

Atoms, molecules and stoichiometry

A-Level Chemistry 9701 · Topic 2 revision notes

Everything from the 7 lessons of this topic on a few pages: the key idea of each lesson, the diagram to remember, the points to learn and the traps examiners set. Read it, cover it, test yourself.

1. Relative masses

2. The mole and the Avogadro constant

3. Formulae and equations

4. Empirical and molecular formulae

5. Reacting masses and limiting reagents

6. Volumes of gases

7. Solutions and titrations

1 Relative masses

Syllabus 2.1

All relative masses are measured against 1/12 of the mass of one atom of carbon-12 (the unified atomic mass unit, u). Relative isotopic mass is the mass of one atom of an isotope on that scale. Relative atomic mass A_r is the **weighted mean** mass of the atoms of an element. Relative molecular mass M_r adds the A_r values in a molecule; for giant ionic compounds the same sum is called relative formula mass. None of them has units.

abundance / %

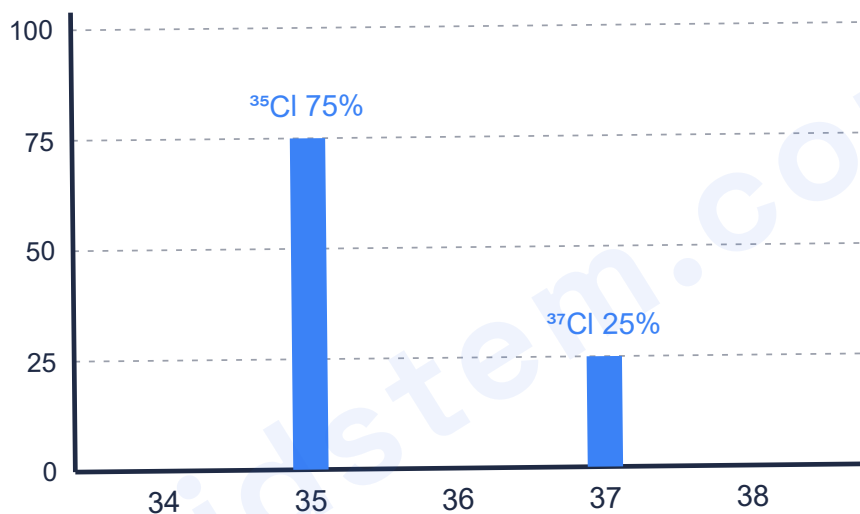


Fig. 1: the mass spectrum of chlorine atoms and the weighted mean it gives

Everything is compared with carbon-12.

- ✓ **Standard:** 1/12 of the mass of one ^{12}C atom.
- ✓ **A_r :** sum of (mass $\times$ abundance) $\div$ total abundance.
- ✓ **M_r :** add the A_r values; a number outside a bracket multiplies everything inside.
- ✓ **No units:** relative masses are ratios.

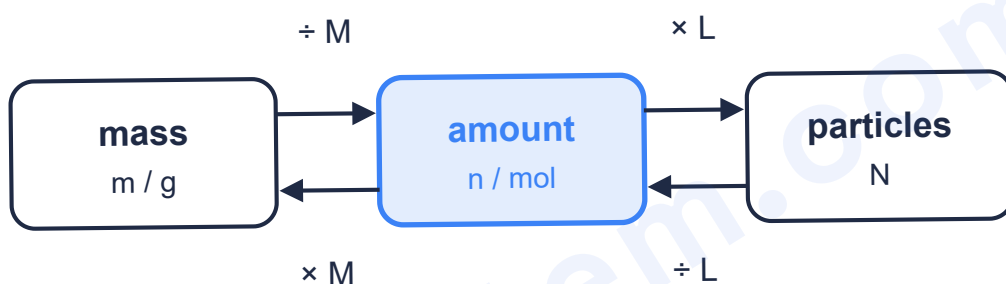
Watch out!

A molecule such as Cl_2 gives **three** molecular ion peaks, at m/z 70, 72 and 74, because each atom can be either isotope. With 75% ^{35}Cl and 25% ^{37}Cl the chances are 0.75×0.75 , $2 \times 0.75 \times 0.25$ and 0.25×0.25 , a ratio of 9 : 6 : 1. Do not forget the factor of 2 for the mixed molecule, which can form two ways.

2 The mole and the Avogadro constant

Syllabus 2.2

One mole is the amount of substance that contains 6.02×10^{23} particles, the Avogadro constant L . That number is chosen so that one mole of carbon-12 atoms has a mass of exactly 12 g, which makes the molar mass M of any substance in g mol^{-1} numerically equal to its relative mass. So $n = m \div M$ and $N = n \times L$. Always say which particle you are counting: atoms, molecules, ions or formula units.



