers'.

In the example above the numbers in front of the charges of the ions (3 and 2) are swapped over and become the multipliers in the formula (2 and 3).

Easy when you know how!

Your notes

Your notes

Worked Example

Balance the following equation:

magnesium + oxygen → magnesium oxide

Answer:

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

$$Mg + O_2 \rightarrow MgO$$

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

	Mg	O
Reactants	1	2
Products	1	1

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

$$2Mg + O_2 \rightarrow 2MgO$$

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

$$2Mg\ (s) + O_2\ (g) \rightarrow 2MgO\ (s)$$

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

1. Balance the following equation

zinc + copper(II) sulfate → zinc sulfate + copper

2. Write down the ionic equation for the above reaction

Your notes

Answer 1:

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

$$Zn + CuSO_4 \rightarrow ZnSO_4 + Cu$$

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

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

$$Zn\,(s) + CuSO_4\,(aq) \rightarrow ZnSO_4\,(aq) + Cu\,(s)$$

Answer 2:

Step 1: The full chemical equation for the reaction is

$$Zn\,(s) + CuSO_4\,(aq) \rightarrow ZnSO_4\,(aq) + Cu\,(s)$$

Step 2: Break down reactants into their respective ions

$$Zn\,(s) + Cu^{2+} + SO_4^{2-}\,(aq) \rightarrow Zn^{2+} + SO_4^{2-}\,(aq) + Cu\,(s)$$

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

$$Zn\,(s) + Cu^{2+} + \cancel{SO_4^{2-}}\,(aq) \rightarrow Zn^{2+} + \cancel{SO_4^{2-}}\,(aq) + Cu\,(s)$$

$$Zn\,(s) + Cu^{2+}(aq) \rightarrow Zn^{2+}\,(aq) + Cu\,(s)$$

Experimental Observations & Equations

- Chemical equations give information about the reaction that is taking place
  - Balanced equations show the number of particles participating in the reaction and the number of products being formed
  - Balanced equations can be used to calculate the number of moles involved in reactions
  - Balanced equations can, also, be used to calculate masses and volumes involved in reactions
  - Ionic equations only show the reacting particles
  - Ionic equations allow you to identify spectator ion

Types of reaction

- Chemical equations can be used to determine the type of reaction taking place

Displacement reactions

$$Br_2\,(aq) + 2KI\,(aq) \rightarrow I_2\,(aq) + 2KBr\,(aq)$$

- In this reaction, the more reactive bromine **displaces** the less reactive iodide in potassium iodide
- This can also be seen in the ionic equation for the reaction

$$Br_2\,(aq) + 2I^-\,(aq) \rightarrow I_2\,(aq) + 2Br^-\,(aq)$$

Examiner Tips and Tricks

The use of chemical equations can help identify risks and hazards in the reaction and suggest appropriate precautions where necessary

For example, the use of aqueous bromine in the above example should suggest the potential use of a fume cupboard and nitrile gloves because:

- Bromine liquid is **toxic**, **corrosive** and **harmful to the environment**
- Bromine water with a concentration of 0.2 mol dm^3 is corrosive
- With a concentration of between 0.06 mol dm^3 and 0.2 mol dm^3, bromine water is an **irritant**
- Only below concentrations of 0.06 mol dm^3 is bromine water considered a **low hazard**

Neutralisation reactions

- These can be identified by the presence of reactant acids and bases as well as the formation of a **neutral solution** salt and water (and sometimes other compounds such as carbon dioxide)

$$HCl\,(aq) + NaOH\,(aq) \rightarrow NaCl\,(aq) + H_2O\,(l)$$

$$Na_2CO_3\,(aq) + 2HNO_3\,(aq) \rightarrow 2NaNO_3\,(aq) + H_2O\,(l) + CO_2\,(g)$$

- The ionic equations can more clearly demonstrate the neutralisation of an acid and a base:

$$H^+\,(aq) + OH^-\,(aq) \rightarrow H_2O\,(l)$$

$$2H^+\,(aq) + CO_3^{2-}\,(aq) \rightarrow H_2O\,(l) + CO_2\,(g)$$

Examiner Tips and Tricks

For neutralisation reactions, the main hazards are linked to:

Your notes

- The concentration of the acid
- The type of acid
  - This could mean **strong**, e.g. HCl, or **weak**, e.g. CH_3COOH
  - This could also mean **monoprotic**, e.g. HNO_3, **diprotic**, e.g. H_2SO_4, or **triprotic**, e.g. H_3PO_4
- The concentration of the base
- The strength of the base
- The physical state of the base, e.g. NaOH (s) is arguably considered more corrosive than a high concentration solution of NaOH (aq)

Precipitation reactions

- These are shown by the reaction of two aqueous solutions to form products which include one solid

$$BaCl_2\,(aq) + Na_2SO_4\,(aq) \rightarrow BaSO_4\,(s) + 2NaCl\,(aq)$$

- The ionic equation shows the precipitation reactions more clearly as there are no other products considered

$$Ba^{2+}\,(aq) + SO_4^{\,2-}\,(aq) \rightarrow BaSO_4\,(s)$$

Examiner Tips and Tricks

A precipitation reaction is a clear example of where consideration for further practical procedures is most obvious

The formation of a solid product should tell you that any purification of the product should include filtering or decanting as a minimum

Your notes

Empirical & Molecular

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.

