Chemical formulas and the mole concept

ELEMENTS

All substances are made up of one or more elements. An element cannot be broken down by any chemical process into simpler substances. There are just over 100 known elements. The smallest part of an element is called an atom.

Names of the first 20 elements

Atomic Number	Name	Symbol	Relative atomic mass
1	hydrogen	H	1.01
2	helium	He	4.00
3	lithium	Li	6.94
4	beryllium	Be	9.01
5	boron	B	10.81
6	carbon	C	12.01
7	nitrogen	N	14.01
8	oxygen	O	16.00
9	fluorine	F	19.00
10	neon	Ne	20.18
11	sodium	Na	22.99
12	magnesium	Mg	24.31
13	aluminium	Al	26.98
14	silicon	Si	28.09
15	phosphorus	P	30.97
16	sulfur	S	32.06
17	chlorine	Cl	35.45
18	argon	Ar	39.95
19	potassium	K	39.10
20	calcium	Ca	40.08

COMPOUNDS

Some substances are made up of a single element although there may be more than one atom of the element in a particle of the substance. Oxygen is diatomic, that is, a molecule of oxygen contains two oxygen atoms. A compound contains more than one element. For example, a molecule of water contains two hydrogen atoms and one oxygen atom. Water is a compound not an element because it can be broken down chemically into its constituent elements: hydrogen and oxygen.

FORMULAS OF COMPOUNDS

Compounds can be described by different chemical formulas.

Empirical formula (literally the formula obtained by experiment)
This shows the simplest whole number ratio of atoms of each element in a particle of the substance. It can be obtained by either knowing the mass of each element in the compound or from the percentage composition by mass of the compound. The percentage composition can be converted directly into mass by assuming 100 g of the compound are taken.

Example: A compound contains 40.00% carbon, 6.73% hydrogen and 53.27% oxygen by mass, determine the empirical formula.

	Amount /mol	Ratio	
C	40.00/12.01 = 3.33	1	Empirical formula
H	6.73/1.01 = 6.66	2	$= CH_2O$
O	53.27/16.00 = 3.33	1	

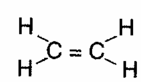
Molecular formula
For molecules this is much more useful as it shows the actual number of atoms of each element in a molecule of the substance. It can be obtained from the empirical formula if the molar mass of the compound is also known.
Methanal CH_2O (M_r =30), ethanoic acid $C_2H_4O_2$ (M_r = 60) and glucose $C_6H_{12}O_6$ (M_r = 180) are different substances with different molecular formulas but all with the same empirical formula CH_2O. Note that subscripts are used to show the number of atoms of each element in the compound.

Structural formula
This shows the arrangement of atoms and bonds within a molecule and is particularly useful in organic chemistry.

The three different formulas can be illustrated using ethene:

CH_2 — empirical formula

C_2H_4 — molecular formula



(can also be written $H_2C{=}CH_2$)

structural formula

MOLE CONCEPT AND AVOGADRO'S CONSTANT

A single atom of an element has an extremely small mass. For example an atom of carbon-12 has a mass of 1.993×10^{-23} g. This is far too small to weigh. A more convenient amount to weigh is 12.00 g. 12.00 g of carbon-12 contains 6.02×10^{23} atoms of carbon-12. This number is known as Avogadro's constant (N_A or L).
Chemists measure amounts of substances in moles. A mole is the amount of substance that contains L particles of that substance. The mass of one mole of **any** substance is known as the **molar mass** and has the symbol M. For example, hydrogen atoms have $\frac{1}{12}$ of the mass of carbon-12 atoms so a mole of hydrogen atoms contains 6.02×10^{23} hydrogen atoms and has a mass of 1.01 g. In reality elements are made up of a mixture of isotopes.
The **relative atomic mass** of an element A_r is the weighted mean of all the naturally occurring isotopes of the element relative to carbon-12. This explains why the relative atomic masses given for the elements above are not whole numbers. The units of molar mass are g mol^{-1} but relative molar masses M_r have no units. For molecules **relative molecular mass** is used. For example, the M_r of glucose, $C_6H_{12}O_6 = (6 \times 12.01) + (12 \times 1.01) + (6 \times 16.00) = 180.18$. For ionic compounds the term **relative formula mass** is used.
Be careful to distinguish between the words **mole** and **molecule**. A molecule of hydrogen gas contains two atoms of hydrogen and has the formula H_2. A mole of hydrogen gas contains 6.02×10^{23} hydrogen molecules made up of two moles (1.20×10^{24}) of hydrogen atoms.

