Atoms, molecules and stoichiometry

A-Level Chemistry

Relative masses of atoms and molecules

Atoms 原子 are far too light to weigh in grams, so we compare every mass to one standard. The standard is the **unified atomic mass unit** 统一原子质量单位 (symbol u), defined as exactly one twelfth of the mass of one carbon-12 atom.

Using this unit, we state masses as simple numbers:

- the **relative atomic mass** 相对原子质量 A_r of an element is the average mass of its atoms compared with $\frac{1}{12}$ of a carbon-12 atom. It is an average over all the **isotopes** 同位素, weighted by how common each one is.
- the **relative isotopic mass** 相对同位素质量 is the mass of one atom of a single isotope, compared with $\frac{1}{12}$ of a carbon-12 atom.
- the **relative molecular mass** 相对分子质量 M_r of a **molecule** 分子 is the sum of the relative atomic masses of all its atoms.
- the **relative formula mass** 相对式量 is the same idea for a substance that is not made of molecules (such as an ionic compound). Add up the relative atomic masses shown in the formula.

$$A_r = \frac{(75 \times 35) + (25 \times 37)}{100} = 35.5$$

Relative atomic mass is a weighted average: chlorine's two isotopes (75% ^{35}Cl, 25% ^{37}Cl) average to $A_r = 35.5$

To find A_r from isotope data, multiply each isotope mass by its percentage, add these up, and divide by 100.

Worked example. Chlorine is 75% ^{35}Cl and 25% ^{37}Cl. Find its relative atomic mass.

$$A_r = \frac{(75 \times 35) + (25 \times 37)}{100} = \frac{2625 + 925}{100} = 35.5.$$

Worked example. A mass spectrometer shows copper is 69.2% ^{63}Cu and 30.8% ^{65}Cu. Find its relative atomic mass.

$$A_r = \frac{(69.2 \times 63) + (30.8 \times 65)}{100} = \frac{4359.6 + 2002.0}{100} = 63.6.$$

The mole and the Avogadro constant

A modern electronic balance measures mass — the basis of mole calculations.

Chemists count particles in groups called moles, just as we count eggs in dozens.

One **mole** 摩尔 (symbol mol) is the amount of substance that contains the same number of particles as there are atoms in exactly 12 g of carbon-12. That number is the **Avogadro constant** 阿伏伽德罗常量:

$$N_A = 6.02 \times 10^{23}\ \text{mol}^{-1}$$

So one mole of anything contains 6.02×10^{23} particles. The particles may be atoms, molecules or **ions** 离子 — always say which.

The mass of one mole in grams equals the relative mass (A_r or M_r). This is the **molar mass** 摩尔质量, with units g mol^{-1}. The key equation is:

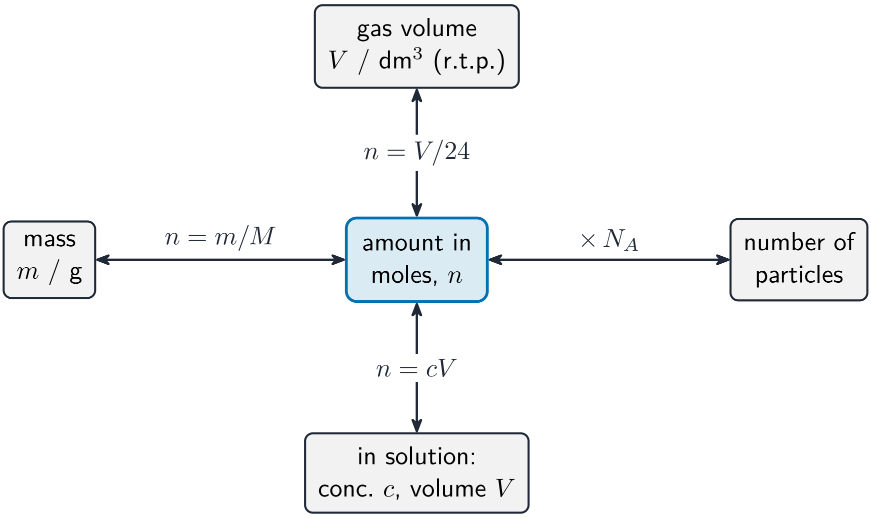
$$n = \frac{m}{M}$$

where n is the amount in moles, m is the mass in grams, and M is the molar mass.

