IB DP CHEMISTRY

Structure 1: Models of the Particulate Nature of Matter

Structure 1.4 · The Mole

Counting Particles by Mass

Revision Notes · Standard and Higher Level

Fahad H. Ahmad

+92 323 509 4443 | Megalecture.com

Original notes prepared for the IB Diploma Programme Chemistry course (2025 syllabus)

What the syllabus requires

Structure 1.4 is the quantitative heart of the course: it turns the invisible world of atoms and molecules into masses, volumes and concentrations you can weigh and measure in the laboratory. Nearly every calculation you meet, from titrations to yields, rests on the ideas below. Use this list as a final checklist.

Understanding	You should be able to...
Avogadro's constant and the mole	State that one mole contains 6.02×10^{23} particles; use N_A to convert between amount (mol) and number of particles.
Molar mass	Relate mass, amount and molar mass through $n = m/M$; find the molar mass from a chemical formula.
Empirical and molecular formulae	Determine an empirical formula from composition data, and a molecular formula from the empirical formula and M_r.
Mole ratios in equations	Read a balanced equation as a ratio of amounts, and carry out reacting-mass calculations.
Yield and limiting reagent	Identify the limiting reagent; calculate theoretical yield, percentage yield and atom economy.
Concentration	Express concentration in mol dm^{-3} and g dm^{-3}; carry out dilution and titration calculations.
Gas volumes	Apply Avogadro's law and the molar volume of a gas to relate amounts and volumes of gases.

> **Exam note:** Structure 1.4 is common to SL and HL. Higher Level questions are longer and combine several of these steps in one problem, so a reliable, written-out method matters more than mental shortcuts. HL-only extensions are flagged with (HL) in these notes.

1. The mole and Avogadro's constant

Atoms are far too small and too numerous to count one by one, so chemists count them in a standard-sized package called the **mole** (symbol mol), exactly as a shopkeeper counts eggs in dozens. One mole is the amount of substance that contains as many particles as there are in this fixed number:

$$\textbf{Avogadro's constant, } N_A = 6.02 \times 10^{23} \text{ mol}^{-1}$$

The particles may be atoms, molecules, ions, electrons or formula units — you must always state *what* the particles are. The quantity measured in moles is called the **amount of substance**, symbol *n*. The link between an amount and the actual number of particles *N* is:

$$N = n \times N_A \text{ and therefore } n = N / N_A$$

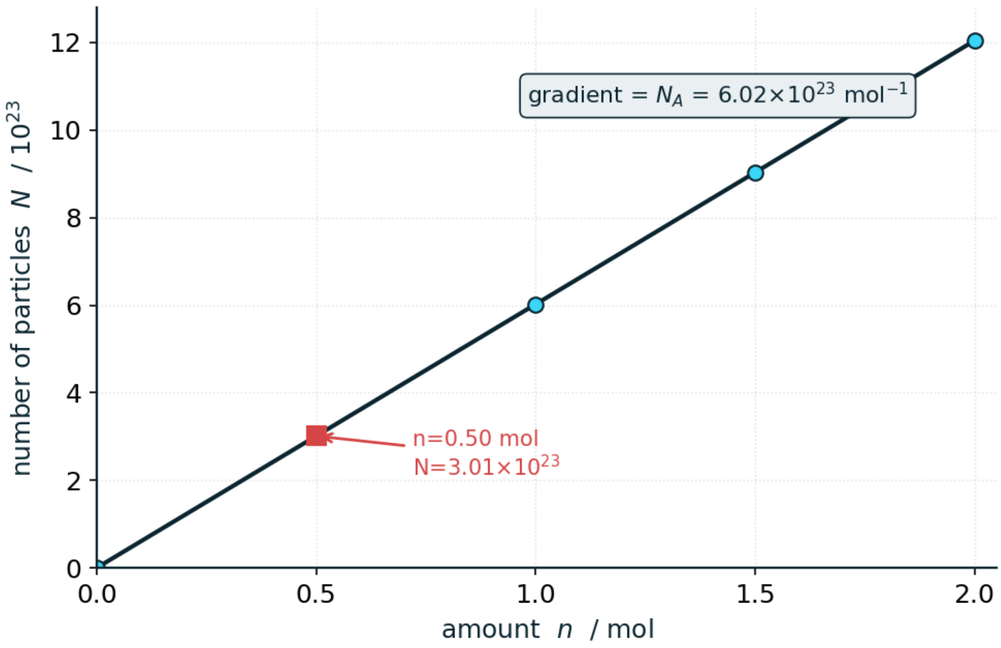

Figure 1. Number of particles is proportional to amount: $N = n \times N_A$. The straight line through the origin has gradient $N_A = 6.02 \times 10^{23}\ mol^{-1}$; at n = 0.50 mol, $N = 3.01 \times 10^{23}$ particles.

