AQA | Year 12 chemistry

Amount of substance

Complete notes

Clear explanations, precise definitions and worked examples for the whole topic. Use the contents or PDF bookmarks to find a section. TEST IT references point to the matching questions in the separate topic Questions & answers pack.

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Relative masses & moles

1. Relative atomic and molecular masses

SPEC 3.1.2.1

CRACK IT

Atoms are too small for ordinary gram measurements to be convenient. Relative masses compare them with a shared reference: **one-twelfth of the mass of one carbon-12 atom**.

Relative isotopic mass describes an atom of one particular isotope. Relative atomic mass, A_r, is a weighted mean for the element, allowing for its isotope abundances.

Because each relative mass is a ratio of two masses, it has no unit. Keep that separate from molar mass, which is normally expressed in g mol^{-1}. The definitions below give the precise exam wording.

Use the A_r values on the Periodic Table supplied with the question. These are given to one decimal place, for example Cl = 35.5. Keep any more precise isotopic masses explicitly given in a mass-spectrum question.

DEFINITIONS & KEY TERMS

Relative atomic mass, A_r

The weighted mean mass of an atom of an element relative to one-twelfth of the mass of one carbon-12 atom.

Relative molecular mass, M_r

The mean mass of a molecule relative to one-twelfth of the mass of one carbon-12 atom.

Relative formula mass

The sum of the relative atomic masses in the formula unit of an ionic compound. Ionic substances do not contain separate molecules.

Molar mass

The mass per mole of specified entities. Its unit is g mol^{-1}; its numerical value matches the corresponding relative mass.

$$A_r = \Sigma(\text{isotopic mass} \times \text{abundance}) / \Sigma(\text{abundances})$$

A_r relative atomic mass; no unit; **Σ** sum of all the indicated contributions.

EXAM TRAP An ordinary mean assumes equal abundances. Use each isotope's actual abundance. Do not attach g mol^{-1} to A_r or M_r.

TEST IT

Try questions 1, 2 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Define relative masses precisely and calculate a weighted mean.

2. Calculate formula masses, including brackets

SPEC 3.1.2.1

CRACK IT

The formula tells you how many atoms of each element are present. To find a relative molecular or formula mass, add the A_r contribution of **every atom in the formula**.

1. Write down how many atoms of each element are present.

2. Multiply the count of each element by its A_r.

3. Add the contributions.

Brackets are the usual trap. In $Al_2(SO_4)_3$, the outside 3 multiplies both S and O, giving $Al_2S_3O_{12}$. It does not multiply the Al.

Use relative molecular mass for discrete molecules. For compounds such as ionic solids that do not contain molecules, use relative formula mass. Give no unit for a relative mass. The same numerical value used as a molar mass has units of g mol^{-1}.

WORKED EXAMPLE

Sulfuric acid

Find $M_r(H_2SO_4)$. Use H 1.0, S 32.1 and O 16.0.

Worked answer

Relative molecular/formula mass = sum of the A_r contributions of every atom

Quantity	H	S	O
Number	2	1	4
A_r	1.0	32.1	16.0
Contribution	Contribution = atom count × A_r 2.0	Contribution = atom count × A_r 32.1	Contribution = atom count × A_r 64.0

$M_r = 2(1.0) + 32.1 + 4(16.0) = 98.1$

M_r = 98.1, with no unit.

WORKED EXAMPLE

Calcium nitrate

Find the relative formula mass of $Ca(NO_3)_2$. Use Ca 40.1, N 14.0 and O 16.0.

Worked answer

The formula contains one Ca, two N and six O atoms.

Relative molecular/formula mass = sum of the A_r contributions of every atom

40.1 + 2(14.0) + 6(16.0) = 164.1

Relative formula mass, M_r = 164.1, with no unit.

EXAM TRAP The outside 2 in $Ca(NO_3)_2$ multiplies both N and O. It does not multiply Ca.

TEST IT

Try question 3 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Count every atom in a formula and distinguish relative mass from molar mass.

3. The mole and the Avogadro constant

SPEC 3.1.2.2

CRACK IT

A mole is a unit for measuring amount of substance, rather like a dozen is a unit for counting items. You can have one mole, two moles or half a mole.

KEY DEFINITION

The mole and the Avogadro constant do different jobs. **mol is the unit; L tells you how many specified particles there are per mole.** Think of “dozen” and 12: the word names the counting unit, while the number tells you how many items it contains.

Use **$L = 6.022 \times 10^{23}\ mol^{-1}$**, rounded to four significant figures. So 1 mol contains approximately 6.022×10^{23} specified particles. Use a different value if a question explicitly supplies one.

The amount of substance has symbol n and unit mol. Name what you are counting: atoms, molecules, formula units, ions or electrons. One mole of each contains the same number of entities, but their masses differ. One mole of O_2 molecules contains two moles of oxygen atoms.

Concept	What it means	Think of a dozen
Mole (mol)	The unit used to measure amount of substance. You can have 1 mol, 2 mol or part of a mole.	The word “dozen” names a counting unit.
Avogadro constant, L	The number of specified particles per mole. Use L = 6.022×10^{23} mol^{-1} (4 significant figures).	12 tells you how many items are in one dozen; L tells you how many particles are in one mole.

$N = nL$; $L = 6.022 \times 10^{23}$ mol^{-1}

N is the number of particles, such as atoms, molecules, ions, formula units or electrons. **n** is the amount of substance in mol, and **L** is the Avogadro constant in mol^{-1}.

EXAM TRAP Always complete the phrase “moles of ...”. One mole of O_2 molecules and one mole of O atoms describe different quantities.

TEST IT

Try question 4 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Explain a mole and name the entities counted.

4. Choose the correct particle or entity

SPEC 3.1.2.2

CRACK IT

Before using a formula, decide **what the question wants you to count**. A molecule, an atom and an ion are not interchangeable labels.

Use molecules for substances made of separate molecules, such as water. For an ionic compound such as NaCl, use formula units rather than molecules.

Then look inside the formula. One H_2O molecule contains two H atoms and one O atom. One formula unit of an ionic compound may contain more than one of a particular ion. Apply that multiplier only when the question asks for those component particles.

Substance or symbol	Entity to count
Fe	Atoms
O_2, CO_2, H_2O	Molecules
NaCl, $MgCl_2$	Formula units
Na^+, Cl^-, SO_4^{2-}	Ions
Transferred charge in a half-equation	Electrons

WORKED EXAMPLE

One sample, three different amounts

A sample contains 0.250 mol H_2O. Find the amount in moles of molecules, hydrogen atoms and all atoms.

Worked answer

Quantity	H_2O molecules	H atoms	All atoms
Multiplier	1	2	2 + 1 = 3
Amount / mol	0.250	0.500	0.750

State the target entity beside every amount.

EXAM TRAP NaCl is an ionic lattice: “NaCl molecules” is the wrong entity. An ion such as SO_4^{2-} counts as one ion, even though it contains five atoms.

TEST IT

Try question 5 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Distinguish molecules, atoms, formula units and ions before calculating.

Mass–mole–particle calculations

5. Convert between mass and moles

SPEC 3.1.2.2

CRACK IT

KEY DEFINITION

Use the relative molecular or formula mass, M_r, in mass-to-moles calculations. M_r has **no unit**. Its numerical value is the same as the mass of one mole in grams: $M_r(H_2SO_4) = 98.1$ means one mole of H_2SO_4 has a mass of 98.1 g.

1. Add the A_r contributions in the formula to find M_r.

2. With mass in grams, divide by M_r to find amount in moles: $n = m/M_r$.

3. To find mass in grams, multiply the amount in moles by M_r: $m = nM_r$.

These are numerical calculation rules using mass in g and amount in moles. For atoms, use A_r instead. Molar mass is the mass per mole and has unit g mol^{-1}; M_r itself remains unitless.

Compare with one mole to check your answer. If $M_r(CaCO_3) = 100.1$, then 0.350 mol must have a mass below 100.1 g.

$n = m/M_r$; $m = nM_r$; $M_r = m/n$

M_r relative molecular or formula mass; no unit; **m** mass of the specified sample or substance, in g; **n** amount of the specified substance or particles, in mol.

WORKED EXAMPLE

Mass to moles

Calculate the number of moles in 9.81 g H_2SO_4; $M_r = 98.1$.

Worked answer

$n = m/M_r$
$n = 9.81 / 98.1 = 0.100$ mol

0.100 mol H_2SO_4.

WORKED EXAMPLE

Moles to mass

Calculate the mass of 0.350 mol $CaCO_3$; $M_r = 100.1$.

Worked answer

$m = n \times M_r$
$m = 0.350 \times 100.1 = 35.035$ g

35.0 g $CaCO_3$ to three significant figures.

TEST IT

Try question 6 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Use $n = m/M_r$ and $m = nM_r$ with the correct units.

6. Convert between moles and particles

SPEC 3.1.2.2

CRACK IT

The Avogadro constant, L, connects amount in moles with particle number. Use $L = 6.022 \times 10^{23}$ mol^{-1} unless a question supplies another value.

- **Moles to particles:** multiply by L, using $N = nL$.

- **Particles to moles:** divide by L, using n = N/L.

N is the number of particles and has no unit. The amount of substance, n, is measured in mol. Label the answer with the entity, such as molecules or chloride ions. L has unit mol^{-1} because it gives the number of particles per mole.

If the target is an atom or ion within a formula, include its formula multiplier as well.

N = nL; n = N/L

L Avogadro constant, 6.022×10^{23} mol^{-1}; **N** number of the specified particles; a count with no unit; **n** amount of the specified substance or particles, in mol.

WORKED EXAMPLE

Count ammonia molecules

How many molecules are in 0.0750 mol NH_3?

Use L = 6.022×10^{23} mol^{-1}.

Worked answer

N = nL
N = $0.0750 \times 6.022 \times 10^{23} = 4.5165 \times 10^{22}$

4.52×10^{22} NH_3 molecules.

WORKED EXAMPLE

Count an amount of neon

Find the amount in moles represented by 1.204×10^{24} Ne atoms.

Use L = 6.022×10^{23} mol^{-1}.

Worked answer

n = $(1.204 \times 10^{24}) / (6.022 \times 10^{23})$

2.000 mol Ne atoms to four significant figures.

EXAM TRAP Use brackets around the full denominator when entering a power of ten. A small fraction of a mole still contains an enormous number of particles.

TEST IT

Try question 7 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Multiply or divide by the Avogadro constant in the correct direction.

7. Count atoms, ions and electrons

SPEC 3.1.2.2

CRACK IT

The amount of a compound is not automatically the amount of every particle inside it. Use the formula to count how many of the requested particles occur in one molecule or formula unit.

1. Find the amount in moles of the stated substance.

2. Multiply by the number of target atoms or ions in each formula.

3. Use N = nL if the question asks for the actual particle number.

For electron counts, use atomic number and ionic charge first. Al^{3+} has 13 - 3 = 10 electrons; Cl^{-} has 17 + 1 = 18. Multiply the amount of those ions by their electron count, then by L.

Write the entity beside intermediate amounts. This makes it easier to spot an incorrect multiplier.

One formula unit of $Al_2(SO_4)_3$ represents	Count
Al^{3+} ions	2
SO_4^{2-} ions	3
All ions	5
O atoms	12
All atoms	2 + 3 + 12 = 17

WORKED EXAMPLE

Ions from aluminium sulfate

For 0.120 mol $Al_2(SO_4)_3$, find the amounts in moles of each ion and the total number of ions.

Use L = 6.022×10^{23} mol^{-1}.

Worked answer

Moles of aluminium ions = moles of $Al_2(SO_4)_3$ × aluminium ions per formula unit
$n(Al^{3+}) = 2 \times 0.120 = 0.240$ mol

Moles of sulfate ions = moles of $Al_2(SO_4)_3$ × sulfate ions per formula unit
$n(SO_4^{2-}) = 3 \times 0.120 = 0.360$ mol

N(total ions) = nL
$N(\text{total ions}) = (0.240 + 0.360) \times 6.022 \times 10^{23}$

3.61×10^{23} ions in total.

EXAM TRAP Apply a subscript multiplier once. If you already have moles of oxygen atoms, do not multiply by the oxygen subscript again.

TEST IT

Try question 8 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Apply formula subscripts once and use atomic number and charge to count electrons.

8. Use the mass–mole–particle route

SPEC 3.1.2.2

CRACK IT

For a mass-to-particles question, make two clear moves: **mass to moles, then moles to particles**.