Chemical reactions and equations

PROPERTIES OF CHEMICAL REACTIONS

In all chemical reactions:

- new substances are formed.
- bonds in the reactants are broken and bonds in the products are formed resulting in an energy change between the reacting system and its surroundings.
- there is a fixed relationship between the number of particles of reactants and products resulting in no overall change in mass – this is known as the stoichiometry of the reaction.

CHEMICAL EQUATIONS

Chemical reactions can be represented by chemical equations. Reactants are written on the left hand side and products on the right hand side. The number of moles of each element must be the same on both sides in a balanced chemical equation, e.g. the reaction of nitric acid (one of the acids present in acid rain) with calcium carbonate (the main constituent of marble statues).

$$\underbrace{\underset{\text{calcium carbonate}}{CaCO_3(s)} + \underset{\text{nitric acid}}{2HNO_3(aq)}}_{\text{REACTANTS}} \longrightarrow \underbrace{\underset{\text{calcium nitrate}}{Ca(NO_3)_2(aq)} + \underset{\text{carbon dioxide}}{CO_2(g)} + \underset{\text{water}}{H_2O(l)}}_{\text{PRODUCTS}}$$

STATE SYMBOLS

Because the physical state that the reactants and products are in can affect both the rate of the reaction and the overall energy change it is good practice to include the state symbols in the equation.

(s) – solid (l) – liquid (g) – gas (aq) – in aqueous solution

→ OR ⇌

A single arrow → is used if the reaction goes to completion. Sometimes the reaction conditions are written on the arrow:

e.g. $$C_2H_4(g) + H_2(g) \xrightarrow{\text{Ni catalyst, 180 °C}} C_2H_6(g)$$

Reversible arrows are used for reactions where both the reactants and products are present in the equilibrium mixture:

e.g. $$3H_2(g) + N_2(g) \underset{\text{250 atm}}{\overset{\text{Fe(s), 550 °C}}{\rightleftharpoons}} 2NH_3(g)$$

COEFFICIENTS AND MOLAR RATIO

The coefficient refers to the number in front of each reactant and product in the equation. The coefficients give information on the molar ratio. In the first example above, two moles of nitric acid react with one mole of calcium carbonate to produce one mole of calcium nitrate, one mole of carbon dioxide and one mole of water. In the reaction between hydrogen and nitrogen above, three moles of hydrogen gas react with one mole of nitrogen gas to produce two moles of ammonia gas.

IONIC EQUATIONS

Because ionic compounds are completely dissociated in solution it is sometimes better to use ionic equations. For example, when silver nitrate solution is added to sodium chloride solution a precipitate of silver chloride is formed.

$$Ag^+(aq) + NO_3^-(aq) + Na^+(aq) + Cl^-(aq) \longrightarrow AgCl(s) + Na^+(aq) + NO_3^-(aq)$$

$Na^+(aq)$ and $NO_3^-(aq)$ are spectator ions and do not take part in the reaction. So the ionic equation becomes:

$$Ag^+(aq) + Cl^-(aq) \longrightarrow AgCl(s)$$

From this we can deduce that any soluble silver salt will react with any soluble chloride to form a precipitate of silver chloride.

Mass and gaseous volume relationships

MEASUREMENT OF MOLAR QUANTITIES

In the laboratory moles can conveniently be measured using either mass or volume depending on the substances involved.

SOLIDS

Normally measured by weighing to obtain the mass.

1.000 kg = 1000 g

When weighing a substance the mass should be recorded to show the accuracy of the balance. For example, exactly 16 g of a substance would be recorded as 16.00 g on a balance weighing to + or – 0.01 g but as 16.000 g on a balance weighing to + or – 0.001 g.

LIQUIDS

Pure liquids may be weighed or the volume recorded.
The density of the liquid = $\frac{\text{mass}}{\text{volume}}$ and is usually expressed in g cm^{-3}.

GASES

Mass or volume may be used for gases.

SOLUTIONS

Volume is usually used for solutions.

1.000 litre = 1.000 dm^3 = 1000 cm^3

Concentration is the amount of solute (dissolved substance) in a known volume of solution (solute plus solvent). It is expressed either in g dm^{-3} or, more usually, in mol dm^{-3}. A solution of known concentration is known as a *standard solution.*

To prepare a 1.00 mol dm^{-3} solution of sodium hydroxide dissolve 40.00 g of solid sodium hydroxide in distilled water and then make the total volume up to 1.00 dm^3.