M = molar mass in g mol^{-1} ; $L = 6.02 \times 10^{23} \text{ mol}^{-1}$

every route between mass and particles goes through the mole

Fig. 1: the mole sits between mass and number of particles

Go through the mole every time.

- ✓ **$n = m \div M$** with m in grams and M in g mol^{-1} .
- ✓ **$N = n \times L$** with $L = 6.02 \times 10^{23} \text{ mol}^{-1}$.
- ✓ **Name the particle:** atoms, molecules, ions or formula units.
- ✓ **Multiply up** by the number of atoms or ions in each formula.

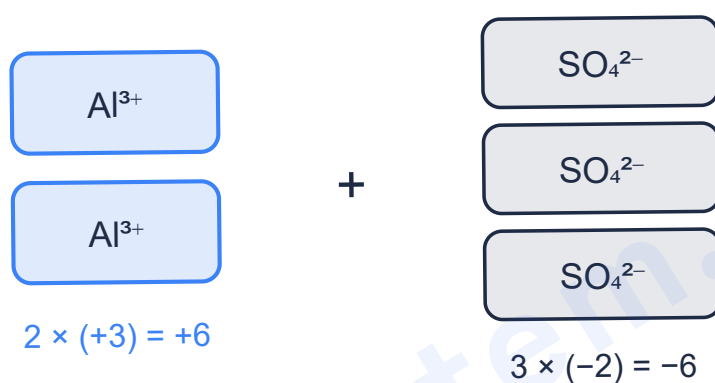
Watch out!

When a question asks for the number of **atoms** or **ions**, multiply the number of formula units by how many of that particle each one contains. 0.100 mol of MgCl_2 contains 0.200 mol of chloride ions, not 0.100 mol.

3 Formulae and equations

Syllabus 2.3

In an ionic compound the total positive charge equals the total negative charge, so Al^{3+} and SO_4^{2-} combine 2 : 3 as $\text{Al}_2(\text{SO}_4)_3$. A balanced equation has the same number of each atom on both sides; balance only with the large numbers in front, never by changing a formula. An ionic equation shows only the species that change, and its charges must balance as well as its atoms.



total charge 0, so the formula is $\text{Al}_2(\text{SO}_4)_3$

Fig. 1: charges cancel to fix the formula of aluminium sulfate

Formula first, balance second.

- ✓ **Ionic formula:** total positive charge = total negative charge.
- ✓ **Brackets** round a polyatomic ion when there is more than one.
- ✓ **Balance with coefficients only;** leave O and H to last in combustion.
- ✓ **Ionic equation:** drop spectators; atoms and charge must both balance.

Watch out!

Never balance an equation by changing a subscript. Writing H_2O_2 to make $\text{H}_2 + \text{O}_2 \rightarrow \text{H}_2\text{O}$ balance turns water into hydrogen peroxide, a different substance. And an ionic equation that balances atoms but not charge is still wrong: check the total charge on each side.

4 Empirical and molecular formulae

Syllabus 2.3

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 of each element in one molecule. To find the empirical formula, divide each mass or percentage by A_r and then divide by the smallest answer. The molecular formula is $n \times$ the empirical formula, where $n = M_r \div \text{empirical formula mass}$.

step	C	H	O
% by mass	40.0	6.7	53.3
$\div A_r$	3.33	6.7	3.33
$\div$ smallest	1.00	2.01	1.00
ratio	1	2	1

empirical formula CH_2O (mass 30.0)

$M_r = 180$, so $n = 180 \div 30.0 = 6$: molecular formula $\text{C}_6\text{H}_{12}\text{O}_6$

Fig. 1: from percentages to glucose in four steps

Divide, divide, scale.

- ✓ **Divide by A_r** , then by the smallest value.
- ✓ **Scale** ratios ending in .5, .33 or .67; never round them away.
- ✓ **$n = M_r \div \text{empirical formula mass}$** gives the molecular formula.
- ✓ **Combustion:** C from CO_2 (12/44), H from H_2O (2/18), O by difference.