So 1 mol of water contains 6.02×10^{23} water molecules; 2 mol of sodium contains $2 \times 6.02 \times 10^{23} = 1.20 \times 10^{24}$ sodium atoms. Because a formula unit is built from several atoms, one mole of a compound contains several moles of atoms — a point worth watching.

Worked example 1 — amount and number of particles

(a) How many atoms are in 0.250 mol of iron? (b) A sample of carbon dioxide contains 3.01×10^{23} molecules. What amount, in mol, is this?

(a) $N = n \times N_A = 0.250 \times 6.02 \times 10^{23}$ = **1.51×10^{23} atoms**.

(b) $n = N / N_A = (3.01 \times 10^{23}) / (6.02 \times 10^{23})$ = **0.500 mol**.

Follow-up: that 0.500 mol of CO_2 contains 0.500 × 3 = 1.50 mol of atoms (one C and two O per molecule), i.e. 9.03×10^{23} atoms in total.

Watch the particles: "How many ions in 1 mol of $MgCl_2$?" is not 1 mole of ions. Each formula unit gives one Mg^{2+} and two Cl^-, so 1 mol of $MgCl_2$ contains 3 mol of ions.

2. Molar mass and the mass–mole link

The **relative atomic mass** A_r of an element is the average mass of its atoms relative to one-twelfth the mass of a carbon-12 atom; it has no units. The **relative formula mass** M_r (called relative molecular mass for molecules) is found by adding the A_r values of every atom in the formula.

The **molar mass** M is the mass of one mole of a substance. Its great convenience is that, numerically, M equals M_r — but molar mass carries the unit g mol^{-1}. For example $M_r(H_2O) = 18.02$, so $M(H_2O) = 18.02$ g mol^{-1}. The central working equation of the whole topic is:

$n = m / M$ (amount = mass in g ÷ molar mass in g mol^{-1})

These three relationships — mass to amount, amount to particles — chain together, letting you convert any of mass, amount and number of particles into any other. Keep the map in your head:

mass (g) ↔ [÷ M] ↔ amount (mol) ↔ [× N_A] ↔ number of particles

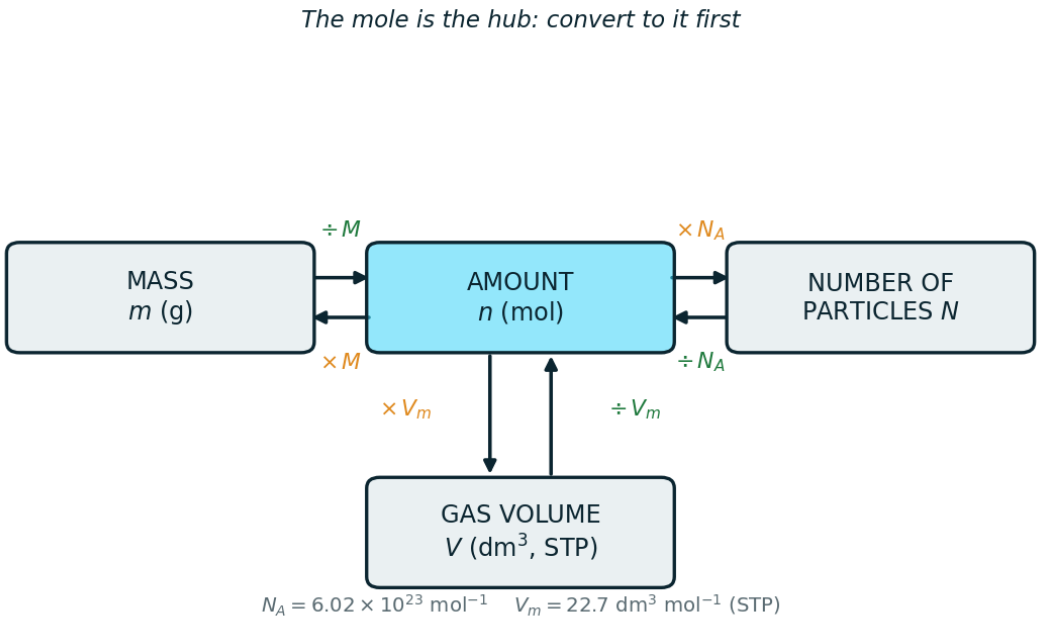

Figure 2. The mole is the hub of every conversion. Divide a mass by the molar mass M to reach moles, then × N_A for particles or × the molar volume V_m = 22.7 dm^3 mol^{-1} for a gas volume at STP; reverse each step with the inverse operation.

Finding a molar mass

Add up the A_r of each atom, multiplied by how many of that atom appear. For hydrated salts, include the water of crystallisation. For example, for $CuSO_4{\cdot}5H_2O$: 63.55 + 32.06 + 4(16.00) + 5(18.02) = 249.71 g mol^{-1}.

Worked example 2 — mass, moles and molecules together

A flask holds 4.40 g of carbon dioxide, CO_2. Find (a) the amount in mol, (b) the number of molecules, (c) the number of oxygen atoms.

$M(CO_2)$ = 12.01 + 2(16.00) = 44.01 g mol^{-1}.

(a) $n = m/M$ = 4.40 / 44.01 = **0.100 mol**.

(b) N = 0.100 × 6.02 × 10^{23} = **6.02 × 10^{22} molecules**.

(c) each molecule has 2 O atoms, so O atoms = 2 × 6.02 × 10^{22} = **1.20 × 10^{23} atoms**.

Worked example 3 — working backwards to a mass

What is the mass of 0.200 mol of sodium hydroxide, NaOH?

M(NaOH) = 22.99 + 16.00 + 1.01 = 40.00 g mol^{-1}.

Rearrange $n = m/M$ to $m = n \times M$ = 0.200 × 40.00 = **8.00 g**.

3. Empirical and molecular formulae

The **empirical formula** is the simplest whole-number ratio of atoms of each element in a compound. The **molecular formula** gives the actual number of atoms in one molecule, and is always a whole-number multiple of the empirical formula. For example glucose is $C_6H_{12}O_6$ (molecular) but CH_2O (empirical); ethane is C_2H_6 but CH_3.

Finding an empirical formula

Whether you are given percentages by mass or actual masses, the recipe is the same:

- 1. Write down the mass (or % treated as grams) of each element.
- 2. Divide each by that element's A_r to get the amount in mol.
- 3. Divide every amount by the smallest of them.
- 4. If the ratios are not yet whole numbers, multiply all by a small integer to clear them.

Worked example 4 — empirical formula from percentages

A compound is 40.0% carbon, 6.7% hydrogen and 53.3% oxygen by mass. Find its empirical formula.

Treat percentages as grams in 100 g:

C: 40.0 / 12.01 = 3.331 mol H: 6.7 / 1.01 = 6.63 mol O: 53.3 / 16.00 = 3.331 mol

Divide by the smallest (3.331): C = 1.00, H = 1.99 ≈ 2, O = 1.00.

Empirical formula = **CH_2O**.

From empirical to molecular formula

You cannot get the molecular formula from composition alone — you also need the relative molecular mass M_r (from, say, a mass spectrum). Find how many empirical units fit inside one molecule:

$$\textbf{whole-number multiple} = M_r \div \textbf{(mass of empirical formula)}$$

Worked example 5 — molecular formula

The compound in Example 4 has M_r = 180. Find its molecular formula.

Mass of the empirical unit CH_2O = 12.01 + 2(1.01) + 16.00 = 30.03.

Multiple = 180 / 30.03 = 5.99 ≈ 6.

Molecular formula = $(CH_2O)_6$ = $\mathbf{C_6H_{12}O_6}$ (glucose).

Percentage composition by mass

The reverse problem — the % by mass of an element in a compound — is often asked in fertiliser and purity questions:

$$\textbf{\% by mass of element} = (\text{total } A_r \text{ of that element} \div M_r) \times 100$$

For instance, the % of nitrogen in ammonium nitrate NH_4NO_3 (M_r = 80.06) is (2 × 14.01 / 80.06) × 100 = 35.0%.