Concentration is often represented by square brackets, e.g.

$$[NaOH(aq)] = 1.00 \text{ mol dm}^{-3}$$

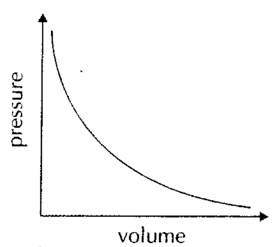
A 25.0 cm^3 sample of this solution contains

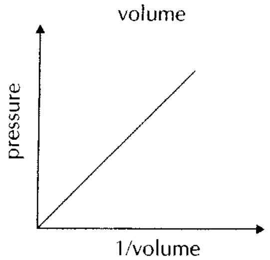
$$1.00 \times \frac{25.0}{1000} = 2.50 \times 10^{-2} \text{ mol of NaOH}$$

CHANGING THE VARIABLES FOR A FIXED MASS OF GAS

$P \propto \frac{1}{V}$ (or PV = constant)

At constant temperature: as the volume decreases the concentration of the particles increases, resulting in more collisions with the container walls. This increase in pressure is inversely proportional to the volume, i.e. doubling the pressure halves the volume.



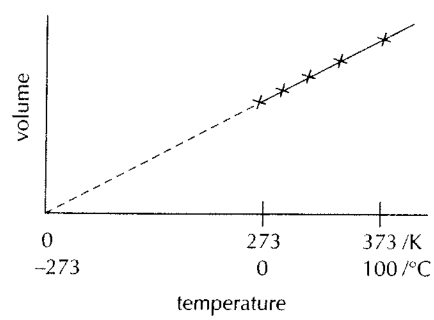


$P \propto T$ (or $\frac{P}{T}$ = constant)

At constant volume: increasing the temperature increases the average kinetic energy so the force with which the particles collide with the container walls increases. Hence pressure increases and is directly proportional to the absolute temperature, i.e. doubling the absolute temperature doubles the pressure.

$V \propto T$ (or $\frac{V}{T}$ = constant)

At constant pressure: at higher temperatures the particles have a greater average velocity so individual particles will collide with the container walls with greater force. To keep the pressure constant there must be fewer collisions per unit area so the volume of the gas must increase. The increase in volume is directly proportional to the absolute temperature, i.e. doubling the absolute temperature doubles the volume.



Extrapolating the graph to zero volume gives the value for absolute zero

IDEAL GAS EQUATION

The different variables for a gas are all related by the ideal gas equation.

$$PV = nRT$$

P = pressure in Pa (N m^{-2})
(1 atm = 1.013 × 10^5 Pa)
T = absolute temperature in K
V = volume in m^3
(1 cm^3 = 1 × 10^{-6} m^3)
n = number of moles
R = gas constant = 8.314 J K^{-1} mol^{-1}

Units

The gas constant can be expressed in different units but it is easier to use SI units.

$$R = \frac{PV}{nT} = \frac{\text{N m}^{-2} \times \text{m}^3}{\text{mol} \times \text{K}} = \text{N m mol}^{-1}\text{ K}^{-1}$$

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

Real gases

An ideal gas exactly obeys the gas laws. Real gases do have some attractive forces between the particles and the particles themselves do occupy some space so they do not exactly obey the laws. If they did they could never condense into liquids. A gas behaves most like an ideal gas at high temperatures and low pressures.

Molar volume of a gas and calculations

MOLAR VOLUME OF A GAS

The ideal gas equation depends on the amount of gas (number of moles of gas) but not on the nature of the gas. Avogadro's Law states that equal volumes of different gases at the same temperature and pressure contain the same number of moles. From this it follows that one mole of any gas will occupy the same volume at the same temperature and pressure. This is known as the **molar volume of a gas**. At 273K and 1.013×10^5 Pa (1 atm.) pressure this volume is 2.24×10^{-2} m^3 (22.4 dm^3 or 22 400 cm^3).

When the mass of a particular gas is fixed (nR is constant) a useful expression to convert the pressure, temperature and volume under one set of conditions (1) to another set of conditions (2) is:

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

In this expression there is no need to convert to SI units as long as the same units for pressure and volume are used on both sides of the equation. However do not forget that T refers to the absolute temperature and must be in kelvin.