1. Divide mass in grams by M_r to find moles of the substance. For atoms, use A_r.

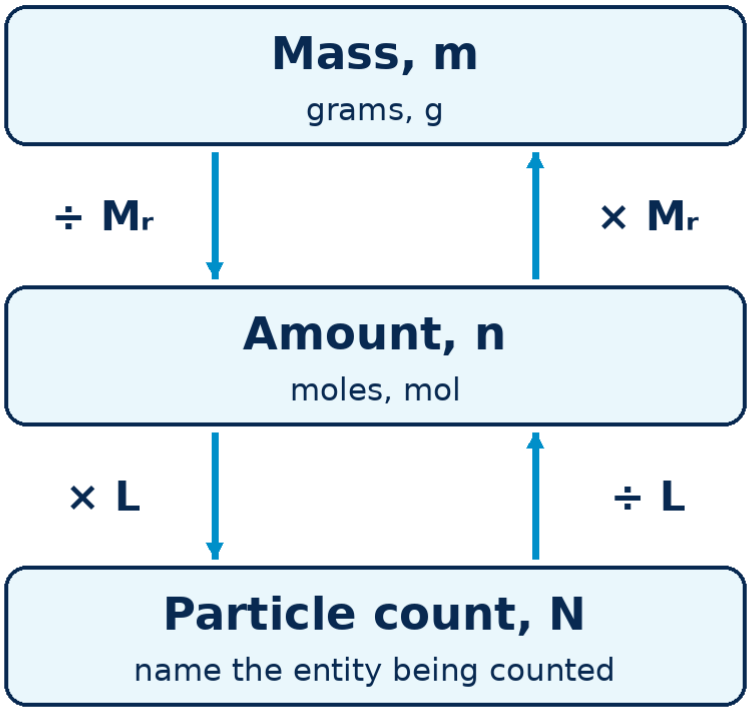
2. If needed, use the formula to find moles of the particular atom or ion being counted.

3. Multiply that mole amount by L.

For molecules or formula units, $N = (m/M_r)L$ when m is in grams. If you need a component particle, include its formula multiplier. Writing both stages makes the target easier to track.

Mass → divide by M_r → moles → multiply by L → particles

Use moles as the bridge



M_r has no unit; use mass in grams.

$L = 6.022 \times 10^{23}$ mol^{-1}

For atoms, use A_r in place of M_r.

For a component atom or ion, include its formula multiplier.

WORKED EXAMPLE

Chloride ions in sodium chloride

How many chloride ions are represented by 5.85 g NaCl? M_r(NaCl) = 58.5; L = 6.022×10^{23} mol^{-1}.

Worked answer

1. n(NaCl) = m/M_r
n(NaCl) = 5.85 / 58.5 = 0.100 mol.

2. Each formula unit represents one Cl^- ion, so n(Cl^-) = 0.100 mol.

3. N(Cl^-) = nL
N(Cl^-) = $0.100 \times 6.022 \times 10^{23}$.

6.02×10^{22} chloride ions.

EXAM TRAP A mass comparison alone does not tell you which sample contains more molecules, atoms or ions. First account for molar mass, then the target-entity multiplier.

TEST IT

Try questions 9, 10 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Connect a measured mass to a specified particle count.

9. Reverse the route and find an unknown relative molecular mass

SPEC 3.1.2.2

CRACK IT

A reverse calculation follows the same relationships in the opposite direction. Start with the target and the information you have.

1. Divide a particle count by L to find moles.

2. Undo any formula multiplier if you need moles of the whole compound.

3. To find mass in grams, use $m = nM_r$.

4. To find an unknown M_r, divide mass in grams by amount in moles: $M_r = m/n$. Give no unit for M_r.

Label the substance and entity at each step. Keep the full calculator value of the amount until the final answer.

WORKED EXAMPLE

Particles to mass

Find the mass of 3.01×10^{22} CO_2 molecules. $M_r(CO_2) = 44.0$.

Use $L = 6.022 \times 10^{23}$ mol^{-1}.

Worked answer

$n = (3.01 \times 10^{22}) / (6.022 \times 10^{23}) = 0.0499834...$ mol

$m = n \times M_r$
$m = 0.0499834... \times 44.0$

2.20 g CO_2.

WORKED EXAMPLE

Find an unknown relative molecular mass

A 1.83 g molecular sample contains 2.50×10^{22} molecules.

Calculate the relative molecular mass, M_r, of the substance. Use $L = 6.022 \times 10^{23}$ mol^{-1}.

Worked answer

$n = (2.50 \times 10^{22}) / (6.022 \times 10^{23}) = 0.0415144...$ mol

$M_r = m/n = 1.83 / 0.0415144...$

M_r = 44.1 with no unit.

EXAM TRAP Retain the full calculator value of n. Molar mass is mass per mole, not the mass of the sample.

TEST IT

Try questions 11, 12 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Move from particles to moles before finding mass or relative molecular mass.

10. Standard form, units and final checks

SPEC 3.1.2.1–3.1.2.2; mathematical skills

CRACK IT

A good method can still lose marks through units, powers of ten or early rounding. Make a final check part of every calculation.

• Keep the calculator's full value during intermediate steps. Round only the final answer.

• Use sensible significant figures from the measured or supplied data. Exact subscripts and equation coefficients do not limit them.

• Check the unit and the entity: mol, g, atoms and molecules describe different answers.

• Check the direction. Dividing by a large molar mass should give fewer moles for a fixed mass.

In standard form, one non-zero digit comes before the decimal point. For example, 0.003045 mol = 3.045×10^{-3} mol. At three significant figures, 7.849×10^{22} becomes 7.85×10^{22}.

EXAM TRAP If dividing by L produces a tiny particle count from an ordinary laboratory sample, recheck the direction. Changing the calculation to multiplication is necessary when moving from moles to particles.

TEST IT

Try question 13 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Finish calculations with a correct unit, particle label and appropriate precision.

Equations & reacting masses

11. Balance equations without changing formulae

SPEC 3.1.2.5

CRACK IT

A reaction rearranges atoms; it does not create or destroy them. A balanced equation must therefore have the same number of atoms of each element on both sides.

1. Write the correct formulae before balancing.

2. Count the atoms on each side. Start with an element appearing in one reactant and one product if possible.

3. Change the coefficients in front of whole formulae. A coefficient multiplies every atom in that formula.

4. Recount every element, use the smallest whole-number coefficients and check the state symbols.

Never change a subscript to make the numbers balance. Changing H_2O to H_2O_2 would change the substance, not balance the original reaction.

State	Meaning
(s)	Solid
(l)	Liquid
(g)	Gas
(aq)	Dissolved in water

WORKED EXAMPLE

Aluminium burns in oxygen

Balance $Al + O_2 \rightarrow Al_2O_3$.

Worked answer

Two Al_2O_3 formula units contain six O atoms, so use three O_2 molecules. This requires four Al atoms.

$4Al(s) + 3O_2(g) \rightarrow 2Al_2O_3(s)$

Al: 4 each side; O: 6 each side.

WORKED EXAMPLE

Neutralisation

Balance $Ca(OH)_2 + HCl \rightarrow CaCl_2 + H_2O$.

Worked answer

$Ca(OH)_2 + 2HCl \rightarrow CaCl_2 + 2H_2O$

Ca 1; O 2; H 4; Cl 2 on each side.

EXAM TRAP Changing MgO to MgO_2 changes the substance. It does not balance the reaction that was given.

TEST IT

Try question 14 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Balance atoms and charge using coefficients and correct state symbols.

12. Write full and net ionic equations

SPEC 3.1.2.5

CRACK IT

An ionic equation removes the ions that are only watching the reaction. These **spectator ions** appear unchanged on both sides.

1. Start with the balanced full equation, including state symbols.

2. Separate appropriate aqueous ionic substances, strong acids and strong alkalis into their ions. Keep the coefficients.

3. Keep solids, liquids, gases and undissociated molecular substances intact. An (aq) label alone does not mean every substance should be split.

4. Cancel spectator ions that are identical on both sides.

5. Check both atom numbers and total charge.

For a strong acid reacting with a strong alkali, the reacting particles are $H^+(aq)$ and $OH^-(aq)$, which form water. The remaining ions do not need to appear in the net equation.

WORKED EXAMPLE

A silver chloride precipitate

Write the ionic equation for $AgNO_3(aq) + NaCl(aq)$.

Worked answer

$AgNO_3(aq) + NaCl(aq) \rightarrow AgCl(s) + NaNO_3(aq)$

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

Na^+ and NO_3^- are spectator ions.

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

$H^+(aq) + OH^-(aq) \rightarrow H_2O(l)$

EXAM TRAP Do not separate a precipitate into aqueous ions. The solid is the product of the change.

TEST IT

Try question 15 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Separate appropriate aqueous species and cancel spectator ions.

13. Calculate reacting masses with a grid

SPEC 3.1.2.5

CRACK IT

A reacting-mass calculation has one important bridge: the balanced equation connects **moles of one substance to moles of another**.

The coefficients in a balanced equation compare **moles, not masses**. In the grid, work across the amount row using these coefficients before converting back to mass.

1. Write the balanced equation above your grid.

2. Put in the known mass and the relevant A_r or M_r values, with no units on relative masses.

3. Divide mass in grams by the relative mass to reach the moles row.

4. Use the equation coefficients to find moles of the other substance.

5. Multiply by its relative mass to find mass in grams.

The grid also works backwards from a product mass. Use M_r for molecules or formula units, and A_r for atoms. Keep mass in grams and amount in moles.

Known mass ÷ M_r → known moles × coefficient ratio → wanted moles × M_r → wanted mass

M_r relative molecular or formula mass; no unit.

WORKED EXAMPLE

Magnesium to magnesium oxide

$2Mg + O_2 \rightarrow 2MgO$. Find the mass of MgO from 4.86 g Mg in excess O_2. $A_r(Mg) = 24.3$; $M_r(MgO) = 40.3$.

Worked answer

Quantity	Mg	O_2	MgO
Mass / g	4.86	In excess	8.06
A_r or M_r (no unit)	24.3	32.0	40.3
Amount / mol	$n = m/A_r$ 4.86/24.3 = 0.200	Not needed	n = n(known) × equation ratio 0.200 × 2/2 = 0.200

$m(MgO) = n \times M_r$
$m(MgO) = 0.200 \times 40.3$

8.06 g MgO.

WORKED EXAMPLE

Oxygen from peroxide

$2H_2O_2 \rightarrow 2H_2O + O_2$. Find the mass of oxygen from 6.80 g H_2O_2. $M_r(H_2O_2) = 34.0$; $M_r(O_2) = 32.0$.

Worked answer

Quantity	H_2O_2	O_2
Mass / g	6.80	3.20
A_r or M_r (no unit)	34.0	32.0
Amount / mol	$n = m/M_r$ $6.80/34.0 = 0.200$	$n = n(\text{known}) \times \text{equation ratio}$ $0.200 \times 1/2 = 0.100$

$m(O_2) = n \times M_r$
$m(O_2) = 0.100 \times 32.0$

3.20 g O_2.

EXAM TRAP A 2 : 1 coefficient ratio changes 0.200 mol into 0.100 mol. Do not apply it directly to 6.80 g.

TEST IT

Try questions 16, 17 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Convert mass to moles, apply the equation ratio, then convert back to mass.

14. Work backwards and calculate purity

SPEC 3.1.2.5

CRACK IT

If a product mass is given, work back through the balanced equation to find how much reactant produced it. The route is the same as before, just travelled in the other direction.

For purity, distinguish the **mass of pure reacting substance** from the mass of the whole sample. Impurities contribute to the sample mass but, in the stated method, do not contribute to the measured reaction.

1. Use the product data to find moles of the pure reactant.

2. Convert those moles into the mass of pure reactant.

3. Divide by the total sample mass and multiply by 100.

Percentage purity = mass of pure substance / mass of impure sample × 100

WORKED EXAMPLE

Iron oxide required

$Fe_2O_3 + 3CO \rightarrow 2Fe + 3CO_2$. Calculate the mass of Fe_2O_3 required to produce 11.16 g Fe.
$A_r(Fe) = 55.8$; $M_r(Fe_2O_3) = 159.6$.

Worked answer

Quantity	Fe_2O_3	Fe
Mass / g	15.96	11.16
A_r or M_r (no unit)	159.6	55.8
Amount / mol	n = n(known) × equation ratio 0.200 × 1/2 = 0.100	$n = m/A_r$ 11.16/55.8 = 0.200

$m(Fe_2O_3) = n \times M_r$
$m(Fe_2O_3) = 0.100 \times 159.6 = 15.96$ g

15.96 g, or 16.0 g at three significant figures.