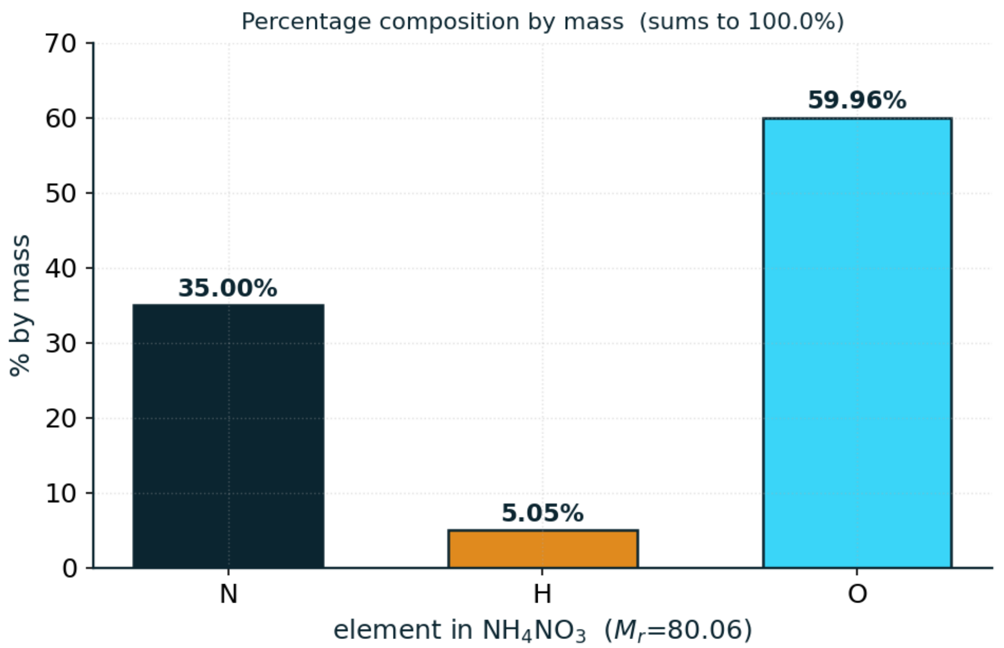

Figure 3. Percentage composition by mass of ammonium nitrate NH_4NO_3: N 35.00%, H 5.05%, O 59.96% — the three shares add to 100%. The nitrogen figure is what fertiliser labels quote.

Common pitfall: Empirical and molecular formulae are not interchangeable. If a question gives you M_r, it almost always wants the molecular formula — stopping at the empirical formula throws away marks.

4. The mole in chemical reactions

A balanced equation is a recipe written in moles. The large coefficients (the **stoichiometric coefficients**) give the ratio in which substances react and form — the **mole ratio**. They say nothing directly about masses, because different substances have different molar masses.

Consider the synthesis of ammonia:

$$N_2(g) + 3H_2(g) \rightarrow 2NH_3(g)$$

This reads: 1 mol of N_2 reacts with 3 mol of H_2 to give 2 mol of NH_3. The ratios 1 : 3 : 2 are the key to every reacting-mass calculation. The standard method is a three-step loop:

- 1. Convert the known mass to an amount with $n = m/M$.
- 2. Use the mole ratio from the equation to find the amount of the substance you want.
- 3. Convert that amount back to a mass with $m = n \times M$.

Worked example 6 — reacting masses

Magnesium burns in oxygen: $2Mg(s) + O_2(g) \rightarrow 2MgO(s)$. Calculate the mass of oxygen that reacts with 4.86 g of magnesium, and the mass of magnesium oxide formed.

Step 1: $n(Mg) = 4.86 / 24.31 = 0.200$ mol.

Step 2: ratio Mg : O_2 : MgO = 2 : 1 : 2. So $n(O_2) = 0.200 / 2 = 0.100$ mol, and $n(MgO) = 0.200$ mol.

Step 3: $m(O_2) = 0.100 \times 32.00 =$ **3.20 g**; $m(MgO) = 0.200 \times 40.31 =$ **8.06 g**.

Check: mass is conserved, 4.86 + 3.20 = 8.06 g. ✓

5. Limiting reagent, yield and atom economy

When reactants are not mixed in the exact ratio of the equation, one runs out first and stops the reaction. That reactant is the **limiting reagent**; it determines how much product can form. The others are in **excess** and some is left over.

To find the limiting reagent, convert every reactant to moles, then divide each amount by its coefficient in the equation. The smallest result marks the limiting reagent. Always base product calculations on the limiting reagent.