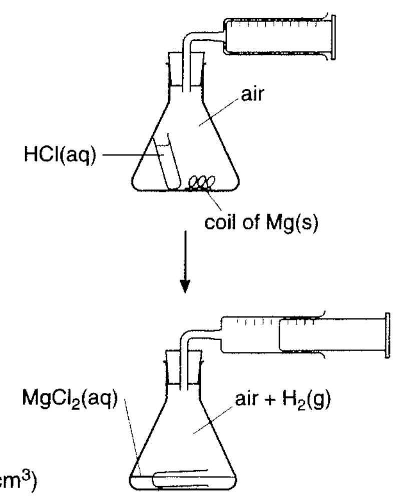
CALCULATIONS FROM EQUATIONS

Work methodically.

Step 1. Write down the correct formulas for all the reactants and products.
Step 2. Balance the equation to obtain the correct stoichiometry of the reaction.
Step 3. If the amounts of all reactants are known work out which are in **excess** and which one is the limiting reagent. By knowing the **limiting reagent** the maximum **yield** of any of the products can be determined.
Step 4. Work out the number of moles of the substance required.
Step 5. Convert the number of moles into the mass or volume.
Step 6. Express the answer to the correct number of significant figures and include the appropriate units.

WORKED EXAMPLES

(a) Calculate the volume of hydrogen gas evolved at 273 K and 1 atm pressure when 0.623 g of magnesium reacts with 27.3 cm^3 of 1.25 mol dm^{-3} hydrochloric acid.



Equation:

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

A_r for Mg = 24.31. Amount of Mg present $= \frac{0.623}{24.31} = 2.56 \times 10^{-2}$ mol

Amount of HCl present $= 1.25 \times \frac{27.3}{1000} = 3.41 \times 10^{-2}$ mol

From the equation $2 \times 2.56 \times 10^{-2} = 5.12 \times 10^{-2}$ mol of HCl would be required to react with all of the magnesium.

Therefore the magnesium is in excess and the limiting reagent is the hydrochloric acid.

The maximum amount of hydrogen produced $= \frac{3.41 \times 10^{-2}}{2} = 1.705 \times 10^{-2}$ mol

Volume of hydrogen at 273 K, 1 atm $= 1.705 \times 10^{-2} \times 22.4 = 0.382$ dm^3 (or 382 cm^3)

(b) Calculate the volume occupied by the hydrogen evolved In the example above if it had been collected at 22 °C and at a pressure of 1.12 atm.

Step 1. Express the temperature as an absolute temperature
22 °C = 295 K

Step 2. Convert the pressure to SI units
1.12 atm. $= 1.12 \times 1.103 \times 10^5 = 1.135 \times 10^5$ Pa

Step 3. Apply the ideal gas equation pV = nRT
$1.135 \times 10^5 \times V = 1.705 \times 10^{-2} \times 8.314 \times 295$

$$V = \frac{1.705 \times 10^{-2} \times 8.314 \times 295}{1.135 \times 10^5} = 3.69 \times 10^{-4}\ m^3\ (369\ cm^3)$$

This could also be solved using $\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$

(there is now no need to change the units of P and V to SI units)

$$V_2 = V_1 \times \frac{P_1}{P_2} \times \frac{T_2}{T_1} = 382 \times \frac{1}{1.12} \times \frac{295}{273} = 369\ cm^3$$

(c) The actual volume of hydrogen collected under these conditions was 342 cm^3. Determine the percentage yield.

Step 1. Use the mole ratio from the equation and the amounts of reactants to determine the limiting reagent and hence theoretical maximum yield. From part (a) theoretical yield = 382 cm^3

Step 2. Apply the relationship:

$$\text{Percentage yield} = \frac{\text{Experimental yield}}{\text{Theoretical yield}} \times 100$$

$$\text{Percentage yield} = \frac{342}{382} \times 100 = 89.5\%$$

IB QUESTIONS – QUANTITATIVE CHEMISTRY

1. What is the mass in grams of one molecule of ethanoic acid CH_3COOH?

A. 0.1 **B.** 3.6×10^{25} **C.** 1×10^{-22} **D.** 60

2. Which is not a true statement?

A. One mole of methane contains four moles of hydrogen atoms

B. One mole of ^{12}C has a mass of 12.00 g

C. One mole of hydrogen gas contains 6.02×10^{23} atoms of hydrogen

D. One mole of methane contains 75% of carbon by mass

3. A pure compound contains 24 g of carbon, 4 g of hydrogen and 32 g of oxygen.

No other elements are present. What is the empirical formula of the compound?