WORKED EXAMPLE

Calcium carbonate purity

A 5.00 g impure $CaCO_3$ sample gives 1.76 g CO_2 with excess acid. $CaCO_3 + 2HCl \rightarrow CaCl_2 + CO_2 + H_2O$. $M_r(CO_2) = 44.0$; $M_r(CaCO_3) = 100.1$.

Calculate the percentage purity by mass of the calcium carbonate sample. Assume the impurities do not react with the acid.

Worked answer

Quantity	$CaCO_3$	CO_2
Mass / g	4.004 pure	1.76
A_r or M_r (no unit)	100.1	44.0
Amount / mol	0.0400	$n = m/M_r$ 1.76/44.0 = 0.0400

Percentage purity = (mass of pure substance ÷ mass of sample) × 100
Purity = 4.004 / 5.00 × 100

80.1% $CaCO_3$ by mass.

EXAM TRAP The impurities must not contribute to the measured reaction. Excess reagent ensures the sample substance controls the product amount.

TEST IT

Try questions 18, 19 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Find a required reactant mass or the pure fraction of an impure sample.

Limiting reactants & linked reactions

15. Find the limiting reactant and excess remaining

SPEC 3.1.2.5

CRACK IT

KEY DEFINITION

The limiting reactant is the one that runs out first. Once it is used up, no more product can form, even if some of the other reactant remains.

A **coefficient** is a big number written in front of an element or compound in a balanced equation. It multiplies the whole formula. If no number is written, the coefficient is 1. For example, in **$2Al + 3Cl_2 \rightarrow 2AlCl_3$**, the coefficients are 2, 3 and 2.

1. Convert each supplied reactant quantity into moles.

2. Divide each mole amount by its own coefficient in the balanced equation.

3. The smaller value identifies the limiting reactant and sets the maximum product amount.

4. To find excess left over, use the limiting amount to calculate how much of the other reactant reacts. Subtract that from its starting amount, then convert to mass if needed.

Compare n/coefficient, not the original masses or the mole amounts alone. Different coefficients mean different reaction requirements.

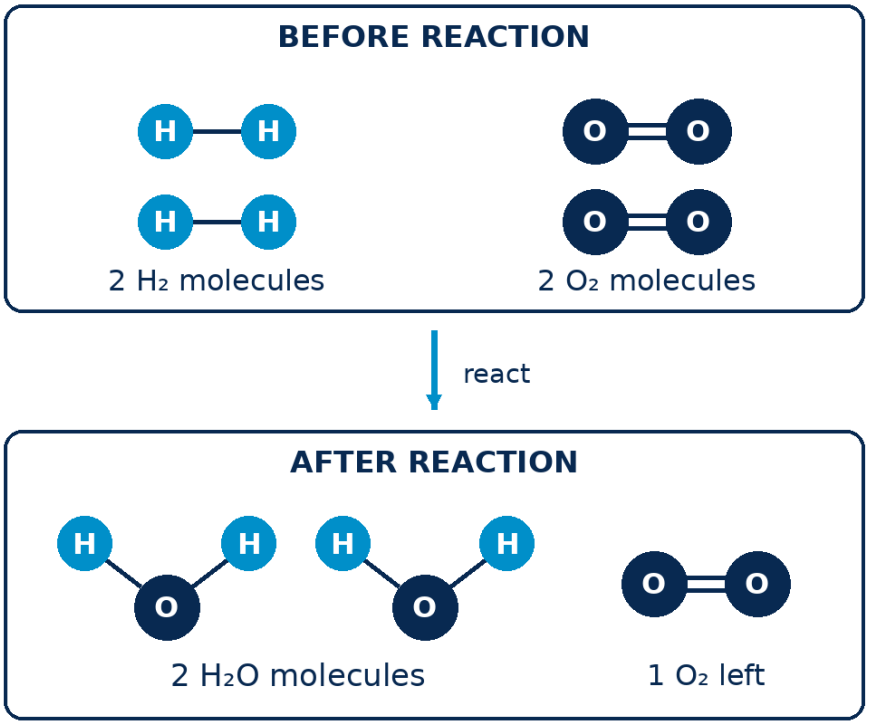
Dividing by a coefficient counts how many complete reaction groups a supply can support. For $2Al + 3Cl_2 \rightarrow 2AlCl_3$, each group needs 2 mol Al and 3 mol Cl_2. The supply supporting fewer complete groups runs out first.

Reaction amount = n(reactant) / its balanced-equation coefficient

n amount of the specified substance or particles, in mol.

Which reactant runs out?

$2H_2 + O_2 \rightarrow 2H_2O$



H_2 is limiting: it is all used up.
O_2 is in excess: some remains.

Molecule model; atom sizes are not to scale.

WORKED EXAMPLE

Aluminium and chlorine

$2Al + 3Cl_2 \rightarrow 2AlCl_3$. Mix 2.70 g Al with 7.10 g Cl_2. Use A_r or M_r values Al 27.0, Cl_2 71.0 and $AlCl_3$ 133.5.

Identify the limiting reactant. Calculate the maximum mass of $AlCl_3$ formed and the mass of the excess reactant remaining.

Worked answer

Quantity	Al initially	Cl_2 initially	$AlCl_3$ formed
Mass / g	2.70	7.10	8.90
A_r or M_r (no unit)	27.0	71.0	133.5
Amount / mol	$n = m/A_r$ $n = 2.70/27.0 = 0.100$	$n = m/M_r$ $n = 7.10/71.0 = 0.100$	n = n(known) × equation ratio $0.100 \times 2/3 = 0.066666...$
Amount ÷ coefficient / mol	Comparison value = n/coefficient $0.100/2 = 0.0500$	Comparison value = n/coefficient $0.100/3 = 0.033333...$: smaller, so limiting	Not compared

$m(AlCl_3) = n \times M_r$
$m(AlCl_3) = (0.100 \times 2/3) \times 133.5 = 8.90$ g

n(Al left) = n(initial) − n(reacted)
n(Al left) = 0.100 − 0.066666... = 0.033333... mol

$m(Al\ left) = n \times A_r$
m(Al left) = 0.033333... × 27.0 = 0.900 g

Cl_2 is limiting; 8.90 g $AlCl_3$ forms and 0.900 g Al remains.

EXAM TRAP The smaller initial number of moles is not automatically limiting. The coefficient demand matters. Do not round 0.066666... to 0.067 before multiplying by 133.5.

TEST IT

Try question 20 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Compare n/coefficient and use the limiting reactant to calculate product.

16. Link reactions and check the full calculation route

SPEC 3.1.2.4–3.1.2.5

CRACK IT

In a sequence of reactions, the product of one stage can become a reactant in the next. Carry its **mole amount** forward, then use the next balanced equation.

1. Finish the mole-ratio step for reaction 1.

2. Label the amount of intermediate formed.

3. Use that amount in reaction 2 and apply its own coefficient ratio.

4. If two reactant amounts are supplied in the second stage, check the limiting reactant again.

Do not carry one coefficient ratio across the whole chain unless you have first combined the equations correctly. Labelled intermediate amounts make the working easier to check.

WORKED EXAMPLE

Limestone to calcium chloride

Stage 1: $CaCO_3 \rightarrow CaO + CO_2$. Stage 2: $CaO + 2HCl \rightarrow CaCl_2 + H_2O$. Find the mass of HCl needed for the CaO from 10.01 g $CaCO_3$. $M_r(CaCO_3) = 100.1$; $M_r(HCl) = 36.5$.

Worked answer

Quantity	$CaCO_3$	CaO intermediate	HCl
Mass / g	10.01	Not needed	7.30
A_r or M_r (no unit)	100.1	56.1	36.5
Amount / mol	$n = m/M_r$ $n = 10.01/100.1 = 0.100$	$n = n(\text{known}) \times \text{equation ratio}$ $0.100 \times 1/1 = 0.100$	$n = n(\text{known}) \times \text{equation ratio}$ $0.100 \times 2/1 = 0.200$

$m(HCl) = n \times M_r$
$m(HCl) = 0.200 \times 36.5$

7.30 g HCl.

Quantity	Reacting mass	Limiting reactant	Empirical formula	Molecular formula	Water of crystallisation	Linked reactions
Starting route	Known mass → moles → equation ratio → mass	Calculate n/coefficient for each	Mass/A_r, then divide by smallest	M_r/empirical-formula mass	Mass lost and anhydrous salt → two amounts	Moles of shared intermediate

Quantity	Reacting mass	Limiting reactant	Empirical formula	Molecular formula	Water of crystallisation	Linked reactions
Check	Correct species and balanced equation	Use the smaller result	Scale all fractional values	Whole-number multiplier	Constant mass; correct residue	Transfer complete; second-stage limiting reactant

WORKED EXAMPLE

Keep calculator precision

A calculation gives 0.066666... mol $AlCl_3$. M_r = 133.5.

Calculate the mass of $AlCl_3$ to three significant figures, retaining the unrounded number of moles. Show how rounding the number of moles to 0.067 mol too early changes the calculated mass.

Worked answer

Correct: 0.066666... × 133.5 = 8.90 g

Premature rounding: 0.067 × 133.5 = 8.9445 g

Retain the unrounded amount and report 8.90 g.

EXAM TRAP Coefficients act between mole amounts. A direct mass calculation is only valid if the molar-mass factors are included as well.

TEST IT

Try questions 21, 22, 23 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Carry an intermediate amount through two equations and diagnose invalid methods.

Empirical & molecular formulae

17. Find empirical formulae from masses and percentages

SPEC 3.1.2.4

CRACK IT

An empirical formula gives the **simplest whole-number ratio of atoms**. A mass ratio is not an atom ratio because different atoms have different masses.

1. Find the mass of each element. For percentages, assume a 100 g sample so each percentage becomes grams.

2. Divide each mass by its A_r to find moles.

3. Divide every mole amount by the smallest one.

4. If a simple fraction remains, multiply the entire ratio to obtain whole numbers.

5. Use those whole numbers as the formula subscripts.

Do not round 1 : 1.5 to 1 : 2. Multiply both values by 2 to get **2 : 3**. For a ratio of **1 : 1.33…**, multiply both by 3 to get **3 : 4**. This may look like 1 : 1.3 if rounded too early, so keep the full calculator values when choosing the multiplier.

WORKED EXAMPLE

Magnesium oxide

A compound contains 0.486 g Mg and 0.320 g O. Use A_r(Mg) = 24.3 and A_r(O) = 16.0.

Determine the empirical formula of the compound.

Worked answer

Quantity	Mg	O
Mass / g	0.486	0.320
A_r	24.3	16.0
Amount / mol	$n = m/A_r$ $n = 0.486/24.3 = 0.0200$	$n = m/A_r$ $n = 0.320/16.0 = 0.0200$
÷ smallest	Ratio = amount ÷ smallest amount $0.0200/0.0200 = 1$	Ratio = amount ÷ smallest amount $0.0200/0.0200 = 1$
Whole-number ratio	1	1

Empirical formula: MgO.

WORKED EXAMPLE

Percentage composition

A compound contains 40.0% carbon, 6.67% hydrogen and 53.33% oxygen by mass. Determine its empirical formula. Use A_r(C) = 12.0, A_r(H) = 1.0 and A_r(O) = 16.0.

Worked answer

Quantity	C	H	O
Mass / g	40.0	6.67	53.33
A_r	12.0	1.0	16.0
Amount / mol	n = m/A_r n = 40.0/12.0 = 3.333...	n = m/A_r n = 6.67/1.0 = 6.67	n = m/A_r n = 53.33/16.0 = 3.333...
÷ smallest	Ratio = amount ÷ smallest amount 3.333.../3.333... = 1	Ratio = amount ÷ smallest amount 6.67/3.333... = 2	Ratio = amount ÷ smallest amount 3.333.../3.333... = 1
Whole-number ratio	1	2	1

Empirical formula: CH_2O.

Ratio containing	Multiply every part by	Example
1.5	2	1 : 1.5 → 2 : 3
1.333...	3	1 : 1.333... → 3 : 4
1.25	4	1 : 1.25 → 4 : 5
1.667...	3	1 : 1.667... → 3 : 5

WORKED EXAMPLE

Recognise a half ratio

A phosphorus oxide is 43.6% P and 56.4% O. Use A_r(P) = 31.0 and A_r(O) = 16.0.

Determine the empirical formula of the phosphorus oxide from these percentages by mass.

Worked answer

Quantity	P	O
Mass / g	43.6	56.4
A_r	31.0	16.0
Amount / mol	n = m/A_r n = 43.6/31.0 = 1.40645…	n = m/A_r n = 56.4/16.0 = 3.525
÷ smallest	Ratio = amount ÷ smallest amount 1.40645…/1.40645… = 1	2.506… ≈ 2.5
Whole-number ratio	2	5

Empirical formula: P_2O_5.