Worked example. How many moles are in 8.0 g of methane, CH_4? (A_r: C = 12, H = 1.)

The molar mass is $M = 12 + 4(1) = 16$ g mol^{-1}, so

$$n = \frac{m}{M} = \frac{8.0}{16} = 0.50 \text{ mol}.$$



The mole is the hub of every amount calculation: convert to mass ($n = m/M$), particles ($\times N_A$), gas volume ($n = V/24$) or solution ($n = cV$)

Formulas

A **compound** 化合物 is a substance made of two or more elements chemically joined.

Charges and formulas of ionic compounds

In an **ionic compound** 离子化合物 the total positive charge balances the total negative charge, so the compound is neutral overall.

You can predict the charge of many ions from the element's position in the Periodic Table:

Group	**1**	**2**	**13**	**15**	**16**	**17**
Usual ion charge	+1	+2	+3	−3	−2	−1

Hydrogen forms H^+, and the Group 18 noble gases do not normally form ions.

Some ions you must know by name and formula:

Name	Formula
nitrate	NO_3^-
carbonate	CO_3^{2-}
sulfate	SO_4^{2-}
hydroxide	OH^-
ammonium	NH_4^+
zinc	Zn^{2+}
silver	Ag^+
hydrogencarbonate	HCO_3^-
phosphate	PO_4^{3-}

For a metal that can have more than one charge, a Roman numeral shows the **oxidation number** 氧化数. For example, iron(II) is Fe^{2+} and iron(III) is Fe^{3+}. To write a formula, balance the charges: iron(III) oxide is Fe_2O_3, because two Fe^{3+} balance three O^{2-}.

Equations and state symbols

A chemical equation must be **balanced** 配平 — the same number of each kind of atom on both sides. Add **state symbols** 状态符号 to show the state of each species: (s) solid, (l) liquid, (g) gas, and (aq) **aqueous** 水溶液 (dissolved in water).

An **ionic equation** 离子方程式 shows only the ions and molecules that actually change. The ions that do not change are **spectator ions** 旁观离子, and you leave them out. For example, the reaction that forms silver chloride is:

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

Empirical and molecular formulas

The **empirical formula** 实验式 is the simplest whole-number ratio of the atoms of each element in a compound. The **molecular formula** 分子式 shows the actual number of atoms of each element in one molecule.

For example, ethane has empirical formula CH_3 but molecular formula C_2H_6.

Hydrated and anhydrous solids

Some solids hold water inside their crystals. This water is the **water of crystallisation** 结晶水. A solid that contains it is **hydrated** 水合的; the same solid with the water removed is **anhydrous** 无水的.

For example, hydrated copper(II) sulfate is $CuSO_4 \cdot 5H_2O$. Heating it drives off the water to leave anhydrous $CuSO_4$.

Calculating empirical and molecular formulas

To find the empirical formula from masses (or percentages by mass):

1. divide each element's mass by its A_r to get the moles.
2. divide all the mole values by the smallest one.
3. round to the nearest whole numbers — that ratio is the empirical formula.

To get the molecular formula, you also need M_r. Find how many times the empirical formula mass fits into M_r, then multiply the formula by that number.

Worked example. A compound is 40.0% carbon, 6.7% hydrogen and 53.3% oxygen by mass. Find its empirical formula. (A_r: C = 12, H = 1, O = 16.)

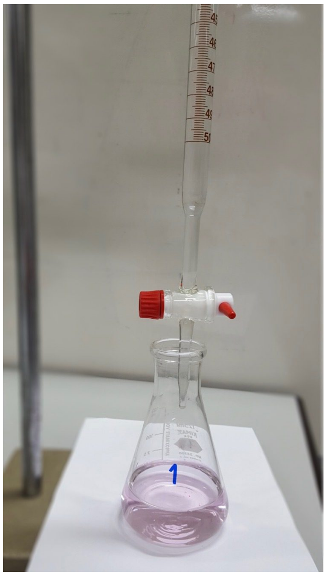
Take 100 g and divide each mass by its A_r to get moles: C = 40.0/12 = 3.33, H = 6.7/1 = 6.7, O = 53.3/16 = 3.33. Dividing through by the smallest (3.33) gives a ratio C : H : O = 1 : 2 : 1, so the empirical formula is CH_2O.

element	% by mass	$\div A_r \to$ moles	$\div$ smallest (3.33)	ratio
C	40.0	$40.0/12 = 3.33$	1.0	1
H	6.7	$6.7/1 = 6.7$	2.0	2
O	53.3	$53.3/16 = 3.33$	1.0	1

empirical formula CH_2O - if $M_r = 180$, it fits $180/30 = 6$ times: molecular formula $C_6H_{12}O_6$

The empirical-formula recipe: divide by Ar, divide by the smallest, read off the ratio

Reacting masses and volumes



A titration finds reacting volumes precisely.

