Atoms, molecules and stoichiometry

Relative masses, the mole and the Avogadro constant, writing formulas and equations, empirical and molecular formulas, and reacting-mass, gas-volume and solution calculations.

2.1 Relative masses of atoms and molecules

The **unified atomic mass unit** (u) is one twelfth of the mass of one atom of carbon-12.

- **Relative atomic mass**, A_r: the weighted mean mass of an atom of the element compared with one twelfth of the mass of a carbon-12 atom.
- **Relative isotopic mass**: the mass of an atom of an isotope compared with one twelfth of the mass of a carbon-12 atom.
- **Relative molecular mass**, M_r: the weighted mean mass of a molecule compared with one twelfth of the mass of a carbon-12 atom. For ionic compounds use **relative formula mass**.

None of these has units.

Weighted averages and the meaning of molar mass

Relative mass is a ratio, whereas molar mass is the mass of one mole and has units. A sample with $M_r = 44.0$ has a molar mass of 44.0 g mol^{-1} when expressed in grams. An ionic lattice has no separate molecules, so speak of formula units and relative formula mass for NaCl rather than "NaCl molecules".

Worked example: a fictional element has isotope masses 62.0 and 64.0 with abundances 70.0% and 30.0%. Its $A_r = (62.0 \times 70.0 + 64.0 \times 30.0)/100 = 62.6$. If the average were 62.4 instead, let the fraction of the lighter isotope be x: $62x + 64(1 - x) = 62.4$, giving $x = 0.800$. Thus the lighter isotope is 80.0% abundant. A simple average is valid only for equal abundances.

> **TRY IT**
>
> An element has equal amounts of isotopes of relative masses 10.0 and 11.0. Find its relative atomic mass, and explain whether an individual atom can have that nucleon number.

Answer: $A_r = 10.5$, without units. Individual atoms have integer nucleon numbers; 10.5 is the sample's weighted mean relative mass.

2.2 The mole and the Avogadro constant

One **mole** of a substance contains 6.02×10^{23} particles (atoms, molecules, ions or electrons). This number per mole is the **Avogadro constant**, $L = 6.02 \times 10^{23}$ mol^{-1}.

Note Academy

$n = \frac{m}{M_r} \qquad N = nL$

The molar mass is in g mol^{-1}.

Count the specified particles

A mole is an amount, not a mass or a volume. Always identify the entities being counted. One mole of O_2 contains one mole of molecules but two moles of oxygen atoms. One mole of $MgCl_2$ contains one mole of formula units and, when fully dissociated, gives one mole of magnesium ions and two moles of chloride ions.

Worked example: 4.40 g CO_2 has $n = 4.40/44.0 = 0.100$ mol molecules. It therefore contains 6.02×10^{22} molecules, 1.20×10^{23} oxygen atoms and 1.81×10^{23} atoms in total. Multiply the number of molecules by the number of relevant atoms **per molecule**; do not divide by the atomic mass again.

> **TRY IT**
>
> How many chloride ions are produced by complete dissociation of 0.0250 mol $CaCl_2$?

Answer: $n(Cl^-) = 2(0.0250) = 0.0500$ mol, so $N = 0.0500(6.02 \times 10^{23}) = 3.01 \times 10^{22}$ ions.

2.3 Formulas

Ions and ionic formulas

Predict the ionic charge from the group: Group 1 gives +1, Group 2 +2, Group 13 +3, Group 15 −3, Group 16 −2 and Group 17 −1. A Roman numeral gives the oxidation number, so iron(III) is Fe^{3+}. Know these ions:

$NO_3^-, CO_3^{2-}, SO_4^{2-}, PO_4^{3-}, HCO_3^-, OH^-, NH_4^+, Zn^{2+}, Ag^+$.

Balance the charges: aluminium sulfate is $Al_2(SO_4)_3$.

Equations

A balanced equation has the same number of each atom (and the same total charge) on both sides, with state symbols (s), (l), (g) and (aq). In **ionic equations** leave out the **spectator ions**.

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

Note Academy

Empirical and molecular formulas

The **empirical formula** is the simplest whole-number ratio of the atoms of each element in a compound. The **molecular formula** is the actual number of atoms in a molecule.

> TRY IT
>
> A compound is 40.0% C, 6.7% H and 53.3% O by mass, with $M_r = 180$. Find its empirical and molecular formulas.

Divide by A_r: C 3.33, H 6.7, O 3.33. Divide by the smallest: C 1, H 2, O 1. The empirical formula is CH_2O (mass 30). Since $180/30 = 6$, the molecular formula is $C_6H_{12}O_6$.

A **hydrated** salt contains **water of crystallisation**; the **anhydrous** salt has none. For $CuSO_4 \cdot xH_2O$, find x from the ratio of the moles of H_2O lost to the moles of anhydrous salt left.

Empirical-formula and hydrate calculations

Mass percentages describe masses, not atom ratios. Assume 100 g if only percentages are given, divide each mass by the appropriate atomic mass, then divide all mole amounts by the smallest. If the ratios are 1 : 1.5, multiply **both** by two; rounding 1.5 to two changes the compound. The empirical-formula mass must divide the molecular mass by a positive integer before a molecular formula is assigned.

Worked example — hydrate: heating 2.50 g of a hydrated salt leaves 1.60 g anhydrous $CuSO_4$ ($M_r = 160$). Water lost is 0.90 g, or $0.90/18.0 = 0.050$ mol. Anhydrous salt is $1.60/160 = 0.0100$ mol. Their ratio is 5 : 1, giving $CuSO_4 \cdot 5H_2O$. Use the **mass lost** for water and the final residue for the salt. The interpretation assumes only water is lost and the salt itself does not decompose.