WORKED EXAMPLE

Find an unknown metal

A metal chloride MCl_2 contains 0.486 g M and 1.420 g Cl. A_r(Cl) = 35.5.

Calculate the relative atomic mass of M and identify the metal.

Worked answer

n(Cl atoms) = m/A_r
n(Cl atoms) = 1.420/35.5 = 0.0400 mol

n(M) = n(Cl atoms)/2
n(M) = 0.0400/2 = 0.0200 mol

A_r(metal) = m/n
A_r(metal) = 0.486/0.0200 = 24.3

A_r(M) = 24.3, so the metal is magnesium.

EXAM TRAP Do not round 1.5 to 2. Multiply the whole ratio. Experimental ratios need to be close to simple fractions, not forced into an arbitrary formula.

TEST IT

Try question 24 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Turn mass data into a simplest whole-number atom ratio.

18. Find an oxide formula from heating data

SPEC 3.1.2.4–3.1.2.5

CRACK IT

When a metal forms an oxide, the solid gains oxygen and its mass increases. First subtract the empty crucible mass so you are comparing the substances, not the apparatus.

The increase is the mass of oxygen gained, provided no solid is lost and the expected oxide is the only product. Convert the metal and oxygen masses to moles, then find their simplest ratio.

1. Heat, cool and weigh again until consecutive masses agree within the balance’s resolution.

2. Allow the apparatus to cool before weighing; hot apparatus gives unreliable readings.

3. Keep the lid slightly open so oxygen can enter while loss of solid is reduced.

Incomplete oxidation makes the apparent oxygen gain too small, so the calculated oxygen-to-metal ratio is too low. Keep heating, cooling and weighing until the mass stops increasing. This is evidence that all the metal has reacted with oxygen.

WORKED EXAMPLE

Copper reacts with oxygen

Crucible mass 24.800 g; crucible + Cu 26.070 g; crucible + oxide 26.390 g. Use A_r(Cu) = 63.5 and A_r(O) = 16.0.

The copper is heated in oxygen to constant mass. Use the measurements to determine the empirical formula of the copper oxide.

Worked answer

m(Cu) = 26.070 − 24.800 = 1.270 g

m(O) = 26.390 − 26.070 = 0.320 g

Quantity	Cu	O
Mass / g	1.270	0.320
A_r	63.5	16.0
Amount / mol	n = m/A_r n = 1.270/63.5 = 0.0200	n = m/A_r n = 0.320/16.0 = 0.0200
÷ smallest	Ratio = amount ÷ smallest amount 0.0200/0.0200 = 1	Ratio = amount ÷ smallest amount 0.0200/0.0200 = 1
Whole-number ratio	1	1

Empirical formula: CuO.

EXAM TRAP Repeated heating, cooling and weighing gives constant mass when consecutive readings agree. It does not by itself establish the identity or purity of a solid.

TEST IT

Try question 25 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Use mass gain to find oxygen and evaluate constant-mass measurements.

19. Use relative mass to find a molecular formula

SPEC 3.1.2.4

CRACK IT

KEY DEFINITION

The empirical formula gives the simplest atom ratio. The molecular formula gives the **actual numbers of atoms in one molecule**, so it is a whole-number multiple of the empirical formula.

1. Find the empirical formula first. If composition is given as percentages, begin with a 100 g sample.

2. Add the A_r contributions to find the empirical-formula mass.

3. Divide the supplied M_r by the empirical-formula mass.

4. Multiply every empirical-formula subscript by that whole-number multiplier.

Check that the final molecular formula adds up to the supplied M_r. The multiplier applies to every element, not just the last one.

Multiplier = M_r / empirical-formula mass

M_r relative molecular or formula mass; no unit.

WORKED EXAMPLE

A carbohydrate

Empirical formula CH_2O; M_r = 180.0. Use C 12.0, H 1.0 and O 16.0.

Determine the molecular formula of the carbohydrate.

Worked answer

Empirical-formula mass = 12.0 + 2(1.0) + 16.0 = 30.0

Multiplier = M_r/empirical-formula mass

Multiplier = 180.0/30.0 = 6

Molecular formula: $C_6H_{12}O_6$.

WORKED EXAMPLE

Phosphorus oxide

Empirical formula P_2O_5; M_r = 284.0. Use P 31.0 and O 16.0.

Determine the molecular formula of the phosphorus oxide.

Worked answer

Empirical-formula mass = 2(31.0) + 5(16.0) = 142.0

Multiplier = M_r/empirical-formula mass

Multiplier = 284.0/142.0 = 2

Molecular formula: P_4O_{10}.

EXAM TRAP Multiply every subscript. A non-integer multiplier far from a whole number signals a wrong formula, wrong mass or calculation error.

TEST IT

Try question 26 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Multiply an empirical formula by a whole-number factor.

20. Find a formula from combustion products

SPEC 3.1.2.4

CRACK IT

Complete combustion lets you count carbon and hydrogen through the products they form. For a compound containing only C, H and O, all its carbon enters CO_2 and all its hydrogen enters H_2O.

1. Find moles of CO_2. Each mole contains one mole of C atoms, so $n(C) = n(CO_2)$.

2. Find moles of H_2O. Each mole contains two moles of H atoms, so $n(H) = 2n(H_2O)$.

3. Convert the C and H amounts into masses. Subtract them from the original sample mass to find the oxygen originally in the compound.

4. Convert that oxygen mass to moles, then find the empirical atom ratio.

Oxygen in the combustion products also comes from the oxygen gas used in the reaction. That is why you cannot simply count it all as oxygen from the sample. If M_r is supplied, use it to find the molecular formula.

$$n(C) = n(CO_2); n(H) = 2n(H_2O)$$

n amount of the specified substance or particles, in mol.

$$m(\text{O in compound}) = \text{sample mass} - m(C) - m(H)$$

m mass of the specified sample or substance, in g.

WORKED EXAMPLE

A CHO compound

A 0.460 g sample gives 0.880 g CO_2 and 0.540 g H_2O. Use $M_r(CO_2) = 44.0$ and $M_r(H_2O) = 18.0$; $A_r(C) = 12.0$, H = 1.0, O = 16.0.

The compound contains carbon, hydrogen and oxygen only and is burned completely. Determine its empirical formula.

Worked answer

$n(C) = m(CO_2)/M_r(CO_2)$
$n(C) = 0.880/44.0 = 0.0200$ mol; $m(C) = n \times A_r$
$m(C) = 0.0200 \times 12.0 = 0.240$ g

$n(H) = 2m(H_2O)/M_r(H_2O)$
$n(H) = 2 \times 0.540/18.0 = 0.0600$ mol; $m(H) = 0.0600$ g

$m(O) = 0.460 - 0.240 - 0.060 = 0.160$ g

Quantity	C	H	O
Mass / g	0.240	0.0600	0.160
A_r	12.0	1.0	16.0
Amount / mol	$n = m/A_r$ $n = 0.240/12.0 = 0.0200$	$n = m/A_r$ $n = 0.0600/1.0 = 0.0600$	$n = m/A_r$ $n = 0.160/16.0 = 0.0100$
÷ smallest	Ratio = amount ÷ smallest amount 0.0200/0.0100 = 2	Ratio = amount ÷ smallest amount 0.0600/0.0100 = 6	Ratio = amount ÷ smallest amount 0.0100/0.0100 = 1
Whole-number ratio	2	6	1

Empirical formula: C_2H_6O.

EXAM TRAP Mass difference is valid only when the compound contains no other elements. Do not count all oxygen in the combustion products as oxygen from the original compound.

TEST IT

Try questions 27, 28 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Use carbon dioxide and water to recover carbon and hydrogen amounts.

Hydrated salts

21. Water of crystallisation and heating errors

SPEC 3.1.2.4–3.1.2.5

CRACK IT

A hydrated salt has water molecules in a fixed ratio within its crystal structure. This is **water of crystallisation**; it is not simply a salt dissolved in water.

DEFINITIONS & KEY TERMS

Hydrated salt

A salt containing water molecules as part of its crystal structure.

Water of crystallisation

Water molecules present in a fixed ratio within the crystal structure of a salt.

Anhydrous salt

A salt containing no water of crystallisation.

In salt·xH_2O, x tells you how many water molecules occur per formula unit of salt. Heating can remove that water and leave an anhydrous salt.

1. Find the mass of anhydrous salt left after heating.

2. Find the mass of water lost by subtracting the final sample mass from the initial sample mass.

3. Convert salt and water masses separately into moles.

4. Divide moles of water by moles of salt to find x.

Check the stated chemistry: this method assumes that the loss is water and that the residue is the intended anhydrous salt.

1. Weigh the empty crucible and then the crucible containing hydrated salt.

2. Heat gently at first to avoid spitting, then sufficiently to remove water without decomposing the salt.

3. Cool and weigh; repeat heating, cooling and weighing to constant mass.

4. Use the salt-left and water-lost mole amounts to calculate x.

$$m(\text{water}) = m(\text{hydrated salt}) - m(\text{anhydrous salt})$$

m mass of the specified sample or substance, in g.

$$x = n(\text{water}) / n(\text{anhydrous salt})$$

n amount of the specified substance or particles, in mol; **x** number of water molecules per formula unit of the anhydrous salt; a whole-number ratio with no unit.

WORKED EXAMPLE

Copper sulfate hydrate

2.496 g $CuSO_4 \cdot xH_2O$ leaves 1.596 g $CuSO_4$. $M_r(CuSO_4) = 159.6$; $M_r(H_2O) = 18.0$.

The hydrate is heated until all its water of crystallisation is removed. Determine x and calculate the relative formula mass of the hydrated salt.

Worked answer

Quantity	$CuSO_4$	H_2O lost
Mass / g	1.596	Mass of water = mass before heating − mass after heating 2.496 − 1.596 = 0.900
A_r or M_r (no unit)	159.6	18.0
Amount / mol	$n = m/M_r$ n = 1.596/159.6 = 0.0100	0.0500

$x = n(H_2O)/n(\text{anhydrous salt})$
$x = 0.0500/0.0100 = 5$

$CuSO_4 \cdot 5H_2O$; relative formula mass = 159.6 + 5(18.0) = 249.6.

WORKED EXAMPLE

Use constant mass

Crucible 19.840 g; with hydrated $MgSO_4$ 22.304 g. After heating: 21.068, 21.044, 21.044 g. Use $M_r(MgSO_4) = 120.4$ and $M_r(H_2O) = 18.0$.

Each mass after heating includes the crucible. Use the final constant mass to determine x in $MgSO_4 \cdot xH_2O$.

Worked answer

Hydrate mass = 22.304 − 19.840 = 2.464 g

Anhydrous mass = 21.044 − 19.840 = 1.204 g

Quantity	$MgSO_4$	H_2O lost
Mass / g	1.204	Mass of water = mass before heating − mass after heating 22.304 − 21.044 = 1.260
A_r or M_r (no unit)	120.4	18.0
Amount / mol	$n = m/M_r$ n = 1.204/120.4 = 0.0100	0.0700

x = n(H_2O)/n(anhydrous salt)
x = 0.0700/0.0100

$MgSO_4 \cdot 7H_2O$.

Problem	Effect on residue and apparent water loss	Effect on x
Incomplete dehydration or water reabsorbed	Residue too heavy; apparent water loss too small	Too low
Solid lost by spitting	Residue too light; mass loss wrongly treated as water	Too high
Salt decomposes as well as losing water	Extra mass loss wrongly treated as water; wrong residue assumption	Usually too high under the assumed-salt calculation

WORKED EXAMPLE

Why incomplete heating lowers x

1.722 g $CaSO_4 \cdot 2H_2O$ should leave 1.362 g $CaSO_4$, but 0.090 g water remains. $M_r(CaSO_4)$ = 136.2; $M_r(H_2O)$ = 18.0.

Calculate the apparent value of x that would be obtained if the wet residue were incorrectly treated as anhydrous $CaSO_4$. State whether this value is higher or lower than the true value.

Worked answer

Measured residue = 1.362 + 0.090 = 1.452 g

Apparent water loss = 1.722 − 1.452 = 0.270 g

Apparent x = (0.270/18.0) / (1.452/136.2) = 1.407…

Apparent x = 1.41, too low. Do not force this to a whole number.

WORKED EXAMPLE

Water percentage in a hydrate

A $CuSO_4$ hydrate contains 36.06% water. $M_r(CuSO_4)$ = 159.6; $M_r(H_2O)$ = 18.0.

Determine x in $CuSO_4 \cdot xH_2O$ from this percentage by mass.