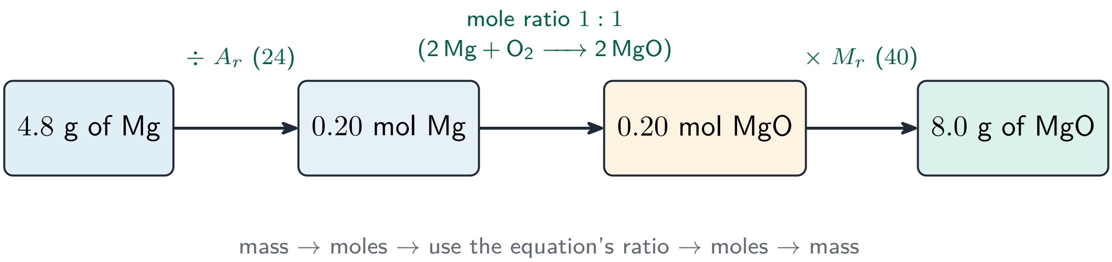
Reacting masses and percentage yield

The numbers in front of each species in a balanced equation give the mole ratio — this is the **stoichiometry** 化学计量. To find a reacting mass: change the known mass to moles, use the mole ratio to find the moles you want, then change back to mass.

Worked example. What mass of magnesium oxide forms when 4.8 g of magnesium burns completely? $2Mg + O_2 \rightarrow 2MgO$. ($A_r$: Mg = 24, O = 16.)

Moles of Mg = 4.8/24 = 0.20 mol. The ratio Mg : MgO is 1 : 1, so 0.20 mol of MgO forms. Its molar mass is 24 + 16 = 40 g mol^{-1}, so

$$m = nM = 0.20 \times 40 = 8.0 \text{ g}.$$



The mole bridge: mass to moles, ratio, then back to mass

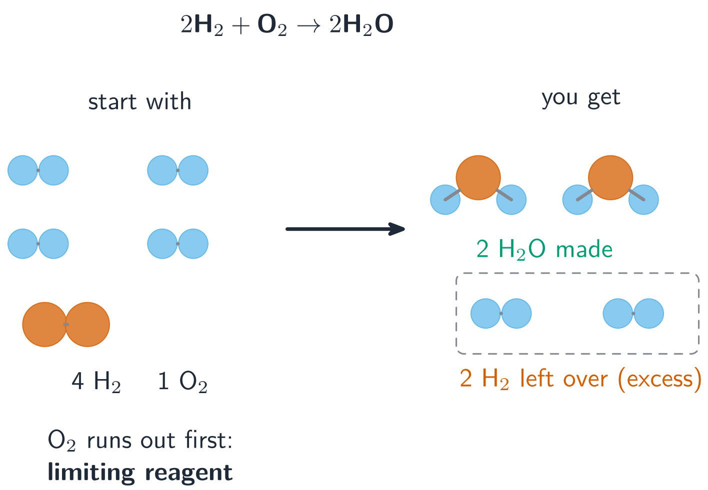
In real reactions you usually get less product than the maximum. The **percentage yield** 产率 compares the amount you actually made with the most you could make:

$$\text{percentage yield} = \frac{\text{actual amount of product}}{\text{maximum possible amount}} \times 100\%$$

Limiting and excess reagent

When two reactants are mixed, one usually runs out first. The **limiting reagent** 限量试剂 is the one that runs out — it decides how much product forms. The other is the **excess reagent** 过量试剂, because there is more than enough of it. Always base the calculation on the limiting reagent.

To find it: work out the moles of each reactant, divide each by its number in the equation, and the smallest result is the limiting reagent.