When an ionic formula is needed, balance total charges in their smallest ratio. For calcium phosphate, three Ca^{2+} ions balance two PO_4^{3-} ions, giving $Ca_3(PO_4)_2$. Brackets apply to the whole polyatomic ion. In ionic equations, cancel ions only if they remain chemically unchanged and in the same state; do not cancel the ions making up a precipitate.

> TRY IT
>
> A compound contains 2.40 g Mg and 1.60 g O. Find its empirical formula using $A_r(Mg) = 24.0$ and $A_r(O) = 16.0$.

Answer: Each amount is 0.100 mol, so the ratio is 1 : 1 and the formula is MgO. The unequal masses do not mean unequal atom numbers.

2.4 Reacting masses and volumes (of solutions and gases)

Use the mole ratio in the balanced equation.

Note Academy

- **Solutions:** $n = cV$, with c in mol dm^{-3} and V in dm^3 (cm^3 ÷ 1000).
- **Gases:** at room temperature and pressure (rtp) one mole of any gas occupies **24 dm^3** (24 000 cm^3). At other conditions use $pV = nRT$.
- **Percentage yield** $= \dfrac{\text{actual yield}}{\text{theoretical yield}} \times 100$.
- The **limiting reagent** is used up first and decides the amount of product. The other reagent is in **excess**.

> **TRY IT**
>
> 2.00 g of $CaCO_3$ reacts with 50.0 cm^3 of 1.00 mol dm^{-3} HCl. What volume of CO_2 forms at rtp?

$CaCO_3 + 2HCl \rightarrow CaCl_2 + H_2O + CO_2$. Moles of $CaCO_3 = 2.00/100 = 0.0200$. Moles of HCl $= 0.0500$, which would need 0.0250 mol $CaCO_3$, so $CaCO_3$ is limiting. $V = 0.0200 \times 24 = 0.480$ dm^3.

> **Significant figures: give the final answer to the same number of significant figures as the least precise data in the question, or the number asked for. Do not round during the working; round only at the end.**

You can also deduce **stoichiometric relationships** from data. If 0.0100 mol of A reacts with 0.0300 mol of B, the ratio is 1 : 3.

A reliable sequence for quantitative questions

Write and balance the reaction first. Convert every supplied quantity into moles, use the equation to compare amounts, and finally convert the relevant product moles into the requested mass, volume or concentration. Coefficients relate **moles**, never gram masses directly. The ratio applies to gases by volume only when their temperature and pressure are the same.

Worked example — titration: 25.0 cm^3 H_2SO_4 requires 20.0 cm^3 of 0.150 mol dm^{-3} NaOH for complete neutralisation. The equation is $H_2SO_4 + 2NaOH \rightarrow Na_2SO_4 + 2H_2O$. Moles NaOH are $0.150(0.0200) = 0.00300$; moles acid are half this, 0.00150. Acid concentration is $0.00150/0.0250 = 0.0600$ mol dm^{-3}. State the 1 : 2 relationship explicitly so the factor of two is visible.

Worked example — back titration: 1.00 g of an impure $CaCO_3$ sample is treated with 25.0 cm^3 of 1.00 mol dm^{-3} HCl. The excess acid requires 10.0 cm^3 of 0.500 mol dm^{-3} NaOH. Initially HCl is 0.0250 mol; excess HCl is $0.0100(0.500) = 0.00500$ mol. The carbonate consumed 0.0200 mol HCl, hence 0.0100 mol $CaCO_3$, or 1.00 g using $M_r = 100$. Under these illustrative data the sample is 100% carbonate. A different residue mass would change the calculated purity; do not treat the excess acid as the acid consumed by carbonate.

Note Academy

Worked example — yield: 0.0500 mol of a limiting reactant should give 0.0500 mol of a product with molar mass 88.0 g mol^{-1}. The theoretical mass is 4.40 g. Recovering 3.30 g gives $3.30/4.40 \times 100 = 75.0\%$ yield. A yield over 100% suggests impurities, retained solvent or a measurement/calculation error, not creation of extra product.

For dilution of an unreacted solute, moles are conserved: $c_1V_1 = c_2V_2$. Mixing reacting solutions requires a reaction calculation first; this dilution shortcut alone cannot account for a reagent being consumed.

> **TRY IT**
>
> 10.0 cm^3 of 0.200 mol dm^{-3} sodium carbonate completely neutralises an acid. Find the moles of HCl required and the volume of 0.100 mol dm^{-3} HCl needed.

Answer: $Na_2CO_3 + 2HCl \rightarrow 2NaCl + CO_2 + H_2O$. Carbonate is 0.00200 mol, requiring 0.00400 mol HCl. Volume $= n/c = 0.0400$ dm³ = **40.0 cm³**.

Exam check: show conversions, the mole ratio and the final units. For a limiting-reagent question compare $n/\text{coefficient}$ for each reagent. For a practical calculation, distinguish a measured titre from the total volume in the flask, and use the mean of concordant titres rather than automatically averaging a rough result.

References and further reading

Scope follows section 2 of the **Cambridge 9701 syllabus for 2025–2027**. **Chemguide's Cambridge topic index** links to alternative explanations. The worked exercises and added diagrams are original teaching examples; numerical examples are illustrative unless a specific source is identified.

Note Academy