Worked answer

Use 100 g: 36.06 g water and 63.94 g anhydrous salt.

Quantity	$CuSO_4$	H_2O
Mass / g	63.94	36.06
A_r or M_r (no unit)	159.6	18.0
Amount / mol	$n = m/M_r$ $n = 63.94/159.6 = 0.400626…$	$n = m/M_r$ $n = 36.06/18.0 = 2.00333…$

$x = n(H_2O)/n(\text{anhydrous salt})$
$x = (36.06/18.0)/(63.94/159.6) = 5.0005…$

$CuSO_4 \cdot 5H_2O$.

EXAM TRAP Heat, cool and weigh until consecutive readings agree. This is evidence that all the water has been driven off. Check that the residue is the intended anhydrous salt, and keep it dry while it cools.

TEST IT

Try questions 29, 30 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Find x in salt·xH₂O and explain how practical errors change x.

Concentration & dilution

22. Solution concentration and mass concentration

SPEC 3.1.2.2

CRACK IT

Concentration tells you how much solute is present in a given volume of **solution**. Use the final solution volume, not the volume of water added.

For concentration in mol dm^{-3}, use c = n/V with V in dm^3. Divide cm^3 by 1000 to convert to dm^3.

Mass concentration tells you grams of solute per dm^3. Calculate mass divided by solution volume, or multiply concentration in mol dm^{-3} by M_r to get mass concentration in g dm^{-3}.

Write the concentration unit before choosing the calculation. mol dm^{-3} and g dm^{-3} describe different quantities.

$$n = cV;\ c = n/V;\ V = n/c$$

V solution volume, in dm^3 when concentration is in mol dm^{-3}; **c** concentration of the specified solute, in mol dm^{-3}; **n** amount of the specified substance or particles, in mol.

Quantity	Unit
n	mol
c	mol dm^{-3}
V in n = cV	dm^3

$$V / dm^3 = V / cm^3 \div 1000$$

V solution volume, in dm^3 when concentration is in mol dm^{-3}.

WORKED EXAMPLE

Amount in an aliquot

Calculate the number of moles in 25.0 cm^3 of 0.200 mol dm^{-3} NaCl.

Worked answer

$V(dm^3) = V(cm^3)/1000$
$V = 25.0/1000 = 0.0250\ dm^3$

$n = cV$
$n = 0.200 \times 0.0250$

0.00500 mol NaCl.

WORKED EXAMPLE

Find the required volume

What volume of 0.150 mol dm^{-3} KNO_3 contains 0.0120 mol?

Worked answer

$V = n/c$
$V = 0.0120/0.150 = 0.0800\ dm^3$

80.0 cm^3.

Mass concentration / g dm^{-3} = cM_r = mass / solution volume

M_r relative molecular or formula mass; no unit; **c** concentration of the specified solute, in mol dm^{-3}.

WORKED EXAMPLE

Mass and molar concentration

5.85 g NaCl is dissolved and made up to 500.0 cm^3. M_r(NaCl) = 58.5.

Calculate the solution concentration in mol dm^{-3} and in g dm^{-3}.

Worked answer

$n = m/M_r$
$n = 5.85/58.5 = 0.100$ mol; $V = 0.5000$ dm^3

$c = n/V$
$c = 0.100/0.5000 = 0.200$ mol dm^{-3}

Mass concentration = mass of solute ÷ solution volume
Mass concentration = $5.85/0.5000 = 11.7$ g dm^{-3}

0.200 mol dm^{-3}; 11.7 g dm^{-3}.

WORKED EXAMPLE

Mass needed for a solution

Prepare 250.0 cm^3 of 0.0800 mol dm^{-3} KCl. M_r(KCl) = 74.6.

Calculate the mass of KCl needed.

Worked answer

$n = cV$
$n = 0.0800 \times 0.2500 = 0.0200$ mol

$m = n \times M_r$
$m = 0.0200 \times 74.6 = 1.492$ g

1.49 g KCl.

EXAM TRAP A g dm^{-3} value is not a mol dm^{-3} value. Divide mass concentration by M_r to obtain molar concentration.

TEST IT

Try questions 31, 32 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Use solution volume in dm^3 and connect concentration with mass.

23. Dilute a solution accurately

SPEC 3.1.2.2

CRACK IT

Adding water spreads the same amount of solute through a larger volume. The concentration falls, but the solute's mole amount stays the same, assuming no reaction or loss.

That gives $c_1V_1 = c_2V_2$. The volumes must use matching units. If the stock volume is unknown, rearrange first to find the volume you need to measure.

1. Measure the required stock solution with suitable volumetric apparatus.

2. Transfer it completely to a volumetric flask.

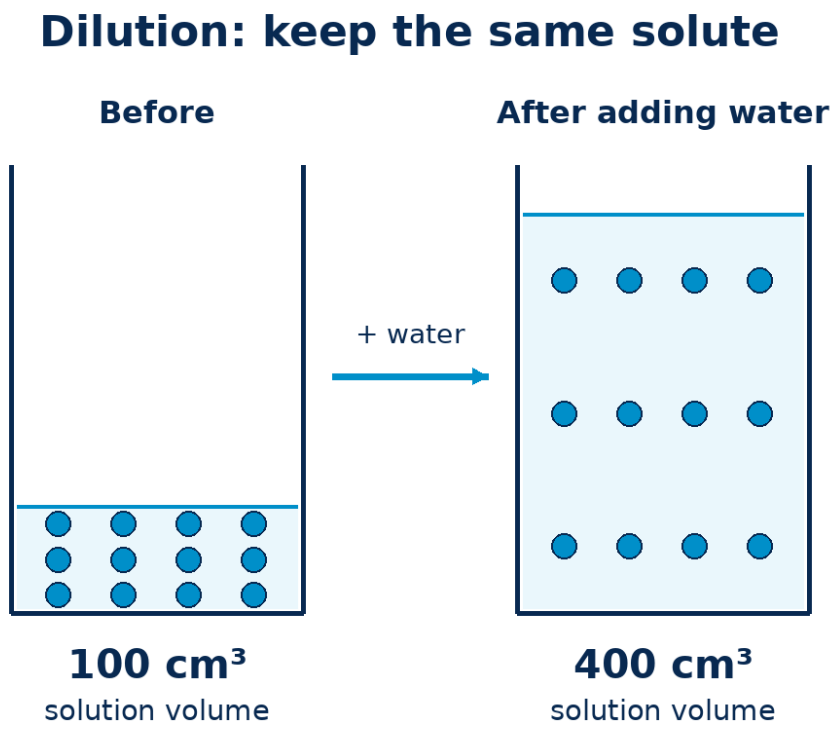
3. Add deionised water to the calibration mark, using drops near the end.

4. Stopper and invert repeatedly to mix.

Make up to the required **final volume**. Do not simply add that volume of water to the stock solution.

$$c_1V_1 = c_2V_2$$

V_1 volume of stock solution used; use matching units for both volumes; V_2 final solution volume; use matching units for both volumes; c_1 initial stock concentration, in mol dm^{-3}; c_2 final diluted concentration, in mol dm^{-3}.



WORKED EXAMPLE

Find the diluted concentration

Dilute 20.0 cm^3 of 0.500 mol dm^{-3} solution to 100.0 cm^3.

Calculate the concentration of the diluted solution in mol dm^{-3}.

Worked answer

$c_2 = c_1V_1/V_2$

$c_2 = (0.500 \times 20.0)/100.0$

0.100 mol dm^{-3}.

WORKED EXAMPLE

Measure the stock volume

Prepare 250.0 cm^3 of 0.0400 mol dm^{-3} solution from 0.200 mol dm^{-3} stock.

Calculate the volume of stock solution needed, in cm^3, and state the final volume after dilution.

Worked answer

$V_1 = c_2V_2/c_1$

$V_1 = (0.0400 \times 250.0)/0.200$

Measure 50.0 cm^3 stock, then make up to a final volume of 250.0 cm^3.

EXAM TRAP Make up to the final volume. Do not add that whole volume of water to the stock; the total would be too large and the solution too dilute.

TEST IT

Try question 33 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Conserve solute amount while changing the final solution volume.

24. Prepare a standard solution

SPEC 3.1.2.5; Required Practical 1

CRACK IT

KEY DEFINITION

A standard solution has an accurately known concentration. To prepare one, both the mass of solute and the final solution volume must be accurate.

1. Calculate the required mass of a suitable pure, dry, stable solid. Weigh it accurately, using weighing by difference where appropriate.

2. Dissolve the solid fully in deionised water in a beaker, stirring with a glass rod.

3. Transfer the solution through a funnel into the volumetric flask.

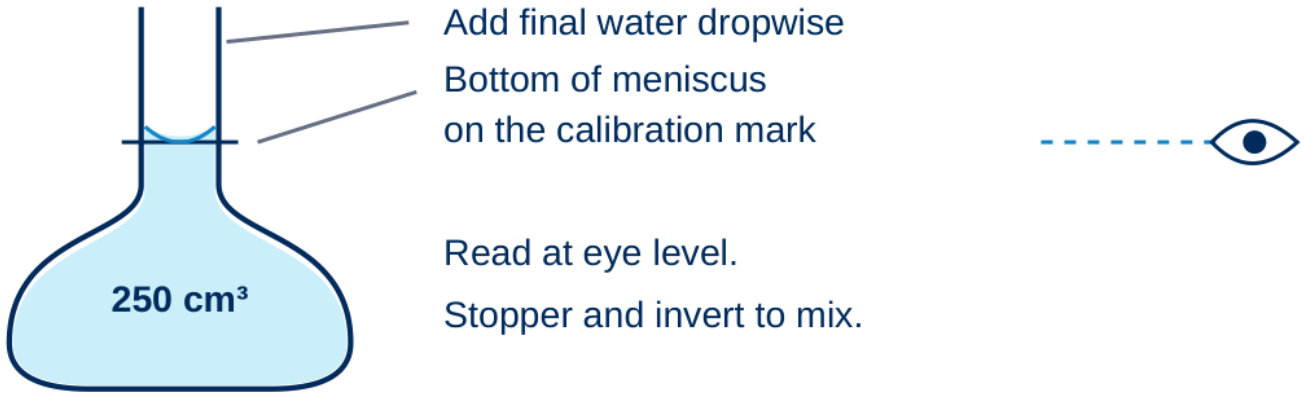
4. Rinse the beaker, rod and funnel into the flask. This transfers solute that would otherwise be left behind.

5. Let a warm solution cool to room temperature. Add water nearly to the mark, then dropwise until the bottom of the meniscus is on the mark at eye level.

6. Stopper and invert repeatedly, then label the solution.

KEY DEFINITION

Quantitative transfer means transferring all the measured solute. A volumetric flask is calibrated to contain its stated volume at the calibration temperature.



WORKED EXAMPLE

Sodium carbonate standard

Prepare 250.0 cm^3 of 0.0500 mol dm^{-3} anhydrous Na_2CO_3. M_r = 106.0.

Calculate the mass of anhydrous sodium carbonate needed.

Worked answer

n = cV
n = 0.0500 × 0.2500 = 0.0125 mol

$m = n \times M_r$
m = 0.0125 × 106.0

Target mass = 1.325 g. Use the actual recorded mass to calculate the precise concentration.

EXAM TRAP Do not add 250.0 cm^3 water to the solid. Make the total solution volume 250.0 cm^3. If you overshoot the calibration mark, removing some solution does not restore the intended concentration.

TEST IT

Try question 34 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Prepare an accurately known concentration using quantitative transfer.

Titrations & practical technique

25. Carry out an acid–base titration

SPEC 3.1.2.5; Required Practical 1

CRACK IT

A titration finds the volume of one solution needed to react with a measured portion of another. The burette delivers the titrant; the conical flask holds the solution being analysed.

1. Rinse the burette with deionised water, then its own solution. Fill it and run solution through the tip to remove air bubbles. Remove the filling funnel.

2. Rinse the pipette with deionised water, then the solution it will measure. Use a pipette filler to transfer a fixed aliquot (a measured portion of the solution) to the conical flask.