Worked example 7 — limiting reagent and percentage yield

In the Haber process 28.0 g of N_2 is mixed with 10.0 g of H_2: $N_2 + 3H_2 \rightarrow 2NH_3$. (a) Identify the limiting reagent. (b) Find the theoretical mass of ammonia. (c) If 24.0 g of NH_3 is actually collected, find the percentage yield.

$n(N_2) = 28.0 / 28.02 = 1.00$ mol; $n(H_2) = 10.0 / 2.02 = 4.95$ mol.

Divide by coefficients: $N_2 \rightarrow 1.00 / 1 = 1.00$; $H_2 \rightarrow 4.95 / 3 = 1.65$. The smaller is N_2, so **N_2 is limiting** (hydrogen is in excess).

(b) $n(NH_3) = 2 \times n(N_2) = 2.00$ mol; $m = 2.00 \times 17.04 =$ **34.1 g** (theoretical yield).

(c) percentage yield = $(24.0 / 34.1) \times 100 =$ **70.4%**.

Percentage yield and atom economy

These two measures answer different questions. **Percentage yield** asks how much of the possible product you actually obtained — it measures the efficiency of a particular experiment. **Atom economy** asks how much of the reactant mass ends up in the useful product rather than in waste — it measures how green the reaction is in principle. A reaction can have a high yield yet a poor atom economy.

$$\textbf{\% yield = (actual yield ÷ theoretical yield)} \times \textbf{100}$$

$$\textbf{\% atom economy} = (\mathbf{M_r}\textbf{ of desired product ÷ sum of }\mathbf{M_r}\textbf{ of all products}) \times \mathbf{100}$$

Worked example 8 — atom economy

Iron is extracted in the blast furnace by $Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$. Calculate the atom economy for producing iron.

Desired product: 2Fe = 2 × 55.85 = 111.70.

All products: $2Fe + 3CO_2$ = 111.70 + 3(44.01) = 111.70 + 132.03 = 243.73.

Atom economy = (111.70 / 243.73) × 100 = **45.8%**. The rest of the mass leaves as CO_2.

6. Concentration of solutions

The **concentration** of a solution is the amount of solute dissolved per unit volume of solution. Square brackets, e.g. [HCl], denote concentration in mol dm^{-3}. Two units are used:

$$\boldsymbol{c = n / V} \textbf{ (in mol dm}^{-3}\textbf{, with } \boldsymbol{V} \textbf{ in dm}^{3}\textbf{) mass concentration = } \boldsymbol{m / V} \textbf{ (in g dm}^{-3}\textbf{)}$$

The two are linked by the molar mass: concentration in g dm^{-3} = concentration in mol dm^{-3} × *M*. The single most common slip in the whole topic is the volume unit: **1 dm^3 = 1000 cm^3**, so always divide a volume in cm^3 by 1000 before using it.

Worked example 9 — concentration and dilution

(a) 5.85 g of sodium chloride is dissolved to make 250 cm^3 of solution. Find the concentration in mol dm^{-3}. (b) 25.0 cm^3 of this solution is then diluted to 100.0 cm^3. Find the new concentration.

(a) *M*(NaCl) = 22.99 + 35.45 = 58.44 g mol^{-1}; *n* = 5.85 / 58.44 = 0.100 mol. *V* = 250 / 1000 = 0.250 dm^3.

$c = n/V$ = 0.100 / 0.250 = **0.400 mol dm^{-3}**.

(b) Dilution keeps the amount of solute constant, so $\boldsymbol{c_1V_1 = c_2V_2}$:

c_2 = (0.400 × 25.0) / 100.0 = **0.100 mol dm^{-3}**. Diluting fourfold cuts the concentration to a quarter, as expected.

Parts per million (ppm)

Very dilute concentrations, such as pollutants in water, are quoted in **parts per million**: the mass of solute per million units of the same mass of solution. Since 1 dm^3 of dilute aqueous solution has a mass close to 1000 g, 1 ppm ≈ 1 mg per dm^3.

$$\textbf{ppm} = \textbf{(mass of solute} \div \textbf{mass of solution)} \times 10^6$$

7. Volumetric analysis (titrations)

A titration measures the volume of one solution that exactly reacts with a known volume of another, allowing an unknown concentration to be found. In an acid–base titration the end point is shown by an indicator. The calculation is simply a reacting-mole problem in which amounts come from $n = c \times V$:

- 1. Find the amount of the known solution: $n = c \times V$ (V in dm^3).
- 2. Use the equation's mole ratio to find the amount of the unknown.
- 3. Divide by its volume to get its concentration: $c = n / V$.