Answer:

	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_2O	

- 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

Your notes

Worked Example

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

Answer:

	Carbon	Hydrogen
Note the % by mass of each element	85.7	14.3
Divide the % by atomic masses	$= \frac{85.7}{12.0}$ $= 7.142$ mol	$= \frac{14.3}{1.00}$ $= 14.3$ 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	

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 formula 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 $C_4H_{10}S$ 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 x 4) + (H x 10) + (S x 1)
  - Relative empirical mass = (12.0 x 4) + (1.0 x 10) + (32.1 x 1)
  - Relative empirical mass = 90.1

Step 2: Divide relative formula 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

- $(C_4 \times 2) + (H_{10} \times 2) + (S \times 2) = (C_8) + (H_{20}) + (S_2)$
  - Molecular Formula of **X** is $C_8H_{20}S_2$

Percentage Composition by Mass

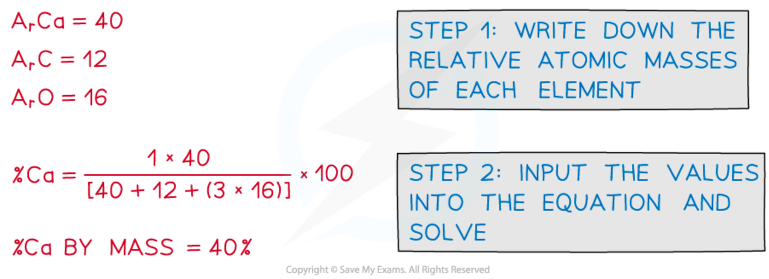
- The percentage by mass of an element in a compound can be calculated using the following equation:

$$\%\ \text{mass of an element} = \frac{A_r \times \text{number of atoms of the element}}{M_r \text{ of the compound}} \times 100$$

Worked Example

Calculate the percentage by mass of calcium in calcium carbonate, $CaCO_3$

Answer:



Water of Crystallisation

- **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 $CuSO_4{\cdot}5H_2O$
- 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**

Your notes

- E.g. cobalt(II) chloride can be hydrated by **six** or **two** water molecules
  - $CoCl_2 \cdot 6H_2O$ or $CoCl_2 \cdot 2H_2O$
- The conversion of anhydrous compounds to hydrated compounds is reversible by heating the hydrated salt:

$$\text{Hydrated:} \quad CuSO_4{\bullet}5H_2O \rightleftharpoons CuSO_4 + 5H_2O \quad \text{:Anhydrous}$$

- 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

Your notes

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: $CuSO_4$ = 159.6, H_2O = 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	$CuSO_4{\bullet}7H_2O$	

Ideal Gas Equation

- The **ideal gas equation** is:

$$PV = nRT$$

- P = pressure in pascals (Pa)
  - V = volume in cubic metres (m^3)
  - n = the amount of substance in moles (mol)
  - R = the gas constant, which is given in the Data Booklet as 8.31 J mol^{-1} K^{-1}

- T = temperature in Kelvin (K)

Examiner Tips and Tricks

There are several calculations in Chemistry where you need to convert the units to or from SI units

The ideal gas equation has three:

1. Pressure is often quoted in kPa but the calculation needs pressure in Pa
    - kPa to Pa = multiply by 1000 or 10^3
2. Volume is usually quoted in cm^3 or dm^3 but the calculation needs volume in m^3
    - cm^3 to m^3 = divide by 1000000 or multiply by 10^{-6}
    - dm^3 to m^3 = divide by 1000 or multiply by 10^{-3}
3. Temperature can be quoted in Kelvin or Celsius
    - Celsius to Kelvin = + 273

This is why you should always show your working! Examiners can't take all of your marks for one error, if you show your working then they should check through for errors and award marks accordingly

- The ideal gas equation can be used to find the amount of moles in a gaseous substance
    - It can also be used for volatile liquids at temperatures above their boiling point
- If the mass of the substance is known, then the molar mass can be calculated
    - This can then be used with empirical formula data to determine the molecular formula of a compound

Worked Example

An unknown compound was analysed and found to contain 66.7% of carbon, 11.1% hydrogen and the remainder was oxygen

0.135 g of the unknown compound had a volume of 56.0 cm^3 at a temperature of 90 °C and a pressure of 101 kPa

Determine the molecular formula of the unknown compound

Answer

Step 1: Calculate the number of moles of carbon, hydrogen and oxygen

Carbon: $\frac{66.7}{12.0}$ = 5.558 moles	Hydrogen: $\frac{11.1}{1.00}$ = 11.1 moles	Oxygen: $\frac{(100 - 66.7 - 11.1)}{16.0}$ = 1.3875 moles

Step 2: Divide by the smallest answer to get the ratio

Carbon: $\frac{5.558}{1.3875} = 4$	Hydrogen: $\frac{11.1}{1.3875} = 8$	Oxygen: $\frac{1.3875}{1.3875} = 1$

Step 3: State the empirical formula

- The empirical formula is C_4H_8O

Step 4: Calculate the amount in moles, using $PV = nRT$

- $n = \frac{PV}{RT} = \frac{(101 \times 10^3) \times (56.0 \times 10^{-6})}{8.31 \times (90 + 273)} = 1.875 \times 10^{-3}$ moles

Step 5: Calculate the molar mass

- Molar mass $= \frac{0.135}{1.875 \times 10^{-3}} = 72$

Step 6: Deduce the molecular formula

- The empirical formula, C_4H_8O, has a mass of (4 x 12.0) + (8 x 1.0) + 16.0 = 72.0
  - Therefore, the molecular formula is also C_4H_8O

Your notes