3. Let a standard transfer pipette drain. Do not blow out the drop designed to remain in it.

4. Add a few drops of a suitable indicator and place the flask on a white tile.

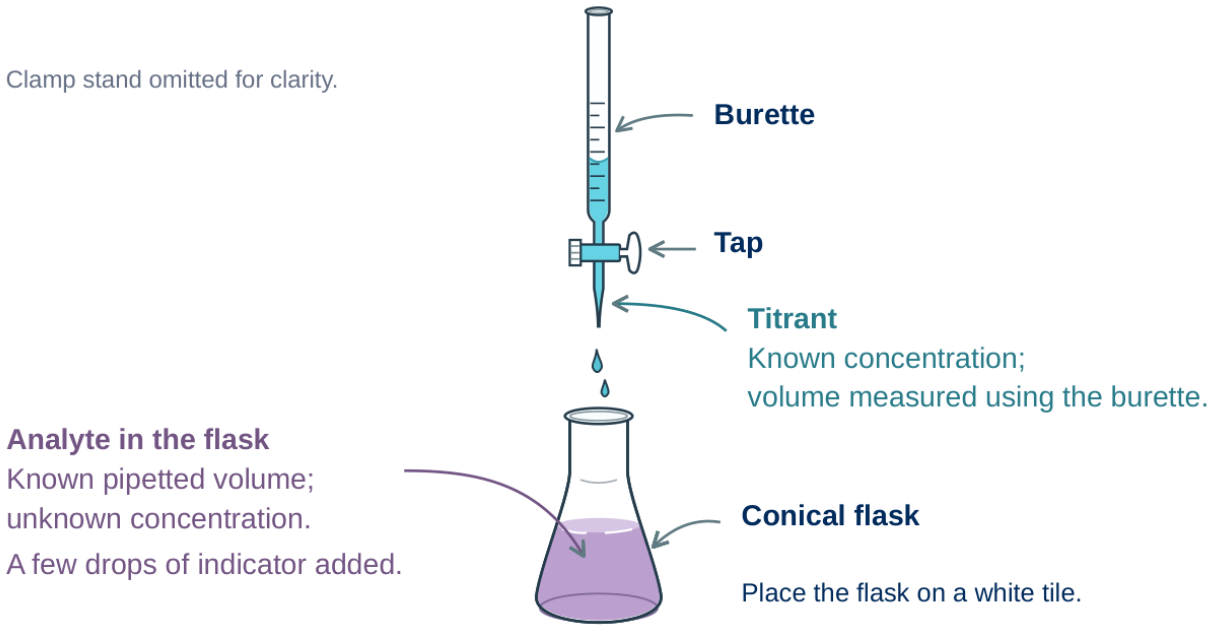
5. Read the burette meniscus at eye level and record the initial reading.

6. Do a rough titration to locate the endpoint. Repeat with fresh aliquots (measured portions), swirling and adding dropwise near the endpoint.

7. Wash splashes down the flask walls with deionised water. This changes volume but not the amount of solute being titrated.

8. Record the final reading and calculate final minus initial. Repeat until you obtain concordant titres (within 0.1 cm^3 of each other).

Record burette readings to two decimal places, normally to the nearest 0.05 cm^3 on a scale graduated every 0.10 cm^3. Use eye protection, a pipette filler and the laboratory risk assessment.



DEFINITIONS & KEY TERMS

End point

The observed indicator colour change.

Equivalence point

The point at which the reactants have been mixed in their exact stoichiometric ratio.

WORKED EXAMPLE

Choose an indicator

Choose a suitable indicator for (a) HCl added to NaOH and (b) complete neutralisation of Na_2CO_3 by HCl. State the colour change at the endpoint for each, starting with the alkali in the conical flask.

Worked answer

• HCl added to NaOH: phenolphthalein changes from pink to just colourless at the endpoint.

• Complete neutralisation of Na_2CO_3 by HCl: methyl orange changes from yellow towards the first persistent orange endpoint.

Choose an indicator whose colour change is close to equivalence.

EXAM TRAP Water left in the pipette or burette dilutes the solution being measured. Water in the conical flask changes total volume but not the moles already delivered. A transfer pipette is calibrated to leave its final drop behind.

TEST IT

Try question 35 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Explain the apparatus, rinsing and endpoint technique used in a titration.

26. Read a burette and choose concordant titres

SPEC Required Practical 1; mathematical skills

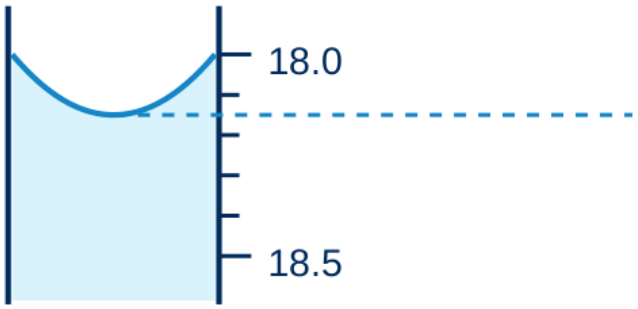
CRACK IT

A burette scale increases **downwards**. The titre is the volume delivered, so subtract the initial reading from the final reading.

Read the bottom of a clear solution's meniscus at eye level. For a burette graduated every 0.10 cm^3, estimate to the nearest 0.05 cm^3 and record two decimal places.

Concordant titres (within 0.1 cm^3 of each other) agree closely enough to use in the mean. Use a different tolerance if the question supplies one. Compare the titres themselves, not just the final readings.

Leave out the rough titre and justified outliers when finding the mean. If no set is concordant, more titrations are needed; do not choose an unsupported average.



Read the lowest point

Here: 18.15 cm³

Scale increases downwards.

Titre = final burette reading − initial burette reading

WORKED EXAMPLE

Select the reliable pair

The following burette readings were recorded during a titration. All readings are in cm³.

Reading / cm³	Rough	1	2	3
Initial	0.20	0.30	0.20	0.45
Final	25.00	24.45	24.70	24.65

Calculate all four titres. Select the concordant accurate titres and calculate their mean, reporting it to two decimal places. Treat accurate titres that differ by no more than 0.10 cm³ as concordant.

Worked answer

Reading / cm^3	Rough	1	2	3
Final	25.00	24.45	24.70	24.65
Initial	0.20	0.30	0.20	0.45
Titre	24.80	24.15	24.50	24.20

Titres 1 and 3 differ by 0.05 cm^3. The rough titre and run 2 are excluded.

Mean = (24.15 + 24.20)/2 = 24.175 cm^3

Report 24.18 cm^3. Retain the unrounded mean for later calculations.

EXAM TRAP A trailing zero in 24.20 records the measurement precision. Do not average the rough result simply because it looks close.

TEST IT

Try questions 36, 37 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Calculate titres from two readings and justify the mean used.

27. Calculate a concentration from a titre

SPEC 3.1.2.2; 3.1.2.5; Required Practical 1

CRACK IT

Use a grid with the reacting substances across the top and **c (concentration), V (volume) and n (amount in moles)** down the side. Add the coefficients from the balanced equation below the mole row.

1. Write the balanced equation and fill in the known concentrations and volumes. Convert each volume to dm^3 by dividing its cm^3 value by 1000.

2. Start in the column with both c and V known. Use n = cV to fill its mole row.

3. Work across the mole row using the equation ratio: divide by the known substance's coefficient, then multiply by the other substance's coefficient.

4. Work up the unknown substance's column: use c = n/V, dividing by that substance's **own** solution volume in dm^3.

5. Give the concentration unit and round only the final answer.

Keep substance names beside the numbers. The burette volume and pipette volume belong to different solutions and cannot be swapped.

WORKED EXAMPLE

Sodium carbonate and hydrochloric acid

25.0 cm^3 of Na_2CO_3 solution requires 20.0 cm^3 of 0.100 mol dm^{-3} HCl solution for complete neutralisation. $Na_2CO_3 + 2HCl \rightarrow 2NaCl + CO_2 + H_2O$.

Calculate the concentration of the sodium carbonate solution in mol dm^{-3}.

Worked answer

$Na_2CO_3 + 2HCl \rightarrow 2NaCl + CO_2 + H_2O$. Start with HCl, whose concentration and volume are known. The 1 : 2 ratio means the carbonate has half as many moles.

Quantity	Na_2CO_3	HCl
Concentration, c / mol dm^{-3}	c = n/V 0.00100/0.0250 = **0.0400**	0.100
Volume, V / dm^3	25.0/1000 = 0.0250	20.0/1000 = 0.0200
Amount, n / mol	0.00200/2 = 0.00100	n = cV 0.100 × 0.0200 = 0.00200
Coefficient (mole ratio)	1	2

The Na_2CO_3 concentration is 0.0400 mol dm^{-3}.

WORKED EXAMPLE

A one-to-one neutralisation

25.0 cm^3 of HNO_3 solution requires 22.4 cm^3 of 0.125 mol dm^{-3} KOH solution for complete neutralisation. $HNO_3 + KOH \rightarrow KNO_3 + H_2O$.

Calculate the concentration of the nitric acid solution in mol dm^{-3}.

Worked answer

$HNO_3 + KOH \rightarrow KNO_3 + H_2O$. The 1 : 1 ratio gives equal moles at the end point.

Quantity	HNO_3	KOH
Concentration, c / mol dm^{-3}	c = n/V 0.00280/0.0250 = **0.112**	0.125
Volume, V / dm^3	25.0/1000 = 0.0250	22.4/1000 = 0.0224
Amount, n / mol	0.00280	n = cV 0.125 × 0.0224 = 0.00280
Coefficient (mole ratio)	1	1

The HNO_3 concentration is 0.112 mol dm^{-3}.

EXAM TRAP Do not set acid and alkali moles equal unless the equation ratio is 1 : 1. Use the volume of the solution whose concentration you are finding in the final c = n/V step.

TEST IT

Try question 38 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Use the balanced-equation ratio between known and unknown solution amounts.

28. Titrate a diluted sample

SPEC 3.1.2.2; 3.1.2.5

CRACK IT

A titration of a diluted sample first tells you about the **diluted solution**. You still need to work back to the original sample.

KEY DEFINITION

An aliquot is a measured portion taken from a well-mixed solution. To scale its mole amount to the full flask, multiply by whole-flask volume divided by aliquot volume.

For example, a 100.0 cm^3 flask contains four 25.0 cm^3 aliquots. If one contains 0.00200 mol acid, the whole flask contains 4 × 0.00200 = 0.00800 mol.

Those moles came from the original 0.0100 dm^3 sample, so its concentration is 0.00800/0.0100 = 0.800 mol dm^{-3}. Alternatively, multiply the diluted concentration by the dilution factor.

$$c_1V_1 = c_2V_2$$

V_1 volume taken from the original solution to make the dilution, in cm^3 or dm^3; V_2 final total volume of the diluted solution, in the same units as V_1; c_1 concentration of the original solution before dilution, in mol dm^{-3}; c_2 concentration of the diluted solution, in mol dm^{-3}.

1 means before dilution; 2 means after dilution. Adding water changes the concentration and volume, but not the number of moles of solute. Use the same units for both volumes: either both cm^3 or both dm^3. The final volume is the total volume of the diluted solution, not the volume of water added.

First use the titration and balanced-equation mole ratio to find the diluted concentration. Then use the dilution equation to work back to the original concentration. The volume of the aliquot titrated is not the final dilution volume.

WORKED EXAMPLE

Vinegar after dilution

10.0 cm^3 vinegar is diluted to 100.0 cm^3. A 25.0 cm^3 aliquot of the diluted vinegar requires 20.0 cm^3 of 0.100 mol dm^{-3} NaOH solution for complete neutralisation. $CH_3COOH + NaOH \rightarrow CH_3COONa + H_2O$. $M_r(CH_3COOH) = 60.0$.

Calculate the concentration of ethanoic acid in the original vinegar in mol dm^{-3} and g dm^{-3}.

Worked answer

An aliquot is a measured portion: here it is 25.0 cm^3 of the diluted vinegar. $CH_3COOH + NaOH \rightarrow CH_3COONa + H_2O$.

Quantity	CH_3COOH (diluted)	NaOH
Concentration, c / mol dm^{-3}	c = n/V 0.00200/0.0250 = 0.0800	0.100
Volume, V / dm^3	25.0/1000 = 0.0250	20.0/1000 = 0.0200
Amount, n / mol	0.00200 (1 : 1 ratio)	n = cV 0.100 × 0.0200 = 0.00200
Coefficient (mole ratio)	1	1

Dilution factor = final dilution volume/original sample volume = 100.0/10.0 = 10.0.

Original concentration = diluted concentration × dilution factor = 0.0800 × 10.0 = **0.800 mol dm^{-3}**.

Mass concentration = c × M_r = 0.800 × 60.0 = **48.0 g dm^{-3}**.

EXAM TRAP Do not apply both the dilution factor and the whole-flask factor to the same quantity without tracking what that quantity represents.

TEST IT

Try question 39 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Distinguish the original sample, final flask volume and titrated aliquot.

29. Titration uncertainty and error direction

SPEC Required Practical 1; mathematical skills

CRACK IT

A titre uses two measurements: an initial and a final burette reading. In this treatment, add their absolute uncertainties to obtain the titre uncertainty.