Worked example 10 — acid–base titration

25.00 cm^3 of sodium hydroxide solution is exactly neutralised by 22.40 cm^3 of 0.100 mol dm^{-3} hydrochloric acid. Find the concentration of the NaOH.

Equation: $NaOH + HCl \rightarrow NaCl + H_2O$ (ratio 1 : 1).

$n(\text{HCl}) = c \times V = 0.100 \times (22.40 / 1000) = 2.240 \times 10^{-3}$ mol.

Ratio 1 : 1, so $n(\text{NaOH}) = 2.240 \times 10^{-3}$ mol.

$c(\text{NaOH}) = n/V = (2.240 \times 10^{-3}) / (25.00 / 1000) =$ **0.0896 mol dm^{-3}**.

Ratio matters: For $H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$ the ratio is 1 : 2, so the amount of acid is *half* the amount of alkali. Read the coefficients before dividing — not every neutralisation is 1 : 1.

8. Gas volumes in reactions

Avogadro's law states that equal volumes of gases, measured at the same temperature and pressure, contain equal numbers of molecules. A powerful consequence follows: for reacting gases, the mole ratio is also the ratio of gas volumes. So in $N_2 + 3H_2 \rightarrow 2NH_3$, 50 cm^3 of nitrogen reacts with 150 cm^3 of hydrogen to give 100 cm^3 of ammonia — no molar masses needed.

Because one mole of any gas occupies the same volume under the same conditions, we define the **molar volume** V_m. At STP (273 K and 100 kPa) the molar volume of an ideal gas is 22.7 dm^3 mol^{-1} (given in the data booklet). This provides a direct mass–volume bridge for gases:

$$\boldsymbol{n = V / V_m} \textbf{ (at STP: } \boldsymbol{n = V} \textbf{ in } \mathbf{dm^3} \div \textbf{22.7)}$$

Worked example 11 — volume of gas produced

Calculate the volume of carbon dioxide, measured at STP, produced when 10.0 g of calcium carbonate is fully decomposed: $CaCO_3(s) \rightarrow CaO(s) + CO_2(g)$.

$M(CaCO_3) = 40.08 + 12.01 + 3(16.00) = 100.09\ g\ mol^{-1}$.

$n(CaCO_3) = 10.0 / 100.09 = 0.0999$ mol; ratio 1 : 1, so $n(CO_2) = 0.0999$ mol.

$V = n \times V_m = 0.0999 \times 22.7 =$ **2.27 dm³** ($2270\ cm^3$).

(HL) Beyond STP: When a gas is not at STP you cannot use a fixed molar volume. Use the ideal gas equation $pV = nRT$ instead (Structure 1.5), with p in Pa, V in m^3, T in K and R = 8.31 $J\ K^{-1}\ mol^{-1}$.

9. Common pitfalls

- Stopping at the empirical formula when M_r is given and the molecular formula is wanted.
- Treating grams as though they were moles — always convert with $n = m/M$ first.
- Forgetting the mole ratio: coefficients in the equation must be used, not a blind 1 : 1.
- Volume unit errors: mixing cm^3 and dm^3 (divide cm^3 by 1000).
- Basing yield or product amounts on the excess reagent instead of the limiting reagent.
- Counting molecules when the question asks for atoms or ions (multiply by the number in the formula).
- Using $V_m = 22.7\ dm^3\ mol^{-1}$ for a gas not at STP, or for a solid/liquid.
- Quoting more significant figures than the data allow (3 s.f. is usually right).

10. Quick reference — formulae

Quantity wanted	Formula
Number of particles	$N = n \times N_A$ ($N_A = 6.02 \times 10^{23}\ mol^{-1}$)
Amount from mass	$n = m / M$
Mass from amount	$m = n \times M$
Molecular formula	molecular = empirical × (M_r ÷ empirical mass)
% by mass of element	(total A_r of element ÷ M_r) × 100
Percentage yield	(actual ÷ theoretical yield) × 100
Atom economy	(M_r desired product ÷ M_r all products) × 100
Concentration	$c = n / V$ ($mol\ dm^{-3}$, V in dm^3)
Dilution	$c_1V_1 = c_2V_2$
Amount of gas at STP	$n = V / 22.7$ (V in dm^3)

Useful constants: $N_A = 6.02 \times 10^{23}$ mol^{-1}; molar volume at STP = 22.7 dm^3 mol^{-1}; 1 dm^3 = 1000 cm^3. All are in the IB data booklet.