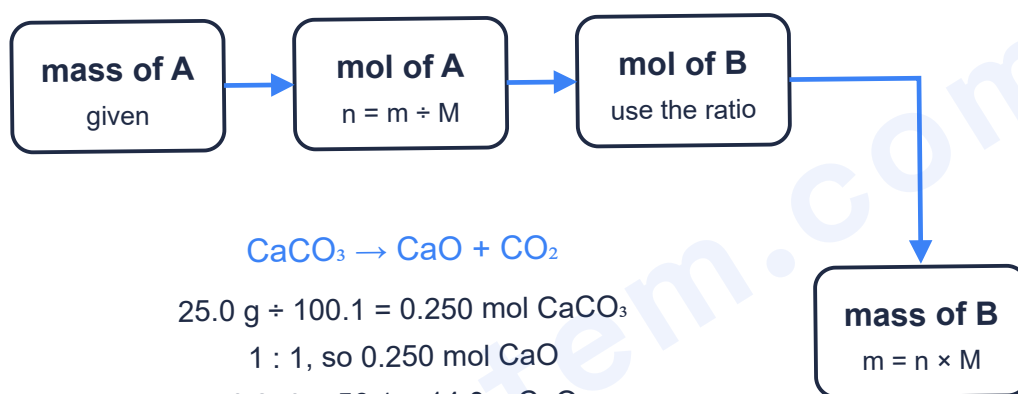
Watch out!

Do not round a ratio like 1 : 1.5 to 1 : 2 or 1 : 1.33 to 1 : 1. Those are real ratios of 2 : 3 and 3 : 4, and rounding them early gives the wrong formula (Fe_2O_3 is 1 : 1.5). In the hydrate experiment, heat to **constant mass**: if some water remains, the water lost is too small and x comes out too low.

5 Reacting masses and limiting reagents

Syllabus 2.4

Mass of A $\rightarrow$ moles of A (divide by M) $\rightarrow$ moles of B (use the equation's ratio) $\rightarrow$ mass of B (multiply by M). The limiting reagent is the reactant that is completely used up; it sets the maximum amount of product, and the other reactant is in excess. Percentage yield = actual yield $\div$ theoretical yield $\times 100$, with the theoretical yield calculated from the limiting reagent.



you never compare masses directly: the equation counts particles

Fig. 1: the three-step route through the mole

Moles in, ratio, moles out.

- ✓ **Mass** $\rightarrow$ **moles**: $n = m \div M$.
- ✓ **Ratio**: from the balanced equation, never from masses.
- ✓ **Limiting reagent**: smallest (moles $\div$ coefficient).
- ✓ **% yield** = actual $\div$ theoretical (from the limiting reagent) $\times 100$.

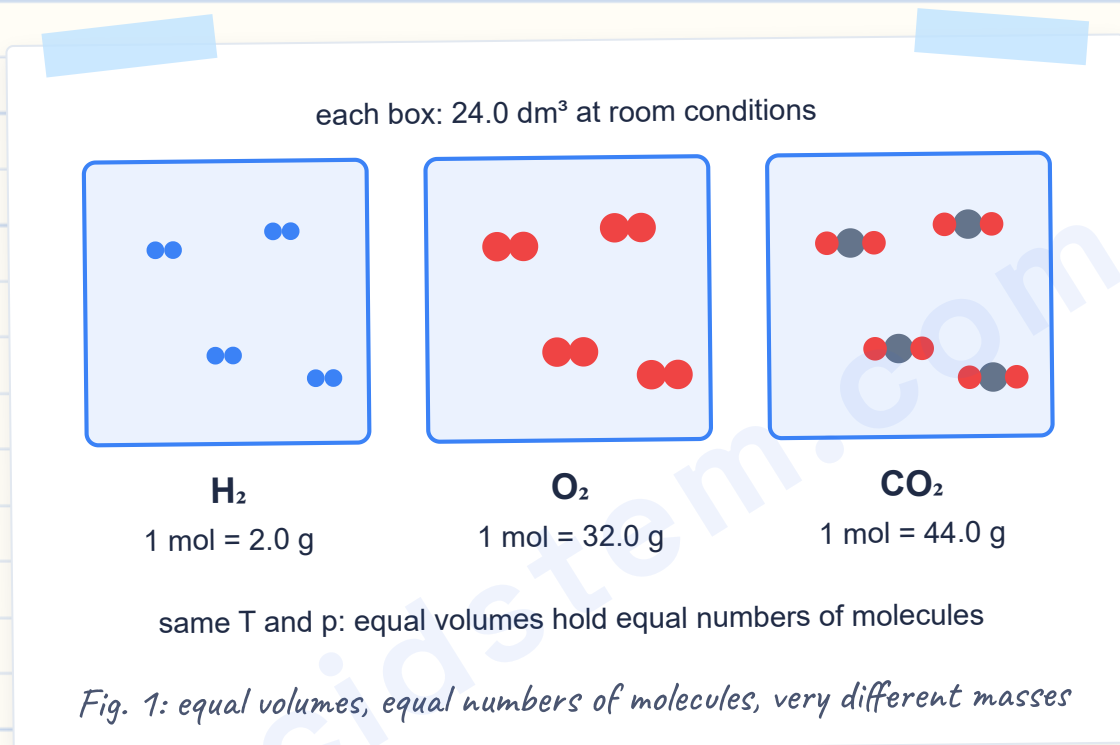
Watch out!