To find percentage uncertainty, divide the absolute uncertainty by the measured titre and multiply by 100. With the same apparatus, a larger titre gives a smaller percentage uncertainty.

A **directional error** is a mistake that makes a result too high or too low. For example, consistently adding acid past the end point makes the recorded titre too large. If that titre is used to calculate an unknown alkali concentration, the concentration comes out too high.

Explain the chain: what went wrong → whether the titre is too large or too small → how that changes the calculated result. This is different from uncertainty, which describes the range of values consistent with a measurement; it does not by itself tell you which way the result is wrong.

Use the uncertainty stated in the question. Two reading uncertainties alone give ±0.10 cm^3 when each is ±0.05 cm^3. A total including a further ±0.05 cm^3 end-point judgement is ±0.15 cm^3. Do not add the end-point term twice.

Percentage uncertainty = absolute uncertainty / measured value × 100

WORKED EXAMPLE

Two readings contribute

A titre is 20.00 cm^3 and each reading has uncertainty ±0.05 cm^3.

Calculate the absolute and percentage uncertainty in the titre from the two burette readings. Then calculate the percentage uncertainty when a further endpoint uncertainty of ±0.05 cm^3 is included.

Worked answer

Absolute uncertainty = 0.05 + 0.05 = 0.10 cm^3

Percentage uncertainty = (absolute uncertainty ÷ measured value) × 100
Percentage uncertainty = 0.10/20.00 × 100 = 0.50%

If endpoint judgement contributes a further ±0.05 cm^3, use total ±0.15 cm^3.

0.15/20.00 × 100 = 0.75%

0.50% for the readings alone; 0.75% including the stated endpoint uncertainty.

DEFINITIONS & KEY TERMS

Precision

How closely repeated measurements agree.

Accuracy

How close a result is to the true or accepted value.

Random error

A varying effect that causes scatter.

Systematic error

A consistent effect that shifts results in one direction.

Known acid in burette; unknown alkali in flask	Effect	Calculated alkali concentration
Burette wet with water	Acid diluted; larger titre needed; stated acid concentration overestimates moles	Too high
Pipette wet with water	Aliquot diluted; fewer alkali moles; smaller titre	Too low
Conical flask wet with deionised water	Aliquot moles unchanged	Unchanged
Initial air bubble disappears from burette jet	Some measured volume fills jet rather than reaching flask	Too high
Endpoint consistently overshot	Recorded titre larger than needed	Too high

EXAM TRAP Concordant titres (within 0.1 cm^3 of each other) show precision. They do not remove a systematic error or prove accuracy. Explain the chain: what changes → effect on titre → effect on calculated quantity.

TEST IT

Try questions 40, 41 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Calculate uncertainty and connect practical errors to the reported result.

30. Use a titration to calculate percentage purity

SPEC 3.1.2.2; 3.1.2.5

CRACK IT

A titration can find how much pure reacting substance was present in an impure sample. Keep track of whether each amount refers to an aliquot or the whole prepared solution.

1. Use the titre and known concentration to find moles of titrant.

2. Apply the equation ratio to find moles of the sample substance in the aliquot.

3. Scale up to the whole flask using the flask-volume/aliquot-volume ratio.

4. Convert to mass of pure substance, then divide by the original sample mass and multiply by 100.

This method assumes that the impurities do not react with the titrant or interfere with the endpoint.

WORKED EXAMPLE

Potassium carbonate purity

2.00 g of an impure K_2CO_3 sample is made up to 250.0 cm^3. A 25.0 cm^3 aliquot of this solution requires 20.0 cm^3 of 0.100 mol dm^{-3} HCl solution for complete neutralisation. $K_2CO_3 + 2HCl \rightarrow 2KCl + CO_2 + H_2O$. $M_r(K_2CO_3) = 138.2$.

Calculate the percentage purity by mass of the potassium carbonate sample. Assume the impurities do not react with hydrochloric acid.

Worked answer

$K_2CO_3 + 2HCl \rightarrow 2KCl + CO_2 + H_2O$. The grid describes the titrated portion.

Quantity	K_2CO_3 aliquot	HCl
Concentration, c / mol dm^{-3}	Not needed for purity	0.100
Volume, V / dm^3	25.0/1000 = 0.0250	20.0/1000 = 0.0200
Amount, n / mol	0.00200/2 = 0.00100	n = cV 0.100 × 0.0200 = 0.00200
Coefficient (mole ratio)	1	2

Moles in the full flask = moles in aliquot × flask volume/aliquot volume = 0.00100 × 250.0/25.0 = 0.0100 mol.

Mass of K_2CO_3 = n × M_r = 0.0100 × 138.2 = 1.382 g.

Percentage purity = pure mass/sample mass × 100 = 1.382/2.00 × 100 = **69.1%**.

EXAM TRAP Dividing the pure mass in one aliquot by the whole sample mass misses the flask/aliquot factor. Overshooting the endpoint gives too much apparent carbonate and a purity that is too high.

TEST IT

Try question 42 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Scale an aliquot result to the whole sample before calculating purity.

31. Link titration, purity, gas and process calculations

SPEC 3.1.2.2–3.1.2.3; 3.1.2.5; Required Practical 1

CRACK IT

A long calculation becomes more manageable when every amount has a label: which substance, and which part of the sample? Distinguish an aliquot, the whole flask, the original sample and a production batch.

Start with the requested quantity and write an equation containing it. Work backwards through any missing quantities, then carry full calculator values through the forward calculation.

In a back titration, find the reagent left over and subtract it from the known amount originally added. Only the difference reacted with the sample. Apply the sample-reaction ratio after that subtraction.

In a standardisation chain, the concentration found in the first titration becomes data for the second. Do not round it prematurely.

Quantity	Solution amount or concentration	Another substance's amount	Gas amount or volume	Purity	Yield	Atom economy
Start with	n = cV or c = n/V	Balanced-equation coefficient ratio	pV = nRT	Pure mass/sample mass × 100	Actual/theoretical × 100	Balanced formula masses and coefficients
Check	Solution volume in dm^3	Limiting reactant used	Pa, m^3, K and supplied R	Whole sample, not one aliquot	Same product and units	All reactants; desired product identified

WORKED EXAMPLE

Diagnose a plausible-looking answer

A student writes n = 0.100 × 25.0 = 2.50 mol for 25.0 cm^3 of 0.100 mol dm^{-3} solution.

Identify the error, calculate the correct number of moles and state the factor by which the student's answer is too large.

Worked answer

The equation is suitable, but the volume must be in dm^3.

Correct n = cV
n = 0.100 × 0.0250 = 0.00250 mol

The student's amount is 1000 times too large.

EXAM TRAP Keep theoretical and measured gas amounts separate. For a production batch, first remove any inert fraction before calculating a theoretical product mass. Do not include that inert fraction in an equation-based atom-economy denominator.

WORKED EXAMPLE

Carry a concentration into a second titration

25.00 cm^3 of 0.04000 mol dm^{-3} Na_2CO_3 solution requires 20.00 cm^3 of HCl solution for complete neutralisation. Then 18.00 cm^3 of this HCl solution completely neutralises 25.00 cm^3 of NaOH solution.

Calculate the concentrations of the HCl and NaOH solutions in mol dm^{-3}. The reactions are $Na_2CO_3 + 2HCl \rightarrow 2NaCl + CO_2 + H_2O$ and $HCl + NaOH \rightarrow NaCl + H_2O$.

Worked answer

First titration: find the HCl concentration. $Na_2CO_3 + 2HCl \rightarrow 2NaCl + CO_2 + H_2O$.

Quantity	Na_2CO_3	HCl
Concentration, c / mol dm^{-3}	0.04000	c = n/V 0.002000/0.02000 = 0.1000
Volume, V / dm^3	25.00/1000 = 0.02500	20.00/1000 = 0.02000
Amount, n / mol	n = cV 0.04000 × 0.02500 = 0.001000	0.001000 × 2 = 0.002000
Coefficient (mole ratio)	1	2

Second titration: use that HCl to find the NaOH concentration. $HCl + NaOH \rightarrow NaCl + H_2O$.

Quantity	HCl	NaOH
Concentration, c / mol dm^{-3}	0.1000	c = n/V 0.001800/0.02500 = **0.07200**
Volume, V / dm^3	18.00/1000 = 0.01800	25.00/1000 = 0.02500
Amount, n / mol	n = cV 0.1000 × 0.01800 = 0.001800	0.001800 (1 : 1 ratio)
Coefficient (mole ratio)	1	1

The NaOH concentration is 0.07200 mol dm^{-3}.

WORKED EXAMPLE

Find what reacted by measuring what is left

0.500 g impure MgO reacts with 40.00 cm^3 of 0.5000 mol dm^{-3} HCl. All the hydrochloric acid remaining after the reaction is completely neutralised by 12.00 cm^3 of 0.2000 mol dm^{-3} NaOH solution. Use M_r(MgO) = 40.3.

Calculate the percentage purity by mass of MgO in the sample. Assume the impurities do not react. The reactions are $MgO + 2HCl \rightarrow MgCl_2 + H_2O$ and $HCl + NaOH \rightarrow NaCl + H_2O$.

Worked answer

$HCl + NaOH \rightarrow NaCl + H_2O$. The back titration measures the acid left after MgO reacts.

Quantity	HCl added	NaOH titre	HCl left
Concentration, c / mol dm^{-3}	0.5000	0.2000	Not needed
Volume, V / dm^3	40.00/1000 = 0.04000	12.00/1000 = 0.01200	Not needed
Amount, n / mol	n = cV 0.5000 × 0.04000 = 0.02000	n = cV 0.2000 × 0.01200 = 0.002400	Same moles as NaOH 0.002400
Coefficient (mole ratio)	Not compared	1	1

Moles of HCl consumed = initial − remaining = 0.02000 − 0.002400 = 0.01760 mol.

$MgO + 2HCl \rightarrow MgCl_2 + H_2O$: MgO : HCl = 1 : 2. Moles of MgO = 0.01760/2 = 0.008800 mol.

Pure mass = n × M_r = 0.008800 × 40.3 = 0.35464 g. Percentage purity = pure mass/sample mass × 100 = 0.35464/0.500 × 100 = **70.9%**.

TEST IT

Try questions 43, 44, 45 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Choose a valid sequence, preserve units and audit the final result.

Gas calculations

32. The ideal gas equation and gas molar mass

SPEC 3.1.2.3

CRACK IT

The ideal gas equation connects pressure, volume, temperature and amount. Write pV = nRT, then rearrange for the quantity you need.

1. Use pressure in Pa, volume in m^3 and temperature in K when using R = 8.31 J mol^{-1} K^{-1}.

2. Convert before substituting: add 273 to temperature in °C for these school calculations, and use 1 $dm^3 = 10^{-3}$ m^3 or 1 $cm^3 = 10^{-6}$ m^3.

3. Calculate the amount in moles. If mass is supplied, use M_r = m/n to find relative molecular mass, using mass in grams.

The ideal-gas model is a better approximation at low pressure and high temperature. The particles then occupy a smaller fraction of the volume, and attractions have less effect.

pV = nRT; n = pV/RT; V = nRT/p; p = nRT/V; T = pV/nR

R gas constant, 8.31 J mol^{-1} K^{-1}, unless the question supplies a different value; **T** absolute temperature of the gas, in K; **V** gas volume, in m^3 in the ideal gas equation; **n** amount of the specified substance or particles, in mol; **p** gas pressure, in Pa in the ideal gas equation.

Conversion	Operation
kPa → Pa	× 1000
cm^3 → m^3	÷ 1 000 000
dm^3 → m^3	÷ 1000
°C → K	Add 273, or 273.15 if the question precision requires it

WORKED EXAMPLE

Convert before substituting

Convert 250 cm^3, 100 kPa and 27 °C to SI units.

Worked answer

V = 2.50 × 10^{-4} m^3; p = 100 000 Pa; T ≈ 300 K

Solution-volume conversions differ: 25.0 cm^3 = 0.0250 dm^3 in n = cV, but 2.50 × 10^{-5} m^3 in pV = nRT.

WORKED EXAMPLE

Amount of gas

Find the number of moles in 250 cm^3 at 100 kPa and 300 K. R = 8.31 J mol^{-1} K^{-1}.

Worked answer

n = pV/(RT)
n = (100 000 × 2.50 × 10^{-4})/(8.31 × 300) = 0.010028… mol

0.0100 mol gas.

WORKED EXAMPLE

Gas volume

Find the volume of 0.0200 mol gas at 298 K and 101 kPa. R = 8.31 J mol^{-1} K^{-1}.