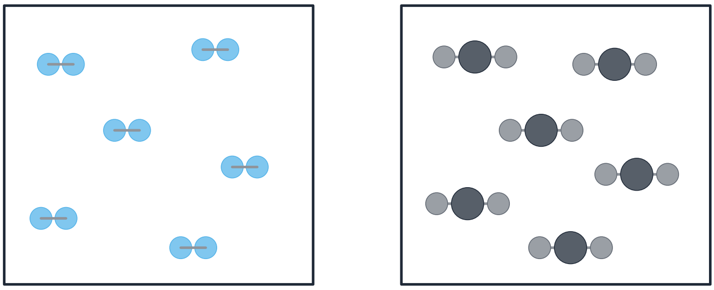
The limiting reagent runs out first and decides how much product forms; the leftover reactant is in excess

Volumes of gases

At the same temperature and pressure, equal volumes of any gases contain equal numbers of molecules. At room temperature and pressure (r.t.p.), one mole of any gas takes up 24.0 dm^3, so:

$$n = \frac{V}{24.0} \qquad (V \text{ in dm}^3 \text{ at r.t.p.})$$

same volume, same temperature and pressure



hydrogen, H_2 carbon dioxide, CO_2

the same **number** of molecules (6 each), even though CO_2 is bigger

Equal volumes of gases at the same temperature and pressure hold equal numbers of molecules, whatever the gas

This is used when burning **hydrocarbons** 碳氢化合物 (compounds of only carbon and hydrogen), where you compare gas volumes.

Volumes and concentrations of solutions

The **concentration** 浓度 of a solution is the amount of **solute** 溶质 in each cubic decimetre of **solution** 溶液, measured in mol dm^{-3}:

$$n = c \times V$$

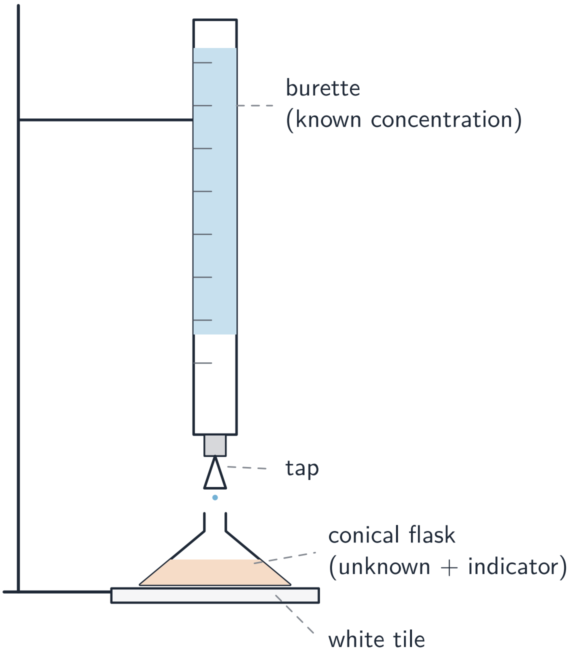
where c is the concentration and V is the volume in dm^3. Remember that 1000 cm^3 = 1 dm^3.

Worked example. In a titration, 25.0 cm^3 of sodium hydroxide solution is exactly neutralised by 20.0 cm^3 of 0.100 mol dm^{-3} hydrochloric acid: $NaOH + HCl \rightarrow NaCl + H_2O$. Find the concentration of the sodium hydroxide.

Moles of HCl $= cV = 0.100 \times \dfrac{20.0}{1000} = 2.00 \times 10^{-3}$ mol. The ratio is 1 : 1, so there are 2.00×10^{-3} mol of NaOH in 25.0 cm^3:

$$c = \frac{n}{V} = \frac{2.00 \times 10^{-3}}{25.0/1000} = 0.0800 \text{ mol dm}^{-3}.$$

This is the basis of a **titration** 滴定, where you find an unknown concentration by reacting it with a solution whose concentration you already know.



In a titration a burette adds a solution of known concentration to the unknown in the conical flask, until the indicator changes

Significant figures

Give your answer to a sensible number of **significant figures** 有效数字 — usually match the data in the question. Do not write more digits than the data supports, and do not round so early that you lose accuracy.

Exam tips

- Convert volumes to dm^3 **before** using concentration ($25.0\ cm^3 = 0.0250\ dm^3$); the missing ÷1000 is the most common titration error.
- Use the **balancing numbers** as the mole ratio between species — never the M_r values.
- Empirical formula: divide each mass/percentage by A_r, then by the **smallest**, then scale to whole numbers; use M_r to reach the molecular formula.
- For gases at r.t.p. use volume = moles × 24 dm^3; quote the equation you use every time.
- Give the answer to the same **significant figures** as the data (usually 3) and always include units.