Use the ratio from the equation, not a ratio of masses, and always work the theoretical yield from the **limiting** reagent. If you use the reagent in excess, the answer will be too big and the percentage yield too small.

6 Volumes of gases

Syllabus 2.4

Equal volumes of gases at the same temperature and pressure contain equal numbers of molecules. So one mole of any gas occupies the same volume: 24.0 dm^3 at room conditions, the Data Booklet value. Amount of gas $n = V \div 24.0$ with V in dm^3 (or $V \div 24\,000$ with V in cm^3). For reactions between gases, the volume ratio equals the mole ratio in the equation.



Same T and p, same volume per mole.

- ✓ **$n = V \div 24.0$** with V in dm^3 at room conditions.
- ✓ **cm^3 to dm^3 :** divide by 1000.
- ✓ **Gas reactions:** volume ratio = mole ratio.
- ✓ **Combustion:** water is liquid; NaOH removes CO_2 .

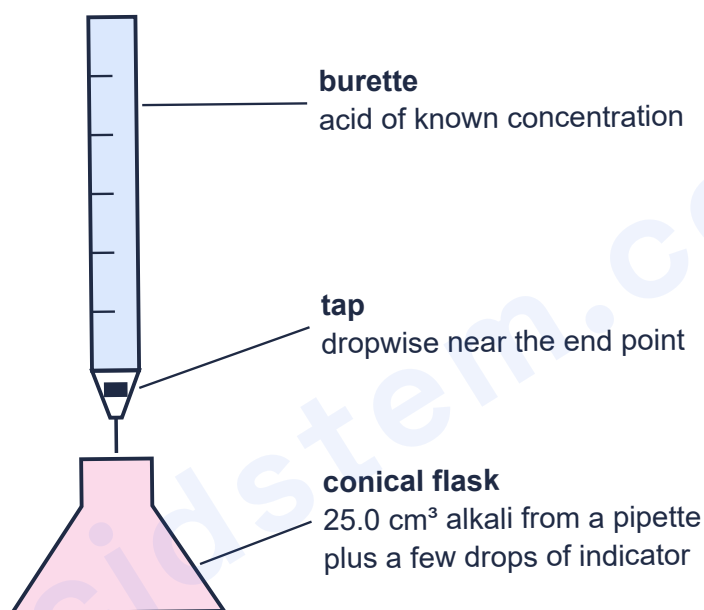
Watch out!

Watch the units: $1 \text{ dm}^3 = 1000 \text{ cm}^3$, so use 24.0 with dm^3 and 24 000 with cm^3 . Water formed in a combustion reaction is a liquid at room temperature, so it does **not** count in the final gas volume. And the molar volume applies only to gases, never to solids, liquids or solutions.

7 Solutions and titrations

Syllabus 2.4

Concentration $c = n \div V$, in mol dm^{-3} with V in dm^3 . So $n = c \times V$, remembering that V in cm^3 must be divided by 1000. Concentration in $\text{g dm}^{-3} = c \times M$. In a titration: find the moles of the solution of known concentration, use the mole ratio from the equation, then divide by the volume of the other solution. Use the mean of concordant titres, those within 0.10 cm^3 of each other.



titre = final – initial reading; repeat until two agree within 0.10 cm^3

Fig. 1: an acid-base titration

$$n = c \times V, \text{ with } V \text{ in } \text{dm}^3.$$

- ✓ **$\text{cm}^3 \rightarrow \text{dm}^3$:** divide by 1000.
- ✓ **Known solution first:** moles, then the equation's ratio.
- ✓ **Scale up** if the titrated sample was a fraction of a larger volume.
- ✓ **Mean of concordant titres** only, within 0.10 cm^3 .

Watch out!

Two slips cost the most marks: using a volume in cm^3 as if it were in dm^3 (answers 1000 times too big), and ignoring the mole ratio when the acid is diprotic, as with H_2SO_4 . Also leave out the rough titre and any titre not within 0.10 cm^3 of the others when you take the mean.