A. $C_2H_4O_2$ **B.** CH_2O **C.** CH_4O **D.** CHO

4. Which one of the following statements about SO_2 is/are correct?

I. One mole of SO_2 contains 1.8×10^{24} atoms

II. One mole of SO_2 has a mass of 64 g

A. Both I and II **B.** Neither I nor II **C.** I only **D.** II only

5. What is the empirical formula for the compound $C_6H_5(OH)_2$?

A. C_6H_6O **B.** $C_6H_5O_2H_2$ **C.** C_6H_7O **D.** $C_6H_7O_2$

6. Phosphorus burns in oxygen to produce phosphorus pentoxide P_4O_{10}.

What is the sum of the coefficients in the balanced equation?

$\_P_4(s) + \_O_2(g) \rightarrow \_P_4O_{10}(s)$

A. 3 **B.** 5 **C.** 6 **D.** 7

7. Magnesium reacts with hydrochloric acid according to the following equation:

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

What mass of hydrogen will be obtained if 100 cm^3 of 2.00 mol dm^{-3} HCl are added to 4.86 g of magnesium?

A. 0.2g **B.** 0.4g **C.** 0.8g **D.** 2.0g

8. Butane burns in oxygen according to the equation below.

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

If 11.6 g of butane is burned in 11.6 g of oxygen which is the limiting reagent?

A. Butane **C.** Neither

B. Oxygen **D.** Oxygen and butane

9. When 250 cm^3 of 3.00 mol dm^{-3} HCl(aq) is added to 350 cm^3 of 2.00 mol dm^{-3} HCl(aq) the concentration of the solution of hydrochloric acid obtained in mol dm^{-3} is:

A. 2.42 **B.** 1.45 **C.** 2.90 **D.** 2.50

10. Sulfuric acid and sodium hydroxide react together according to the equation:

$H_2SO_4(aq) + 2NaOH(aq) \rightarrow Na_2SO_4(aq) + 2H_2O(l)$

What volume of 0.250 mol dm^{-3} NaOH is required to neutralise exactly 25.0 cm^3 of 0.125 mol dm^{-3} H_2SO_4?

A. 25.0 cm^3 **B.** 12.5 cm^3 **C.** 50 cm^3 **D.** 6.25 cm^3

11. Separate samples of two gases, each containing a pure substance, are found to have the same density under the same conditions of temperature and pressure. Which statement about these two samples **must** be correct?

A. They have the same volume

B. They have the same relative molecular mass

C. There are equal numbers of moles of gas in the two samples

D. They condense at the same temperature

12. Which expression represents the density of a gas sample of relative molar mass, M_r, at temperature T, and pressure, P?

A. $\frac{PM_r}{T}$ **C.** $\frac{PM_r}{RT}$

B. $\frac{RT}{PM_r}$ **D.** $\frac{RM_r}{PT}$

13. A 250 cm^3 sample of an unknown gas has a mass of 1.42 g at 35 °C and 0.85 atmospheres. Which expression gives its molar mass, M_r? (R = 82.05 cm^3 atm K^{-1} mol^{-1})

A. $\frac{1.42 \times 82.05 \times 35}{0.25 \times 0.85}$ **C.** $\frac{1.42 \times 250 \times 0.85}{82.05 \times 308}$

B. $\frac{1.42 \times 82.05 \times 308}{0.25 \times 0.85}$ **D.** $\frac{1.42 \times 82.05 \times 308}{250 \times 0.85}$

14. Aspirin, $C_9H_8O_4$, is made by reacting ethanoic anhydride, $C_4H_6O_3$ (M_r = 102.1), with 2-hydroxybenzoic acid (M_r = 138.1), according to the equation:

$2C_7H_6O_3 + C_4H_6O_3 \rightarrow 2C_9H_8O_4 + H_2O$

(a) If 15.0 g 2-hydroxybenzoic acid is reacted with 15.0 g ethanoic acid, determine the limiting reagent in this reaction.

(b) Calculate the maximum mass of aspirin that could be obtained in this reaction.

(c) If the mass obtained in this experiment was 13.7 g, calculate the percentage yield of aspirin.

15. 14.48 g of a metal sulfate with the formula M_2SO_4 were dissolved in water. Excess barium nitrate solution was added in order to precipitate all the sulfate ions in the form of barium sulfate. 9.336 g of precipitate was obtained.

(a) Calculate the amount of barium sulfate $BaSO_4$ precipitated.

(b) Calculate the amount of sulfate ions present in the 14.48 g of M_2SO_4.

(c) What is the relative molar mass of M_2SO_4?

(d) Calculate the relative atomic mass of M and hence identify the metal.