11. Test yourself

Attempt all ten without notes, then check against the full worked solutions that follow. Use A_r values to 2 decimal places.

1. Calculate the number of atoms in 12.0 g of magnesium (A_r = 24.31).

2. Find the mass of 0.150 mol of sodium carbonate, Na_2CO_3.

3. A hydrocarbon is 82.7% C and 17.3% H by mass and has M_r = 58. Find its molecular formula.

4. What mass of calcium oxide forms when 25.0 g of calcium carbonate is fully heated? $CaCO_3 \rightarrow CaO + CO_2$.

5. 8.00 g of sodium hydroxide is dissolved and made up to 500 cm^3. Find the concentration in mol dm^{-3}.

6. What volume of a 0.250 mol dm^{-3} solution contains 0.0500 mol of solute?

7. For $2H_2 + O_2 \rightarrow 2H_2O$, what volume of oxygen at STP reacts exactly with 4.00 g of hydrogen?

8. 20.00 cm^3 of sulfuric acid is neutralised by 25.60 cm^3 of 0.150 mol dm^{-3} NaOH. $H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$. Find the concentration of the acid.

9. In $4Fe + 3O_2 \rightarrow 2Fe_2O_3$, 11.2 g of iron reacts with 6.00 g of oxygen. Identify the limiting reagent and find the mass of Fe_2O_3 formed.

10. Calculate the percentage by mass of nitrogen in ammonium nitrate, NH_4NO_3.

Worked answers

1. n = 12.0 / 24.31 = 0.4936 mol; N = 0.4936 × 6.02 × 10^{23} = **2.97 × 10^{23} atoms**.

2. $M(Na_2CO_3)$ = 2(22.99) + 12.01 + 3(16.00) = 105.99 g mol^{-1}; m = 0.150 × 105.99 = **15.9 g**.

3. C: 82.7 / 12.01 = 6.886; H: 17.3 / 1.01 = 17.13. Divide by 6.886: C = 1, H = 2.49, so × 2 gives C_2H_5 (empirical mass 29.07). 58 / 29.07 = 2.0, so molecular formula = **C_4H_{10}**.

4. $n(CaCO_3)$ = 25.0 / 100.09 = 0.2498 mol; ratio 1 : 1, so n(CaO) = 0.2498 mol. m = 0.2498 × 56.08 = **14.0 g**.

5. M(NaOH) = 40.00 g mol^{-1}; n = 8.00 / 40.00 = 0.200 mol; V = 0.500 dm^3; c = 0.200 / 0.500 = **0.400 mol dm^{-3}**.

6. $V = n / c$ = 0.0500 / 0.250 = 0.200 dm^3 = **200 cm^3**.

7. $n(H_2)$ = 4.00 / 2.02 = 1.98 mol; ratio $H_2 : O_2$ = 2 : 1, so $n(O_2)$ = 0.990 mol. V = 0.990 × 22.7 = **22.5 dm^3**.

8. n(NaOH) = 0.150 × (25.60 / 1000) = 3.84 × 10^{-3} mol; ratio 2 : 1, so $n(H_2SO_4)$ = 1.92 × 10^{-3} mol. c = 1.92 × 10^{-3} / (20.00 / 1000) = **0.0960 mol dm^{-3}**.

9. n(Fe) = 11.2 / 55.85 = 0.2005 mol; $n(O_2)$ = 6.00 / 32.00 = 0.1875 mol. Divide by coefficients: Fe → 0.2005 / 4 = 0.0501; O_2 → 0.1875 / 3 = 0.0625. Smaller is Fe, so **Fe is limiting**. $n(Fe_2O_3)$ = 0.2005 × 2/4 = 0.1003 mol; M = 159.70; m = 0.1003 × 159.70 = **16.0 g**.

10. $M(NH_4NO_3)$ = 2(14.01) + 4(1.01) + 3(16.00) = 80.06; N is 2 × 14.01 = 28.02. % = (28.02 / 80.06) × 100 = **35.0%**.