Give your answer in m^3 and cm^3.

Worked answer

V = nRT/p
V = (0.0200 × 8.31 × 298)/101 000 = 4.90372... × 10^{-4} m^3

490 cm^3.

M_r = m/n = mRT/pV

M_r relative molecular or formula mass; no unit; **R** gas constant, 8.31 J mol^{-1} K^{-1}, unless the question supplies a different value; **T** absolute temperature of the gas, in K; **V** gas volume, in m^3 in the ideal gas equation; **m** mass of the specified sample or substance, in g; **n** amount of the specified substance or particles, in mol; **p** gas pressure, in Pa in the ideal gas equation.

WORKED EXAMPLE

Relative molecular mass of a vapour

A 0.180 g vapour occupies 100 cm^3 at 100 kPa and 400 K. R = 8.31 J mol^{-1} K^{-1}.

Calculate the relative molecular mass, M_r, of the vapour.

Worked answer

n = pV/(RT)
n = (100 000 × 1.00 × 10^{-4})/(8.31 × 400) = 0.00300842... mol

M_r = m/n
M_r = 0.180/0.00300842...

M_r = 59.8 with no unit.

WORKED EXAMPLE

Relative molecular mass from gas density

A gas has density 1.20 g dm^{-3} at 100 kPa and 300 K.

Calculate the relative molecular mass, M_r, of the gas. Use R = 8.31 J mol^{-1} K^{-1}.

Worked answer

Choose 1.00 dm^3, which is 0.00100 m^3 and has mass 1.20 g.

n = pV/(RT)
n = (100 000 × 0.00100)/(8.31 × 300) = 0.0401123... mol

M_r = m/n
M_r = 1.20/0.0401123...

M_r = 29.9.

EXAM TRAP Use mass in grams and amount in moles to calculate the unitless relative molecular mass, M_r. A vapour experiment assumes all the sample vaporises, none is lost and the measured volume contains only that gas.

TEST IT

Try question 46 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Use SI gas units and calculate gas amount, volume and molar mass.

33. Gas volumes at the same temperature and pressure

SPEC 3.1.2.3; 3.1.2.5

CRACK IT

For gases at the **same temperature and pressure**, volume is proportional to amount in moles. This lets you use balanced-equation coefficients as gas-volume ratios.

Check both conditions before using the shortcut. It does not turn the equation coefficients into volume ratios for liquids or solids.

If a molar gas volume V_m is supplied, use $n = V/V_m$ with matching volume units. For example, with V_m = 24.0 dm^3 mol^{-1}, first convert 120 cm^3 to 0.120 dm^3. Then n = 0.120/24.0 = 0.00500 mol.

WORKED EXAMPLE

Carbon monoxide combustion

$2CO(g) + O_2(g) \rightarrow 2CO_2(g)$. Mix 60.0 cm^3 CO with 50.0 cm^3 O_2 at the same temperature and pressure.

Identify the limiting reactant and calculate the volume of each gas present after complete reaction, measured at the original temperature and pressure.

Worked answer

$2CO + O_2 \rightarrow 2CO_2$. At the same temperature and pressure, gas volumes are proportional to moles. Divide each starting reactant volume by its coefficient; the smaller value identifies the limiting reactant.

Quantity	CO	O_2	CO_2
Initial volume / cm^3	60.0	50.0	0
Coefficient	2	1	2
Volume ÷ coefficient / cm^3	60.0/2 = **30.0 (smaller)**	50.0/1 = 50.0	Product: not compared
Volume used or formed / cm^3	30.0 × 2 = 60.0 used	30.0 × 1 = 30.0 used	30.0 × 2 = 60.0 formed
Final volume / cm^3	60.0 − 60.0 = 0	50.0 − 30.0 = **20.0**	**60.0**

CO is limiting. The final mixture contains 20.0 cm^3 O_2 and 60.0 cm^3 CO_2; no CO remains.

WORKED EXAMPLE

Ammonia volume

$N_2 + 3H_2 \rightarrow 2NH_3$. What volume of NH_3 is formed from 90.0 cm^3 H_2 with excess N_2 at the same conditions?

Worked answer

$V(NH_3) = V(\text{known gas}) \times \text{coefficient(target)/coefficient(known gas)}$
$V(NH_3) = 90.0 \times 2/3$

60.0 cm^3 NH_3.

EXAM TRAP Do not assume a gas always occupies 24.0 dm^3 mol^{-1}. Use the stated molar volume, matching conditions, or pV = nRT.

TEST IT

Try question 47 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Use gas-volume ratios only when temperature and pressure match.

34. Combine solution amounts, limiting reactants and gases

SPEC 3.1.2.2–3.1.2.3; 3.1.2.5

CRACK IT

A reaction involving a solid, a solution and a gas still uses the same mole-ratio bridge. Each starting quantity just has a different route to moles.

1. Use $n = m/M_r$ for the solid and $n = cV$ for the solution, with V in dm^3.

2. If both reactant quantities are supplied, check which is limiting.

3. Use the limiting amount and balanced equation to find moles of gas.

4. Convert the gas amount to volume using $pV = nRT$ or a supplied molar gas volume.

Do not calculate a gas volume from a reactant that is actually in excess. The reactant that runs out sets the maximum amount of gas.

WORKED EXAMPLE

Magnesium with hydrochloric acid

0.300 g Mg reacts with 20.0 cm^3 of 1.00 mol dm^{-3} HCl. Mg + 2HCl → $MgCl_2$ + H_2. A_r(Mg) = 24.3. Find the maximum H_2 volume at 100 kPa and 298 K; R = 8.31 J mol^{-1} K^{-1}.

Worked answer

Mg + 2HCl → $MgCl_2$ + H_2. Compare the starting moles divided by each coefficient.

Quantity	Mg	HCl
Mass / g	0.300	Not needed
A_r or M_r (no unit)	24.3	Not needed
Concentration, c / mol dm^{-3}	Solid	1.00
Volume, V / dm^3	Solid	20.0/1000 = 0.0200
Amount, n / mol	n = m/A_r 0.300/24.3 = 0.012345…	n = cV 1.00 × 0.0200 = 0.0200
Coefficient	1	2
n ÷ coefficient / mol	0.012345…/1	0.0200/2 = **0.0100 (smaller)**

HCl is limiting. HCl : H_2 = 2 : 1, so n(H_2) = 0.0200/2 = 0.0100 mol.

V = nRT/p = (0.0100 × 8.31 × 298)/100000 = 2.47638 × 10^{-4} m^3 = **248 cm^3 H_2**.

EXAM TRAP Do not use all of the magnesium to calculate hydrogen when there is insufficient acid to react with it.

TEST IT

Try question 48 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Find the limiting reactant before calculating a gas volume.

Yield & atom economy

35. Percentage yield, including gas measurements

SPEC 3.1.2.3; 3.1.2.5

CRACK IT

KEY DEFINITION

The theoretical yield is the maximum amount of desired product predicted by the balanced equation. The actual yield is what you recover from the experiment.

1. Calculate the theoretical yield from the limiting reactant.

2. Divide actual yield by theoretical yield and multiply by 100.

3. Compare matching quantities: mass with mass, amount with amount, or suitable gas volumes measured under matching conditions.

A reaction may be incomplete, competing reactions may form other products, or product may be lost during transfer and purification.

A result above 100% suggests an apparent product mass that is too high, for example because the product is wet or impure. It does not mean more pure product formed than the theoretical maximum.

Percentage yield = actual amount of product / theoretical amount of product × 100

WORKED EXAMPLE

Calcium oxide yield

$CaCO_3 \rightarrow CaO + CO_2$. 10.01 g $CaCO_3$ gives 4.49 g CaO. $M_r(CaCO_3) = 100.1$; $M_r(CaO) = 56.1$.

Calculate the percentage yield of calcium oxide.

Worked answer

$n(CaCO_3) = m/M_r$
$n(CaCO_3) = 10.01/100.1 = 0.100$ mol

Theoretical CaO mass = 0.100 × 56.1 = 5.61 g

Percentage yield = (actual yield ÷ theoretical yield) × 100
Yield = 4.49/5.61 × 100

80.0% yield.

WORKED EXAMPLE

Predict an actual mass

A process has theoretical product mass 12.0 g and expected yield 75.0%.

Calculate the expected actual mass of product.

Worked answer

Actual mass = 12.0 × 75.0/100

9.00 g product.

WORKED EXAMPLE

Yield from measured oxygen

$2H_2O_2 \rightarrow 2H_2O + O_2$. 20.0 cm^3 of 0.500 mol dm^{-3} H_2O_2 releases 100 cm^3 dry O_2 at 100 kPa and 300 K. R = 8.31 J mol^{-1} K^{-1}.

Calculate the percentage yield of oxygen.

Worked answer

Route	Calculation	O_2 amount / mol
Theoretical from reactant	$n(H_2O_2) = 0.500 \times 0.0200 = 0.0100$; then × 1/2	0.00500
Actual from gas	$n = (100\,000 \times 1.00 \times 10^{-4})/(8.31 \times 300)$	0.0040112…

Percentage yield = (actual yield ÷ theoretical yield) × 100
Yield = 0.0040112…/0.00500 × 100

80.2% yield.

EXAM TRAP Wet or impure product can give an apparent yield above 100%. A gas leak makes the measured yield too low. If gas is collected over water, use the dry-gas pressure with any required correction supplied or justified.

TEST IT

Try question 49 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Compare the actual product with the theoretical amount from the limiting reactant.

36. Atom economy and choosing a reaction route

SPEC 3.1.2.5

CRACK IT

Atom economy asks how much of the reactant mass is directed into the **chosen desired product** by the balanced equation. Percentage yield asks how much of that product is actually recovered.

Use the formula-mass contribution of the desired product, including its coefficient, divided by the total reactant formula-mass contributions, also including coefficients. Multiply by 100.

Conservation of mass means the denominator can also be the total formula-mass contribution of all products. Do not include catalysts, solvents or arbitrary excess quantities.

A high atom economy can reduce waste, but choosing a sustainable process also needs energy use, hazards, raw-material cost and supply, renewability, rate, yield, separation and recycling to be considered. A useful by-product may also affect the choice.

Atom economy = coefficient × M_r of desired product / Σ(coefficient × M_r of each reactant) × 100

M_r relative molecular or formula mass; no unit; **Σ** sum of all the indicated contributions.

WORKED EXAMPLE

Sodium carbonate from hydrogen carbonate

$2NaHCO_3 \rightarrow Na_2CO_3 + CO_2 + H_2O$. Desired product: Na_2CO_3. Use $M_r(NaHCO_3) = 84.0$ and $M_r(Na_2CO_3) = 106.0$.

Calculate the percentage atom economy for producing sodium carbonate.

Worked answer

Atom economy = (total relative mass of desired product ÷ total relative mass of reactants) × 100
Atom economy = 106.0/(2 × 84.0) × 100

63.1%.

WORKED EXAMPLE

Changing the desired product

$CaCO_3 + 2HCl \rightarrow CaCl_2 + CO_2 + H_2O$. A_r or M_r values: $CaCO_3$ 100.1, HCl 36.5, $CaCl_2$ 111.1, CO_2 44.0.

Calculate the percentage atom economy first when $CaCl_2$ is the desired product, and then when CO_2 is the desired product.

Worked answer

Total reactant formula mass = 100.1 + 2(36.5) = 173.1

For $CaCl_2$: 111.1/173.1 × 100 = 64.2%

For CO_2: 44.0/173.1 × 100 = 25.4%

The same equation has a different atom economy for a different desired product.

Measure	What it compares	Source of information
Yield	Actual product with theoretical product	Experiment and stoichiometry
Atom economy	Desired-product mass with total stoichiometric reactant mass	Balanced equation

WORKED EXAMPLE

Choose between routes

Route A: 100% atom economy, 70% yield, high energy demand and hazardous solvent. Route B: 65% atom economy, 95% yield, lower energy demand and a recoverable by-product.

Compare the two routes using atom economy, yield, energy demand and waste. Explain why atom economy alone cannot establish which route is preferable.

Worked answer

A incorporates more reactant mass into the desired product in principle. B recovers a greater fraction of its theoretical product and may have lower energy and waste-handling costs. A useful recommendation must state which priorities matter and use evidence from the data.

Neither percentage alone establishes the better route.

EXAM TRAP A reaction can have 100% atom economy and a low yield: the equation permits all atoms to enter the product, while the experiment may not produce or recover all of it.

TEST IT

Try questions 50, 51 in the matching topic Questions & answers pack. Attempt them before checking the worked answers at the back.

DONE WHEN Calculate equation-based atom economy and distinguish it from experimental yield.